8.0 Appendices

Contents

8.1 Chemical shift assignments of EcDHFR: $NADP^+$: Folate complex in the presence of co-solvents

The below tables present the NMR chemical shift data for EcDHFR: $NADP^+$: Folate complex in the presence of 17% glycerol **(Table 8.1.1)**, 17% methanol **(Table 8.1.2)** and buffer only or no co-solvent **(Table 8.1.3)**. The method of assignment is presented in the main text **(Chapter 4.0)**.

8.1.1 Chemical shift assignments of EcDHFR: NADP+: Folate complex with 17 % glycerol co-solvent

Table 8.1.1 Average chemical shifts (ppm) of nuclei in EcDHFR: $NADP^+$: Folate complex under the standard NMR buffer conditions in the presence of 17% glycerol co-solvent (by final volume) from nuclear magnetic resonance spectroscopy measured at 298.3 K. Assign Name in the colour red refers to tentative chemical shift assignments for ligand and co-factor, where applicable, for which assignment confidence is low.

17% Glycerol Shift (ppm)	SD	Assign Name	Residue	Isotope
171.15	0.000	C	1Met	13C
2.29	0.003	Hba	1Met	1H
2.38	0.002	Hbb	1Met	1H
55.42	0.061	Ca	1Met	13C
32.90	0.000	Cb	1Met	13C
4.22	0.012	Ha	1Met	1H
2.57	0.021	Hga	1Met	1H
2.64	0.024	Hgb	1Met	1H
30.13	0.146	Cg	1Met	13C
173.75	0.000	C	2Ile	13C
14.03	0.021	Cd1	2Ile	13C
39.32	0.000	Cb	2Ile	13C

29.04	0.000	Cg1	2Ile	13C
1.02	0.006	Hg1a	2Ile	1H
61.42	0.076	Ca	2Ile	13C
1.02	0.004	Hd1*	2Ile	1H
1.85	0.002	Hg1b	2Ile	1H
18.03	0.009	Cg2	2Ile	13C
1.95	0.010	Hb	2Ile	1H
4.61	0.015	Ha	2Ile	1H
124.60	0.111	N	2Ile	15N
9.50	0.019	H	2Ile	1H
0.90	0.020	Hg2*	2Ile	1H
173.41	0.000	C	3Ser	13C
3.80	0.011	Hba	3Ser	1H
65.53	0.000	Cb	3Ser	13C
56.29	0.028	Ca	3Ser	13C
4.19	0.002	Hbb	3Ser	1H
5.95	0.004	Ha	3Ser	1H
125.86	0.112	N	3Ser	15N
9.39	0.008	H	3Ser	1H
29.83	0.000	Cg	4Leu	13C
175.10	0.000	C	4Leu	13C
1.92	0.003	Hg	4Leu	1H
26.40	0.000	Cdb	4Leu	13C
25.57	0.000	Cda	4Leu	13C
0.95	0.005	Hda*	4Leu	1H
53.77	0.003	Ca	4Leu	13C
1.85	0.003	Hbb	4Leu	1H
1.66	0.013	Hba	4Leu	1H
43.84	0.070	Cb	4Leu	13C
0.98	0.010	Hdb*	4Leu	1H
5.59	0.006	Ha	4Leu	1H
121.76	0.132	N	4Leu	15N
8.57	0.011	H	4Leu	1H
172.22	0.000	C	5Ile	13C
43.16	0.023	Cb	5Ile	13C
2.23	0.003	Hg1a	5Ile	1H
2.32	0.001	Hg1b	5Ile	1H
16.54	0.022	Cd1	5Ile	13C
15.50	0.012	Cg2	5Ile	13C
27.75	0.000	Cg1	5Ile	13C
58.01	0.074	Ca	5Ile	13C
1.22	0.011	Hb	5Ile	1H

1.18	0.010	Hd1*	5Ile	1H
6.02	0.017	Ha	5Ile	1H
0.38	0.016	Hg2*	5Ile	1H
8.60	0.009	H	5Ile	1H
120.11	0.190	N	5Ile	15N
175.06	0.000	C	6Ala	13C
25.91	0.017	Cb	6Ala	13C
52.70	0.020	Ca	6Ala	13C
4.98	0.010	Ha	6Ala	1H
126.55	0.159	N	6Ala	15N
8.64	0.008	H	6Ala	1H
0.65	0.032	Hb*	6Ala	1H
174.97	0.000	C	7Ala	13C
21.11	0.035	Cb	7Ala	13C
50.61	0.059	Ca	7Ala	13C
5.03	0.005	Ha	7Ala	1H
1.48	0.002	Hb*	7Ala	1H
175.19	0.000	C	8Leu	13C
29.06	0.062	Cg	8Leu	13C
1.36	0.004	Hba	8Leu	1H
9.13	0.022	H	8Leu	1H
123.28	0.064	N	8Leu	15N
1.37	0.005	Hg	8Leu	1H
25.70	0.034	Cda	8Leu	13C
54.05	0.021	Ca	8Leu	13C
4.74	0.011	Ha	8Leu	1H
45.54	0.000	Cb	8Leu	13C
1.49	0.006	Hbb	8Leu	1H
0.43	0.001	Hdb*	8Leu	1H
0.29	0.003	Hda*	8Leu	1H
175.79	0.000	C	9Ala	13C
19.48	0.000	Cb	9Ala	13C
5.09	0.003	Ha	9Ala	1H
49.84	0.052	Ca	9Ala	13C
125.81	0.174	N	9Ala	15N
8.50	0.017	H	9Ala	1H
1.49	0.014	Hb*	9Ala	1H
177.77	0.000	C	10Val	13C
31.75	0.050	Cb	10Val	13C
21.53	0.052	Cgb	10Val	13C
23.35	0.004	Cga	10Val	13C
65.02	0.077	Ca	10Val	13C

2.18	0.010	Hb	10Val	1H
1.04	0.018	Hga*	10Val	1H
1.04	0.021	Hgb*	10Val	1H
3.80	0.020	Ha	10Val	1H
117.89	0.108	N	10Val	15N
7.60	0.010	H	10Val	1H
174.74	0.000	C	11Asp	13C
56.08	0.084	Ca	11Asp	13C
122.88	0.075	N	11Asp	15N
9.11	0.009	H	11Asp	1H
4.38	0.016	Ha	11Asp	1H
2.87	0.043	Hba	11Asp	1H
3.13	0.003	Hbb	11Asp	1H
39.04	0.028	Cb	11Asp	13C
2.23	0.000	Hba	12Arg	1H
175.80	0.000	C	12Arg	13C
7.15	0.000	He	12Arg	1H
119.18	0.000	Ne	12Arg	15N
27.57	0.000	Cb	12Arg	13C
43.38	0.000	Cd	12Arg	13C
2.57	0.001	Hbb	12Arg	1H
57.57	0.091	Ca	12Arg	13C
1.63	0.005	Hga	12Arg	1H
3.46	0.001	Hdb	12Arg	1H
3.24	0.001	Hda	12Arg	1H
28.16	0.000	Cg	12Arg	13C
107.14	0.090	N	12Arg	15N
1.78	0.019	Hgb	12Arg	1H
3.72	0.030	Ha	12Arg	1H
8.53	0.011	H	12Arg	1H
176.80	0.000	C	13Val	13C
19.09	0.004	Cga	119Val	13C
32.97	0.082	Cb	13Val	13C
21.96	0.000	Cgb	119Val	13C
65.70	0.102	Ca	13Val	13C
3.62	0.012	Ha	13Val	1H
1.22	0.018	Hgb*	13Val	1H
1.94	0.037	Hb	13Val	1H
0.97	0.020	Hga*	13Val	1H
120.61	0.116	N	13Val	15N
7.16	0.014	H	13Val	1H
0.74	0.000	Hg2*	14Ile	1H

41.79	0.000	Cb	14Ile	13C
14.03	0.000	Cd1	14Ile	13C
1.67	0.000	Hb	14Ile	1H
17.71	0.000	Cg2	14Ile	13C
61.40	0.000	Ca	14Ile	13C
4.36	0.005	Ha	14Ile	1H
0.59	0.007	Hg1b	14Ile	1H
0.19	0.004	Hg1a	14Ile	1H
26.63	0.000	Cg1	14Ile	13C
169.71	0.000	C	15Gly	13C
109.66	0.273	N	15Gly	15N
7.55	0.014	H	15Gly	1H
4.49	0.009	Hab	15Gly	1H
4.22	0.010	Haa	15Gly	1H
45.94	0.077	Ca	15Gly	13C
174.67	0.000	C	16Met	13C
2.06	0.000	Hga	16Met	1H
2.20	0.000	Hgb	16Met	1H
18.59	0.074	Ce	16Met	13C
1.96	0.024	He*	16Met	1H
31.55	0.117	Cg	16Met	13C
2.52	0.010	Hba	16Met	1H
2.60	0.003	Hbb	16Met	1H
34.94	0.077	Cb	16Met	13C
4.59	0.011	Ha	16Met	1H
55.49	0.106	Ca	16Met	13C
119.29	0.089	N	16Met	15N
8.59	0.009	H	16Met	1H
36.60	0.000	Cg	17Glu	13C
27.31	0.000	Cb	17Glu	13C
175.38	0.000	C	17Glu	13C
173.39	0.000	C	18Asn	13C
6.75	0.000	Hd2a	18Asn	1H
7.56	0.000	Hd2b	18Asn	1H
110.06	0.024	Nd2	18Asn	15N
114.67	0.183	N	18Asn	15N
9.47	0.012	H	18Asn	1H
54.17	0.040	Ca	18Asn	13C
3.10	0.007	Hbb	18Asn	1H
4.23	0.004	Ha	18Asn	1H
2.48	0.003	Hba	18Asn	1H
38.87	0.049	Cb	18Asn	13C

176.03	0.000	C	19Ala	13C
21.65	0.002	Cb	19Ala	13C
50.53	0.052	Ca	19Ala	13C
4.49	0.016	Ha	19Ala	1H
1.29	0.018	Hb*	19Ala	1H
120.97	0.082	N	19Ala	15N
7.72	0.007	H	19Ala	1H
40.90	0.000	Cb	20Met	13C
175.17	0.000	C	20Met	13C
52.33	0.000	Ca	20Met	13C
17.08	0.060	Ce	20Met	13C
1.93	0.025	He*	20Met	1H
119.86	0.151	N	20Met	15N
8.33	0.022	H	20Met	1H
173.64	0.000	C	21Pro	13C
132.55	0.000	Ne1	22Trp	15N
10.57	0.000	He1	22Trp	1H
173.86	0.000	C	22Trp	13C
57.26	0.000	Ca	22Trp	13C
7.44	0.018	H	22Trp	1H
116.26	0.152	N	22Trp	15N
7.57	0.000	Hd2b	23Asn	1H
6.87	0.000	Hd2a	23Asn	1H
172.41	0.000	C	23Asn	13C
9.01	0.001	H	23Asn	1H
117.26	0.095	N	23Asn	15N
53.66	0.000	Ca	23Asn	13C
4.91	0.000	Ha	23Asn	1H
112.14	0.000	Nd2	23Asn	15N
40.44	0.000	Cb	23Asn	13C
2.62	0.003	Hba	23Asn	1H
2.92	0.002	Hbb	23Asn	1H
173.94	0.000	C	24Leu	13C
25.92	0.000	Cdb	24Leu	13C
125.05	0.063	N	24Leu	15N
9.54	0.010	H	24Leu	1H
0.83	0.002	Hdb*	24Leu	1H
51.36	0.030	Ca	24Leu	13C
26.73	0.097	Cda	24Leu	13C
1.52	0.002	Hg	24Leu	1H
0.42	0.002	Hda*	24Leu	1H
1.65	0.003	Hbb	24Leu	1H

1.09	0.002	Hba	24Leu	1H
5.30	0.004	Ha	24Leu	1H
44.49	0.000	Cb	24Leu	13C
179.47	0.000	C	25Pro	13C
27.96	0.000	Cg	25Pro	13C
65.51	0.060	Ca	25Pro	13C
2.01	0.002	Hgb	25Pro	1H
3.73	0.004	Hdb	25Pro	1H
2.01	0.002	Hga	25Pro	1H
4.56	0.016	Ha	25Pro	1H
50.62	0.035	Cd	25Pro	13C
3.47	0.004	Hda	25Pro	1H
2.44	0.016	Hbb	25Pro	1H
1.76	0.011	Hba	25Pro	1H
31.34	0.040	Cb	25Pro	13C
181.56	0.000	C	26Ala	13C
19.11	0.000	Cb	26Ala	13C
55.26	0.054	Ca	26Ala	13C
4.18	0.013	Ha	26Ala	1H
1.31	0.012	Hb*	26Ala	1H
120.21	0.069	N	26Ala	15N
9.30	0.013	H	26Ala	1H
177.29	0.000	C	27Asp	13C
2.93	0.006	Hbb	27Asp	1H
56.40	0.038	Ca	27Asp	13C
43.71	0.047	Cb	27Asp	13C
2.12	0.009	Hba	27Asp	1H
4.92	0.010	Ha	27Asp	1H
118.42	0.067	N	27Asp	15N
7.47	0.010	H	27Asp	1H
179.01	0.000	C	28Leu	13C
24.90	0.048	Cdb	28Leu	13C
27.14	0.000	Cg	28Leu	13C
57.53	0.069	Ca	28Leu	13C
22.21	0.034	Cda	28Leu	13C
3.98	0.006	Ha	28Leu	1H
40.85	0.041	Cb	28Leu	13C
121.19	0.102	N	28Leu	15N
1.69	0.007	Hbb	28Leu	1H
1.32	0.007	Hba	28Leu	1H
0.54	0.006	Hdb*	28Leu	1H
1.49	0.011	Hg	28Leu	1H

0.09	0.008	Hda*	28Leu	1H
7.61	0.010	H	28Leu	1H
180.37	0.000	C	29Ala	13C
17.54	0.000	Cb	29Ala	13C
55.17	0.007	Ca	29Ala	13C
1.22	0.010	Hb*	29Ala	1H
4.19	0.015	Ha	29Ala	1H
120.62	0.131	N	29Ala	15N
7.87	0.009	H	29Ala	1H
6.75	0.000	He3	30Trp	1H
177.82	0.000	C	30Trp	13C
128.01	0.000	Cd1	30Trp	13C
7.13	0.012	Hd1	30Trp	1H
3.48	0.003	Hbb	30Trp	1H
60.21	0.089	Ca	30Trp	13C
29.13	0.087	Cb	30Trp	13C
4.03	0.005	Ha	30Trp	1H
130.35	0.071	Ne1	30Trp	15N
10.51	0.008	He1	30Trp	1H
2.73	0.008	Hba	30Trp	1H
124.08	0.059	N	30Trp	15N
7.45	0.008	H	30Trp	1H
178.39	0.000	C	31Phe	13C
123.51	0.085	N	31Phe	15N
3.26	0.001	Hbb	31Phe	1H
38.14	0.029	Cb	31Phe	13C
61.34	0.086	Ca	31Phe	13C
9.05	0.019	H	31Phe	1H
3.60	0.001	Ha	31Phe	1H
2.67	0.007	Hba	31Phe	1H
177.77	0.000	C	32Lys	13C
32.41	0.000	Cb	32Lys	13C
42.26	0.000	Ce	32Lys	13C
1.93	0.005	Hbb	32Lys	1H
25.01	0.000	Cg	32Lys	13C
1.82	0.022	Hba	32Lys	1H
2.83	0.014	Hea	32Lys	1H
1.37	0.000	Hgb	32Lys	1H
1.17	0.003	Hga	32Lys	1H
30.04	0.000	Cd	32Lys	13C
1.67	0.016	Hda	32Lys	1H
2.84	0.003	Heb	32Lys	1H

1.67	0.016	Hdb	32Lys	1H
124.31	0.145	N	32Lys	15N
8.70	0.012	H	32Lys	1H
60.29	0.078	Ca	32Lys	13C
3.40	0.009	Ha	32Lys	1H
178.26	0.000	C	33Arg	13C
121.67	0.000	Ne	33Arg	15N
7.12	0.005	He	33Arg	1H
43.76	0.004	Cd	33Arg	13C
59.10	0.048	Ca	33Arg	13C
117.11	0.146	N	33Arg	15N
2.99	0.003	Hdb	33Arg	1H
1.75	0.011	Hbb	33Arg	1H
1.29	0.017	Hga	33Arg	1H
3.72	0.002	Ha	33Arg	1H
29.71	0.000	Cb	33Arg	13C
26.47	0.109	Cg	33Arg	13C
1.46	0.039	Hgb	33Arg	1H
1.51	0.012	Hba	33Arg	1H
8.11	0.017	H	33Arg	1H
2.98	0.012	Hda	33Arg	1H
173.95	0.000	C	34Asn	13C
39.16	0.000	Cb	34Asn	13C
1.44	0.000	Hbb	34Asn	1H
1.31	0.002	Hba	34Asn	1H
54.33	0.159	Ca	34Asn	13C
4.15	0.015	Ha	34Asn	1H
111.35	0.061	N	34Asn	15N
7.08	0.008	H	34Asn	1H
173.23	0.000	C	35Thr	13C
70.45	0.012	Cb	35Thr	13C
20.92	0.043	Cg2	35Thr	13C
3.40	0.004	Hb	35Thr	1H
61.99	0.057	Ca	35Thr	13C
3.90	0.007	Ha	35Thr	1H
0.13	0.013	Hg2*	35Thr	1H
107.23	0.056	N	35Thr	15N
7.14	0.006	H	35Thr	1H
176.39	0.000	C	36Leu	13C
26.64	0.029	Cdb	36Leu	13C
24.57	0.080	Cda	36Leu	13C
57.04	0.062	Ca	36Leu	13C

1.59	0.003	Hdb*	36Leu	1H
3.40	0.018	Ha	36Leu	1H
121.70	0.099	N	36Leu	15N
1.36	0.082	Hba	36Leu	1H
0.77	0.022	Hda*	36Leu	1H
1.47	0.027	Hbb	36Leu	1H
42.30	0.059	Cb	36Leu	13C
7.52	0.015	H	36Leu	1H
173.43	0.000	C	37Asp	13C
55.01	0.030	Ca	37Asp	13C
4.35	0.011	Ha	37Asp	1H
37.43	0.012	Cb	37Asp	13C
2.98	0.016	Hbb	37Asp	1H
2.98	0.016	Hba	37Asp	1H
113.05	0.054	N	37Asp	15N
7.90	0.023	H	37Asp	1H
33.89	0.000	Cb	38Lys	13C
172.52	0.000	C	38Lys	13C
1.20	0.000	[Hga]	38Lys	1H
1.44	0.000	Hba	38Lys	1H
1.06	0.000	[Hgb]	38Lys	1H
1.79	0.000	Hbb	38Lys	1H
4.70	0.000	Ha	38Lys	1H
53.99	0.000	Ca	38Lys	13C
119.38	0.048	N	38Lys	15N
7.91	0.011	H	38Lys	1H
32.21	0.000	Cb	39Pro	13C
2.14	0.000	Hbb	39Pro	1H
1.96	0.000	Hba	39Pro	1H
175.72	0.000	C	39Pro	13C
28.86	0.000	Cg	39Pro	13C
2.10	0.000	Hga	39Pro	1H
2.19	0.018	Hgb	39Pro	1H
5.04	0.004	Ha	39Pro	1H
62.22	0.029	Ca	39Pro	13C
3.84	0.004	Hda	39Pro	1H
4.04	0.005	Hdb	39Pro	1H
49.15	0.047	Cd	39Pro	13C
173.54	0.000	C	40Val	13C
34.09	0.052	Cb	40Val	13C
21.30	0.103	Cgb	136Val	13C
18.45	0.058	Cga	136Val	13C

56.70	0.144	Ca	40Val	13C
5.58	0.002	Ha	40Val	1H
1.85	0.001	Hb	40Val	1H
0.84	0.007	Hgb*	40Val	1H
0.63	0.014	Hga*	40Val	1H
112.91	0.039	N	40Val	15N
8.75	0.006	H	40Val	1H
174.76	0.000	C	41Ile	13C
40.62	0.060	Cb	41Ile	13C
4.82	0.010	Ha	41Ile	1H
17.52	0.000	Cg2	41Ile	13C
0.40	0.013	Hg2*	41Ile	1H
0.42	0.004	Hg1a	41Ile	1H
59.56	0.055	Ca	41Ile	13C
27.46	0.000	Cg1	41Ile	13C
1.31	0.018	Hg1b	41Ile	1H
1.07	0.029	Hb	41Ile	1H
14.81	0.020	Cd1	41Ile	13C
121.52	0.173	N	41Ile	15N
8.45	0.006	H	41Ile	1H
0.39	0.025	Hd1*	41Ile	1H
174.33	0.000	C	42Met	13C
31.75	0.013	Cg	42Met	13C
18.35	0.047	Ce	42Met	13C
1.80	0.025	He*	42Met	1H
2.10	0.007	Hga	42Met	1H
2.53	0.005	Hgb	42Met	1H
52.12	0.045	Ca	42Met	13C
2.04	0.018	Hbb	42Met	1H
40.45	0.051	Cb	42Met	13C
1.76	0.018	Hba	42Met	1H
123.92	0.111	N	42Met	15N
9.09	0.007	H	42Met	1H
5.76	0.016	Ha	42Met	1H
175.40	0.000	C	43Gly	13C
4.36	0.014	Hab	43Gly	1H
4.12	0.012	Haa	43Gly	1H
44.35	0.067	Ca	43Gly	13C
105.62	0.121	N	43Gly	15N
9.22	0.011	H	43Gly	1H
30.12	0.000	Cb	44Arg	13C
42.72	0.000	Cd	44Arg	13C

1.57	0.000	Hba	44Arg	1H
1.66	0.000	Hbb	44Arg	1H
25.21	0.000	Cg	44Arg	13C
1.32	0.000	Hgb	44Arg	1H
2.77	0.000	Hda	44Arg	1H
2.83	0.000	Hdb	44Arg	1H
3.34	0.000	Ha	44Arg	1H
1.00	0.000	Hga	44Arg	1H
60.92	0.000	Ca	44Arg	13C
178.30	0.000	C	44Arg	13C
7.66	0.008	H	44Arg	1H
119.15	0.127	N	44Arg	15N
4.32	0.000	Ha	45His	1H
58.13	0.000	Ca	45His	13C
178.02	0.000	C	45His	13C
4.24	0.000	Ha	45His	1H
1.85	0.000	Hbb	45His	1H
1.74	0.000	Hba	45His	1H
27.00	0.000	Cb	45His	13C
7.43	0.005	H	45His	1H
112.89	0.098	N	45His	15N
7.02	0.003	Hd1	45His	1H
119.24	0.000	N	46Thr	15N
8.08	0.000	H	46Thr	1H
176.10	0.000	C	46Thr	13C
4.30	0.001	Ha	46Thr	1H
20.94	0.082	Cg2	46Thr	13C
68.50	0.000	Cb	46Thr	13C
1.41	0.007	Hg2*	46Thr	1H
3.94	0.008	Hb	46Thr	1H
7.28	0.000	He3	47Trp	1H
10.25	0.000	He1	47Trp	1H
127.98	0.000	Ne1	47Trp	15N
7.25	0.000	Hd1	47Trp	1H
124.55	0.211	N	47Trp	15N
8.35	0.002	H	47Trp	1H
3.32	0.003	Hba	47Trp	1H
3.46	0.007	Hbb	47Trp	1H
60.09	0.093	Ca	47Trp	13C
30.10	0.004	Cb	47Trp	13C
4.66	0.003	Ha	47Trp	1H
8.05	0.000	H	48Glu	1H

178.18	0.000	C	48Glu	13C
59.08	0.060	Ca	48Glu	13C
3.45	0.004	Ha	48Glu	1H
2.24	0.002	Hbb	48Glu	1H
1.94	0.003	Hba	48Glu	1H
28.85	0.000	Cb	48Glu	13C
2.32	0.008	Hga	48Glu	1H
2.85	0.023	Hgb	48Glu	1H
37.47	0.106	Cg	48Glu	13C
175.01	0.000	C	49Ser	13C
4.04	0.001	Hbb	49Ser	1H
7.78	0.017	H	49Ser	1H
113.94	0.045	N	49Ser	15N
63.60	0.000	Cb	49Ser	13C
3.99	0.020	Hba	49Ser	1H
4.20	0.004	Ha	49Ser	1H
60.55	0.111	Ca	49Ser	13C
178.68	0.000	C	50Ile	13C
17.51	0.051	Cg2	50Ile	13C
38.93	0.020	Cb	50Ile	13C
14.41	0.033	Cd1	50Ile	13C
64.95	0.020	Ca	50Ile	13C
27.58	0.041	Cg1	50Ile	13C
0.42	0.014	Hg2*	50Ile	1H
1.60	0.018	Hg1b	50Ile	1H
7.64	0.006	H	50Ile	1H
122.57	0.127	N	50Ile	15N
3.51	0.016	Ha	50Ile	1H
1.38	0.013	Hb	50Ile	1H
0.41	0.009	Hd1*	50Ile	1H
0.06	0.020	Hg1a	50Ile	1H
172.45	0.000	C	51Gly	13C
3.62	0.030	Hab	51Gly	1H
104.18	0.059	N	51Gly	15N
2.93	0.035	Haa	51Gly	1H
45.80	0.137	Ca	51Gly	13C
7.57	0.013	H	51Gly	1H
2.97	0.011	Hdb	52Arg	1H
43.53	0.086	Cd	52Arg	13C
2.97	0.011	Hda	52Arg	1H
53.20	0.006	Ca	52Arg	13C
24.83	0.000	Cg	52Arg	13C

4.41	0.012	Ha	52Arg	1H
1.30	0.015	Hgb	52Arg	1H
1.23	0.016	Hga	52Arg	1H
28.61	0.000	Cb	52Arg	13C
1.64	0.008	Hba	52Arg	1H
1.92	0.013	Hbb	52Arg	1H
115.89	0.079	N	52Arg	15N
6.80	0.005	H	52Arg	1H
49.47	0.000	Cd	53Pro	13C
1.94	0.000	Hbb	53Pro	1H
31.40	0.000	Cb	53Pro	13C
1.67	0.000	Hba	53Pro	1H
3.59	0.000	Hdb	53Pro	1H
3.57	0.000	Hda	53Pro	1H
3.96	0.000	Ha	53Pro	1H
28.06	0.000	Cg	53Pro	13C
1.73	0.000	Hga	53Pro	1H
2.01	0.000	Hgb	53Pro	1H
61.75	0.000	Ca	53Pro	13C
176.94	0.000	C	53Pro	13C
176.06	0.000	C	54Leu	13C
21.98	0.000	Cda	54Leu	13C
26.32	0.000	Cdb	54Leu	13C
26.32	0.000	Cg	54Leu	13C
52.02	0.049	Ca	54Leu	13C
1.64	0.007	Hbb	54Leu	1H
1.64	0.006	Hg	54Leu	1H
40.60	0.077	Cb	54Leu	13C
0.84	0.018	Hdb*	54Leu	1H
0.86	0.023	Hba	54Leu	1H
0.49	0.003	Hda*	54Leu	1H
4.44	0.007	Ha	54Leu	1H
9.47	0.006	H	54Leu	1H
126.04	0.226	N	54Leu	15N
172.82	0.000	C	56Gly	13C
112.79	0.000	N	56Gly	15N
7.46	0.004	H	56Gly	1H
3.72	0.017	Haa	56Gly	1H
3.86	0.014	Hab	56Gly	1H
46.69	0.059	Ca	56Gly	13C
28.03	0.000	Cg	57Arg	13C
1.24	0.000	Hga	57Arg	1H

2.74	0.000	Hgb	57Arg	1H
174.40	0.000	C	57Arg	13C
54.53	0.053	Ca	57Arg	13C
43.17	0.000	Cd	57Arg	13C
2.71	0.008	Hdb	57Arg	1H
2.36	0.004	Hda	57Arg	1H
4.40	0.003	Ha	57Arg	1H
1.93	0.005	Hbb	57Arg	1H
1.29	0.003	Hba	57Arg	1H
35.98	0.000	Cb	57Arg	13C
7.26	0.005	H	57Arg	1H
118.03	0.051	N	57Arg	15N
174.94	0.000	C	58Lys	13C
29.64	0.000	Cd	58Lys	13C
1.59	0.000	Hdb	58Lys	1H
1.59	0.000	Hda	58Lys	1H
2.83	0.025	Heb	58Lys	1H
32.55	0.000	Cb	58Lys	13C
123.65	0.144	N	58Lys	15N
42.07	0.000	Ce	58Lys	13C
1.59	0.001	Hba	58Lys	1H
1.64	0.001	Hbb	58Lys	1H
7.46	0.008	H	58Lys	1H
56.12	0.059	Ca	58Lys	13C
2.81	0.026	Hea	58Lys	1H
4.41	0.007	Ha	58Lys	1H
1.33	0.002	Hgb	58Lys	1H
1.10	0.002	Hga	58Lys	1H
25.24	0.000	Cg	58Lys	13C
173.36	0.000	Cg	59Asn	13C
172.50	0.000	C	59Asn	13C
108.94	0.012	Nd2	59Asn	15N
7.43	0.001	Hd2b	59Asn	1H
4.69	0.037	Ha	59Asn	1H
6.66	0.011	Hd2a	59Asn	1H
40.85	0.090	Cb	59Asn	13C
126.67	0.052	N	59Asn	15N
53.43	0.027	Ca	59Asn	13C
9.16	0.004	H	59Asn	1H
1.77	0.008	Hba	59Asn	1H
2.84	0.014	Hbb	59Asn	1H
0.56	0.000	Hg1a	60Ile	1H

172.43	0.000	C	60Ile	13C
39.40	0.039	Cb	60Ile	13C
19.16	0.030	Cg2	60Ile	13C
60.11	0.077	Ca	60Ile	13C
16.38	0.034	Cd1	60Ile	13C
28.28	0.042	Cg1	60Ile	13C
1.71	0.011	Hb	60Ile	1H
1.24	0.012	Hg1b	60Ile	1H
4.37	0.011	Ha	60Ile	1H
126.35	0.141	N	60Ile	15N
8.74	0.010	H	60Ile	1H
0.59	0.005	Hg2*	60Ile	1H
0.65	0.023	Hd1*	60Ile	1H
175.40	0.000	C	61Ile	13C
37.50	0.054	Cb	61Ile	13C
12.21	0.010	Cd1	61Ile	13C
19.44	0.054	Cg2	61Ile	13C
58.17	0.089	Ca	61Ile	13C
0.00	0.006	Hg1a	61Ile	1H
28.09	0.023	Cg1	61Ile	13C
-0.39	0.010	Hd1*	61Ile	1H
4.46	0.009	Ha	61Ile	1H
0.54	0.020	Hb	61Ile	1H
-0.44	0.005	Hg1b	61Ile	1H
0.15	0.018	Hg2*	61Ile	1H
127.51	0.125	N	61Ile	15N
8.85	0.008	H	61Ile	1H
26.85	0.000	Cg	62Leu	13C
175.56	0.000	C	62Leu	13C
26.34	0.019	Cdb	62Leu	13C
0.57	0.032	Hg	62Leu	1H
24.87	0.036	Cda	62Leu	13C
53.66	0.013	Ca	62Leu	13C
-0.08	0.026	Hda*	62Leu	1H
125.76	0.145	N	62Leu	15N
0.66	0.024	Hbb	62Leu	1H
8.37	0.008	H	62Leu	1H
43.16	0.050	Cb	62Leu	13C
4.35	0.018	Ha	62Leu	1H
0.19	0.027	Hdb*	62Leu	1H
-0.11	0.028	Hba	62Leu	1H
174.06	0.000	C	63Ser	13C

4.38	0.024	Hbb	63Ser	1H
3.81	0.009	Hba	63Ser	1H
58.69	0.119	Ca	63Ser	13C
64.62	0.066	Cb	63Ser	13C
5.26	0.007	Ha	63Ser	1H
115.52	0.080	N	63Ser	15N
8.70	0.014	H	63Ser	1H
174.71	0.000	C	64Ser	13C
64.41	0.038	Cb	64Ser	13C
4.03	0.002	Hbb	64Ser	1H
3.96	0.004	Hba	64Ser	1H
60.51	0.120	Ca	64Ser	13C
4.62	0.016	Ha	64Ser	1H
122.69	0.056	N	64Ser	15N
10.17	0.012	H	64Ser	1H
172.56	0.000	C	65Gln	13C
113.24	0.004	Ne2	65Gln	15N
7.69	0.032	He2b	65Gln	1H
6.80	0.031	He2a	65Gln	1H
53.12	0.070	Ca	65Gln	13C
29.55	0.000	Cb	65Gln	13C
2.09	0.013	Hbb	65Gln	1H
1.76	0.025	Hba	65Gln	1H
4.65	0.008	Ha	65Gln	1H
122.82	0.152	N	65Gln	15N
8.63	0.012	H	65Gln	1H
2.25	0.009	Hga	65Gln	1H
2.41	0.020	Hgb	65Gln	1H
33.88	0.069	Cg	65Gln	13C
177.05	0.009	C	66Pro	13C
62.80	0.055	Ca	66Pro	13C
27.77	0.000	Cg	66Pro	13C
1.97	0.011	Hgb	66Pro	1H
1.85	0.015	Hga	66Pro	1H
3.49	0.025	Hda	66Pro	1H
3.66	0.019	Hdb	66Pro	1H
50.26	0.089	Cd	66Pro	13C
2.14	0.017	Hbb	66Pro	1H
3.98	0.024	Ha	66Pro	1H
1.54	0.027	Hba	66Pro	1H
31.87	0.062	Cb	66Pro	13C
42.68	0.041	Ca	67Gly	13C

2.02	0.004	Hab	67Gly	1H
1.73	0.017	Haa	67Gly	1H
7.68	0.014	H	67Gly	1H
108.77	0.190	N	67Gly	15N
21.24	0.015	Cg2	68Thr	13C
174.12	0.022	C	68Thr	13C
60.28	0.048	Ca	68Thr	13C
69.18	0.080	Cb	68Thr	13C
0.93	0.024	Hg2*	68Thr	1H
4.50	0.031	Hb	68Thr	1H
4.22	0.029	Ha	68Thr	1H
105.87	0.027	N	68Thr	15N
5.92	0.016	H	68Thr	1H
176.24	0.000	C	69Asp	13C
55.17	0.017	Ca	69Asp	13C
44.10	0.000	Cb	69Asp	13C
3.13	0.009	Hbb	69Asp	1H
3.01	0.030	Hba	69Asp	1H
4.81	0.026	Ha	69Asp	1H
120.18	0.079	N	69Asp	15N
7.31	0.007	H	69Asp	1H
176.93	0.000	C	70Asp	13C
40.29	0.000	Cb	70Asp	13C
4.82	0.015	Ha	70Asp	1H
55.08	0.030	Ca	70Asp	13C
2.76	0.015	Hba	70Asp	1H
2.88	0.021	Hbb	70Asp	1H
126.66	0.121	N	70Asp	15N
8.88	0.006	H	70Asp	1H
175.64	0.000	C	71Arg	13C
31.55	0.000	Cb	71Arg	13C
1.80	0.010	Hba	71Arg	1H
43.68	0.088	Cd	71Arg	13C
1.97	0.011	Hbb	71Arg	1H
57.40	0.018	Ca	71Arg	13C
3.10	0.022	Hda	71Arg	1H
3.41	0.019	Hdb	71Arg	1H
1.97	0.012	Hgb	71Arg	1H
1.80	0.006	Hga	71Arg	1H
4.20	0.020	Ha	71Arg	1H
26.08	0.058	Cg	71Arg	13C
118.12	0.048	N	71Arg	15N

8.88	0.006	H	71Arg	1H
172.91	0.000	C	72Val	13C
23.05	0.141	Cgb	13Val	13C
33.44	0.031	Cb	72Val	13C
22.01	0.078	Cga	13Val	13C
58.29	0.040	Ca	72Val	13C
4.57	0.018	Ha	72Val	1H
1.40	0.011	Hb	72Val	1H
0.35	0.023	Hgb*	72Val	1H
-0.44	0.031	Hga*	72Val	1H
108.14	0.032	N	72Val	15N
7.23	0.018	H	72Val	1H
171.88	0.000	C	73Thr	13C
70.38	0.015	Cb	73Thr	13C
21.12	0.000	Cg2	73Thr	13C
3.85	0.006	Hb	73Thr	1H
62.92	0.090	Ca	73Thr	13C
1.08	0.023	Hg2*	73Thr	1H
4.33	0.025	Ha	73Thr	1H
117.08	0.038	N	73Thr	15N
7.92	0.006	H	73Thr	1H
130.28	0.000	Ne1	74Trp	15N
176.50	0.000	C	74Trp	13C
7.32	0.000	He3	74Trp	1H
7.11	0.004	Hd1	74Trp	1H
56.14	0.023	Ca	74Trp	13C
5.06	0.015	Ha	74Trp	1H
2.84	0.010	Hba	74Trp	1H
3.50	0.009	Hbb	74Trp	1H
10.22	0.029	He1	74Trp	1H
29.06	0.084	Cb	74Trp	13C
128.84	0.107	N	74Trp	15N
8.75	0.020	H	74Trp	1H
174.85	0.000	C	75Val	13C
22.32	0.023	Cga	40Val	13C
35.84	0.045	Cb	75Val	13C
58.84	0.040	Ca	75Val	13C
4.84	0.019	Ha	75Val	1H
0.70	0.025	Hgb*	75Val	1H
2.12	0.029	Hb	75Val	1H
19.82	0.031	Cgb	40Val	13C
116.27	0.040	N	75Val	15N

9.17	0.007	H	75Val	1H
0.48	0.032	Hga*	75Val	1H
1.75	0.000	Hdb	76Lys	1H
1.68	0.001	Hda	76Lys	1H
55.52	0.001	Ca	76Lys	13C
29.46	0.000	Cd	76Lys	13C
42.07	0.000	Ce	76Lys	13C
175.58	0.012	C	76Lys	13C
2.87	0.002	Hea	76Lys	1H
2.95	0.002	Heb	76Lys	1H
2.05	0.004	Hbb	76Lys	1H
1.86	0.005	Hba	76Lys	1H
1.47	0.004	Hga	76Lys	1H
34.24	0.040	Cb	76Lys	13C
1.73	0.014	Hgb	76Lys	1H
24.37	0.061	Cg	76Lys	13C
5.09	0.009	Ha	76Lys	1H
115.91	0.092	N	76Lys	15N
8.30	0.006	H	76Lys	1H
174.01	0.000	C	77Ser	13C
66.35	0.000	Cb	77Ser	13C
4.10	0.002	Hba	77Ser	1H
4.29	0.000	Hbb	77Ser	1H
57.05	0.010	Ca	77Ser	13C
4.89	0.058	Ha	77Ser	1H
108.69	0.120	N	77Ser	15N
7.22	0.005	H	77Ser	1H
177.12	0.000	C	78Val	13C
122.61	0.098	N	78Val	15N
8.91	0.005	H	78Val	1H
31.62	0.086	Cb	78Val	13C
67.17	0.045	Ca	78Val	13C
22.89	0.005	Cgb	72Val	13C
16.87	0.032	Cga	72Val	13C
3.37	0.035	Ha	78Val	1H
1.85	0.022	Hb	78Val	1H
0.69	0.031	Hgb*	78Val	1H
0.38	0.040	Hga*	78Val	1H
39.58	0.000	Cb	79Asp	13C
2.48	0.000	Hba	79Asp	1H
179.66	0.000	C	79Asp	13C
2.57	0.001	Hbb	79Asp	1H

57.78	0.106	Ca	79Asp	13C
4.35	0.016	Ha	79Asp	1H
117.96	0.030	N	79Asp	15N
8.46	0.005	H	79Asp	1H
178.90	0.000	C	80Glu	13C
120.72	0.103	N	80Glu	15N
2.25	0.006	Hga	80Glu	1H
36.91	0.042	Cg	80Glu	13C
7.97	0.010	H	80Glu	1H
59.19	0.043	Ca	80Glu	13C
2.04	0.022	Hbb	80Glu	1H
2.37	0.006	Hgb	80Glu	1H
30.71	0.000	Cb	80Glu	13C
2.01	0.022	Hba	80Glu	1H
3.97	0.003	Ha	80Glu	1H
17.83	0.000	Cb	81Ala	13C
177.92	0.000	C	81Ala	13C
55.57	0.051	Ca	81Ala	13C
3.89	0.023	Ha	81Ala	1H
1.49	0.025	Hb*	81Ala	1H
8.22	0.007	H	81Ala	1H
122.33	0.083	N	81Ala	15N
180.34	0.000	C	82Ile	13C
115.90	0.054	N	82Ile	15N
8.00	0.011	H	82Ile	1H
38.37	0.102	Cb	82Ile	13C
13.28	0.013	Cd1	82Ile	13C
65.48	0.064	Ca	82Ile	13C
29.59	0.055	Cg1	82Ile	13C
3.67	0.007	Ha	82Ile	1H
0.90	0.017	Hd1*	82Ile	1H
1.07	0.018	Hg1a	82Ile	1H
2.03	0.018	Hg1b	82Ile	1H
1.92	0.020	Hb	82Ile	1H
16.98	0.077	Cg2	82Ile	13C
0.86	0.027	Hg2*	82Ile	1H
17.74	0.000	Cb	83Ala	13C
180.37	0.000	C	83Ala	13C
1.49	0.015	Hb*	83Ala	1H
4.11	0.015	Ha	83Ala	1H
55.19	0.030	Ca	83Ala	13C
8.18	0.006	H	83Ala	1H

124.08	0.098	N	83Ala	15N
177.96	0.000	C	84Ala	13C
18.12	0.044	Cb	84Ala	13C
4.10	0.002	Ha	84Ala	1H
1.43	0.002	Hb*	84Ala	1H
119.38	0.153	N	84Ala	15N
53.77	0.075	Ca	84Ala	13C
8.07	0.011	H	84Ala	1H
175.42	0.000	C	85Cys	13C
114.50	0.119	N	85Cys	15N
61.87	0.070	Ca	85Cys	13C
2.46	0.004	Hba	85Cys	1H
3.32	0.006	Hbb	85Cys	1H
3.95	0.008	Ha	85Cys	1H
7.43	0.005	H	85Cys	1H
27.96	0.058	Cb	85Cys	13C
173.27	0.000	C	86Gly	13C
3.89	0.015	Hab	86Gly	1H
3.75	0.013	Haa	86Gly	1H
45.20	0.045	Ca	86Gly	13C
103.03	0.057	N	86Gly	15N
7.24	0.026	H	86Gly	1H
175.23	0.000	C	87Asp	13C
122.33	0.049	N	87Asp	15N
53.40	0.057	Ca	87Asp	13C
4.71	0.012	Ha	87Asp	1H
8.51	0.027	H	87Asp	1H
2.47	0.006	Hba	87Asp	1H
2.70	0.014	Hbb	87Asp	1H
39.60	0.068	Cb	87Asp	13C
4.09	0.000	Ha	88Val	1H
58.27	0.000	Ca	88Val	13C
22.41	0.015	Cgb	75Val	13C
32.14	0.024	Cb	88Val	13C
114.24	0.064	N	88Val	15N
7.24	0.029	H	88Val	1H
0.98	0.010	Hgb*	88Val	1H
2.39	0.014	Hb	88Val	1H
18.36	0.023	Cga	75Val	13C
0.59	0.029	Hga*	88Val	1H
177.63	0.000	C	89Pro	13C
50.77	0.000	Cd	89Pro	13C

3.81	0.008	Hdb	89Pro	1H
3.81	0.008	Hda	89Pro	1H
27.51	0.000	Cg	89Pro	13C
64.70	0.053	Ca	89Pro	13C
32.13	0.000	Cb	89Pro	13C
1.98	0.011	Hga	89Pro	1H
2.35	0.007	Hbb	89Pro	1H
2.15	0.016	Hgb	89Pro	1H
1.89	0.016	Hba	89Pro	1H
4.33	0.021	Ha	89Pro	1H
173.34	0.000	C	90Glu	13C
33.02	0.000	Cb	90Glu	13C
36.17	0.000	Cg	90Glu	13C
1.78	0.002	Hbb	90Glu	1H
1.91	0.001	Hga	90Glu	1H
1.64	0.013	Hba	90Glu	1H
2.18	0.019	Hgb	90Glu	1H
4.92	0.011	Ha	90Glu	1H
55.88	0.069	Ca	90Glu	13C
116.90	0.069	N	90Glu	15N
7.76	0.005	H	90Glu	1H
173.90	0.000	C	91Ile	13C
130.03	0.184	N	91Ile	15N
41.35	0.033	Cb	91Ile	13C
14.07	0.032	Cd1	91Ile	13C
8.78	0.011	H	91Ile	1H
61.20	0.056	Ca	91Ile	13C
1.63	0.002	Hg1b	91Ile	1H
0.78	0.002	Hg1a	91Ile	1H
0.93	0.024	Hd1*	91Ile	1H
27.88	0.000	Cg1	91Ile	13C
17.90	0.045	Cg2	91Ile	13C
1.72	0.012	Hb	91Ile	1H
3.85	0.011	Ha	91Ile	1H
0.76	0.031	Hg2*	91Ile	1H
32.05	0.000	Cg	92Met	13C
173.98	0.000	C	92Met	13C
2.14	0.000	Hgb	92Met	1H
2.07	0.000	Hga	92Met	1H
30.13	0.017	Cb	92Met	13C
17.03	0.020	Ce	92Met	13C
2.07	0.025	He*	92Met	1H

2.30	0.001	Hbb	92Met	1H
1.33	0.003	Hba	92Met	1H
121.91	0.106	N	92Met	15N
7.89	0.004	H	92Met	1H
5.22	0.007	Ha	92Met	1H
51.83	0.077	Ca	92Met	13C
176.86	0.000	C	93Val	13C
62.28	0.068	Ca	93Val	13C
31.48	0.063	Cb	93Val	13C
22.82	0.184	Cgb	78Val	13C
4.32	0.006	Ha	93Val	1H
2.26	0.007	Hb	93Val	1H
20.25	0.056	Cga	78Val	13C
9.41	0.009	H	93Val	1H
124.94	0.101	N	93Val	15N
0.58	0.021	Hgb*	93Val	1H
0.16	0.029	Hga*	93Val	1H
174.20	0.000	C	94Ile	13C
119.56	0.015	N	94Ile	15N
8.97	0.008	H	94Ile	1H
17.55	0.054	Cg2	94Ile	13C
15.74	0.048	Cd1	94Ile	13C
60.66	0.039	Ca	94Ile	13C
39.05	0.043	Cb	94Ile	13C
28.00	0.000	Cg1	94Ile	13C
1.83	0.004	Hg1b	94Ile	1H
0.98	0.012	Hg2*	94Ile	1H
1.06	0.009	Hg1a	94Ile	1H
2.89	0.007	Hb	94Ile	1H
1.02	0.045	Hd1*	94Ile	1H
5.67	0.006	Ha	94Ile	1H
174.16	0.000	C	95Gly	13C
3.88	0.011	Hab	95Gly	1H
1.97	0.006	Haa	95Gly	1H
41.28	0.074	Ca	95Gly	13C
6.19	0.006	H	95Gly	1H
102.88	0.113	N	95Gly	15N
2.85	0.000	Haa	96Gly	1H
2.95	0.005	Hab	96Gly	1H
46.71	0.005	Ca	96Gly	13C
8.22	0.006	H	96Gly	1H
111.60	0.218	N	96Gly	15N

174.73	0.000	C	97Gly	13C
4.01	0.013	Hab	97Gly	1H
3.62	0.007	Haa	97Gly	1H
49.10	0.055	Ca	97Gly	13C
180.68	0.000	C	98Arg	13C
8.87	0.000	He	98Arg	1H
83.68	0.000	Ne	98Arg	15N
122.08	0.060	N	98Arg	15N
9.22	0.024	H	98Arg	1H
2.23	0.018	Hbb	98Arg	1H
29.68	0.072	Cb	98Arg	13C
58.41	0.106	Ca	98Arg	13C
2.11	0.020	Hba	98Arg	1H
1.81	0.003	Hga	98Arg	1H
1.90	0.002	Hgb	98Arg	1H
27.40	0.000	Cg	98Arg	13C
3.22	0.014	Hda	98Arg	1H
3.35	0.011	Hdb	98Arg	1H
4.28	0.008	Ha	98Arg	1H
43.05	0.040	Cd	98Arg	13C
178.59	0.000	C	99Val	13C
31.67	0.104	Cb	99Val	13C
21.84	0.035	Cgb	88Val	13C
17.99	0.042	Cga	88Val	13C
0.66	0.005	Hga*	99Val	1H
68.10	0.028	Ca	99Val	13C
0.99	0.007	Hgb*	99Val	1H
122.00	0.140	N	99Val	15N
3.73	0.019	Ha	99Val	1H
7.31	0.007	H	99Val	1H
1.72	0.018	Hb	99Val	1H
6.48	0.000	Hd*	100Tyr	1H
6.94	0.000	He*	100Tyr	1H
177.92	0.000	C	100Tyr	13C
2.84	0.014	Hbb	100Tyr	1H
2.37	0.004	Hba	100Tyr	1H
37.84	0.015	Cb	100Tyr	13C
60.37	0.023	Ca	100Tyr	13C
4.26	0.006	Ha	100Tyr	1H
119.44	0.066	N	100Tyr	15N
9.54	0.008	H	100Tyr	1H
178.13	0.000	C	101Glu	13C

116.04	0.131	N	101Glu	15N
36.12	0.000	Cg	101Glu	13C
8.08	0.015	H	101Glu	1H
2.33	0.004	Hga	101Glu	1H
2.42	0.003	Hgb	101Glu	1H
60.00	0.051	Ca	101Glu	13C
2.27	0.001	Hbb	101Glu	1H
2.19	0.008	Hba	101Glu	1H
3.74	0.002	Ha	101Glu	1H
29.67	0.000	Cb	101Glu	13C
32.66	0.000	Cb	102Gln	13C
36.40	0.000	Cg	102Gln	13C
4.71	0.000	Ha	102Gln	1H
177.16	0.000	C	102Gln	13C
57.96	0.102	Ca	102Gln	13C
114.15	0.224	N	102Gln	15N
7.19	0.009	H	102Gln	1H
176.89	0.000	C	103Phe	13C
6.93	0.000	He*	103Phe	1H
7.39	0.000	Hd*	103Phe	1H
7.99	0.003	H	103Phe	1H
113.08	0.029	N	103Phe	15N
60.30	0.033	Ca	103Phe	13C
3.09	0.007	Hbb	103Phe	1H
2.85	0.012	Hba	103Phe	1H
4.42	0.004	Ha	103Phe	1H
41.81	0.056	Cb	103Phe	13C
1.16	0.000	Hg	104Leu	1H
8.38	0.007	H	104Leu	1H
123.56	0.137	N	104Leu	15N
24.96	0.009	Cda	104Leu	13C
26.77	0.054	Cda	104Leu	13C
1.81	0.002	Hdb*	104Leu	1H
60.89	0.066	Ca	104Leu	13C
4.33	0.005	Ha	104Leu	1H
1.99	0.004	Hbb	104Leu	1H
1.50	0.002	Hba	104Leu	1H
38.78	0.035	Cb	104Leu	13C
0.93	0.011	Hda*	104Leu	1H
50.47	0.000	Cd	105Pro	13C
31.35	0.000	Cb	105Pro	13C
27.94	0.000	Cg	105Pro	13C

3.80	0.000	Hdb	105Pro	1H
3.42	0.000	Hda	105Pro	1H
1.95	0.000	Hgb	105Pro	1H
1.92	0.000	Hga	105Pro	1H
65.47	0.000	Ca	105Pro	13C
177.13	0.000	C	105Pro	13C
34.54	0.000	Cb	106Lys	13C
4.35	0.000	Ha	106Lys	1H
25.19	0.000	Cg	106Lys	13C
2.16	0.000	Hbb	106Lys	1H
1.82	0.000	Hba	106Lys	1H
41.74	0.000	Ce	106Lys	13C
29.44	0.000	Cd	106Lys	13C
1.51	0.000	Hdb	106Lys	1H
1.34	0.000	Hda	106Lys	1H
2.77	0.000	Heb	106Lys	1H
2.72	0.000	Hea	106Lys	1H
1.42	0.000	Hga	106Lys	1H
175.84	0.000	C	106Lys	13C
55.38	0.021	Ca	106Lys	13C
112.64	0.039	N	106Lys	15N
7.44	0.018	H	106Lys	1H
177.26	0.000	C	107Ala	13C
52.37	0.034	Ca	107Ala	13C
122.19	0.069	N	107Ala	15N
4.61	0.023	Ha	107Ala	1H
7.93	0.010	H	107Ala	1H
21.36	0.066	Cb	107Ala	13C
1.74	0.026	Hb*	107Ala	1H
174.82	0.012	C	108Gln	13C
6.89	0.035	He2a	108Gln	1H
112.70	0.016	Ne2	108Gln	15N
7.72	0.046	He2b	108Gln	1H
55.87	0.015	Ca	108Gln	13C
31.67	0.081	Cb	108Gln	13C
2.39	0.025	Hbb	108Gln	1H
2.17	0.022	Hba	108Gln	1H
4.60	0.023	Ha	108Gln	1H
118.33	0.060	N	108Gln	15N
9.23	0.019	H	108Gln	1H
2.49	0.017	Hga	108Gln	1H
2.58	0.023	Hgb	108Gln	1H

34.87	0.070	Cg	108Gln	13C
173.93	0.000	C	109Lys	13C
30.37	0.024	Cd	109Lys	13C
1.49	0.003	Hda	109Lys	1H
56.07	0.051	Ca	109Lys	13C
1.38	0.007	Hgb	109Lys	1H
120.38	0.112	N	109Lys	15N
2.23	0.007	Hbb	109Lys	1H
36.94	0.045	Cb	109Lys	13C
1.92	0.003	Hba	109Lys	1H
1.49	0.009	Hdb	109Lys	1H
7.79	0.006	H	109Lys	1H
2.75	0.017	Heb	109Lys	1H
5.72	0.016	Ha	109Lys	1H
1.10	0.006	Hga	109Lys	1H
25.95	0.025	Cg	109Lys	13C
2.51	0.020	Hea	109Lys	1H
42.59	0.046	Ce	109Lys	13C
174.71	0.000	C	110Leu	13C
121.77	0.062	N	110Leu	15N
25.12	0.076	Cdb	110Leu	13C
23.60	0.016	Cda	110Leu	13C
9.04	0.008	H	110Leu	1H
0.53	0.004	Hdb*	110Leu	1H
52.97	0.076	Ca	110Leu	13C
0.65	0.008	Hba	110Leu	1H
5.15	0.008	Ha	110Leu	1H
44.52	0.074	Cb	110Leu	13C
1.32	0.012	Hbb	110Leu	1H
-0.81	0.024	Hda*	110Leu	1H
174.85	0.000	C	111Tyr	13C
6.74	0.000	Hd*	111Tyr	1H
6.50	0.000	He*	111Tyr	1H
2.63	0.009	Hba	111Tyr	1H
3.27	0.006	Hbb	111Tyr	1H
38.30	0.136	Cb	111Tyr	13C
56.08	0.076	Ca	111Tyr	13C
5.24	0.012	Ha	111Tyr	1H
9.49	0.010	H	111Tyr	1H
122.48	0.194	N	111Tyr	15N
1.08	0.000	Hg	112Leu	1H
9.60	0.018	H	112Leu	1H

123.35	0.167	N	112Leu	15N
26.06	0.047	Cdb	112Leu	13C
22.09	0.051	Cda	112Leu	13C
52.84	0.090	Ca	112Leu	13C
0.35	0.032	Hba	112Leu	1H
1.48	0.012	Hbb	112Leu	1H
0.30	0.021	Hdb*	112Leu	1H
44.69	0.035	Cb	112Leu	13C
-0.03	0.015	Hda*	112Leu	1H
5.36	0.006	Ha	112Leu	1H
173.17	0.000	C	113Thr	13C
1.40	0.000	Hg2*	113Thr	1H
59.98	0.017	Ca	113Thr	13C
69.13	0.000	Cb	113Thr	13C
5.14	0.018	Ha	113Thr	1H
3.96	0.002	Hb	113Thr	1H
6.69	0.000	Hd2	114His	1H
29.39	0.000	Cb	114His	13C
174.97	0.000	C	114His	13C
9.25	0.012	H	114His	1H
126.41	0.073	N	114His	15N
4.86	0.003	Ha	114His	1H
54.19	0.007	Ca	114His	13C
176.68	0.000	C	115Ile	13C
39.87	0.022	Cb	115Ile	13C
60.81	0.002	Ca	115Ile	13C
12.86	0.012	Cd1	115Ile	13C
0.86	0.007	Hg1b	115Ile	1H
17.39	0.111	Cg2	115Ile	13C
-0.03	0.016	Hg1a	115Ile	1H
4.05	0.003	Ha	115Ile	1H
26.69	0.000	Cg1	115Ile	13C
0.78	0.018	Hb	115Ile	1H
9.12	0.011	H	115Ile	1H
126.98	0.196	N	115Ile	15N
-0.92	0.014	Hd1*	115Ile	1H
0.18	0.011	Hg2*	115Ile	1H
173.68	0.000	C	116Asp	13C
53.36	0.088	Ca	116Asp	13C
4.67	0.032	Ha	116Asp	1H
129.90	0.123	N	116Asp	15N
2.55	0.017	Hba	116Asp	1H

2.74	0.030	Hbb	116Asp	1H
8.36	0.030	H	116Asp	1H
38.53	0.107	Cb	116Asp	13C
174.43	0.000	C	117Ala	13C
20.48	0.000	Cb	117Ala	13C
51.41	0.196	Ca	117Ala	13C
4.44	0.009	Ha	117Ala	1H
0.49	0.002	Hb*	117Ala	1H
124.21	0.126	N	117Ala	15N
7.75	0.014	H	117Ala	1H
36.58	0.000	Cg	118Glu	13C
2.20	0.002	Hgb	118Glu	1H
8.59	0.004	H	118Glu	1H
124.09	0.033	N	118Glu	15N
2.03	0.024	Hga	118Glu	1H
55.39	0.172	Ca	118Glu	13C
4.60	0.003	Ha	118Glu	1H
1.87	0.002	Hba	118Glu	1H
1.99	0.002	Hbb	118Glu	1H
29.22	0.000	Cb	118Glu	13C
174.75	0.000	C	119Val	13C
35.37	0.060	Cb	119Val	13C
118.69	0.109	N	119Val	15N
8.16	0.011	H	119Val	1H
22.34	0.045	Cgb	93Val	13C
20.39	0.029	Cga	93Val	13C
58.60	0.048	Ca	119Val	13C
2.14	0.003	Hb	119Val	1H
0.84	0.002	Hga*	119Val	1H
0.94	0.002	Hgb*	119Val	1H
4.65	0.005	Ha	119Val	1H
1.92	0.000	Hba	120Glu	1H
175.69	0.000	C	120Glu	13C
30.10	0.000	Cb	120Glu	13C
36.30	0.000	Cg	120Glu	13C
2.29	0.000	Hga	120Glu	1H
2.33	0.012	Hgb	120Glu	1H
8.40	0.007	H	120Glu	1H
123.93	0.118	N	120Glu	15N
1.98	0.029	Hbb	120Glu	1H
4.37	0.009	Ha	120Glu	1H
56.28	0.010	Ca	120Glu	13C

4.94	0.000	Hab	121Gly	1H
172.61	0.000	C	121Gly	13C
3.78	0.005	Haa	121Gly	1H
46.02	0.062	Ca	121Gly	13C
8.40	0.010	H	121Gly	1H
106.49	0.084	N	121Gly	15N
116.33	0.158	N	122Asp	15N
52.51	0.017	Ca	122Asp	13C
8.59	0.011	H	122Asp	1H
4.92	0.003	Ha	122Asp	1H
2.70	0.005	Hba	122Asp	1H
41.82	0.123	Cb	122Asp	13C
3.19	0.018	Hbb	122Asp	1H
7.45	0.000	H	123Thr	1H
113.82	0.000	N	123Thr	15N
8.34	0.000	H	124His	1H
117.81	0.000	N	124His	15N
173.66	0.000	C	124His	13C
7.40	0.000	Hd2	124His	1H
56.35	0.041	Ca	124His	13C
5.49	0.003	Ha	124His	1H
2.74	0.009	Hba	124His	1H
3.14	0.003	Hbb	124His	1H
33.24	0.222	Cb	124His	13C
6.89	0.000	Hd*	125Phe	1H
7.07	0.000	He*	125Phe	1H
41.28	0.000	Cb	125Phe	13C
2.82	0.004	Hba	125Phe	1H
2.91	0.001	Hbb	125Phe	1H
124.82	0.022	N	125Phe	15N
56.63	0.085	Ca	125Phe	13C
9.14	0.021	H	125Phe	1H
4.47	0.002	Ha	125Phe	1H
1.53	0.005	Hda	126Pro	1H
27.23	0.028	Cg	126Pro	13C
62.52	0.053	Ca	126Pro	13C
1.41	0.004	Hgb	126Pro	1H
1.10	0.005	Hga	126Pro	1H
3.19	0.008	Hdb	126Pro	1H
49.90	0.033	Cd	126Pro	13C
2.17	0.015	Hbb	126Pro	1H
31.83	0.010	Cb	126Pro	13C

1.66	0.023	Hba	126Pro	1H
4.29	0.020	Ha	126Pro	1H
54.58	0.056	Ca	127Asp	13C
117.61	0.080	N	127Asp	15N
4.31	0.029	Ha	127Asp	1H
8.08	0.025	H	127Asp	1H
2.56	0.015	Hbb	127Asp	1H
2.38	0.011	Hba	127Asp	1H
40.56	0.121	Cb	127Asp	13C
6.31	0.000	He*	128Tyr	1H
6.82	0.000	Hd*	128Tyr	1H
4.79	0.002	Ha	128Tyr	1H
55.60	0.063	Ca	128Tyr	13C
2.76	0.001	Hba	128Tyr	1H
3.03	0.002	Hbb	128Tyr	1H
7.48	0.026	H	128Tyr	1H
118.97	0.248	N	128Tyr	15N
39.40	0.036	Cb	128Tyr	13C
29.61	0.000	Cb	129Glu	13C
1.92	0.000	Hba	129Glu	1H
173.34	0.000	C	129Glu	13C
2.15	0.002	Hga	129Glu	1H
36.15	0.000	Cg	129Glu	13C
2.30	0.001	Hgb	129Glu	1H
123.02	0.102	N	129Glu	15N
8.77	0.004	H	129Glu	1H
53.17	0.037	Ca	129Glu	13C
4.60	0.002	Ha	129Glu	1H
178.28	0.000	C	130Pro	13C
51.03	0.000	Cd	130Pro	13C
3.80	0.025	Hda	130Pro	1H
3.83	0.000	Hdb	130Pro	1H
2.04	0.003	Hgb	130Pro	1H
65.86	0.029	Ca	130Pro	13C
2.04	0.003	Hba	130Pro	1H
27.20	0.000	Cg	130Pro	13C
1.78	0.002	Hga	130Pro	1H
32.09	0.000	Cb	130Pro	13C
2.40	0.002	Hbb	130Pro	1H
4.34	0.004	Ha	130Pro	1H
176.91	0.000	C	131Asp	13C
2.60	0.008	Hba	131Asp	1H

2.71	0.004	Hbb	131Asp	1H
40.14	0.085	Cb	131Asp	13C
4.57	0.005	Ha	131Asp	1H
56.38	0.088	Ca	131Asp	13C
9.07	0.011	H	131Asp	1H
114.74	0.080	N	131Asp	15N
174.91	0.000	C	132Asp	13C
118.07	0.100	N	132Asp	15N
55.08	0.096	Ca	132Asp	13C
8.17	0.009	H	132Asp	1H
4.55	0.003	Ha	132Asp	1H
2.32	0.006	Hba	132Asp	1H
41.38	0.083	Cb	132Asp	13C
2.87	0.017	Hbb	132Asp	1H
7.84	0.000	He3	133Trp	1H
7.86	0.000	Hd1	133Trp	1H
128.17	0.000	Ne1	133Trp	15N
10.35	0.000	He1	133Trp	1H
173.83	0.000	C	133Trp	13C
129.21	0.000	Cd1	133Trp	13C
119.56	0.081	N	133Trp	15N
56.13	0.041	Ca	133Trp	13C
7.80	0.012	H	133Trp	1H
2.92	0.005	Hba	133Trp	1H
34.09	0.079	Cb	133Trp	13C
3.15	0.006	Hbb	133Trp	1H
4.89	0.006	Ha	133Trp	1H
2.07	0.000	Hga	134Glu	1H
175.69	0.000	C	134Glu	13C
35.62	0.000	Cg	134Glu	13C
2.13	0.000	Hgb	134Glu	1H
32.49	0.000	Cb	134Glu	13C
1.84	0.002	Hba	134Glu	1H
2.06	0.001	Hbb	134Glu	1H
54.34	0.115	Ca	134Glu	13C
4.69	0.022	Ha	134Glu	1H
122.46	0.139	N	134Glu	15N
9.58	0.007	H	134Glu	1H
62.19	0.000	Cb	135Ser	13C
3.80	0.000	Hba	135Ser	1H
3.89	0.002	Hbb	135Ser	1H
4.86	0.019	Ha	135Ser	1H

58.62	0.029	Ca	135Ser	13C
121.34	0.029	N	135Ser	15N
9.04	0.010	H	135Ser	1H
175.58	0.000	C	136Val	13C
121.48	0.135	N	136Val	15N
9.08	0.009	H	136Val	1H
61.07	0.076	Ca	136Val	13C
4.67	0.007	Ha	136Val	1H
32.50	0.099	Cb	136Val	13C
22.05	0.155	Cga	99Val	13C
24.47	0.108	Cgb	99Val	13C
2.42	0.017	Hb	136Val	1H
0.91	0.028	Hgb*	136Val	1H
0.80	0.033	Hga*	136Val	1H
2.62	0.000	Hba	137Phe	1H
7.32	0.000	He*	137Phe	1H
173.11	0.000	C	137Phe	13C
7.18	0.000	Hd*	137Phe	1H
58.57	0.041	Ca	137Phe	13C
4.72	0.002	Ha	137Phe	1H
123.36	0.068	N	137Phe	15N
7.87	0.017	H	137Phe	1H
42.92	0.025	Cb	137Phe	13C
3.45	0.002	Hbb	137Phe	1H
173.09	0.000	C	138Ser	13C
7.51	0.031	H	138Ser	1H
119.41	0.208	N	138Ser	15N
57.13	0.015	Ca	138Ser	13C
5.26	0.005	Ha	138Ser	1H
3.43	0.005	Hba	138Ser	1H
3.58	0.006	Hbb	138Ser	1H
64.84	0.028	Cb	138Ser	13C
4.20	0.001	Ha	139Glu	1H
2.14	0.003	Hbb	139Glu	1H
1.85	0.000	Hba	139Glu	1H
172.85	0.000	C	139Glu	13C
2.13	0.008	Hgb	139Glu	1H
1.68	0.003	Hga	139Glu	1H
35.01	0.000	Cb	139Glu	13C
37.30	0.065	Cg	139Glu	13C
56.32	0.070	Ca	139Glu	13C
125.05	0.131	N	139Glu	15N

8.69	0.004	H	139Glu	1H
6.83	0.000	Hd*	140Phe	1H
7.11	0.000	He*	140Phe	1H
174.03	0.000	C	140Phe	13C
129.35	0.078	N	140Phe	15N
8.68	0.031	H	140Phe	1H
58.68	0.025	Ca	140Phe	13C
2.80	0.002	Hbb	140Phe	1H
4.12	0.005	Ha	140Phe	1H
2.68	0.001	Hba	140Phe	1H
40.67	0.011	Cb	140Phe	13C
2.28	0.000	Hbb	141His	1H
172.15	0.000	C	141His	13C
119.31	0.000	Cd2	141His	13C
6.09	0.001	Hd2	141His	1H
0.94	0.003	Hba	141His	1H
123.19	0.173	N	141His	15N
54.24	0.034	Ca	141His	13C
7.96	0.025	H	141His	1H
31.13	0.036	Cb	141His	13C
4.09	0.016	Ha	141His	1H
175.84	0.000	C	142Asp	13C
53.25	0.072	Ca	142Asp	13C
4.50	0.007	Ha	142Asp	1H
120.36	0.161	N	142Asp	15N
7.99	0.023	H	142Asp	1H
2.78	0.021	Hbb	142Asp	1H
2.38	0.017	Hba	142Asp	1H
42.38	0.117	Cb	142Asp	13C
176.70	0.000	C	143Ala	13C
122.56	0.152	N	143Ala	15N
18.96	0.029	Cb	143Ala	13C
52.73	0.002	Ca	143Ala	13C
8.09	0.025	H	143Ala	1H
4.01	0.038	Ha	143Ala	1H
1.23	0.014	Hb*	143Ala	1H
175.67	0.000	C	144Asp	13C
53.17	0.020	Ca	144Asp	13C
41.43	0.000	Cb	144Asp	13C
3.20	0.015	Hbb	144Asp	1H
2.80	0.013	Hba	144Asp	1H
4.61	0.019	Ha	144Asp	1H

8.91	0.021	H	144Asp	1H
120.25	0.114	N	144Asp	15N
54.94	0.000	Ca	145Ala	13C
178.51	0.000	C	145Ala	13C
18.43	0.024	Cb	145Ala	13C
4.06	0.012	Ha	145Ala	1H
1.39	0.036	Hb*	145Ala	1H
8.19	0.008	H	145Ala	1H
117.66	0.075	N	145Ala	15N
31.06	0.000	Cb	146Gln	13C
174.64	0.000	C	146Gln	13C
113.04	0.035	N	146Gln	15N
2.01	0.000	Hbb	146Gln	1H
9.79	0.001	He2b	146Gln	1H
7.08	0.002	He2a	146Gln	1H
8.02	0.002	H	146Gln	1H
34.90	0.067	Cg	146Gln	13C
112.83	0.015	Ne2	146Gln	15N
1.99	0.015	Hba	146Gln	1H
2.31	0.008	Hgb	146Gln	1H
2.31	0.008	Hga	146Gln	1H
56.61	0.172	Ca	146Gln	13C
4.38	0.019	Ha	146Gln	1H
7.02	0.000	Hd2a	147Asn	1H
8.42	0.000	Hd2b	147Asn	1H
174.20	0.000	C	147Asn	13C
116.77	0.021	Nd2	147Asn	15N
119.54	0.069	N	147Asn	15N
5.28	0.013	Ha	147Asn	1H
52.89	0.133	Ca	147Asn	13C
2.92	0.007	Hbb	147Asn	1H
2.42	0.013	Hba	147Asn	1H
8.14	0.014	H	147Asn	1H
41.13	0.000	Cb	147Asn	13C
172.89	0.000	C	148Ser	13C
117.40	0.120	N	148Ser	15N
8.95	0.012	H	148Ser	1H
61.38	0.143	Ca	148Ser	13C
3.92	0.002	Hbb	148Ser	1H
3.83	0.005	Hba	148Ser	1H
63.43	0.000	Cb	148Ser	13C
4.03	0.005	Ha	148Ser	1H

173.31	0.000	C	149His	13C
117.67	0.168	N	149His	15N
55.19	0.021	Ca	149His	13C
35.30	0.032	Cb	149His	13C
2.27	0.003	Hba	149His	1H
7.06	0.003	H	149His	1H
4.94	0.043	Ha	149His	1H
3.17	0.015	Hbb	149His	1H
173.10	0.000	C	150Ser	13C
64.05	0.000	Cb	150Ser	13C
4.16	0.004	Hbb	150Ser	1H
4.36	0.004	Ha	150Ser	1H
4.06	0.012	Hba	150Ser	1H
58.72	0.095	Ca	150Ser	13C
113.49	0.111	N	150Ser	15N
8.68	0.009	H	150Ser	1H
171.93	0.000	C	151Tyr	13C
115.12	0.314	N	151Tyr	15N
7.65	0.004	H	151Tyr	1H
54.81	0.016	Ca	151Tyr	13C
39.08	0.073	Cb	151Tyr	13C
1.84	0.011	Hba	151Tyr	1H
5.28	0.022	Ha	151Tyr	1H
2.59	0.030	Hbb	151Tyr	1H
29.97	0.000	Cb	152Cys	13C
54.87	0.000	Ca	152Cys	13C
174.33	0.000	C	152Cys	13C
8.24	0.008	H	152Cys	1H
118.16	0.162	N	152Cys	15N
55.44	0.000	Ca	153Phe	13C
175.02	0.000	C	153Phe	13C
5.05	0.002	Ha	153Phe	1H
1.99	0.009	Hba	153Phe	1H
8.45	0.023	H	153Phe	1H
128.73	0.073	N	153Phe	15N
40.41	0.000	Cb	153Phe	13C
2.41	0.007	Hbb	153Phe	1H
36.79	0.000	Cg	154Glu	13C
2.20	0.000	Hga	154Glu	1H
2.50	0.000	Hgb	154Glu	1H
9.80	0.025	H	154Glu	1H
35.03	0.000	Cb	154Glu	13C

124.21	0.177	N	154Glu	15N
1.99	0.001	Hba	154Glu	1H
2.12	0.004	Hbb	154Glu	1H
5.52	0.002	Ha	154Glu	1H
54.49	0.000	Ca	154Glu	13C
27.58	0.000	Cg1	155Ile	13C
8.63	0.000	H	155Ile	1H
124.13	0.000	N	155Ile	15N
174.87	0.000	C	155Ile	13C
0.98	0.002	Hg1a	155Ile	1H
1.91	0.003	Hg1b	155Ile	1H
40.45	0.093	Cb	155Ile	13C
17.25	0.029	Cg2	155Ile	13C
1.65	0.003	Hb	155Ile	1H
60.16	0.038	Ca	155Ile	13C
5.28	0.005	Ha	155Ile	1H
13.43	0.023	Cd1	155Ile	13C
0.63	0.030	Hd1*	155Ile	1H
0.40	0.031	Hg2*	155Ile	1H
175.70	0.000	C	156Leu	13C
25.35	0.077	Cdb	156Leu	13C
28.29	0.117	Cg	156Leu	13C
53.35	0.094	Ca	156Leu	13C
9.34	0.016	H	156Leu	1H
126.33	0.132	N	156Leu	15N
1.40	0.027	Hba	156Leu	1H
1.69	0.015	Hbb	156Leu	1H
0.84	0.007	Hdb*	156Leu	1H
26.28	0.053	Cda	156Leu	13C
45.55	0.076	Cb	156Leu	13C
5.69	0.008	Ha	156Leu	1H
1.50	0.020	Hg	156Leu	1H
0.58	0.021	Hda*	156Leu	1H
175.93	0.000	C	157Glu	13C
37.19	0.000	Cg	157Glu	13C
2.34	0.015	Hgb	157Glu	1H
54.64	0.074	Ca	157Glu	13C
2.29	0.033	Hga	157Glu	1H
1.91	0.013	Hba	157Glu	1H
2.15	0.018	Hbb	157Glu	1H
33.59	0.081	Cb	157Glu	13C
5.39	0.020	Ha	157Glu	1H

119.86	0.052	N	157Glu	15N
9.37	0.014	H	157Glu	1H
176.04	0.000	C	158Arg	13C
6.96	0.017	He	158Arg	1H
102.91	17.802	Ne	158Arg	15N
43.01	0.063	Cd	158Arg	13C
57.30	0.076	Ca	158Arg	13C
1.26	0.005	Hgb	158Arg	1H
27.31	0.048	Cg	158Arg	13C
1.49	0.004	Hbb	158Arg	1H
1.14	0.007	Hba	158Arg	1H
30.60	0.063	Cb	158Arg	13C
3.39	0.025	Ha	158Arg	1H
0.75	0.008	Hga	158Arg	1H
2.75	0.021	Hdb	158Arg	1H
2.75	0.021	Hda	158Arg	1H
126.63	0.122	N	158Arg	15N
8.26	0.009	H	158Arg	1H
43.39	0.070	Cd	159Arg	13C
58.56	0.082	Ca	159Arg	13C
3.12	0.008	Hdb	159Arg	1H
1.50	0.026	Hgb	159Arg	1H
1.40	0.040	Hga	159Arg	1H
1.38	0.020	Hba	159Arg	1H
3.11	0.018	Hda	159Arg	1H
3.97	0.031	Ha	159Arg	1H
131.35	0.169	N	159Arg	15N
1.71	0.026	Hbb	159Arg	1H
8.00	0.010	H	159Arg	1H
28.46	0.065	Cg	159Arg	13C
31.18	0.137	Cb	159Arg	13C

8.1.2 Chemical shift assignments of EcDHFR: NADP+: Folate complex with 17 % methanol co-solvent

Table 8.1.2 Average chemical shifts (ppm) of nuclei in EcDHFR: $NADP^+$: Folate complex under the standard NMR buffer conditions in the presence of 17% methanol co-solvent (by final volume) from nuclear magnetic resonance spectroscopy measured at 298.3 K. Assign Name in the colour red refers to tentative chemical shift assignments for ligand and co-factor, for which assignment confidence is low.

17 % Methanol chemical Shift (ppm)	SD	Assign Name	Residue	Isotope
171.56	0.000	C	1Met	13C
2.35	0.009	Hbb	1Met	1H
55.19	0.025	Ca	1Met	13C
32.70	0.004	Cb	1Met	13C
2.29	0.019	Hba	1Met	1H
4.17	0.016	Ha	1Met	1H
2.65	0.013	Hgb	1Met	1H
2.56	0.012	Hga	1Met	1H
30.18	0.042	Cg	1Met	13C
0.99	0.000	Hg1a	2Ile	1H
29.07	0.000	Cg1	2Ile	13C
173.91	0.000	C	2Ile	13C
1.80	0.017	Hg1b	2Ile	1H
13.90	0.024	Cd1	2Ile	13C
0.98	0.010	Hd1*	2Ile	1H
61.28	0.076	Ca	2Ile	13C
124.60	0.153	N	2Ile	15N
39.22	0.147	Cb	2Ile	13C
9.45	0.019	H	2Ile	1H
4.59	0.013	Ha	2Ile	1H
1.93	0.012	Hb	2Ile	1H
17.96	0.084	Cg2	2Ile	13C
0.88	0.007	Hg2*	2Ile	1H
173.54	0.000	C	3Ser	13C

125.93	0.044	N	3Ser	15N
9.35	0.032	H	3Ser	1H
3.76	0.006	Hba	3Ser	1H
56.17	0.047	Ca	3Ser	13C
4.17	0.013	Hbb	3Ser	1H
5.95	0.008	Ha	3Ser	1H
65.43	0.059	Cb	3Ser	13C
175.15	0.000	C	4Leu	13C
29.73	0.000	Cg	4Leu	13C
1.89	0.013	Hg	4Leu	1H
25.47	0.000	Cda	4Leu	13C
26.27	0.078	Cdb	4Leu	13C
0.92	0.007	Hda*	4Leu	1H
1.82	0.007	Hbb	4Leu	1H
0.95	0.012	Hdb*	4Leu	1H
1.63	0.009	Hba	4Leu	1H
121.80	0.045	N	4Leu	15N
43.70	0.073	Cb	4Leu	13C
53.71	0.059	Ca	4Leu	13C
8.52	0.031	H	4Leu	1H
5.55	0.012	Ha	4Leu	1H
172.22	0.000	C	5Ile	13C
2.30	0.001	Hg1b	5Ile	1H
27.65	0.000	Cg1	5Ile	13C
2.20	0.003	Hg1a	5Ile	1H
43.03	0.100	Cb	5Ile	13C
120.19	0.045	N	5Ile	15N
1.19	0.017	Hb	5Ile	1H
15.32	0.066	Cg2	5Ile	13C
8.54	0.030	H	5Ile	1H
16.42	0.054	Cd1	5Ile	13C
57.91	0.068	Ca	5Ile	13C
1.14	0.007	Hd1*	5Ile	1H
0.35	0.008	Hg2*	5Ile	1H
5.99	0.013	Ha	5Ile	1H
175.06	0.000	C	6Ala	13C
25.78	0.058	Cb	6Ala	13C
126.42	0.061	N	6Ala	15N
52.61	0.035	Ca	6Ala	13C
0.63	0.009	Hb*	6Ala	1H
4.94	0.010	Ha	6Ala	1H
8.60	0.036	H	6Ala	1H

175.12	0.000	C	7Ala	13C
50.43	0.046	Ca	7Ala	13C
4.98	0.020	Ha	7Ala	1H
20.95	0.062	Cb	7Ala	13C
1.44	0.007	Hb*	7Ala	1H
175.19	0.000	C	8Leu	13C
28.96	0.062	Cg	8Leu	13C
25.62	0.030	Cda	8Leu	13C
1.34	0.005	Hg	8Leu	1H
53.95	0.014	Ca	8Leu	13C
4.72	0.019	Ha	8Leu	1H
1.33	0.007	Hba	8Leu	1H
0.26	0.006	Hda*	8Leu	1H
1.46	0.004	Hbb	8Leu	1H
123.39	0.061	N	8Leu	15N
9.13	0.040	H	8Leu	1H
45.43	0.051	Cb	8Leu	13C
26.15	0.057	Cdb	8Leu	13C
0.40	0.005	Hdb*	8Leu	1H
175.95	0.000	C	9Ala	13C
125.68	0.071	N	9Ala	15N
8.47	0.032	H	9Ala	1H
49.75	0.045	Ca	9Ala	13C
5.04	0.013	Ha	9Ala	1H
19.33	0.057	Cb	9Ala	13C
1.44	0.006	Hb*	9Ala	1H
177.77	0.000	C	10Val	13C
31.53	0.175	Cb	10Val	13C
64.99	0.047	Ca	10Val	13C
2.14	0.011	Hb	10Val	1H
118.02	0.050	N	10Val	15N
21.39	0.044	Cga	10Val	13C
3.76	0.005	Ha	10Val	1H
7.56	0.033	H	10Val	1H
0.99	0.010	Hga*	10Val	1H
23.17	0.047	Cgb	10Val	13C
1.01	0.005	Hgb*	10Val	1H
174.71	0.000	C	11Asp	13C
122.77	0.056	N	11Asp	15N
55.95	0.071	Ca	11Asp	13C
4.35	0.007	Ha	11Asp	1H
9.05	0.022	H	11Asp	1H

2.88	0.013	Hba	11Asp	1H
3.10	0.005	Hbb	11Asp	1H
38.96	0.029	Cb	11Asp	13C
28.24	0.000	Cg	12Arg	13C
43.50	0.000	Cd	12Arg	13C
2.25	0.000	Hba	12Arg	1H
3.42	0.000	Hdb	12Arg	1H
83.13	0.000	Ne	12Arg	15N
7.17	0.000	He	12Arg	1H
27.38	0.000	Cb	12Arg	13C
175.78	0.000	C	12Arg	13C
1.76	0.002	Hgb	12Arg	1H
1.60	0.010	Hga	12Arg	1H
3.22	0.007	Hda	12Arg	1H
2.55	0.012	Hbb	12Arg	1H
106.91	0.062	N	12Arg	15N
8.43	0.021	H	12Arg	1H
57.44	0.075	Ca	12Arg	13C
3.70	0.008	Ha	12Arg	1H
176.80	0.000	C	13Val	13C
21.91	0.078	Cga	13Val	13C
32.82	0.119	Cb	13Val	13C
0.93	0.006	Hga*	13Val	1H
1.92	0.005	Hb	13Val	1H
65.52	0.055	Ca	13Val	13C
120.56	0.036	N	13Val	15N
3.59	0.007	Ha	13Val	1H
7.07	0.025	H	13Val	1H
23.11	0.054	Cgb	13Val	13C
1.19	0.007	Hgb*	13Val	1H
0.74	0.000	Hg1a	14Ile	1H
41.95	0.012	Cb	14Ile	13C
14.77	0.072	Cd1	14Ile	13C
59.94	0.014	Ca	14Ile	13C
2.13	0.005	Hb	14Ile	1H
17.66	0.020	Cg2	14Ile	13C
0.46	0.007	Hd1*	14Ile	1H
1.18	0.008	Hg2*	14Ile	1H
5.43	0.012	Ha	14Ile	1H
26.42	0.131	Cg1	14Ile	13C
169.76	0.000	C	15Gly	13C
109.42	0.050	N	15Gly	15N

7.52	0.028	H	15Gly	1H
4.47	0.009	Hab	15Gly	1H
45.83	0.099	Ca	15Gly	13C
4.18	0.020	Haa	15Gly	1H
174.67	0.000	C	16Met	13C
55.39	0.000	Ca	16Met	13C
34.54	0.000	Cb	16Met	13C
4.68	0.028	Ha	16Met	1H
18.40	0.068	Ce	16Met	13C
1.95	0.001	He*	16Met	1H
119.31	0.069	N	16Met	15N
8.53	0.030	H	16Met	1H
27.31	0.000	Cb	17Glu	13C
36.60	0.000	Cg	17Glu	13C
175.33	0.000	C	17Glu	13C
173.39	0.000	C	18Asn	13C
114.30	0.034	N	18Asn	15N
9.44	0.028	H	18Asn	1H
54.07	0.049	Ca	18Asn	13C
4.21	0.003	Ha	18Asn	1H
6.71	0.024	Hd2a	18Asn	1H
38.75	0.073	Cb	18Asn	13C
7.49	0.020	Hd2b	18Asn	1H
2.46	0.018	Hba	18Asn	1H
3.07	0.015	Hbb	18Asn	1H
109.92	0.187	Nd2	18Asn	15N
176.03	0.000	C	19Ala	13C
50.47	0.084	Ca	19Ala	13C
4.45	0.006	Ha	19Ala	1H
120.86	0.078	N	19Ala	15N
7.68	0.029	H	19Ala	1H
21.49	0.077	Cb	19Ala	13C
1.24	0.006	Hb*	19Ala	1H
175.17	0.000	C	20Met	13C
40.71	0.000	Cb	20Met	13C
52.23	0.000	Ca	20Met	13C
119.68	0.048	N	20Met	15N
8.28	0.027	H	20Met	1H
17.12	0.055	Ce	20Met	13C
1.93	0.002	He*	20Met	1H
173.64	0.000	C	21Pro	13C
173.73	0.000	C	22Trp	13C

116.07	0.031	N	22Trp	15N
7.44	0.005	H	22Trp	1H
132.74	0.077	Ne1	22Trp	15N
10.50	0.017	He1	22Trp	1H
7.58	0.000	Hd2b	23Asn	1H
172.43	0.000	C	23Asn	13C
112.29	0.000	Nd2	23Asn	15N
6.83	0.000	Hd2a	23Asn	1H
117.20	0.020	N	23Asn	15N
9.01	0.002	H	23Asn	1H
40.24	0.133	Cb	23Asn	13C
2.60	0.005	Hba	23Asn	1H
2.89	0.006	Hbb	23Asn	1H
4.87	0.012	Ha	23Asn	1H
53.52	0.056	Ca	23Asn	13C
173.94	0.000	C	24Leu	13C
26.62	0.004	Cg	24Leu	13C
1.49	0.014	Hg	24Leu	1H
125.04	0.073	N	24Leu	15N
25.91	0.084	Cdb	24Leu	13C
9.48	0.030	H	24Leu	1H
26.63	0.048	Cda	24Leu	13C
51.23	0.051	Ca	24Leu	13C
1.07	0.005	Hba	24Leu	1H
0.80	0.010	Hdb*	24Leu	1H
1.61	0.014	Hbb	24Leu	1H
5.26	0.015	Ha	24Leu	1H
0.39	0.005	Hda*	24Leu	1H
44.52	0.100	Cb	24Leu	13C
179.46	0.000	C	25Pro	13C
27.86	0.000	Cg	25Pro	13C
31.24	0.047	Cb	25Pro	13C
3.70	0.007	Hdb	25Pro	1H
1.74	0.006	Hba	25Pro	1H
1.98	0.004	Hgb	25Pro	1H
1.98	0.018	Hga	25Pro	1H
50.52	0.035	Cd	25Pro	13C
2.41	0.029	Hbb	25Pro	1H
3.44	0.010	Hda	25Pro	1H
65.38	0.064	Ca	25Pro	13C
4.53	0.008	Ha	25Pro	1H
181.44	0.000	C	26Ala	13C

55.15	0.008	Ca	26Ala	13C
4.14	0.002	Ha	26Ala	1H
19.08	0.094	Cb	26Ala	13C
1.26	0.008	Hb*	26Ala	1H
120.11	0.051	N	26Ala	15N
9.21	0.029	H	26Ala	1H
177.37	0.000	C	27Asp	13C
56.26	0.157	Ca	27Asp	13C
4.89	0.009	Ha	27Asp	1H
2.91	0.014	Hbb	27Asp	1H
118.35	0.059	N	27Asp	15N
2.08	0.011	Hba	27Asp	1H
43.56	0.090	Cb	27Asp	13C
7.41	0.030	H	27Asp	1H
179.01	0.000	C	28Leu	13C
27.04	0.000	Cg	28Leu	13C
1.46	0.004	Hg	28Leu	1H
121.22	0.044	N	28Leu	15N
57.53	0.122	Ca	28Leu	13C
1.65	0.010	Hbb	28Leu	1H
1.29	0.009	Hba	28Leu	1H
7.59	0.036	H	28Leu	1H
3.95	0.009	Ha	28Leu	1H
40.71	0.066	Cb	28Leu	13C
22.08	0.064	Cda	28Leu	13C
0.06	0.007	Hda*	28Leu	1H
24.82	0.063	Cdb	28Leu	13C
0.50	0.005	Hdb*	28Leu	1H
180.37	0.000	C	29Ala	13C
1.19	0.009	Hb*	29Ala	1H
17.39	0.058	Cb	29Ala	13C
55.03	0.044	Ca	29Ala	13C
4.14	0.027	Ha	29Ala	1H
120.66	0.033	N	29Ala	15N
7.84	0.034	H	29Ala	1H
130.50	0.000	Ne1	30Trp	15N
10.52	0.000	He1	30Trp	1H
6.95	0.000	Hd1	30Trp	1H
177.84	0.000	C	30Trp	13C
6.72	0.023	He3	30Trp	1H
3.44	0.015	Hbb	30Trp	1H
60.07	0.081	Ca	30Trp	13C

2.69	0.007	Hba	30Trp	1H
124.04	0.040	N	30Trp	15N
4.00	0.007	Ha	30Trp	1H
29.06	0.090	Cb	30Trp	13C
7.43	0.039	H	30Trp	1H
6.46	0.000	He*	31Phe	1H
178.39	0.000	C	31Phe	13C
2.62	0.015	Hba	31Phe	1H
3.23	0.009	Hbb	31Phe	1H
123.44	0.076	N	31Phe	15N
38.12	0.139	Cb	31Phe	13C
9.04	0.034	H	31Phe	1H
61.29	0.063	Ca	31Phe	13C
3.56	0.007	Ha	31Phe	1H
177.81	0.000	C	32Lys	13C
42.16	0.000	Ce	32Lys	13C
2.80	0.015	Hea	32Lys	1H
1.81	0.011	Hba	32Lys	1H
24.91	0.000	Cg	32Lys	13C
1.90	0.009	Hbb	32Lys	1H
1.14	0.003	Hga	32Lys	1H
29.94	0.000	Cd	32Lys	13C
32.19	0.159	Cb	32Lys	13C
2.81	0.004	Heb	32Lys	1H
1.64	0.016	Hda	32Lys	1H
1.35	0.006	Hgb	32Lys	1H
1.64	0.016	Hdb	32Lys	1H
124.33	0.042	N	32Lys	15N
8.67	0.030	H	32Lys	1H
60.24	0.091	Ca	32Lys	13C
3.36	0.013	Ha	32Lys	1H
85.56	0.000	Ne	33Arg	15N
178.26	0.000	C	33Arg	13C
7.12	0.041	He	33Arg	1H
43.66	0.004	Cd	33Arg	13C
26.26	0.000	Cg	33Arg	13C
1.46	0.010	Hgb	33Arg	1H
2.96	0.008	Hda	33Arg	1H
1.72	0.004	Hbb	33Arg	1H
2.96	0.003	Hdb	33Arg	1H
29.60	0.043	Cb	33Arg	13C
117.18	0.066	N	33Arg	15N

1.48	0.014	Hba	33Arg	1H
1.27	0.005	Hga	33Arg	1H
8.12	0.032	H	33Arg	1H
58.99	0.044	Ca	33Arg	13C
3.70	0.006	Ha	33Arg	1H
174.11	0.000	C	34Asn	13C
1.42	0.002	Hbb	34Asn	1H
1.30	0.012	Hba	34Asn	1H
39.01	0.053	Cb	34Asn	13C
54.17	0.088	Ca	34Asn	13C
4.11	0.013	Ha	34Asn	1H
111.27	0.041	N	34Asn	15N
7.06	0.033	H	34Asn	1H
173.23	0.000	C	35Thr	13C
61.86	0.041	Ca	35Thr	13C
3.86	0.010	Ha	35Thr	1H
107.35	0.035	N	35Thr	15N
70.31	0.045	Cb	35Thr	13C
7.10	0.033	H	35Thr	1H
20.76	0.059	Cg2	35Thr	13C
3.36	0.007	Hb	35Thr	1H
0.09	0.015	Hg2*	35Thr	1H
176.39	0.000	C	36Leu	13C
57.02	0.086	Ca	36Leu	13C
26.61	0.066	Cdb	36Leu	13C
3.38	0.007	Ha	36Leu	1H
1.55	0.009	Hdb*	36Leu	1H
121.87	0.048	N	36Leu	15N
1.31	0.004	Hba	36Leu	1H
1.45	0.008	Hbb	36Leu	1H
24.45	0.042	Cda	36Leu	13C
7.48	0.023	H	36Leu	1H
42.19	0.082	Cb	36Leu	13C
0.74	0.007	Hda*	36Leu	1H
173.47	0.000	C	37Asp	13C
54.91	0.046	Ca	37Asp	13C
4.33	0.008	Ha	37Asp	1H
113.12	0.069	N	37Asp	15N
2.97	0.006	Hbb	37Asp	1H
7.90	0.038	H	37Asp	1H
37.35	0.070	Cb	37Asp	13C
2.96	0.006	Hba	37Asp	1H

1.06	0.000	Hgb	38Lys	1H
1.20	0.000	Hga	38Lys	1H
172.52	0.000	C	38Lys	13C
54.04	0.000	Ca	38Lys	13C
33.70	0.000	Cb	38Lys	13C
1.45	0.000	Hba	38Lys	1H
1.81	0.011	Hbb	38Lys	1H
4.74	0.009	Ha	38Lys	1H
119.22	0.097	N	38Lys	15N
7.85	0.030	H	38Lys	1H
175.75	0.000	C	39Pro	13C
32.02	0.000	Cb	39Pro	13C
28.76	0.000	Cg	39Pro	13C
1.98	0.002	Hba	39Pro	1H
2.14	0.005	Hbb	39Pro	1H
2.07	0.007	Hga	39Pro	1H
2.16	0.015	Hgb	39Pro	1H
3.80	0.011	Hda	39Pro	1H
62.09	0.028	Ca	39Pro	13C
5.00	0.008	Ha	39Pro	1H
3.99	0.015	Hdb	39Pro	1H
49.04	0.044	Cd	39Pro	13C
173.54	0.000	C	40Val	13C
22.22	0.023	Cga	40Val	13C
19.72	0.030	Cgb	40Val	13C
33.91	0.117	Cb	40Val	13C
0.81	0.010	Hgb*	40Val	1H
113.27	0.041	N	40Val	15N
0.60	0.008	Hga*	40Val	1H
1.82	0.008	Hb	40Val	1H
8.71	0.030	H	40Val	1H
56.67	0.076	Ca	40Val	13C
5.54	0.010	Ha	40Val	1H
174.85	0.000	C	41Ile	13C
17.42	0.000	Cg2	41Ile	13C
40.46	0.112	Cb	41Ile	13C
27.36	0.000	Cg1	41Ile	13C
59.51	0.118	Ca	41Ile	13C
0.36	0.004	Hg2*	41Ile	1H
1.06	0.006	Hb	41Ile	1H
0.39	0.009	Hg1a	41Ile	1H
1.28	0.007	Hg1b	41Ile	1H

4.78	0.015	Ha	41Ile	1H
121.67	0.040	N	41Ile	15N
8.42	0.029	H	41Ile	1H
14.63	0.055	Cd1	41Ile	13C
0.38	0.007	Hd1*	41Ile	1H
174.33	0.000	C	42Met	13C
31.65	0.013	Cg	42Met	13C
2.07	0.012	Hga	42Met	1H
2.50	0.014	Hgb	42Met	1H
1.73	0.017	Hba	42Met	1H
1.99	0.013	Hbb	42Met	1H
40.33	0.066	Cb	42Met	13C
1.80	0.002	He*	42Met	1H
18.29	0.019	Ce	42Met	13C
124.03	0.057	N	42Met	15N
9.04	0.027	H	42Met	1H
52.00	0.070	Ca	42Met	13C
5.72	0.012	Ha	42Met	1H
175.40	0.000	C	43Gly	13C
4.33	0.008	Hab	43Gly	1H
105.76	0.044	N	43Gly	15N
4.07	0.010	Haa	43Gly	1H
44.25	0.079	Ca	43Gly	13C
9.19	0.028	H	43Gly	1H
42.72	0.000	Cd	44Arg	13C
1.57	0.000	Hba	44Arg	1H
1.66	0.000	Hbb	44Arg	1H
3.34	0.000	Ha	44Arg	1H
2.77	0.000	Hda	44Arg	1H
2.83	0.000	Hdb	44Arg	1H
1.32	0.000	Hgb	44Arg	1H
25.21	0.000	Cg	44Arg	13C
1.07	0.000	Hga	44Arg	1H
178.55	0.000	C	44Arg	13C
60.92	0.000	Ca	44Arg	13C
29.93	0.000	Cb	44Arg	13C
119.37	0.084	N	44Arg	15N
7.62	0.030	H	44Arg	1H
4.24	0.000	Ha	45His	1H
1.85	0.000	Hbb	45His	1H
178.02	0.000	C	45His	13C
4.32	0.000	Ha	45His	1H

58.13	0.000	Ca	45His	13C
1.75	0.000	Hba	45His	1H
112.56	0.036	N	45His	15N
7.41	0.027	H	45His	1H
176.10	0.000	C	46Thr	13C
119.57	0.000	N	46Thr	15N
8.05	0.026	H	46Thr	1H
3.91	0.009	Hb	46Thr	1H
4.26	0.006	Ha	46Thr	1H
68.56	0.105	Cb	46Thr	13C
20.92	0.092	Cg2	46Thr	13C
1.37	0.008	Hg2*	46Thr	1H
7.20	0.000	Hd1	47Trp	1H
10.27	0.000	He1	47Trp	1H
128.00	0.000	Ne1	47Trp	15N
7.39	0.024	He3	47Trp	1H
3.42	0.013	Hbb	47Trp	1H
29.99	0.026	Cb	47Trp	13C
3.29	0.004	Hba	47Trp	1H
124.54	0.036	N	47Trp	15N
8.33	0.037	H	47Trp	1H
60.00	0.063	Ca	47Trp	13C
4.63	0.006	Ha	47Trp	1H
178.24	0.000	C	48Glu	13C
8.04	0.008	H	48Glu	1H
37.39	0.098	Cg	48Glu	13C
28.74	0.026	Cb	48Glu	13C
2.29	0.004	Hga	48Glu	1H
1.92	0.004	Hba	48Glu	1H
2.21	0.006	Hbb	48Glu	1H
2.83	0.008	Hgb	48Glu	1H
58.93	0.057	Ca	48Glu	13C
3.42	0.006	Ha	48Glu	1H
174.88	0.000	C	49Ser	13C
4.01	0.001	Hbb	49Ser	1H
60.51	0.039	Ca	49Ser	13C
63.47	0.041	Cb	49Ser	13C
3.96	0.006	Hba	49Ser	1H
4.18	0.004	Ha	49Ser	1H
114.10	0.041	N	49Ser	15N
7.76	0.035	H	49Ser	1H
178.65	0.000	C	50Ile	13C

17.44	0.060	Cg2	50Ile	13C
27.48	0.038	Cg1	50Ile	13C
1.56	0.006	Hg1b	50Ile	1H
122.70	0.087	N	50Ile	15N
38.80	0.103	Cb	50Ile	13C
7.58	0.030	H	50Ile	1H
0.03	0.009	Hg1a	50Ile	1H
0.39	0.007	Hg2*	50Ile	1H
14.29	0.059	Cd1	50Ile	13C
64.87	0.059	Ca	50Ile	13C
1.34	0.009	Hb	50Ile	1H
3.47	0.005	Ha	50Ile	1H
0.37	0.012	Hd1*	50Ile	1H
172.45	0.000	C	51Gly	13C
104.16	0.063	N	51Gly	15N
7.57	0.037	H	51Gly	1H
3.59	0.008	Hab	51Gly	1H
2.89	0.010	Haa	51Gly	1H
45.60	0.044	Ca	51Gly	13C
43.43	0.086	Cd	52Arg	13C
2.94	0.010	Hda	52Arg	1H
2.94	0.010	Hdb	52Arg	1H
24.73	0.000	Cg	52Arg	13C
1.27	0.003	Hgb	52Arg	1H
1.20	0.006	Hga	52Arg	1H
1.61	0.003	Hba	52Arg	1H
1.89	0.004	Hbb	52Arg	1H
28.51	0.011	Cb	52Arg	13C
53.11	0.069	Ca	52Arg	13C
4.37	0.010	Ha	52Arg	1H
115.89	0.054	N	52Arg	15N
6.76	0.028	H	52Arg	1H
28.06	0.000	Cg	53Pro	13C
49.47	0.000	Cd	53Pro	13C
1.67	0.000	Hba	53Pro	1H
3.57	0.000	Hda	53Pro	1H
3.61	0.000	Hdb	53Pro	1H
1.73	0.000	Hga	53Pro	1H
2.01	0.000	Hgb	53Pro	1H
3.96	0.000	Ha	53Pro	1H
176.90	0.000	C	53Pro	13C
61.34	0.000	Ca	53Pro	13C

31.21	0.000	Cb	53Pro	13C
1.94	0.003	Hbb	53Pro	1H
176.06	0.000	C	54Leu	13C
26.22	0.000	Cg	54Leu	13C
51.90	0.106	Ca	54Leu	13C
1.62	0.008	Hg	54Leu	1H
26.22	0.051	Cdb	54Leu	13C
21.92	0.041	Cda	54Leu	13C
1.61	0.011	Hbb	54Leu	1H
4.41	0.013	Ha	54Leu	1H
0.80	0.019	Hdb*	54Leu	1H
0.83	0.021	Hba	54Leu	1H
40.48	0.089	Cb	54Leu	13C
0.46	0.007	Hda*	54Leu	1H
125.95	0.055	N	54Leu	15N
9.40	0.030	H	54Leu	1H
172.82	0.000	C	56Gly	13C
7.46	0.004	H	56Gly	1H
112.84	0.004	N	56Gly	15N
3.84	0.006	Hab	56Gly	1H
3.70	0.007	Haa	56Gly	1H
46.49	0.067	Ca	56Gly	13C
28.03	0.000	Cg	57Arg	13C
81.17	0.000	Ne	57Arg	15N
174.44	0.000	C	57Arg	13C
2.68	0.000	Hgb	57Arg	1H
5.75	0.033	He	57Arg	1H
54.42	0.063	Ca	57Arg	13C
43.07	0.000	Cd	57Arg	13C
1.28	0.012	Hga	57Arg	1H
2.33	0.011	Hda	57Arg	1H
4.37	0.006	Ha	57Arg	1H
2.68	0.007	Hdb	57Arg	1H
1.27	0.008	Hba	57Arg	1H
1.90	0.010	Hbb	57Arg	1H
118.11	0.065	N	57Arg	15N
7.22	0.027	H	57Arg	1H
35.86	0.048	Cb	57Arg	13C
174.88	0.000	C	58Lys	13C
1.57	0.000	Hdb	58Lys	1H
29.54	0.000	Cd	58Lys	13C
1.56	0.004	Hda	58Lys	1H

2.80	0.023	Heb	58Lys	1H
41.97	0.000	Ce	58Lys	13C
55.90	0.082	Ca	58Lys	13C
1.62	0.008	Hbb	58Lys	1H
32.38	0.105	Cb	58Lys	13C
2.78	0.024	Hea	58Lys	1H
1.56	0.003	Hba	58Lys	1H
1.31	0.006	Hgb	58Lys	1H
25.14	0.000	Cg	58Lys	13C
4.38	0.006	Ha	58Lys	1H
1.07	0.005	Hga	58Lys	1H
123.28	0.046	N	58Lys	15N
7.35	0.027	H	58Lys	1H
173.36	0.000	Cg	59Asn	13C
172.50	0.000	C	59Asn	13C
4.65	0.008	Ha	59Asn	1H
53.30	0.057	Ca	59Asn	13C
1.74	0.007	Hba	59Asn	1H
40.68	0.091	Cb	59Asn	13C
7.37	0.019	Hd2b	59Asn	1H
2.80	0.005	Hbb	59Asn	1H
126.64	0.050	N	59Asn	15N
6.60	0.018	Hd2a	59Asn	1H
109.21	0.137	Nd2	59Asn	15N
9.12	0.030	H	59Asn	1H
172.47	0.000	C	60Ile	13C
0.56	0.004	Hg1a	60Ile	1H
126.48	0.054	N	60Ile	15N
1.21	0.009	Hg1b	60Ile	1H
39.27	0.131	Cb	60Ile	13C
8.71	0.032	H	60Ile	1H
59.97	0.093	Ca	60Ile	13C
28.13	0.063	Cg1	60Ile	13C
1.67	0.010	Hb	60Ile	1H
4.33	0.011	Ha	60Ile	1H
19.02	0.060	Cg2	60Ile	13C
16.21	0.036	Cd1	60Ile	13C
0.56	0.009	Hg2*	60Ile	1H
0.63	0.006	Hd1*	60Ile	1H
175.41	0.000	C	61Ile	13C
127.64	0.088	N	61Ile	15N
58.07	0.080	Ca	61Ile	13C

-0.47	0.016	Hg1b	61Ile	1H
4.42	0.009	Ha	61Ile	1H
19.37	0.060	Cg2	61Ile	13C
-0.04	0.006	Hg1a	61Ile	1H
27.99	0.033	Cg1	61Ile	13C
8.79	0.031	H	61Ile	1H
0.50	0.006	Hb	61Ile	1H
37.34	0.076	Cb	61Ile	13C
0.11	0.010	Hg2*	61Ile	1H
12.06	0.023	Cd1	61Ile	13C
-0.42	0.006	Hd1*	61Ile	1H
175.58	0.000	C	62Leu	13C
26.22	0.034	Cdb	62Leu	13C
0.52	0.018	Hg	62Leu	1H
125.85	0.031	N	62Leu	15N
0.16	0.012	Hdb*	62Leu	1H
53.56	0.086	Ca	62Leu	13C
8.32	0.031	H	62Leu	1H
4.33	0.005	Ha	62Leu	1H
0.64	0.010	Hbb	62Leu	1H
-0.14	0.020	Hba	62Leu	1H
24.80	0.027	Cda	62Leu	13C
43.05	0.059	Cb	62Leu	13C
-0.11	0.004	Hda*	62Leu	1H
174.15	0.000	C	63Ser	13C
4.35	0.021	Hbb	63Ser	1H
3.78	0.011	Hba	63Ser	1H
64.64	0.095	Cb	63Ser	13C
115.66	0.035	N	63Ser	15N
58.65	0.148	Ca	63Ser	13C
8.64	0.025	H	63Ser	1H
5.22	0.008	Ha	63Ser	1H
174.89	0.000	C	64Ser	13C
3.93	0.006	Hba	64Ser	1H
3.99	0.011	Hbb	64Ser	1H
64.15	0.169	Cb	64Ser	13C
60.47	0.061	Ca	64Ser	13C
4.58	0.005	Ha	64Ser	1H
122.80	0.076	N	64Ser	15N
10.13	0.026	H	64Ser	1H
172.56	0.000	C	65Gln	13C
113.10	0.157	Ne2	65Gln	15N

6.77	0.036	He2a	65Gln	1H
7.70	0.004	He2b	65Gln	1H
53.03	0.046	Ca	65Gln	13C
4.63	0.003	Ha	65Gln	1H
29.44	0.037	Cb	65Gln	13C
1.75	0.005	Hba	65Gln	1H
2.07	0.009	Hbb	65Gln	1H
122.91	0.056	N	65Gln	15N
2.23	0.006	Hga	65Gln	1H
8.63	0.037	H	65Gln	1H
2.40	0.006	Hgb	65Gln	1H
33.96	0.080	Cg	65Gln	13C
176.95	0.000	C	66Pro	13C
62.70	0.085	Ca	66Pro	13C
3.48	0.011	Hda	66Pro	1H
3.65	0.006	Hdb	66Pro	1H
1.83	0.003	Hga	66Pro	1H
1.95	0.005	Hgb	66Pro	1H
50.13	0.092	Cd	66Pro	13C
27.67	0.000	Cg	66Pro	13C
2.12	0.006	Hbb	66Pro	1H
3.97	0.003	Ha	66Pro	1H
31.76	0.095	Cb	66Pro	13C
1.53	0.009	Hba	66Pro	1H
108.80	0.242	N	67Gly	15N
1.68	0.007	Haa	67Gly	1H
7.62	0.019	H	67Gly	1H
1.97	0.020	Hab	67Gly	1H
42.52	0.056	Ca	67Gly	13C
174.13	0.015	C	68Thr	13C
21.14	0.015	Cg2	68Thr	13C
0.90	0.007	Hg2*	68Thr	1H
60.21	0.135	Ca	68Thr	13C
105.74	0.054	N	68Thr	15N
4.17	0.006	Ha	68Thr	1H
69.10	0.056	Cb	68Thr	13C
4.47	0.004	Hb	68Thr	1H
5.90	0.046	H	68Thr	1H
176.26	0.000	C	69Asp	13C
55.01	0.099	Ca	69Asp	13C
43.94	0.092	Cb	69Asp	13C
3.09	0.007	Hbb	69Asp	1H

2.96	0.013	Hba	69Asp	1H
4.76	0.010	Ha	69Asp	1H
120.04	0.039	N	69Asp	15N
7.22	0.024	H	69Asp	1H
176.92	0.000	C	70Asp	13C
54.95	0.048	Ca	70Asp	13C
4.77	0.012	Ha	70Asp	1H
40.16	0.063	Cb	70Asp	13C
2.73	0.008	Hba	70Asp	1H
2.84	0.009	Hbb	70Asp	1H
126.58	0.095	N	70Asp	15N
8.84	0.030	H	70Asp	1H
176.00	0.000	C	71Arg	13C
31.33	0.110	Cb	71Arg	13C
43.58	0.076	Cd	71Arg	13C
1.93	0.011	Hbb	71Arg	1H
1.77	0.014	Hba	71Arg	1H
3.37	0.005	Hdb	71Arg	1H
3.07	0.014	Hda	71Arg	1H
1.76	0.009	Hga	71Arg	1H
1.94	0.016	Hgb	71Arg	1H
57.29	0.067	Ca	71Arg	13C
118.04	0.040	N	71Arg	15N
26.00	0.071	Cg	71Arg	13C
8.82	0.032	H	71Arg	1H
4.16	0.012	Ha	71Arg	1H
172.87	0.000	C	72Val	13C
33.26	0.074	Cb	72Val	13C
108.15	0.044	N	72Val	15N
58.19	0.029	Ca	72Val	13C
1.37	0.007	Hb	72Val	1H
7.17	0.024	H	72Val	1H
4.53	0.006	Ha	72Val	1H
22.77	0.055	Cgb	72Val	13C
16.73	0.035	Cga	72Val	13C
0.32	0.004	Hgb*	72Val	1H
-0.47	0.009	Hga*	72Val	1H
171.94	0.000	C	73Thr	13C
21.02	0.000	Cg2	73Thr	13C
62.79	0.075	Ca	73Thr	13C
4.30	0.009	Ha	73Thr	1H
1.04	0.007	Hg2*	73Thr	1H

117.13	0.038	N	73Thr	15N
7.85	0.032	H	73Thr	1H
70.24	0.045	Cb	73Thr	13C
3.80	0.008	Hb	73Thr	1H
176.52	0.000	C	74Trp	13C
130.21	0.046	Ne1	74Trp	15N
7.12	0.024	Hd1	74Trp	1H
7.39	0.013	He3	74Trp	1H
10.19	0.022	He1	74Trp	1H
55.90	0.086	Ca	74Trp	13C
3.46	0.011	Hbb	74Trp	1H
2.80	0.009	Hba	74Trp	1H
28.93	0.091	Cb	74Trp	13C
128.94	0.136	N	74Trp	15N
5.02	0.011	Ha	74Trp	1H
8.68	0.025	H	74Trp	1H
174.85	0.000	C	75Val	13C
22.31	0.015	Cgb	75Val	13C
58.72	0.084	Ca	75Val	13C
0.66	0.008	Hgb*	75Val	1H
4.79	0.021	Ha	75Val	1H
35.66	0.091	Cb	75Val	13C
18.17	0.078	Cga	75Val	13C
116.37	0.042	N	75Val	15N
2.10	0.007	Hb	75Val	1H
9.13	0.029	H	75Val	1H
0.47	0.007	Hga*	75Val	1H
1.66	0.003	Hda	76Lys	1H
1.73	0.001	Hdb	76Lys	1H
175.59	0.000	C	76Lys	13C
55.45	0.000	Ca	76Lys	13C
41.97	0.000	Ce	76Lys	13C
29.36	0.000	Cd	76Lys	13C
2.92	0.001	Heb	76Lys	1H
2.84	0.001	Hea	76Lys	1H
2.03	0.007	Hbb	76Lys	1H
1.83	0.008	Hba	76Lys	1H
1.44	0.008	Hga	76Lys	1H
34.14	0.065	Cb	76Lys	13C
5.06	0.009	Ha	76Lys	1H
1.69	0.013	Hgb	76Lys	1H
116.03	0.029	N	76Lys	15N

8.29	0.028	H	76Lys	1H
24.22	0.076	Cg	76Lys	13C
174.14	0.000	C	77Ser	13C
56.91	0.041	Ca	77Ser	13C
4.25	0.010	Hbb	77Ser	1H
4.87	0.016	Ha	77Ser	1H
108.84	0.092	N	77Ser	15N
4.06	0.008	Hba	77Ser	1H
7.18	0.029	H	77Ser	1H
66.29	0.075	Cb	77Ser	13C
177.14	0.000	C	78Val	13C
31.52	0.128	Cb	78Val	13C
1.84	0.006	Hb	78Val	1H
22.44	0.043	Cgb	78Val	13C
122.39	0.061	N	78Val	15N
0.69	0.008	Hgb*	78Val	1H
8.89	0.029	H	78Val	1H
67.09	0.056	Ca	78Val	13C
20.15	0.041	Cga	78Val	13C
3.36	0.008	Ha	78Val	1H
0.38	0.006	Hga*	78Val	1H
179.65	0.000	C	79Asp	13C
39.61	0.127	Cb	79Asp	13C
2.45	0.002	Hba	79Asp	1H
2.54	0.011	Hbb	79Asp	1H
57.64	0.076	Ca	79Asp	13C
4.30	0.011	Ha	79Asp	1H
118.07	0.041	N	79Asp	15N
8.38	0.022	H	79Asp	1H
178.84	0.000	C	80Glu	13C
36.81	0.042	Cg	80Glu	13C
1.99	0.022	Hba	80Glu	1H
2.22	0.012	Hga	80Glu	1H
30.61	0.012	Cb	80Glu	13C
2.02	0.020	Hbb	80Glu	1H
2.35	0.009	Hgb	80Glu	1H
120.62	0.106	N	80Glu	15N
59.00	0.071	Ca	80Glu	13C
7.91	0.018	H	80Glu	1H
3.94	0.005	Ha	80Glu	1H
178.00	0.000	C	81Ala	13C
17.81	0.065	Cb	81Ala	13C

1.47	0.013	Hb*	81Ala	1H
122.28	0.063	N	81Ala	15N
55.42	0.076	Ca	81Ala	13C
3.85	0.008	Ha	81Ala	1H
8.15	0.027	H	81Ala	1H
180.34	0.000	C	82Ile	13C
65.29	0.073	Ca	82Ile	13C
29.47	0.019	Cg1	82Ile	13C
38.21	0.129	Cb	82Ile	13C
2.00	0.008	Hg1b	82Ile	1H
1.90	0.008	Hb	82Ile	1H
1.03	0.019	Hg1a	82Ile	1H
3.64	0.007	Ha	82Ile	1H
115.87	0.030	N	82Ile	15N
7.97	0.030	H	82Ile	1H
13.21	0.032	Cd1	82Ile	13C
16.79	0.050	Cg2	82Ile	13C
0.84	0.010	Hg2*	82Ile	1H
0.86	0.006	Hd1*	82Ile	1H
17.55	0.000	Cb	83Ala	13C
180.38	0.000	C	83Ala	13C
55.07	0.038	Ca	83Ala	13C
1.44	0.009	Hb*	83Ala	1H
4.08	0.010	Ha	83Ala	1H
124.20	0.031	N	83Ala	15N
8.14	0.029	H	83Ala	1H
177.96	0.000	C	84Ala	13C
17.90	0.122	Cb	84Ala	13C
1.40	0.010	Hb*	84Ala	1H
53.70	0.103	Ca	84Ala	13C
119.21	0.036	N	84Ala	15N
4.06	0.006	Ha	84Ala	1H
8.06	0.038	H	84Ala	1H
175.42	0.000	C	85Cys	13C
61.76	0.078	Ca	85Cys	13C
3.92	0.012	Ha	85Cys	1H
3.29	0.016	Hbb	85Cys	1H
2.42	0.010	Hba	85Cys	1H
27.86	0.073	Cb	85Cys	13C
114.54	0.040	N	85Cys	15N
7.40	0.031	H	85Cys	1H
173.27	0.000	C	86Gly	13C

102.91	0.035	N	86Gly	15N
3.74	0.006	Haa	86Gly	1H
7.19	0.027	H	86Gly	1H
3.88	0.010	Hab	86Gly	1H
45.07	0.082	Ca	86Gly	13C
175.25	0.000	C	87Asp	13C
53.26	0.096	Ca	87Asp	13C
122.17	0.088	N	87Asp	15N
4.69	0.017	Ha	87Asp	1H
8.49	0.028	H	87Asp	1H
2.44	0.006	Hba	87Asp	1H
2.69	0.006	Hbb	87Asp	1H
39.53	0.086	Cb	87Asp	13C
21.87	0.000	Cgb	88Val	13C
32.04	0.024	Cb	88Val	13C
2.37	0.007	Hb	88Val	1H
4.09	0.003	Ha	88Val	1H
57.97	0.063	Ca	88Val	13C
114.16	0.033	N	88Val	15N
0.94	0.007	Hgb*	88Val	1H
7.18	0.033	H	88Val	1H
17.84	0.048	Cga	88Val	13C
0.58	0.008	Hga*	88Val	1H
177.55	0.000	C	89Pro	13C
50.67	0.000	Cd	89Pro	13C
3.78	0.006	Hdb	89Pro	1H
3.78	0.007	Hda	89Pro	1H
32.03	0.000	Cb	89Pro	13C
27.41	0.000	Cg	89Pro	13C
1.96	0.003	Hga	89Pro	1H
2.32	0.003	Hbb	89Pro	1H
1.86	0.004	Hba	89Pro	1H
2.12	0.006	Hgb	89Pro	1H
64.61	0.097	Ca	89Pro	13C
4.31	0.008	Ha	89Pro	1H
173.40	0.000	C	90Glu	13C
1.75	0.002	Hbb	90Glu	1H
36.07	0.000	Cg	90Glu	13C
1.60	0.006	Hba	90Glu	1H
2.14	0.006	Hgb	90Glu	1H
1.88	0.011	Hga	90Glu	1H
32.79	0.130	Cb	90Glu	13C

55.75	0.084	Ca	90Glu	13C
4.89	0.010	Ha	90Glu	1H
116.90	0.100	N	90Glu	15N
7.71	0.021	H	90Glu	1H
173.93	0.000	C	91Ile	13C
41.21	0.086	Cb	91Ile	13C
1.61	0.002	Hg1b	91Ile	1H
27.78	0.000	Cg1	91Ile	13C
0.75	0.003	Hg1a	91Ile	1H
1.68	0.014	Hb	91Ile	1H
13.91	0.064	Cd1	91Ile	13C
0.91	0.009	Hd1*	91Ile	1H
129.99	0.035	N	91Ile	15N
17.79	0.059	Cg2	91Ile	13C
61.14	0.062	Ca	91Ile	13C
0.75	0.006	Hg2*	91Ile	1H
8.74	0.038	H	91Ile	1H
3.83	0.010	Ha	91Ile	1H
32.05	0.000	Cg	92Met	13C
174.24	0.000	C	92Met	13C
2.06	0.000	He*	92Met	1H
16.95	0.000	Ce	92Met	13C
2.04	0.000	Hga	92Met	1H
30.04	0.018	Cb	92Met	13C
2.08	0.022	Hgb	92Met	1H
2.26	0.017	Hbb	92Met	1H
1.29	0.014	Hba	92Met	1H
121.85	0.044	N	92Met	15N
7.82	0.018	H	92Met	1H
51.70	0.073	Ca	92Met	13C
5.17	0.017	Ha	92Met	1H
176.90	0.000	C	93Val	13C
31.38	0.057	Cb	93Val	13C
2.23	0.006	Hb	93Val	1H
62.12	0.072	Ca	93Val	13C
22.20	0.040	Cgb	93Val	13C
125.03	0.043	N	93Val	15N
0.54	0.009	Hgb*	93Val	1H
9.35	0.031	H	93Val	1H
4.28	0.016	Ha	93Val	1H
20.21	0.067	Cga	93Val	13C
0.13	0.008	Hga*	93Val	1H

174.20	0.000	C	94Ile	13C
27.90	0.000	Cg1	94Ile	13C
38.96	0.048	Cb	94Ile	13C
1.80	0.009	Hg1b	94Ile	1H
119.65	0.028	N	94Ile	15N
2.85	0.011	Hb	94Ile	1H
8.90	0.021	H	94Ile	1H
17.42	0.049	Cg2	94Ile	13C
1.03	0.007	Hg1a	94Ile	1H
60.49	0.050	Ca	94Ile	13C
0.94	0.009	Hg2*	94Ile	1H
5.64	0.008	Ha	94Ile	1H
1.02	0.027	Hd1*	94Ile	1H
15.64	0.031	Cd1	94Ile	13C
174.16	0.000	C	95Gly	13C
41.18	0.069	Ca	95Gly	13C
3.86	0.017	Hab	95Gly	1H
1.94	0.004	Haa	95Gly	1H
103.08	0.035	N	95Gly	15N
6.14	0.025	H	95Gly	1H
2.81	0.016	Haa	96Gly	1H
2.91	0.016	Hab	96Gly	1H
46.43	0.111	Ca	96Gly	13C
111.73	0.033	N	96Gly	15N
8.17	0.029	H	96Gly	1H
174.82	0.000	C	97Gly	13C
3.98	0.014	Hab	97Gly	1H
3.59	0.008	Haa	97Gly	1H
49.09	0.122	Ca	97Gly	13C
180.68	0.000	C	98Arg	13C
8.86	0.000	He	98Arg	1H
83.73	0.000	Ne	98Arg	15N
29.55	0.089	Cb	98Arg	13C
2.20	0.014	Hbb	98Arg	1H
2.08	0.011	Hba	98Arg	1H
3.20	0.016	Hda	98Arg	1H
3.32	0.010	Hdb	98Arg	1H
1.78	0.008	Hga	98Arg	1H
42.95	0.040	Cd	98Arg	13C
1.87	0.007	Hgb	98Arg	1H
122.09	0.057	N	98Arg	15N
27.30	0.055	Cg	98Arg	13C

9.21	0.045	H	98Arg	1H
58.31	0.071	Ca	98Arg	13C
4.24	0.008	Ha	98Arg	1H
178.64	0.000	C	99Val	13C
21.84	0.000	Cga	99Val	13C
31.52	0.029	Cb	99Val	13C
1.70	0.006	Hb	99Val	1H
0.62	0.011	Hga*	99Val	1H
122.16	0.051	N	99Val	15N
7.27	0.031	H	99Val	1H
24.44	0.057	Cgb	99Val	13C
67.97	0.043	Ca	99Val	13C
3.70	0.007	Ha	99Val	1H
0.95	0.010	Hgb*	99Val	1H
178.00	0.000	C	100Tyr	13C
6.96	0.009	He*	100Tyr	1H
60.27	0.053	Ca	100Tyr	13C
6.51	0.010	Hd*	100Tyr	1H
4.28	0.009	Ha	100Tyr	1H
2.40	0.009	Hba	100Tyr	1H
2.82	0.009	Hbb	100Tyr	1H
37.76	0.102	Cb	100Tyr	13C
119.55	0.028	N	100Tyr	15N
9.51	0.041	H	100Tyr	1H
36.02	0.000	Cg	101Glu	13C
2.30	0.005	Hga	101Glu	1H
2.39	0.003	Hgb	101Glu	1H
2.24	0.001	Hbb	101Glu	1H
2.16	0.004	Hba	101Glu	1H
115.97	0.041	N	101Glu	15N
29.57	0.028	Cb	101Glu	13C
8.04	0.033	H	101Glu	1H
59.81	0.078	Ca	101Glu	13C
3.71	0.008	Ha	101Glu	1H
36.40	0.000	Cg	102Gln	13C
4.71	0.000	Ha	102Gln	1H
32.47	0.000	Cb	102Gln	13C
177.20	0.000	C	102Gln	13C
58.11	0.035	Ca	102Gln	13C
113.98	0.068	N	102Gln	15N
7.16	0.033	H	102Gln	1H
176.86	0.000	C	103Phe	13C

2.82	0.012	Hba	103Phe	1H
7.40	0.016	Hd*	103Phe	1H
6.94	0.020	He*	103Phe	1H
3.05	0.011	Hbb	103Phe	1H
60.18	0.050	Ca	103Phe	13C
4.38	0.007	Ha	103Phe	1H
41.71	0.075	Cb	103Phe	13C
113.14	0.053	N	103Phe	15N
7.94	0.028	H	103Phe	1H
1.16	0.000	Hg	104Leu	1H
26.67	0.054	Cda	104Leu	13C
24.86	0.009	Cda	104Leu	13C
1.78	0.003	Hdb*	104Leu	1H
60.79	0.067	Ca	104Leu	13C
1.47	0.004	Hba	104Leu	1H
38.67	0.050	Cb	104Leu	13C
4.30	0.007	Ha	104Leu	1H
1.96	0.003	Hbb	104Leu	1H
123.48	0.059	N	104Leu	15N
0.91	0.005	Hda*	104Leu	1H
8.33	0.030	H	104Leu	1H
50.47	0.000	Cd	105Pro	13C
27.94	0.000	Cg	105Pro	13C
1.92	0.000	Hga	105Pro	1H
3.80	0.000	Hdb	105Pro	1H
65.27	0.000	Ca	105Pro	13C
31.16	0.000	Cb	105Pro	13C
177.03	0.000	C	105Pro	13C
1.96	0.015	Hgb	105Pro	1H
3.44	0.000	Hda	105Pro	1H
175.76	0.000	C	106Lys	13C
25.16	0.099	Cg	106Lys	13C
1.53	0.009	Hdb	106Lys	1H
55.18	0.029	Ca	106Lys	13C
1.38	0.016	Hga	106Lys	1H
41.77	0.074	Ce	106Lys	13C
29.26	0.046	Cd	106Lys	13C
2.76	0.012	Heb	106Lys	1H
4.37	0.005	Ha	106Lys	1H
2.73	0.021	Hea	106Lys	1H
1.83	0.005	Hba	106Lys	1H
34.58	0.101	Cb	106Lys	13C

2.16	0.007	Hbb	106Lys	1H
1.37	0.018	Hda	106Lys	1H
112.59	0.059	N	106Lys	15N
7.41	0.037	H	106Lys	1H
177.27	0.000	C	107Ala	13C
52.24	0.060	Ca	107Ala	13C
4.58	0.012	Ha	107Ala	1H
122.33	0.047	N	107Ala	15N
7.90	0.027	H	107Ala	1H
21.09	0.049	Cb	107Ala	13C
1.73	0.005	Hb*	107Ala	1H
174.80	0.000	C	108Gln	13C
112.79	0.000	Ne2	108Gln	15N
7.70	0.031	He2b	108Gln	1H
6.86	0.024	He2a	108Gln	1H
2.37	0.009	Hbb	108Gln	1H
31.53	0.117	Cb	108Gln	13C
2.14	0.009	Hba	108Gln	1H
55.73	0.060	Ca	108Gln	13C
118.44	0.047	N	108Gln	15N
4.57	0.007	Ha	108Gln	1H
2.48	0.006	Hga	108Gln	1H
2.57	0.006	Hgb	108Gln	1H
9.17	0.033	H	108Gln	1H
34.86	0.131	Cg	108Gln	13C
174.02	0.000	C	109Lys	13C
30.27	0.024	Cd	109Lys	13C
1.46	0.007	Hda	109Lys	1H
1.36	0.007	Hgb	109Lys	1H
2.73	0.006	Heb	109Lys	1H
1.46	0.009	Hdb	109Lys	1H
25.85	0.025	Cg	109Lys	13C
1.07	0.006	Hga	109Lys	1H
2.49	0.009	Hea	109Lys	1H
120.48	0.075	N	109Lys	15N
42.47	0.057	Ce	109Lys	13C
2.20	0.014	Hbb	109Lys	1H
7.74	0.024	H	109Lys	1H
1.89	0.007	Hba	109Lys	1H
55.92	0.059	Ca	109Lys	13C
36.77	0.073	Cb	109Lys	13C
5.68	0.008	Ha	109Lys	1H

174.80	0.000	C	110Leu	13C
24.99	0.086	Cdb	110Leu	13C
0.51	0.008	Hdb*	110Leu	1H
1.29	0.012	Hbb	110Leu	1H
0.61	0.017	Hba	110Leu	1H
44.43	0.075	Cb	110Leu	13C
121.97	0.047	N	110Leu	15N
52.82	0.070	Ca	110Leu	13C
8.98	0.025	H	110Leu	1H
5.12	0.014	Ha	110Leu	1H
23.48	0.025	Cda	110Leu	13C
-0.84	0.007	Hda*	110Leu	1H
6.70	0.000	Hd*	111Tyr	1H
175.02	0.000	C	111Tyr	13C
2.60	0.010	Hba	111Tyr	1H
3.23	0.010	Hbb	111Tyr	1H
122.49	0.072	N	111Tyr	15N
38.09	0.079	Cb	111Tyr	13C
55.85	0.079	Ca	111Tyr	13C
9.43	0.027	H	111Tyr	1H
5.20	0.011	Ha	111Tyr	1H
123.48	0.047	N	112Leu	15N
25.96	0.047	Cdb	112Leu	13C
9.55	0.044	H	112Leu	1H
1.05	0.005	Hg	112Leu	1H
0.27	0.019	Hdb*	112Leu	1H
0.32	0.023	Hba	112Leu	1H
1.47	0.016	Hbb	112Leu	1H
52.75	0.057	Ca	112Leu	13C
5.32	0.010	Ha	112Leu	1H
44.59	0.046	Cb	112Leu	13C
21.99	0.039	Cda	112Leu	13C
-0.07	0.005	Hda*	112Leu	1H
173.15	0.000	C	113Thr	13C
1.37	0.000	Hg2*	113Thr	1H
59.82	0.066	Ca	113Thr	13C
5.11	0.010	Ha	113Thr	1H
68.96	0.078	Cb	113Thr	13C
3.92	0.011	Hb	113Thr	1H
54.09	0.000	Ca	114His	13C
30.30	0.000	Cb	114His	13C
175.20	0.000	C	114His	13C

4.83	0.000	Ha	114His	1H
6.72	0.026	Hd2	114His	1H
126.63	0.092	N	114His	15N
9.19	0.030	H	114His	1H
176.74	0.000	C	115Ile	13C
26.59	0.000	Cg1	115Ile	13C
0.82	0.021	Hg1b	115Ile	1H
-0.06	0.006	Hg1a	115Ile	1H
126.54	0.140	N	115Ile	15N
60.70	0.099	Ca	115Ile	13C
9.03	0.034	H	115Ile	1H
4.01	0.013	Ha	115Ile	1H
39.69	0.072	Cb	115Ile	13C
12.71	0.044	Cd1	115Ile	13C
0.75	0.013	Hb	115Ile	1H
17.27	0.051	Cg2	115Ile	13C
-0.94	0.005	Hd1*	115Ile	1H
0.14	0.007	Hg2*	115Ile	1H
173.75	0.000	C	116Asp	13C
53.17	0.037	Ca	116Asp	13C
38.56	0.051	Cb	116Asp	13C
4.64	0.008	Ha	116Asp	1H
2.50	0.006	Hba	116Asp	1H
2.74	0.005	Hbb	116Asp	1H
129.66	0.066	N	116Asp	15N
8.31	0.027	H	116Asp	1H
174.52	0.000	C	117Ala	13C
51.24	0.141	Ca	117Ala	13C
124.21	0.040	N	117Ala	15N
20.49	0.089	Cb	117Ala	13C
0.46	0.012	Hb*	117Ala	1H
4.39	0.012	Ha	117Ala	1H
7.73	0.031	H	117Ala	1H
36.48	0.000	Cg	118Glu	13C
2.01	0.019	Hga	118Glu	1H
2.16	0.016	Hgb	118Glu	1H
1.96	0.007	Hbb	118Glu	1H
1.85	0.007	Hba	118Glu	1H
55.35	0.109	Ca	118Glu	13C
29.13	0.074	Cb	118Glu	13C
4.56	0.009	Ha	118Glu	1H
124.22	0.031	N	118Glu	15N

8.56	0.030	H	118Glu	1H
174.75	0.000	C	119Val	13C
21.86	0.000	Cgb	119Val	13C
35.24	0.074	Cb	119Val	13C
58.51	0.120	Ca	119Val	13C
118.69	0.053	N	119Val	15N
2.12	0.005	Hb	119Val	1H
4.62	0.008	Ha	119Val	1H
0.91	0.006	Hgb*	119Val	1H
8.12	0.018	H	119Val	1H
18.94	0.096	Cga	119Val	13C
0.80	0.008	Hga*	119Val	1H
175.67	0.000	C	120Glu	13C
1.89	0.001	Hba	120Glu	1H
36.20	0.000	Cg	120Glu	13C
2.26	0.001	Hga	120Glu	1H
29.97	0.042	Cb	120Glu	13C
2.29	0.007	Hgb	120Glu	1H
1.94	0.028	Hbb	120Glu	1H
56.18	0.014	Ca	120Glu	13C
4.34	0.005	Ha	120Glu	1H
123.98	0.061	N	120Glu	15N
8.38	0.031	H	120Glu	1H
172.55	0.000	C	121Gly	13C
4.90	0.013	Hab	121Gly	1H
45.86	0.082	Ca	121Gly	13C
3.75	0.012	Haa	121Gly	1H
106.58	0.062	N	121Gly	15N
8.31	0.025	H	121Gly	1H
2.67	0.005	Hba	122Asp	1H
3.18	0.010	Hbb	122Asp	1H
41.82	0.108	Cb	122Asp	13C
52.38	0.067	Ca	122Asp	13C
4.88	0.010	Ha	122Asp	1H
116.22	0.060	N	122Asp	15N
8.54	0.036	H	122Asp	1H
113.95	0.035	N	123Thr	15N
61.99	0.077	Ca	123Thr	13C
4.70	0.009	Ha	123Thr	1H
72.31	0.050	Cb	123Thr	13C
7.39	0.020	H	123Thr	1H
21.85	0.061	Cg2	123Thr	13C

3.59	0.011	Hb	123Thr	1H
1.36	0.008	Hg2*	123Thr	1H
117.97	0.000	N	124His	15N
7.32	0.003	Hd2	124His	1H
8.28	0.027	H	124His	1H
117.95	0.035	N	124His	15N
3.12	0.008	Hbb	124His	1H
33.12	0.097	Cb	124His	13C
2.74	0.018	Hba	124His	1H
55.99	0.136	Ca	124His	13C
5.47	0.004	Ha	124His	1H
7.07	0.000	He*	125Phe	1H
2.88	0.014	Hbb	125Phe	1H
2.78	0.010	Hba	125Phe	1H
41.18	0.063	Cb	125Phe	13C
6.88	0.019	Hd*	125Phe	1H
56.55	0.090	Ca	125Phe	13C
4.44	0.009	Ha	125Phe	1H
124.83	0.036	N	125Phe	15N
9.11	0.032	H	125Phe	1H
62.42	0.050	Ca	126Pro	13C
1.38	0.005	Hgb	126Pro	1H
27.13	0.028	Cg	126Pro	13C
31.72	0.045	Cb	126Pro	13C
1.64	0.003	Hba	126Pro	1H
2.14	0.006	Hbb	126Pro	1H
1.07	0.006	Hga	126Pro	1H
4.27	0.007	Ha	126Pro	1H
1.48	0.012	Hda	126Pro	1H
3.15	0.012	Hdb	126Pro	1H
49.74	0.056	Cd	126Pro	13C
54.46	0.100	Ca	127Asp	13C
4.30	0.009	Ha	127Asp	1H
2.53	0.004	Hbb	127Asp	1H
2.35	0.006	Hba	127Asp	1H
40.53	0.075	Cb	127Asp	13C
117.66	0.107	N	127Asp	15N
8.05	0.026	H	127Asp	1H
55.56	0.000	Ca	128Tyr	13C
6.34	0.015	He*	128Tyr	1H
4.75	0.010	Ha	128Tyr	1H
6.84	0.022	Hd*	128Tyr	1H

2.74	0.007	Hba	128Tyr	1H
3.00	0.008	Hbb	128Tyr	1H
39.22	0.074	Cb	128Tyr	13C
118.87	0.023	N	128Tyr	15N
7.41	0.015	H	128Tyr	1H
29.42	0.000	Cb	129Glu	13C
1.89	0.000	Hba	129Glu	1H
36.05	0.000	Cg	129Glu	13C
2.27	0.010	Hgb	129Glu	1H
53.07	0.040	Ca	129Glu	13C
2.12	0.016	Hga	129Glu	1H
4.58	0.002	Ha	129Glu	1H
123.13	0.090	N	129Glu	15N
8.77	0.021	H	129Glu	1H
178.20	0.000	C	130Pro	13C
3.77	0.024	Hda	130Pro	1H
50.93	0.000	Cd	130Pro	13C
3.80	0.004	Hdb	130Pro	1H
27.10	0.000	Cg	130Pro	13C
31.99	0.000	Cb	130Pro	13C
1.75	0.005	Hga	130Pro	1H
2.02	0.006	Hba	130Pro	1H
2.37	0.005	Hbb	130Pro	1H
2.02	0.004	Hgb	130Pro	1H
65.71	0.076	Ca	130Pro	13C
4.30	0.011	Ha	130Pro	1H
177.02	0.000	C	131Asp	13C
56.28	0.073	Ca	131Asp	13C
2.68	0.008	Hbb	131Asp	1H
2.57	0.010	Hba	131Asp	1H
40.03	0.061	Cb	131Asp	13C
4.54	0.006	Ha	131Asp	1H
114.76	0.024	N	131Asp	15N
9.01	0.020	H	131Asp	1H
175.00	0.000	C	132Asp	13C
54.98	0.093	Ca	132Asp	13C
2.30	0.006	Hba	132Asp	1H
2.84	0.004	Hbb	132Asp	1H
41.26	0.086	Cb	132Asp	13C
4.53	0.008	Ha	132Asp	1H
118.01	0.058	N	132Asp	15N
8.12	0.030	H	132Asp	1H

7.84	0.000	He3	133Trp	1H
173.84	0.000	C	133Trp	13C
128.05	0.003	Ne1	133Trp	15N
55.95	0.120	Ca	133Trp	13C
7.84	0.024	Hd1	133Trp	1H
10.23	0.052	He1	133Trp	1H
4.85	0.008	Ha	133Trp	1H
119.46	0.051	N	133Trp	15N
7.76	0.029	H	133Trp	1H
3.12	0.010	Hbb	133Trp	1H
2.88	0.010	Hba	133Trp	1H
33.98	0.085	Cb	133Trp	13C
175.84	0.000	C	134Glu	13C
2.04	0.000	Hga	134Glu	1H
35.52	0.000	Cg	134Glu	13C
2.11	0.000	Hgb	134Glu	1H
2.04	0.001	Hbb	134Glu	1H
32.40	0.011	Cb	134Glu	13C
1.81	0.007	Hba	134Glu	1H
54.28	0.059	Ca	134Glu	13C
4.65	0.002	Ha	134Glu	1H
122.58	0.077	N	134Glu	15N
9.53	0.029	H	134Glu	1H
3.83	0.005	Hbb	135Ser	1H
3.77	0.007	Hba	135Ser	1H
58.49	0.045	Ca	135Ser	13C
62.05	0.064	Cb	135Ser	13C
4.81	0.013	Ha	135Ser	1H
121.47	0.074	N	135Ser	15N
8.99	0.027	H	135Ser	1H
175.58	0.000	C	136Val	13C
121.31	0.031	N	136Val	15N
32.42	0.103	Cb	136Val	13C
9.06	0.043	H	136Val	1H
2.40	0.006	Hb	136Val	1H
61.01	0.063	Ca	136Val	13C
4.63	0.014	Ha	136Val	1H
18.31	0.047	Cga	136Val	13C
0.79	0.008	Hga*	136Val	1H
21.07	0.084	Cgb	136Val	13C
0.90	0.009	Hgb*	136Val	1H
7.31	0.000	He*	137Phe	1H

173.17	0.000	C	137Phe	13C
2.59	0.010	Hba	137Phe	1H
7.17	0.022	Hd*	137Phe	1H
3.43	0.006	Hbb	137Phe	1H
42.78	0.069	Cb	137Phe	13C
58.39	0.073	Ca	137Phe	13C
4.69	0.014	Ha	137Phe	1H
123.17	0.036	N	137Phe	15N
7.84	0.035	H	137Phe	1H
173.09	0.000	C	138Ser	13C
3.54	0.012	Hbb	138Ser	1H
3.40	0.007	Hba	138Ser	1H
119.48	0.069	N	138Ser	15N
7.47	0.031	H	138Ser	1H
64.73	0.054	Cb	138Ser	13C
56.95	0.061	Ca	138Ser	13C
5.22	0.011	Ha	138Ser	1H
172.85	0.000	C	139Glu	13C
1.65	0.005	Hga	139Glu	1H
2.10	0.007	Hgb	139Glu	1H
37.20	0.065	Cg	139Glu	13C
1.82	0.012	Hba	139Glu	1H
2.11	0.010	Hbb	139Glu	1H
34.84	0.131	Cb	139Glu	13C
56.37	0.100	Ca	139Glu	13C
4.16	0.009	Ha	139Glu	1H
124.75	0.090	N	139Glu	15N
8.60	0.024	H	139Glu	1H
174.02	0.000	C	140Phe	13C
6.83	0.024	Hd*	140Phe	1H
58.54	0.040	Ca	140Phe	13C
7.09	0.022	He*	140Phe	1H
4.09	0.003	Ha	140Phe	1H
2.65	0.002	Hba	140Phe	1H
2.77	0.003	Hbb	140Phe	1H
40.59	0.078	Cb	140Phe	13C
129.29	0.081	N	140Phe	15N
8.63	0.029	H	140Phe	1H
172.15	0.000	C	141His	13C
6.10	0.038	Hd2	141His	1H
54.20	0.098	Ca	141His	13C
2.20	0.012	Hbb	141His	1H

4.06	0.012	Ha	141His	1H
31.18	0.127	Cb	141His	13C
0.91	0.016	Hba	141His	1H
122.90	0.044	N	141His	15N
7.98	0.040	H	141His	1H
175.84	0.000	C	142Asp	13C
120.31	0.098	N	142Asp	15N
7.98	0.022	H	142Asp	1H
2.76	0.004	Hbb	142Asp	1H
2.35	0.004	Hba	142Asp	1H
53.16	0.058	Ca	142Asp	13C
42.37	0.084	Cb	142Asp	13C
4.46	0.010	Ha	142Asp	1H
176.70	0.000	C	143Ala	13C
52.61	0.046	Ca	143Ala	13C
122.53	0.050	N	143Ala	15N
18.78	0.078	Cb	143Ala	13C
3.95	0.005	Ha	143Ala	1H
8.03	0.027	H	143Ala	1H
1.18	0.006	Hb*	143Ala	1H
175.61	0.000	C	144Asp	13C
53.01	0.091	Ca	144Asp	13C
3.17	0.004	Hbb	144Asp	1H
2.77	0.002	Hba	144Asp	1H
41.29	0.075	Cb	144Asp	13C
4.57	0.006	Ha	144Asp	1H
120.23	0.092	N	144Asp	15N
8.82	0.026	H	144Asp	1H
178.46	0.000	C	145Ala	13C
54.67	0.104	Ca	145Ala	13C
4.03	0.004	Ha	145Ala	1H
117.31	0.083	N	145Ala	15N
8.15	0.030	H	145Ala	1H
18.27	0.073	Cb	145Ala	13C
1.37	0.006	Hb*	145Ala	1H
174.64	0.000	C	146Gln	13C
7.07	0.000	He2a	146Gln	1H
9.77	0.000	He2b	146Gln	1H
1.98	0.001	Hbb	146Gln	1H
112.74	0.008	Ne2	146Gln	15N
30.86	0.077	Cb	146Gln	13C
34.80	0.067	Cg	146Gln	13C

1.98	0.008	Hba	146Gln	1H
2.28	0.008	Hga	146Gln	1H
2.28	0.008	Hgb	146Gln	1H
7.94	0.072	H	146Gln	1H
56.32	0.104	Ca	146Gln	13C
113.12	0.083	N	146Gln	15N
4.37	0.012	Ha	146Gln	1H
174.20	0.000	C	147Asn	13C
116.76	0.012	Nd2	147Asn	15N
8.39	0.042	Hd2b	147Asn	1H
6.98	0.026	Hd2a	147Asn	1H
2.88	0.008	Hbb	147Asn	1H
40.95	0.103	Cb	147Asn	13C
2.40	0.014	Hba	147Asn	1H
52.79	0.070	Ca	147Asn	13C
119.47	0.070	N	147Asn	15N
5.30	0.021	Ha	147Asn	1H
8.13	0.032	H	147Asn	1H
172.89	0.000	C	148Ser	13C
61.34	0.039	Ca	148Ser	13C
3.89	0.002	Hbb	148Ser	1H
63.31	0.036	Cb	148Ser	13C
4.00	0.006	Ha	148Ser	1H
3.81	0.013	Hba	148Ser	1H
117.23	0.024	N	148Ser	15N
8.92	0.031	H	148Ser	1H
6.95	0.000	Hd1	149His	1H
173.30	0.000	C	149His	13C
55.05	0.056	Ca	149His	13C
4.88	0.003	Ha	149His	1H
3.13	0.014	Hbb	149His	1H
34.93	0.139	Cb	149His	13C
2.25	0.010	Hba	149His	1H
117.61	0.040	N	149His	15N
7.02	0.025	H	149His	1H
173.10	0.000	C	150Ser	13C
58.66	0.042	Ca	150Ser	13C
4.33	0.015	Ha	150Ser	1H
4.01	0.010	Hba	150Ser	1H
4.13	0.005	Hbb	150Ser	1H
113.58	0.039	N	150Ser	15N
63.93	0.046	Cb	150Ser	13C

8.60	0.021	H	150Ser	1H
7.12	0.000	Hd*	151Tyr	1H
6.29	0.000	He*	151Tyr	1H
172.06	0.000	C	151Tyr	13C
1.82	0.010	Hba	151Tyr	1H
54.67	0.067	Ca	151Tyr	13C
2.54	0.020	Hbb	151Tyr	1H
38.96	0.119	Cb	151Tyr	13C
5.25	0.014	Ha	151Tyr	1H
115.22	0.057	N	151Tyr	15N
7.62	0.029	H	151Tyr	1H
54.71	0.000	Ca	152Cys	13C
29.78	0.000	Cb	152Cys	13C
174.33	0.000	C	152Cys	13C
118.67	0.041	N	152Cys	15N
8.33	0.044	H	152Cys	1H
55.31	0.000	Ca	153Phe	13C
175.02	0.000	C	153Phe	13C
1.97	0.008	Hba	153Phe	1H
40.31	0.000	Cb	153Phe	13C
5.02	0.006	Ha	153Phe	1H
2.39	0.010	Hbb	153Phe	1H
128.65	0.061	N	153Phe	15N
8.39	0.026	H	153Phe	1H
2.50	0.000	Hgb	154Glu	1H
2.20	0.000	Hga	154Glu	1H
36.79	0.000	Cg	154Glu	13C
1.97	0.003	Hba	154Glu	1H
34.93	0.000	Cb	154Glu	13C
2.10	0.004	Hbb	154Glu	1H
54.39	0.000	Ca	154Glu	13C
5.48	0.015	Ha	154Glu	1H
124.16	0.038	N	154Glu	15N
9.76	0.029	H	154Glu	1H
27.58	0.000	Cg1	155Ile	13C
174.90	0.000	C	155Ile	13C
1.87	0.014	Hg1b	155Ile	1H
0.95	0.006	Hg1a	155Ile	1H
40.29	0.121	Cb	155Ile	13C
1.62	0.006	Hb	155Ile	1H
124.16	0.072	N	155Ile	15N
8.60	0.027	H	155Ile	1H

60.08	0.158	Ca	155Ile	13C
17.20	0.083	Cg2	155Ile	13C
5.24	0.013	Ha	155Ile	1H
13.29	0.041	Cd1	155Ile	13C
0.39	0.010	Hg2*	155Ile	1H
0.61	0.009	Hd1*	155Ile	1H
175.75	0.000	C	156Leu	13C
25.25	0.077	Cdb	156Leu	13C
28.19	0.117	Cg	156Leu	13C
26.16	0.072	Cda	156Leu	13C
126.33	0.061	N	156Leu	15N
1.47	0.009	Hg	156Leu	1H
0.80	0.009	Hdb*	156Leu	1H
1.37	0.016	Hba	156Leu	1H
0.57	0.006	Hda*	156Leu	1H
9.28	0.030	H	156Leu	1H
1.65	0.016	Hbb	156Leu	1H
45.42	0.113	Cb	156Leu	13C
53.22	0.077	Ca	156Leu	13C
5.65	0.012	Ha	156Leu	1H
175.93	0.000	C	157Glu	13C
2.30	0.011	Hgb	157Glu	1H
37.09	0.000	Cg	157Glu	13C
2.25	0.020	Hga	157Glu	1H
1.88	0.010	Hba	157Glu	1H
33.46	0.118	Cb	157Glu	13C
2.11	0.009	Hbb	157Glu	1H
119.89	0.048	N	157Glu	15N
9.29	0.029	H	157Glu	1H
54.52	0.057	Ca	157Glu	13C
5.34	0.008	Ha	157Glu	1H
176.04	0.000	C	158Arg	13C
7.00	0.005	He	158Arg	1H
84.85	0.024	Ne	158Arg	15N
42.91	0.063	Cd	158Arg	13C
27.21	0.048	Cg	158Arg	13C
1.23	0.008	Hgb	158Arg	1H
1.11	0.007	Hba	158Arg	1H
1.46	0.005	Hbb	158Arg	1H
0.72	0.006	Hga	158Arg	1H
2.71	0.009	Hda	158Arg	1H
2.72	0.006	Hdb	158Arg	1H

30.49	0.065	Cb	158Arg	13C
126.60	0.085	N	158Arg	15N
8.21	0.030	H	158Arg	1H
57.06	0.095	Ca	158Arg	13C
3.36	0.008	Ha	158Arg	1H
28.47	0.000	Cg	159Arg	13C
1.51	0.003	Hgb	159Arg	1H
1.42	0.003	Hga	159Arg	1H
43.32	0.061	Cd	159Arg	13C
3.09	0.002	Hdb	159Arg	1H
131.36	0.065	N	159Arg	15N
58.38	0.108	Ca	159Arg	13C
1.37	0.010	Hba	159Arg	1H
1.69	0.014	Hbb	159Arg	1H
3.09	0.005	Hda	159Arg	1H
7.93	0.031	H	159Arg	1H
3.95	0.010	Ha	159Arg	1H
31.17	0.075	Cb	159Arg	13C
8.58	0.003	H7*	160Fol	1H
7.94	0.003	H16*	160Fol	1H
7.07	0.021	H13*	160Fol	1H
7.53	0.010	H12*	160Fol	1H
6.59	0.015	H15*	160Fol	1H
8.12	0.000	H5n*	161Nap	1H
8.58	0.000	H2n*	161Nap	1H
9.09	0.000	H6n*	161Nap	1H
9.79	0.030	H4n*	161Nap	1H
7.48	0.005	H2a*	161Nap	1H
8.33	0.016	H8a*	161Nap	1H

8.1.3 Chemical shift assignments of EcDHFR: $NADP^+$: Folate complex without co-solvent present

Table 8.1.3 Average chemical shifts (ppm) of nuclei in EcDHFR: $NADP^+$: Folate complex under the standard NMR buffer conditions in the presence of no co-solvent or buffer only from nuclear magnetic resonance spectroscopy measured at 298.3 K. Assign Name in the colour red refers to tentative chemical shift assignments for ligand and co-factor, for which assignment confidence is low.

Buffer Chemical Shift (ppm)	SD	Assign Name	Residue	Isotope
55.28	0.094	Ca	1Met	13C
32.72	0.013	Cg	1Met	13C
30.14	0.176	Cb	1Met	13C
4.17	0.008	Ha	1Met	1H
2.55	0.002	Hba	1Met	1H
2.63	0.005	Hbb	1Met	1H
2.26	0.009	Hga	1Met	1H
2.36	0.008	Hgb	1Met	1H
171.15	0.004	C	1Met	13C
124.63	0.043	N	2Ile	15N
9.46	0.009	H	2Ile	1H
61.46	0.056	Ca	2Ile	13C
39.32	0.052	Cb	2Ile	13C
29.07	0.056	Cg1	2Ile	13C
18.09	0.058	Cg2	2Ile	13C
14.04	0.044	Cd1	2Ile	13C
4.57	0.003	Ha	2Ile	1H
1.92	0.008	Hb	2Ile	1H
0.99	0.011	Hg1a	2Ile	1H
1.81	0.005	Hg1b	2Ile	1H
0.87	0.006	Hg2*	2Ile	1H
0.98	0.008	Hd1*	2Ile	1H
173.89	0.039	C	2Ile	13C
126.01	0.042	N	3Ser	15N
9.41	0.006	H	3Ser	1H
56.26	0.038	Ca	3Ser	13C
65.49	0.034	Cb	3Ser	13C
5.95	0.012	Ha	3Ser	1H
4.18	0.004	Hbb	3Ser	1H

3.76	0.007	Hba	3Ser	1H
173.51	0.049	C	3Ser	13C
121.73	0.030	N	4Leu	15N
8.55	0.006	H	4Leu	1H
53.78	0.054	Ca	4Leu	13C
43.79	0.061	Cb	4Leu	13C
5.54	0.007	Ha	4Leu	1H
26.04	0.013	Cdb	4Leu	13C
1.62	0.008	Hba	4Leu	1H
1.81	0.011	Hbb	4Leu	1H
29.75	0.044	Cg	4Leu	13C
1.88	0.006	Hg	4Leu	1H
0.91	0.006	Hda*	4Leu	1H
0.95	0.008	Hdb*	4Leu	1H
175.19	0.032	C	4Leu	13C
25.51	0.069	Cda	4Leu	13C
120.20	0.013	N	5Ile	15N
8.59	0.005	H	5Ile	1H
57.98	0.038	Ca	5Ile	13C
43.10	0.048	Cb	5Ile	13C
5.98	0.011	Ha	5Ile	1H
15.41	0.047	Cg2	5Ile	13C
16.55	0.032	Cd1	5Ile	13C
1.18	0.007	Hb	5Ile	1H
172.39	0.000	C	5Ile	13C
0.33	0.006	Hg2*	5Ile	1H
1.13	0.007	Hd1*	5Ile	1H
27.94	0.056	Cg1	5Ile	13C
2.18	0.001	Hg1a	5Ile	1H
2.25	0.002	Hg1b	5Ile	1H
126.43	0.008	N	6Ala	15N
8.64	0.011	H	6Ala	1H
52.69	0.076	Ca	6Ala	13C
25.80	0.060	Cb	6Ala	13C
4.94	0.005	Ha	6Ala	1H
0.63	0.006	Hb*	6Ala	1H
175.06	0.000	C	6Ala	13C
50.59	0.075	Ca	7Ala	13C
21.04	0.059	Cb	7Ala	13C
4.96	0.009	Ha	7Ala	1H
1.45	0.009	Hb*	7Ala	1H
175.11	0.000	C	7Ala	13C

123.53	0.007	N	8Leu	15N
9.15	0.012	H	8Leu	1H
53.95	0.004	Ca	8Leu	13C
45.48	0.015	Cb	8Leu	13C
4.67	0.003	Ha	8Leu	1H
28.99	0.071	Cg	8Leu	13C
25.99	0.029	Cdb	8Leu	13C
175.43	0.000	C	8Leu	13C
1.48	0.007	Hbb	8Leu	1H
1.32	0.005	Hba	8Leu	1H
0.40	0.007	Hdb*	8Leu	1H
0.23	0.008	Hda*	8Leu	1H
25.56	0.035	Cda	8Leu	13C
1.32	0.002	Hg	8Leu	1H
125.92	0.012	N	9Ala	15N
8.52	0.013	H	9Ala	1H
5.01	0.002	Ha	9Ala	1H
49.86	0.014	Ca	9Ala	13C
19.32	0.030	Cb	9Ala	13C
1.44	0.009	Hb*	9Ala	1H
175.96	0.000	C	9Ala	13C
118.36	0.019	N	10Val	15N
7.59	0.003	H	10Val	1H
65.03	0.066	Ca	10Val	13C
31.75	0.026	Cb	10Val	13C
21.41	0.040	Cga	10Val	13C
23.26	0.033	Cgb	10Val	13C
177.77	0.000	C	10Val	13C
2.11	0.004	Hb	10Val	1H
1.00	0.007	Hgb*	10Val	1H
0.98	0.005	Hga*	10Val	1H
3.76	0.009	Ha	10Val	1H
122.82	0.018	N	11Asp	15N
9.12	0.003	H	11Asp	1H
56.04	0.065	Ca	11Asp	13C
39.08	0.036	Cb	11Asp	13C
4.35	0.007	Ha	11Asp	1H
174.94	0.000	C	11Asp	13C
3.09	0.009	Hbb	11Asp	1H
2.89	0.004	Hba	11Asp	1H
107.33	0.012	N	12Arg	15N
8.50	0.006	H	12Arg	1H

57.49	0.041	Ca	12Arg	13C
27.65	0.021	Cb	12Arg	13C
3.68	0.006	Ha	12Arg	1H
43.46	0.049	Cd	12Arg	13C
175.90	0.012	C	12Arg	13C
2.23	0.007	Hba	12Arg	1H
2.54	0.007	Hbb	12Arg	1H
1.74	0.003	Hgb	12Arg	1H
1.60	0.003	Hga	12Arg	1H
3.22	0.004	Hda	12Arg	1H
3.43	0.003	Hdb	12Arg	1H
28.15	0.070	Cg	12Arg	13C
83.29	0.000	Ne	12Arg	15N
7.15	0.000	He	12Arg	1H
120.64	0.027	N	13Val	15N
7.14	0.007	H	13Val	1H
32.95	0.032	Cb	13Val	13C
65.72	0.046	Ca	13Val	13C
3.58	0.005	Ha	13Val	1H
176.80	0.000	C	13Val	13C
1.91	0.006	Hb	13Val	1H
1.19	0.006	Hgb*	13Val	1H
0.92	0.006	Hga*	13Val	1H
23.21	0.045	Cgb	13Val	13C
21.95	0.040	Cga	13Val	13C
41.72	0.016	Cb	14Ile	13C
1.67	0.008	Hb	14Ile	1H
3.82	0.007	Ha	14Ile	1H
0.74	0.003	Hg2*	14Ile	1H
14.14	0.033	Cd1	14Ile	13C
17.92	0.069	Cg2	14Ile	13C
61.16	0.071	Ca	14Ile	13C
27.88	0.051	Cg1	14Ile	13C
109.37	0.007	N	15Gly	15N
7.55	0.007	H	15Gly	1H
45.89	0.041	Ca	15Gly	13C
169.88	0.000	C	15Gly	13C
4.15	0.000	Haa	15Gly	1H
4.44	0.000	Hab	15Gly	1H
119.28	0.008	N	16Met	15N
8.57	0.003	H	16Met	1H
55.44	0.000	Ca	16Met	13C

34.54	0.000	Cb	16Met	13C
4.74	0.000	Ha	16Met	1H
174.67	0.000	C	16Met	13C
1.93	0.000	He*	16Met	1H
18.55	0.000	Ce	16Met	13C
27.23	0.000	Cb	17Glu	13C
36.52	0.000	Cg	17Glu	13C
175.53	0.000	C	17Glu	13C
114.55	0.006	N	18Asn	15N
9.48	0.010	H	18Asn	1H
38.76	0.065	Cb	18Asn	13C
54.16	0.049	Ca	18Asn	13C
173.56	0.053	C	18Asn	13C
4.20	0.006	Ha	18Asn	1H
3.06	0.005	Hbb	18Asn	1H
2.47	0.002	Hba	18Asn	1H
6.75	0.000	Hd2a	18Asn	1H
110.48	0.017	Nd2	18Asn	15N
7.54	0.000	Hd2b	18Asn	1H
121.12	0.017	N	19Ala	15N
7.71	0.007	H	19Ala	1H
50.57	0.049	Ca	19Ala	13C
21.60	0.035	Cb	19Ala	13C
4.45	0.008	Ha	19Ala	1H
1.24	0.008	Hb*	19Ala	1H
176.05	0.015	C	19Ala	13C
119.83	0.008	N	20Met	15N
8.34	0.009	H	20Met	1H
52.46	0.000	Ca	20Met	13C
40.97	0.000	Cb	20Met	13C
175.17	0.000	C	20Met	13C
17.13	0.023	Ce	20Met	13C
1.89	0.010	He*	20Met	1H
177.92	0.000	C	21Pro	13C
10.56	0.000	He1	22Trp	1H
132.69	0.000	Ne1	22Trp	15N
116.21	0.000	N	22Trp	15N
7.40	0.000	H	22Trp	1H
173.84	0.000	C	22Trp	13C
6.83	0.004	Hd1	22Trp	1H
28.57	0.000	Cb	22Trp	13C
126.44	0.000	Cd1	22Trp	13C

117.38	0.000	N	23Asn	15N
8.98	0.000	H	23Asn	1H
53.63	0.061	Ca	23Asn	13C
40.36	0.021	Cb	23Asn	13C
4.85	0.009	Ha	23Asn	1H
2.61	0.006	Hba	23Asn	1H
2.87	0.005	Hbb	23Asn	1H
112.39	0.000	Nd2	23Asn	15N
7.59	0.000	Hd2b	23Asn	1H
6.84	0.000	Hd2a	23Asn	1H
172.65	0.000	C	23Asn	13C
125.33	0.024	N	24Leu	15N
9.57	0.014	H	24Leu	1H
51.20	0.091	Ca	24Leu	13C
44.50	0.092	Cb	24Leu	13C
5.24	0.006	Ha	24Leu	1H
173.94	0.000	C	24Leu	13C
1.60	0.008	Hbb	24Leu	1H
1.07	0.005	Hba	24Leu	1H
0.39	0.009	Hda*	24Leu	1H
0.79	0.000	Hdb*	24Leu	1H
1.49	0.000	Hg	24Leu	1H
26.71	0.061	Cda	24Leu	13C
25.80	0.054	[1943]	24Leu	13C
65.36	0.076	Ca	25Pro	13C
50.55	0.011	Cd	25Pro	13C
31.28	0.052	Cb	25Pro	13C
27.91	0.010	Cg	25Pro	13C
179.56	0.000	C	25Pro	13C
3.44	0.002	Hda	25Pro	1H
3.67	0.000	Hdb	25Pro	1H
1.74	0.012	Hba	25Pro	1H
2.41	0.008	Hbb	25Pro	1H
1.97	0.021	Hgb	25Pro	1H
1.95	0.019	Hga	25Pro	1H
4.51	0.000	Ha	25Pro	1H
120.31	0.021	N	26Ala	15N
9.29	0.004	H	26Ala	1H
55.11	0.119	Ca	26Ala	13C
19.00	0.070	Cb	26Ala	13C
4.16	0.000	Ha	26Ala	1H
1.25	0.000	Hb*	26Ala	1H

181.60	0.023	C	26Ala	13C
118.54	0.034	N	27Asp	15N
7.48	0.006	H	27Asp	1H
56.40	0.053	Ca	27Asp	13C
43.59	0.081	Cb	27Asp	13C
4.88	0.002	Ha	27Asp	1H
2.07	0.009	Hba	27Asp	1H
2.89	0.008	Hbb	27Asp	1H
177.35	0.000	C	27Asp	13C
121.36	0.029	N	28Leu	15N
7.61	0.007	H	28Leu	1H
3.93	0.004	Ha	28Leu	1H
40.74	0.106	Cb	28Leu	13C
57.60	0.048	Ca	28Leu	13C
1.28	0.003	Hba	28Leu	1H
1.64	0.003	Hbb	28Leu	1H
1.44	0.007	Hg	28Leu	1H
27.08	0.011	Cg	28Leu	13C
24.76	0.070	Cdb	28Leu	13C
22.19	0.089	Cda	28Leu	13C
0.49	0.007	Hdb*	28Leu	1H
0.04	0.003	Hda*	28Leu	1H
178.97	0.017	C	28Leu	13C
120.68	0.006	N	29Ala	15N
7.87	0.009	H	29Ala	1H
17.54	0.135	Cb	29Ala	13C
55.07	0.032	Ca	29Ala	13C
4.15	0.003	Ha	29Ala	1H
180.68	0.034	C	29Ala	13C
1.20	0.048	Hb*	29Ala	1H
124.27	0.014	N	30Trp	15N
7.45	0.010	H	30Trp	1H
29.17	0.053	Cb	30Trp	13C
60.14	0.071	Ca	30Trp	13C
4.01	0.006	Ha	30Trp	1H
2.68	0.007	Hba	30Trp	1H
3.41	0.005	Hbb	30Trp	1H
177.97	0.017	C	30Trp	13C
130.62	0.000	Ne1	30Trp	15N
10.52	0.000	He1	30Trp	1H
6.75	0.000	He3	30Trp	1H
6.97	0.001	Hd1	30Trp	1H

129.25	0.000	Cd1	30Trp	13C
123.60	0.007	N	31Phe	15N
9.05	0.007	H	31Phe	1H
61.37	0.091	Ca	31Phe	13C
38.08	0.033	Cb	31Phe	13C
178.42	0.000	C	31Phe	13C
2.60	0.005	Hba	31Phe	1H
3.21	0.006	Hbb	31Phe	1H
3.55	0.006	Ha	31Phe	1H
124.34	0.041	N	32Lys	15N
8.70	0.006	H	32Lys	1H
60.29	0.063	Ca	32Lys	13C
32.33	0.157	Cb	32Lys	13C
3.34	0.005	Ha	32Lys	1H
42.18	0.000	Ce	32Lys	13C
24.93	0.000	Cg	32Lys	13C
29.96	0.042	Cd	32Lys	13C
177.85	0.001	C	32Lys	13C
1.79	0.018	Hba	32Lys	1H
1.89	0.003	Hbb	32Lys	1H
2.77	0.000	Hea	32Lys	1H
2.81	0.000	Heb	32Lys	1H
1.58	0.001	Hda	32Lys	1H
1.63	0.001	Hdb	32Lys	1H
117.14	0.018	N	33Arg	15N
8.10	0.005	H	33Arg	1H
59.01	0.082	Ca	33Arg	13C
29.64	0.053	Cb	33Arg	13C
43.70	0.014	Cd	33Arg	13C
26.31	0.005	Cg	33Arg	13C
178.49	0.000	C	33Arg	13C
1.47	0.002	Hba	33Arg	1H
1.71	0.002	Hbb	33Arg	1H
3.71	0.006	Ha	33Arg	1H
1.27	0.002	Hga	33Arg	1H
1.41	0.001	Hgb	33Arg	1H
2.96	0.001	Hda	33Arg	1H
2.96	0.001	Hdb	33Arg	1H
7.10	0.000	He	33Arg	1H
85.74	0.000	Ne	33Arg	15N
111.55	0.022	N	34Asn	15N
7.10	0.009	H	34Asn	1H

4.11	0.001	Ha	34Asn	1H
39.06	0.052	Cb	34Asn	13C
54.53	0.040	Ca	34Asn	13C
1.25	0.002	Hba	34Asn	1H
1.35	0.004	Hbb	34Asn	1H
174.07	0.017	C	34Asn	13C
107.40	0.035	N	35Thr	15N
7.14	0.010	H	35Thr	1H
61.91	0.097	Ca	35Thr	13C
70.26	0.127	Cb	35Thr	13C
3.91	0.000	Ha	35Thr	1H
20.86	0.104	Cg2	35Thr	13C
173.28	0.018	C	35Thr	13C
3.34	0.000	Hb	35Thr	1H
0.07	0.000	Hg2*	35Thr	1H
121.84	0.007	N	36Leu	15N
7.52	0.006	H	36Leu	1H
56.92	0.034	Ca	36Leu	13C
42.27	0.081	Cb	36Leu	13C
3.37	0.008	Ha	36Leu	1H
24.39	0.007	Cdb	36Leu	13C
1.31	0.006	Hba	36Leu	1H
1.43	0.006	Hbb	36Leu	1H
26.56	0.015	Cdb	36Leu	13C
1.54	0.006	Hdb*	36Leu	1H
0.73	0.000	Hda*	36Leu	1H
176.54	0.000	C	36Leu	13C
113.28	0.004	N	37Asp	15N
7.89	0.003	H	37Asp	1H
54.95	0.026	Ca	37Asp	13C
37.33	0.222	Cb	37Asp	13C
4.35	0.000	Ha	37Asp	1H
2.97	0.002	Hba	37Asp	1H
173.68	0.017	C	37Asp	13C
2.98	0.000	Hbb	37Asp	1H
119.76	0.007	N	38Lys	15N
7.92	0.011	H	38Lys	1H
54.10	0.000	Ca	38Lys	13C
33.81	0.036	Cb	38Lys	13C
172.52	0.000	C	38Lys	13C
4.76	0.000	Ha	38Lys	1H
1.06	0.000	Hgb	38Lys	1H

1.44	0.002	Hba	38Lys	1H
1.79	0.000	Hbb	38Lys	1H
62.17	0.096	Ca	39Pro	13C
49.04	0.015	Cd	39Pro	13C
32.00	0.015	Cb	39Pro	13C
28.81	0.005	Cg	39Pro	13C
3.97	0.006	Hdb	39Pro	1H
3.79	0.003	Hda	39Pro	1H
2.04	0.000	Hga	39Pro	1H
2.16	0.001	Hgb	39Pro	1H
1.96	0.005	Hba	39Pro	1H
4.97	0.005	Ha	39Pro	1H
2.14	0.009	Hbb	39Pro	1H
175.90	0.000	C	39Pro	13C
113.05	0.017	N	40Val	15N
8.73	0.006	H	40Val	1H
56.54	0.068	Ca	40Val	13C
33.97	0.105	Cb	40Val	13C
5.54	0.007	Ha	40Val	1H
1.81	0.004	Hb	40Val	1H
22.25	0.016	Cga	40Val	13C
19.76	0.002	Cga	40Val	13C
0.80	0.000	Hgb*	40Val	1H
0.59	0.000	Hga*	40Val	1H
173.63	0.017	C	40Val	13C
121.66	0.003	N	41Ile	15N
8.46	0.004	H	41Ile	1H
59.55	0.043	Ca	41Ile	13C
40.53	0.102	Cb	41Ile	13C
4.83	0.000	Ha	41Ile	1H
1.04	0.001	Hb	41Ile	1H
27.39	0.017	Cg1	41Ile	13C
0.39	0.003	Hg1a	41Ile	1H
1.26	0.001	Hg1b	41Ile	1H
17.44	0.010	Cg2	41Ile	13C
14.71	0.001	Cd1	41Ile	13C
0.34	0.000	Hg2*	41Ile	1H
174.94	0.000	C	41Ile	13C
0.43	0.000	Hd1*	41Ile	1H
52.15	0.105	Ca	42Met	13C
40.47	0.206	Cb	42Met	13C
31.50	0.014	Cg	42Met	13C

123.94	0.018	N	42Met	15N
9.08	0.005	H	42Met	1H
5.71	0.008	Ha	42Met	1H
1.72	0.002	Hba	42Met	1H
2.00	0.013	Hbb	42Met	1H
2.48	0.000	Hgb	42Met	1H
2.08	0.000	Hga	42Met	1H
174.46	0.018	C	42Met	13C
1.78	0.000	He*	42Met	1H
18.42	0.000	Ce	42Met	13C
105.74	0.019	N	43Gly	15N
9.22	0.007	H	43Gly	1H
44.37	0.045	Ca	43Gly	13C
4.31	0.004	Hab	43Gly	1H
4.06	0.008	Haa	43Gly	1H
175.58	0.000	C	43Gly	13C
119.32	0.003	N	44Arg	15N
7.66	0.004	H	44Arg	1H
60.78	0.102	Ca	44Arg	13C
30.20	0.062	Cb	44Arg	13C
42.66	0.013	Cd	44Arg	13C
178.49	0.000	C	44Arg	13C
1.57	0.002	Hba	44Arg	1H
1.65	0.010	Hbb	44Arg	1H
3.34	0.000	Ha	44Arg	1H
2.77	0.003	Hda	44Arg	1H
2.83	0.002	Hdb	44Arg	1H
1.32	0.005	Hga	44Arg	1H
25.13	0.015	Cg	44Arg	13C
112.91	0.018	N	45His	15N
7.44	0.007	H	45His	1H
58.04	0.055	Ca	45His	13C
26.92	0.052	Cb	45His	13C
177.99	0.020	C	45His	13C
4.24	0.004	Ha	45His	1H
1.85	0.000	Hbb	45His	1H
1.74	0.000	Hba	45His	1H
119.76	0.034	N	46Thr	15N
8.12	0.015	H	46Thr	1H
68.42	0.000	Cb	46Thr	13C
20.84	0.142	Cg2	46Thr	13C
176.15	0.000	C	46Thr	13C

1.35	0.000	Hg2*	46Thr	1H
3.95	0.000	Hb	46Thr	1H
124.47	0.021	N	47Trp	15N
8.36	0.002	H	47Trp	1H
128.31	0.000	Ne1	47Trp	15N
10.36	0.000	He1	47Trp	1H
30.07	0.070	Cb	47Trp	13C
7.28	0.000	He3	47Trp	1H
7.28	0.003	Hd1	47Trp	1H
4.68	0.000	Ha	47Trp	1H
3.27	0.002	Hba	47Trp	1H
3.38	0.001	Hbb	47Trp	1H
127.30	0.000	Cd1	47Trp	13C
28.60	0.035	Cb	48Glu	13C
59.06	0.106	Ca	48Glu	13C
37.36	0.000	Cg	48Glu	13C
178.32	0.000	C	48Glu	13C
3.41	0.000	Ha	48Glu	1H
8.09	0.000	H	48Glu	1H
2.81	0.000	Hgb	48Glu	1H
2.31	0.000	Hga	48Glu	1H
1.91	0.000	Hba	48Glu	1H
2.18	0.000	Hbb	48Glu	1H
114.21	0.018	N	49Ser	15N
7.79	0.012	H	49Ser	1H
60.36	0.079	Ca	49Ser	13C
63.51	0.071	Cb	49Ser	13C
4.23	0.000	Ha	49Ser	1H
175.17	0.000	C	49Ser	13C
3.95	0.000	Hba	49Ser	1H
4.00	0.000	Hbb	49Ser	1H
122.85	0.039	N	50Ile	15N
7.65	0.006	H	50Ile	1H
65.10	0.056	Ca	50Ile	13C
38.70	0.016	Cb	50Ile	13C
1.35	0.002	Hb	50Ile	1H
3.47	0.000	Ha	50Ile	1H
27.51	0.020	Cg1	50Ile	13C
17.31	0.073	Cg2	50Ile	13C
14.23	0.093	Cd1	50Ile	13C
0.04	0.002	Hg1a	50Ile	1H
1.55	0.004	Hg1b	50Ile	1H

0.38	0.000	Hg2*	50Ile	1H
178.81	0.044	C	50Ile	13C
0.43	0.000	Hd1*	50Ile	1H
104.35	0.008	N	51Gly	15N
7.54	0.008	H	51Gly	1H
3.61	0.006	Hab	51Gly	1H
2.94	0.003	Haa	51Gly	1H
45.72	0.077	Ca	51Gly	13C
172.64	0.006	C	51Gly	13C
116.06	0.031	N	52Arg	15N
6.80	0.003	H	52Arg	1H
53.17	0.019	Ca	52Arg	13C
28.53	0.031	Cb	52Arg	13C
4.37	0.008	Ha	52Arg	1H
1.61	0.002	Hba	52Arg	1H
1.89	0.002	Hbb	52Arg	1H
43.37	0.016	Cd	52Arg	13C
2.93	0.002	Hda	52Arg	1H
2.97	0.001	Hdb	52Arg	1H
24.76	0.000	Cg	52Arg	13C
1.26	0.000	Hgb	52Arg	1H
1.19	0.002	Hga	52Arg	1H
61.69	0.039	Ca	53Pro	13C
31.20	0.095	Cb	53Pro	13C
27.98	0.008	Cg	53Pro	13C
49.41	0.016	Cd	53Pro	13C
1.95	0.005	Hbb	53Pro	1H
1.68	0.008	Hba	53Pro	1H
3.57	0.001	Hda	53Pro	1H
3.61	0.001	Hdb	53Pro	1H
1.73	0.005	Hga	53Pro	1H
2.02	0.012	Hgb	53Pro	1H
3.96	0.000	Ha	53Pro	1H
177.05	0.000	C	53Pro	13C
126.38	0.009	N	54Leu	15N
9.48	0.006	H	54Leu	1H
52.12	0.059	Ca	54Leu	13C
40.52	0.066	Cb	54Leu	13C
4.41	0.004	Ha	54Leu	1H
26.26	0.019	Cdb	54Leu	13C
21.94	0.002	Cda	54Leu	13C
1.61	0.005	Hbb	54Leu	1H

0.84	0.006	Hba	54Leu	1H
0.78	0.009	Hdb*	54Leu	1H
34.18	0.000	Cg	54Leu	13C
0.43	0.004	Hda*	54Leu	1H
176.06	0.000	C	54Leu	13C
46.61	0.018	Ca	56Gly	13C
3.69	0.004	Haa	56Gly	1H
3.85	0.002	Hab	56Gly	1H
173.09	0.000	C	56Gly	13C
118.23	0.011	N	57Arg	15N
7.25	0.012	H	57Arg	1H
35.92	0.026	Cb	57Arg	13C
54.58	0.049	Ca	57Arg	13C
4.36	0.003	Ha	57Arg	1H
27.98	0.004	Cg	57Arg	13C
43.11	0.013	Cd	57Arg	13C
1.90	0.000	Hbb	57Arg	1H
1.29	0.000	Hba	57Arg	1H
2.32	0.001	Hda	57Arg	1H
2.67	0.002	Hdb	57Arg	1H
2.73	0.002	Hgb	57Arg	1H
1.24	0.003	Hga	57Arg	1H
174.47	0.017	C	57Arg	13C
123.76	0.012	N	58Lys	15N
7.48	0.013	H	58Lys	1H
56.12	0.047	Ca	58Lys	13C
32.48	0.115	Cb	58Lys	13C
4.36	0.002	Ha	58Lys	1H
1.55	0.002	Hba	58Lys	1H
1.63	0.005	Hbb	58Lys	1H
29.58	0.013	Cd	58Lys	13C
25.16	0.000	Cg	58Lys	13C
41.99	0.000	Ce	58Lys	13C
174.95	0.078	C	58Lys	13C
2.76	0.003	Hea	58Lys	1H
2.80	0.000	Heb	58Lys	1H
1.30	0.000	Hgb	58Lys	1H
1.05	0.000	Hga	58Lys	1H
1.54	0.000	Hda	58Lys	1H
1.57	0.001	Hdb	58Lys	1H
9.15	0.004	H	59Asn	1H
126.56	0.057	N	59Asn	15N

53.34	0.031	Ca	59Asn	13C
40.65	0.094	Cb	59Asn	13C
4.74	0.000	Ha	59Asn	1H
172.65	0.000	C	59Asn	13C
109.07	0.000	Nd2	59Asn	15N
6.67	0.000	Hd2a	59Asn	1H
7.41	0.000	Hd2b	59Asn	1H
173.36	0.000	Cg	59Asn	13C
2.85	0.000	Hbb	59Asn	1H
1.80	0.000	Hba	59Asn	1H
126.46	0.015	N	60Ile	15N
8.75	0.005	H	60Ile	1H
59.96	0.094	Ca	60Ile	13C
39.26	0.072	Cb	60Ile	13C
28.21	0.005	Cg1	60Ile	13C
19.06	0.061	Cg2	60Ile	13C
16.30	0.013	Cd1	60Ile	13C
172.56	0.000	C	60Ile	13C
4.34	0.000	Ha	60Ile	1H
1.65	0.003	Hb	60Ile	1H
1.19	0.004	Hg1b	60Ile	1H
0.62	0.004	Hd1*	60Ile	1H
0.55	0.011	Hg1a	60Ile	1H
0.55	0.021	Hg2*	60Ile	1H
8.85	0.007	H	61Ile	1H
127.61	0.014	N	61Ile	15N
58.03	0.030	Ca	61Ile	13C
37.22	0.059	Cb	61Ile	13C
4.41	0.005	Ha	61Ile	1H
19.30	0.093	Cg2	61Ile	13C
11.93	0.110	Cd1	61Ile	13C
175.47	0.027	C	61Ile	13C
0.50	0.006	Hb	61Ile	1H
0.09	0.004	Hg2*	61Ile	1H
-0.05	0.006	Hg1a	61Ile	1H
-0.53	0.008	Hg1b	61Ile	1H
28.04	0.044	Cg1	61Ile	13C
-0.42	0.004	Hd1*	61Ile	1H
125.78	0.005	N	62Leu	15N
8.36	0.009	H	62Leu	1H
53.62	0.058	Ca	62Leu	13C
43.09	0.045	Cb	62Leu	13C

4.31	0.008	Ha	62Leu	1H
-0.15	0.012	Hba	62Leu	1H
0.63	0.003	Hbb	62Leu	1H
26.33	0.034	Cdb	62Leu	13C
0.15	0.007	Hdb*	62Leu	1H
0.52	0.001	Hg	62Leu	1H
24.84	0.068	Cda	62Leu	13C
175.69	0.003	C	62Leu	13C
-0.11	0.008	Hda*	62Leu	1H
115.52	0.029	N	63Ser	15N
8.68	0.003	H	63Ser	1H
64.67	0.000	Cb	63Ser	13C
58.69	0.066	Ca	63Ser	13C
5.21	0.000	Ha	63Ser	1H
174.16	0.000	C	63Ser	13C
4.40	0.000	Hbb	63Ser	1H
3.85	0.000	Hba	63Ser	1H
122.82	0.030	N	64Ser	15N
10.19	0.004	H	64Ser	1H
64.20	0.104	Cb	64Ser	13C
60.36	0.060	Ca	64Ser	13C
4.63	0.000	Ha	64Ser	1H
174.99	0.000	C	64Ser	13C
123.02	0.010	N	65Gln	15N
8.63	0.003	H	65Gln	1H
53.06	0.100	Ca	65Gln	13C
29.50	0.049	Cb	65Gln	13C
4.64	0.002	Ha	65Gln	1H
33.89	0.019	Cg	65Gln	13C
1.73	0.000	Hba	65Gln	1H
2.08	0.009	Hbb	65Gln	1H
2.41	0.009	Hgb	65Gln	1H
2.25	0.006	Hga	65Gln	1H
113.36	0.000	Ne2	65Gln	15N
6.83	0.000	He2a	65Gln	1H
7.71	0.000	He2b	65Gln	1H
172.56	0.000	C	65Gln	13C
62.71	0.003	Ca	66Pro	13C
50.24	0.050	Cd	66Pro	13C
31.74	0.039	Cb	66Pro	13C
27.70	0.016	Cg	66Pro	13C
1.51	0.004	Hba	66Pro	1H

2.13	0.004	Hbb	66Pro	1H
1.83	0.005	Hga	66Pro	1H
1.94	0.007	Hgb	66Pro	1H
3.46	0.004	Hda	66Pro	1H
3.65	0.002	Hdb	66Pro	1H
3.96	0.002	Ha	66Pro	1H
177.17	0.000	C	66Pro	13C
42.52	0.114	Ca	67Gly	13C
109.05	0.027	N	67Gly	15N
7.73	0.011	H	67Gly	1H
1.94	0.006	Hab	67Gly	1H
1.68	0.010	Haa	67Gly	1H
106.19	0.041	N	68Thr	15N
5.93	0.022	H	68Thr	1H
60.17	0.113	Ca	68Thr	13C
69.15	0.013	Cb	68Thr	13C
21.03	0.000	Cg2	68Thr	13C
174.29	0.000	C	68Thr	13C
4.17	0.000	Ha	68Thr	1H
4.46	0.000	Hb	68Thr	1H
0.94	0.000	Hg2*	68Thr	1H
120.27	0.001	N	69Asp	15N
7.32	0.005	H	69Asp	1H
55.17	0.027	Ca	69Asp	13C
44.10	0.033	Cb	69Asp	13C
4.74	0.001	Ha	69Asp	1H
3.08	0.001	Hbb	69Asp	1H
2.99	0.006	Hba	69Asp	1H
176.35	0.024	C	69Asp	13C
126.81	0.003	N	70Asp	15N
8.87	0.004	H	70Asp	1H
40.22	0.013	Cb	70Asp	13C
4.76	0.003	Ha	70Asp	1H
2.85	0.006	Hbb	70Asp	1H
55.15	0.026	Ca	70Asp	13C
2.73	0.004	Hba	70Asp	1H
177.15	0.012	C	70Asp	13C
118.33	0.005	N	71Arg	15N
8.86	0.003	H	71Arg	1H
57.45	0.091	Ca	71Arg	13C
31.44	0.024	Cb	71Arg	13C
4.17	0.005	Ha	71Arg	1H

43.65	0.051	Cd	71Arg	13C
25.97	0.017	Cg	71Arg	13C
1.92	0.001	Hgb	71Arg	1H
1.77	0.005	Hga	71Arg	1H
175.97	0.017	C	71Arg	13C
3.38	0.001	Hdb	71Arg	1H
3.08	0.001	Hda	71Arg	1H
108.39	0.010	N	72Val	15N
7.24	0.012	H	72Val	1H
33.24	0.125	Cb	72Val	13C
58.25	0.082	Ca	72Val	13C
4.54	0.001	Ha	72Val	1H
1.36	0.003	Hb	72Val	1H
0.31	0.006	Hgb*	72Val	1H
-0.49	0.002	Hga*	72Val	1H
22.82	0.087	Cgb	72Val	13C
16.81	0.078	Cga	72Val	13C
173.05	0.031	C	72Val	13C
117.27	0.012	N	73Thr	15N
7.92	0.010	H	73Thr	1H
62.96	0.070	Ca	73Thr	13C
70.35	0.020	Cb	73Thr	13C
4.37	0.000	Ha	73Thr	1H
171.99	0.040	C	73Thr	13C
1.10	0.000	Hg2*	73Thr	1H
3.79	0.000	Hb	73Thr	1H
21.18	0.000	Cg2	73Thr	13C
128.89	0.011	N	74Trp	15N
8.78	0.007	H	74Trp	1H
56.11	0.031	Ca	74Trp	13C
28.96	0.066	Cb	74Trp	13C
5.03	0.006	Ha	74Trp	1H
3.46	0.004	Hbb	74Trp	1H
2.79	0.007	Hba	74Trp	1H
130.36	0.000	Ne1	74Trp	15N
10.22	0.000	He1	74Trp	1H
176.67	0.000	C	74Trp	13C
7.13	0.005	Hd1	74Trp	1H
7.38	0.000	He3	74Trp	1H
127.91	0.000	Cd1	74Trp	13C
116.56	0.011	N	75Val	15N
9.18	0.006	H	75Val	1H

35.73	0.028	Cb	75Val	13C
58.78	0.031	Ca	75Val	13C
4.82	0.000	Ha	75Val	1H
2.09	0.005	Hb	75Val	1H
22.32	0.006	Cgb	75Val	13C
18.24	0.010	Cga	75Val	13C
0.45	0.004	Hga*	75Val	1H
0.65	0.000	Hgb*	75Val	1H
174.91	0.047	C	75Val	13C
116.01	0.006	N	76Lys	15N
8.29	0.004	H	76Lys	1H
55.57	0.081	Ca	76Lys	13C
34.14	0.121	Cb	76Lys	13C
5.04	0.005	Ha	76Lys	1H
2.03	0.006	Hbb	76Lys	1H
1.81	0.001	Hba	76Lys	1H
41.97	0.085	Ce	76Lys	13C
29.37	0.020	Cd	76Lys	13C
24.34	0.087	Cg	76Lys	13C
1.64	0.002	Hda	76Lys	1H
1.71	0.001	Hdb	76Lys	1H
2.90	0.001	Heb	76Lys	1H
2.81	0.006	Hea	76Lys	1H
1.42	0.004	Hga	76Lys	1H
175.61	0.034	C	76Lys	13C
1.65	0.000	Hgb	76Lys	1H
108.87	0.016	N	77Ser	15N
7.22	0.007	H	77Ser	1H
66.36	0.175	Cb	77Ser	13C
57.10	0.075	Ca	77Ser	13C
4.86	0.005	Ha	77Ser	1H
4.24	0.000	Hbb	77Ser	1H
4.06	0.010	Hba	77Ser	1H
174.11	0.013	C	77Ser	13C
122.68	0.009	N	78Val	15N
8.93	0.005	H	78Val	1H
67.26	0.094	Ca	78Val	13C
31.50	0.120	Cb	78Val	13C
3.32	0.000	Ha	78Val	1H
1.84	0.003	Hb	78Val	1H
20.07	0.062	Cga	78Val	13C
22.59	0.072	Cgb	78Val	13C

0.66	0.000	Hgb*	78Val	1H
0.35	0.002	Hga*	78Val	1H
177.27	0.002	C	78Val	13C
118.17	0.023	N	79Asp	15N
8.47	0.003	H	79Asp	1H
39.80	0.137	Cb	79Asp	13C
57.80	0.046	Ca	79Asp	13C
4.30	0.005	Ha	79Asp	1H
2.47	0.029	Hba	79Asp	1H
2.55	0.003	Hbb	79Asp	1H
179.92	0.013	C	79Asp	13C
120.79	0.002	N	80Glu	15N
7.97	0.009	H	80Glu	1H
4.04	0.000	Ha	80Glu	1H
59.23	0.060	Ca	80Glu	13C
30.58	0.144	Cb	80Glu	13C
36.83	0.016	Cg	80Glu	13C
1.98	0.003	Hba	80Glu	1H
2.02	0.001	Hbb	80Glu	1H
2.22	0.001	Hga	80Glu	1H
2.36	0.001	Hgb	80Glu	1H
179.14	0.000	C	80Glu	13C
122.72	0.023	N	81Ala	15N
8.23	0.006	H	81Ala	1H
17.85	0.019	Cb	81Ala	13C
55.67	0.085	Ca	81Ala	13C
3.85	0.006	Ha	81Ala	1H
1.47	0.000	Hb*	81Ala	1H
178.01	0.000	C	81Ala	13C
116.13	0.010	N	82Ile	15N
8.03	0.006	H	82Ile	1H
65.52	0.015	Ca	82Ile	13C
38.32	0.027	Cb	82Ile	13C
3.61	0.000	Ha	82Ile	1H
1.87	0.002	Hb	82Ile	1H
29.67	0.014	Cg1	82Ile	13C
16.80	0.055	Cg2	82Ile	13C
13.52	0.037	Cd1	82Ile	13C
1.01	0.002	Hg1a	82Ile	1H
2.01	0.002	Hg1b	82Ile	1H
0.85	0.007	Hd1*	82Ile	1H
0.82	0.005	Hg2*	82Ile	1H

180.49	0.000	C	82Ile	13C
124.16	0.030	N	83Ala	15N
8.17	0.006	H	83Ala	1H
55.15	0.064	Ca	83Ala	13C
17.67	0.030	Cb	83Ala	13C
4.08	0.005	Ha	83Ala	1H
1.42	0.000	Hb*	83Ala	1H
180.48	0.007	C	83Ala	13C
119.44	0.011	N	84Ala	15N
8.04	0.007	H	84Ala	1H
53.87	0.065	Ca	84Ala	13C
17.95	0.055	Cb	84Ala	13C
4.07	0.007	Ha	84Ala	1H
1.39	0.000	Hb*	84Ala	1H
178.04	0.010	C	84Ala	13C
114.62	0.009	N	85Cys	15N
7.43	0.007	H	85Cys	1H
61.84	0.056	Ca	85Cys	13C
27.89	0.146	Cb	85Cys	13C
3.90	0.000	Ha	85Cys	1H
2.42	0.001	Hba	85Cys	1H
3.27	0.001	Hbb	85Cys	1H
175.50	0.013	C	85Cys	13C
7.24	0.007	H	86Gly	1H
103.17	0.001	N	86Gly	15N
45.12	0.040	Ca	86Gly	13C
3.75	0.006	Haa	86Gly	1H
3.89	0.010	Hab	86Gly	1H
173.45	0.034	C	86Gly	13C
122.42	0.013	N	87Asp	15N
8.55	0.005	H	87Asp	1H
39.53	0.047	Cb	87Asp	13C
53.44	0.029	Ca	87Asp	13C
4.75	0.000	Ha	87Asp	1H
2.46	0.007	Hba	87Asp	1H
2.69	0.003	Hbb	87Asp	1H
176.42	1.357	C	87Asp	13C
114.25	0.005	N	88Val	15N
7.23	0.015	H	88Val	1H
58.11	0.126	Ca	88Val	13C
31.85	0.010	Cb	88Val	13C
2.36	0.002	Hb	88Val	1H

21.79	0.000	Cgb	88Val	13C
17.85	0.000	Cga	88Val	13C
4.10	0.011	Ha	88Val	1H
0.93	0.000	Hgb*	88Val	1H
0.56	0.000	Hga*	88Val	1H
177.31	0.000	C	88Val	13C
64.71	0.029	Ca	89Pro	13C
50.70	0.024	Cd	89Pro	13C
32.07	0.025	Cb	89Pro	13C
27.44	0.008	Cg	89Pro	13C
2.32	0.006	Hbb	89Pro	1H
1.84	0.003	Hba	89Pro	1H
2.11	0.002	Hgb	89Pro	1H
1.95	0.002	Hga	89Pro	1H
4.30	0.000	Ha	89Pro	1H
3.79	0.004	Hdb	89Pro	1H
3.74	0.005	Hda	89Pro	1H
177.80	0.000	C	89Pro	13C
117.04	0.018	N	90Glu	15N
7.75	0.006	H	90Glu	1H
55.84	0.060	Ca	90Glu	13C
33.00	0.162	Cb	90Glu	13C
4.88	0.001	Ha	90Glu	1H
1.60	0.001	Hba	90Glu	1H
1.71	0.001	Hbb	90Glu	1H
36.11	0.012	Cg	90Glu	13C
2.14	0.002	Hgb	90Glu	1H
1.86	0.002	Hga	90Glu	1H
173.33	0.000	C	90Glu	13C
130.19	0.012	N	91Ile	15N
8.80	0.011	H	91Ile	1H
61.26	0.025	Ca	91Ile	13C
41.36	0.020	Cb	91Ile	13C
3.81	0.008	Ha	91Ile	1H
17.70	0.004	Cg2	91Ile	13C
14.04	0.003	Cd1	91Ile	13C
27.80	0.020	Cg1	91Ile	13C
1.68	0.003	Hb	91Ile	1H
0.71	0.006	Hg1a	91Ile	1H
1.59	0.003	Hg1b	91Ile	1H
174.06	0.003	C	91Ile	13C
0.79	0.000	Hg2*	91Ile	1H

0.91	0.000	Hd1*	91Ile	1H
121.89	0.024	N	92Met	15N
7.91	0.012	H	92Met	1H
51.84	0.157	Ca	92Met	13C
30.03	0.110	Cb	92Met	13C
5.16	0.008	Ha	92Met	1H
31.94	0.110	Cg	92Met	13C
2.06	0.000	Hba	92Met	1H
2.06	0.000	Hbb	92Met	1H
2.02	0.002	Hga	92Met	1H
174.29	0.031	C	92Met	13C
2.05	0.000	He*	92Met	1H
17.04	0.000	Ce	92Met	13C
2.10	0.002	Hgb	92Met	1H
125.00	0.004	N	93Val	15N
9.39	0.004	H	93Val	1H
61.98	0.070	Ca	93Val	13C
31.26	0.122	Cb	93Val	13C
2.23	0.004	Hb	93Val	1H
22.30	0.005	Cgb	93Val	13C
20.32	0.049	Cga	93Val	13C
4.34	0.000	Ha	93Val	1H
0.52	0.000	Hgb*	93Val	1H
0.12	0.005	Hga*	93Val	1H
176.97	0.011	C	93Val	13C
60.46	0.071	Ca	94Ile	13C
17.43	0.102	Cg2	94Ile	13C
15.61	0.065	Cd1	94Ile	13C
119.70	0.038	N	94Ile	15N
8.97	0.004	H	94Ile	1H
38.92	0.033	Cb	94Ile	13C
5.63	0.010	Ha	94Ile	1H
2.85	0.002	Hb	94Ile	1H
27.92	0.019	Cg1	94Ile	13C
1.01	0.011	Hg1a	94Ile	1H
1.80	0.002	Hg1b	94Ile	1H
0.90	0.020	Hg2*	94Ile	1H
0.97	0.041	Hd1*	94Ile	1H
174.25	0.017	C	94Ile	13C
6.19	0.005	H	95Gly	1H
103.07	0.018	N	95Gly	15N
41.14	0.082	Ca	95Gly	13C

3.81	0.011	Hab	95Gly	1H
1.92	0.006	Haa	95Gly	1H
174.23	0.000	C	95Gly	13C
111.71	0.002	N	96Gly	15N
8.22	0.007	H	96Gly	1H
46.71	0.000	Ca	96Gly	13C
3.95	0.000	Hab	96Gly	1H
2.89	0.000	Haa	96Gly	1H
173.36	0.000	C	96Gly	13C
49.04	0.047	Ca	97Gly	13C
174.90	0.000	C	97Gly	13C
122.32	0.043	N	98Arg	15N
9.23	0.020	H	98Arg	1H
29.47	0.041	Cb	98Arg	13C
58.39	0.106	Ca	98Arg	13C
4.21	0.000	Ha	98Arg	1H
2.20	0.004	Hbb	98Arg	1H
2.09	0.001	Hba	98Arg	1H
27.33	0.017	Cg	98Arg	13C
43.01	0.016	Cd	98Arg	13C
3.15	0.002	Hda	98Arg	1H
3.32	0.001	Hdb	98Arg	1H
1.74	0.000	Hga	98Arg	1H
1.84	0.000	Hgb	98Arg	1H
180.67	0.072	C	98Arg	13C
8.80	0.000	He	98Arg	1H
83.80	0.000	Ne	98Arg	15N
122.15	0.026	N	99Val	15N
7.30	0.008	H	99Val	1H
68.11	0.028	Ca	99Val	13C
31.49	0.036	Cb	99Val	13C
3.67	0.000	Ha	99Val	1H
24.26	0.000	Cgb	99Val	13C
178.69	0.038	C	99Val	13C
1.68	0.000	Hb	99Val	1H
0.94	0.000	Hgb*	99Val	1H
0.60	0.000	Hga*	99Val	1H
22.20	0.000	Cga	99Val	13C
119.56	0.019	N	100Tyr	15N
9.54	0.006	H	100Tyr	1H
60.30	0.048	Ca	100Tyr	13C
37.79	0.070	Cb	100Tyr	13C

4.26	0.004	Ha	100Tyr	1H
178.03	0.011	C	100Tyr	13C
2.40	0.003	Hba	100Tyr	1H
2.80	0.005	Hbb	100Tyr	1H
6.43	0.000	Hd*	100Tyr	1H
6.94	0.000	He*	100Tyr	1H
116.03	0.002	N	101Glu	15N
8.06	0.012	H	101Glu	1H
29.59	0.023	Cb	101Glu	13C
60.06	0.167	Ca	101Glu	13C
36.06	0.006	Cg	101Glu	13C
2.39	0.006	Hgb	101Glu	1H
3.71	0.004	Ha	101Glu	1H
2.30	0.001	Hga	101Glu	1H
2.23	0.000	Hbb	101Glu	1H
2.16	0.000	Hba	101Glu	1H
175.49	0.036	C	101Glu	13C
114.45	0.059	N	102Gln	15N
7.23	0.011	H	102Gln	1H
58.20	0.177	Ca	102Gln	13C
32.70	0.050	Cb	102Gln	13C
36.32	0.000	Cg	102Gln	13C
4.76	0.000	Ha	102Gln	1H
177.34	0.000	C	102Gln	13C
113.29	0.008	N	103Phe	15N
8.00	0.009	H	103Phe	1H
60.27	0.065	Ca	103Phe	13C
41.73	0.095	Cb	103Phe	13C
2.81	0.015	Hba	103Phe	1H
3.05	0.010	Hbb	103Phe	1H
4.38	0.004	Ha	103Phe	1H
175.56	0.994	C	103Phe	13C
7.43	0.009	Hd*	103Phe	1H
6.94	0.002	He*	103Phe	1H
131.63	0.012	Cd*	103Phe	13C
130.18	0.031	Ce*	103Phe	13C
123.55	0.025	N	104Leu	15N
8.38	0.008	H	104Leu	1H
60.81	0.000	Ca	104Leu	13C
38.68	0.074	Cb	104Leu	13C
1.44	0.009	Hba	104Leu	1H
1.97	0.002	Hbb	104Leu	1H

26.81	0.008	Cdb	104Leu	13C
4.28	0.003	Ha	104Leu	1H
0.89	0.000	Hdb*	104Leu	1H
1.16	0.000	Hg	104Leu	1H
0.89	0.000	Hda*	104Leu	1H
24.83	0.000	Cda	104Leu	13C
65.42	0.099	Ca	105Pro	13C
50.44	0.022	Cd	105Pro	13C
31.28	0.044	Cb	105Pro	13C
27.88	0.011	Cg	105Pro	13C
3.76	0.058	Hdb	105Pro	1H
3.43	0.014	Hda	105Pro	1H
177.35	0.000	C	105Pro	13C
1.95	0.000	Hgb	105Pro	1H
1.92	0.000	Hga	105Pro	1H
112.92	0.023	N	106Lys	15N
7.44	0.006	H	106Lys	1H
55.48	0.099	Ca	106Lys	13C
34.58	0.065	Cb	106Lys	13C
4.35	0.001	Ha	106Lys	1H
41.68	0.012	Ce	106Lys	13C
29.38	0.016	Cd	106Lys	13C
25.11	0.000	Cg	106Lys	13C
1.82	0.001	Hba	106Lys	1H
2.16	0.004	Hbb	106Lys	1H
1.34	0.005	Hda	106Lys	1H
1.51	0.001	Hdb	106Lys	1H
2.72	0.001	Hea	106Lys	1H
2.77	0.002	Heb	106Lys	1H
176.01	0.000	C	106Lys	13C
1.42	0.000	Hga	106Lys	1H
122.35	0.004	N	107Ala	15N
7.95	0.005	H	107Ala	1H
21.10	0.109	Cb	107Ala	13C
52.30	0.029	Ca	107Ala	13C
4.56	0.002	Ha	107Ala	1H
1.71	0.004	Hb*	107Ala	1H
177.38	0.000	C	107Ala	13C
118.45	0.019	N	108Gln	15N
9.25	0.004	H	108Gln	1H
55.84	0.094	Ca	108Gln	13C
31.55	0.062	Cb	108Gln	13C

34.82	0.047	Cg	108Gln	13C
4.59	0.005	Ha	108Gln	1H
2.57	0.005	Hgb	108Gln	1H
2.50	0.007	Hga	108Gln	1H
2.13	0.001	Hba	108Gln	1H
2.36	0.003	Hbb	108Gln	1H
174.96	0.000	C	108Gln	13C
7.71	0.000	He2b	108Gln	1H
112.68	0.019	Ne2	108Gln	15N
6.90	0.000	He2a	108Gln	1H
120.78	0.008	N	109Lys	15N
7.80	0.006	H	109Lys	1H
56.15	0.049	Ca	109Lys	13C
36.84	0.050	Cb	109Lys	13C
5.69	0.015	Ha	109Lys	1H
25.94	0.044	Cg	109Lys	13C
30.30	0.006	Cd	109Lys	13C
42.59	0.074	Ce	109Lys	13C
1.90	0.002	Hba	109Lys	1H
2.18	0.001	Hbb	109Lys	1H
1.06	0.008	Hga	109Lys	1H
1.34	0.000	Hgb	109Lys	1H
1.48	0.001	Hdb	109Lys	1H
1.41	0.000	Hda	109Lys	1H
2.48	0.007	Hea	109Lys	1H
2.72	0.001	Heb	109Lys	1H
174.07	0.032	C	109Lys	13C
122.01	0.011	N	110Leu	15N
9.05	0.007	H	110Leu	1H
52.92	0.036	Ca	110Leu	13C
44.47	0.015	Cb	110Leu	13C
5.12	0.011	Ha	110Leu	1H
23.46	0.087	Cda	110Leu	13C
1.27	0.002	Hbb	110Leu	1H
0.60	0.007	Hba	110Leu	1H
0.48	0.000	Hg	110Leu	1H
-0.87	0.001	Hda*	110Leu	1H
174.85	0.000	C	110Leu	13C
122.41	0.009	N	111Tyr	15N
9.48	0.005	H	111Tyr	1H
38.43	0.081	Cb	111Tyr	13C
55.99	0.046	Ca	111Tyr	13C

5.19	0.004	Ha	111Tyr	1H
3.21	0.005	Hbb	111Tyr	1H
2.60	0.021	Hba	111Tyr	1H
175.08	0.002	C	111Tyr	13C
6.76	0.000	Hd*	111Tyr	1H
6.53	0.000	He*	111Tyr	1H
123.57	0.016	N	112Leu	15N
9.60	0.033	H	112Leu	1H
52.81	0.069	Ca	112Leu	13C
44.63	0.053	Cb	112Leu	13C
5.32	0.006	Ha	112Leu	1H
1.47	0.002	Hbb	112Leu	1H
0.29	0.003	Hba	112Leu	1H
22.19	0.015	Cda	112Leu	13C
26.04	0.072	Cdb	112Leu	13C
0.28	0.011	Hdb*	112Leu	1H
1.04	0.002	Hg	112Leu	1H
-0.09	0.003	Hda*	112Leu	1H
60.03	0.008	Ca	113Thr	13C
69.05	0.000	Cb	113Thr	13C
173.48	0.000	C	113Thr	13C
9.26	0.015	H	114His	1H
126.62	0.031	N	114His	15N
54.34	0.259	Ca	114His	13C
29.34	0.246	Cb	114His	13C
4.83	0.002	Ha	114His	1H
175.05	0.000	C	114His	13C
6.70	0.000	Hd2	114His	1H
127.38	0.026	N	115Ile	15N
9.13	0.007	H	115Ile	1H
60.88	0.110	Ca	115Ile	13C
39.52	0.067	Cb	115Ile	13C
3.99	0.000	Ha	115Ile	1H
17.26	0.034	Cg2	115Ile	13C
12.91	0.050	Cd1	115Ile	13C
26.64	0.015	Cg1	115Ile	13C
0.75	0.007	Hb	115Ile	1H
0.80	0.001	Hg1b	115Ile	1H
0.13	0.006	Hg2*	115Ile	1H
-0.06	0.006	Hg1a	115Ile	1H
-0.94	0.005	Hd1*	115Ile	1H
176.72	0.000	C	115Ile	13C

130.15	0.006	N	116Asp	15N
8.35	0.005	H	116Asp	1H
53.65	0.040	Ca	116Asp	13C
38.51	0.062	Cb	116Asp	13C
4.64	0.002	Ha	116Asp	1H
2.55	0.006	Hba	116Asp	1H
2.69	0.008	Hbb	116Asp	1H
173.73	0.000	C	116Asp	13C
124.29	0.015	N	117Ala	15N
7.75	0.008	H	117Ala	1H
51.18	0.097	Ca	117Ala	13C
20.41	0.118	Cb	117Ala	13C
4.38	0.010	Ha	117Ala	1H
0.43	0.004	Hb*	117Ala	1H
174.54	0.000	C	117Ala	13C
124.18	0.010	N	118Glu	15N
8.59	0.006	H	118Glu	1H
55.47	0.151	Ca	118Glu	13C
28.91	0.083	Cb	118Glu	13C
4.54	0.002	Ha	118Glu	1H
36.34	0.139	Cg	118Glu	13C
1.95	0.000	Hbb	118Glu	1H
1.84	0.000	Hba	118Glu	1H
2.02	0.001	Hga	118Glu	1H
2.16	0.002	Hgb	118Glu	1H
175.22	0.000	C	118Glu	13C
118.86	0.000	N	119Val	15N
8.15	0.006	H	119Val	1H
58.57	0.068	Ca	119Val	13C
35.21	0.011	Cb	119Val	13C
21.91	0.059	Cgb	119Val	13C
18.99	0.023	Cga	119Val	13C
2.10	0.004	Hb	119Val	1H
0.91	0.007	Hgb*	119Val	1H
0.80	0.004	Hga*	119Val	1H
174.84	0.000	C	119Val	13C
4.62	0.001	Ha	119Val	1H
56.44	0.011	Ca	120Glu	13C
36.36	0.044	Cg	120Glu	13C
30.03	0.014	Cb	120Glu	13C
124.11	0.030	N	120Glu	15N
8.40	0.004	H	120Glu	1H

4.33	0.003	Ha	120Glu	1H
1.95	0.003	Hbb	120Glu	1H
1.88	0.002	Hba	120Glu	1H
2.25	0.014	Hga	120Glu	1H
2.30	0.005	Hgb	120Glu	1H
175.94	0.013	C	120Glu	13C
106.95	0.016	N	121Gly	15N
8.43	0.009	H	121Gly	1H
46.00	0.063	Ca	121Gly	13C
4.92	0.006	Hab	121Gly	1H
172.73	0.000	C	121Gly	13C
3.73	0.007	Haa	121Gly	1H
116.33	0.020	N	122Asp	15N
8.59	0.014	H	122Asp	1H
41.98	0.079	Cb	122Asp	13C
52.41	0.048	Ca	122Asp	13C
4.89	0.005	Ha	122Asp	1H
3.18	0.003	Hbb	122Asp	1H
2.68	0.006	Hba	122Asp	1H
56.19	0.072	Ca	124His	13C
33.18	0.056	Cb	124His	13C
5.46	0.011	Ha	124His	1H
2.76	0.010	Hba	124His	1H
3.12	0.005	Hbb	124His	1H
7.35	0.000	Hd2	124His	1H
124.99	0.010	N	125Phe	15N
9.15	0.011	H	125Phe	1H
56.84	0.048	Ca	125Phe	13C
41.29	0.045	Cb	125Phe	13C
4.42	0.004	Ha	125Phe	1H
2.87	0.007	Hbb	125Phe	1H
2.78	0.006	Hba	125Phe	1H
7.07	0.000	He*	125Phe	1H
62.54	0.057	Ca	126Pro	13C
31.80	0.030	Cb	126Pro	13C
27.17	0.036	Cg	126Pro	13C
49.84	0.028	Cd	126Pro	13C
1.47	0.008	Hda	126Pro	1H
3.16	0.003	Hdb	126Pro	1H
2.12	0.005	Hbb	126Pro	1H
1.62	0.003	Hba	126Pro	1H
1.37	0.003	Hgb	126Pro	1H

1.05	0.004	Hga	126Pro	1H
4.26	0.005	Ha	126Pro	1H
117.70	0.008	N	127Asp	15N
8.11	0.003	H	127Asp	1H
54.57	0.045	Ca	127Asp	13C
40.66	0.069	Cb	127Asp	13C
4.29	0.007	Ha	127Asp	1H
2.54	0.004	Hbb	127Asp	1H
2.35	0.008	Hba	127Asp	1H
119.16	0.013	N	128Tyr	15N
7.47	0.005	H	128Tyr	1H
55.38	0.040	Ca	128Tyr	13C
39.34	0.038	Cb	128Tyr	13C
4.75	0.000	Ha	128Tyr	1H
2.74	0.007	Hba	128Tyr	1H
2.99	0.005	Hbb	128Tyr	1H
6.84	0.000	Hd*	128Tyr	1H
6.34	0.000	He*	128Tyr	1H
116.87	0.000	Ce*	128Tyr	13C
123.43	0.007	N	129Glu	15N
8.82	0.004	H	129Glu	1H
53.25	0.060	Ca	129Glu	13C
4.54	0.006	Ha	129Glu	1H
29.71	0.038	Cb	129Glu	13C
36.08	0.015	Cg	129Glu	13C
2.27	0.012	Hgb	129Glu	1H
2.10	0.008	Hga	129Glu	1H
2.08	0.000	Hba	129Glu	1H
2.20	0.032	Hbb	129Glu	1H
32.09	0.069	Cb	130Pro	13C
51.07	0.037	Cd	130Pro	13C
65.95	0.021	Ca	130Pro	13C
27.43	0.020	Cg	130Pro	13C
2.37	0.007	Hbb	130Pro	1H
2.00	0.003	Hba	130Pro	1H
1.73	0.006	Hga	130Pro	1H
2.01	0.013	Hgb	130Pro	1H
3.78	0.027	Hda	130Pro	1H
178.39	0.000	C	130Pro	13C
4.29	0.009	Ha	130Pro	1H
114.91	0.047	N	131Asp	15N
9.04	0.004	H	131Asp	1H

56.37	0.039	Ca	131Asp	13C
40.07	0.070	Cb	131Asp	13C
4.53	0.003	Ha	131Asp	1H
2.69	0.006	Hbb	131Asp	1H
2.56	0.004	Hba	131Asp	1H
177.05	0.033	C	131Asp	13C
117.86	0.014	N	132Asp	15N
8.17	0.007	H	132Asp	1H
55.04	0.040	Ca	132Asp	13C
41.28	0.065	Cb	132Asp	13C
4.51	0.007	Ha	132Asp	1H
2.31	0.006	Hba	132Asp	1H
2.86	0.011	Hbb	132Asp	1H
175.05	0.038	C	132Asp	13C
119.65	0.007	N	133Trp	15N
7.80	0.003	H	133Trp	1H
34.00	0.057	Cb	133Trp	13C
56.25	0.018	Ca	133Trp	13C
4.81	0.006	Ha	133Trp	1H
2.89	0.017	Hba	133Trp	1H
3.12	0.009	Hbb	133Trp	1H
128.14	0.000	Ne1	133Trp	15N
10.28	0.000	He1	133Trp	1H
173.97	0.013	C	133Trp	13C
7.84	0.007	Hd1	133Trp	1H
7.84	0.000	He3	133Trp	1H
129.20	0.000	Cd1	133Trp	13C
122.92	0.015	N	134Glu	15N
9.57	0.004	H	134Glu	1H
54.33	0.031	Ca	134Glu	13C
32.39	0.024	Cb	134Glu	13C
4.64	0.004	Ha	134Glu	1H
35.59	0.055	Cg	134Glu	13C
1.80	0.005	Hba	134Glu	1H
2.04	0.003	Hbb	134Glu	1H
2.08	0.017	Hga	134Glu	1H
2.11	0.009	Hgb	134Glu	1H
175.74	0.025	C	134Glu	13C
121.54	0.004	N	135Ser	15N
9.05	0.015	H	135Ser	1H
58.41	0.039	Ca	135Ser	13C
62.09	0.074	Cb	135Ser	13C

4.82	0.001	Ha	135Ser	1H
3.78	0.027	Hba	135Ser	1H
3.85	0.000	Hbb	135Ser	1H
121.54	0.005	N	136Val	15N
9.09	0.015	H	136Val	1H
60.86	0.051	Ca	136Val	13C
32.35	0.054	Cb	136Val	13C
4.65	0.002	Ha	136Val	1H
21.09	0.038	Cgb	136Val	13C
18.31	0.037	Cga	136Val	13C
2.41	0.005	Hb	136Val	1H
0.89	0.008	Hgb*	136Val	1H
0.78	0.005	Hga*	136Val	1H
175.77	0.000	C	136Val	13C
123.61	0.011	N	137Phe	15N
7.89	0.009	H	137Phe	1H
58.48	0.063	Ca	137Phe	13C
42.95	0.050	Cb	137Phe	13C
4.69	0.001	Ha	137Phe	1H
3.44	0.002	Hbb	137Phe	1H
2.62	0.006	Hba	137Phe	1H
173.20	0.000	C	137Phe	13C
7.34	0.000	He*	137Phe	1H
7.21	0.000	Hd*	137Phe	1H
131.61	0.000	Cd*	137Phe	13C
131.68	0.000	Ce*	137Phe	13C
119.70	0.004	N	138Ser	15N
7.55	0.004	H	138Ser	1H
64.68	0.053	Cb	138Ser	13C
57.02	0.038	Ca	138Ser	13C
5.21	0.010	Ha	138Ser	1H
3.49	0.000	Hbb	138Ser	1H
3.43	0.002	Hba	138Ser	1H
173.12	0.000	C	138Ser	13C
8.70	0.009	H	139Glu	1H
125.75	0.002	N	139Glu	15N
56.40	0.040	Ca	139Glu	13C
34.94	0.073	Cb	139Glu	13C
4.15	0.010	Ha	139Glu	1H
37.20	0.053	Cg	139Glu	13C
1.80	0.006	Hba	139Glu	1H
2.09	0.015	Hbb	139Glu	1H

173.01	0.000	C	139Glu	13C
1.62	0.005	Hga	139Glu	1H
2.11	0.007	Hgb	139Glu	1H
129.34	0.017	N	140Phe	15N
8.68	0.008	H	140Phe	1H
58.73	0.062	Ca	140Phe	13C
40.63	0.045	Cb	140Phe	13C
2.64	0.006	Hba	140Phe	1H
4.05	0.003	Ha	140Phe	1H
2.78	0.005	Hbb	140Phe	1H
6.86	0.007	Hd*	140Phe	1H
7.12	0.008	He*	140Phe	1H
174.17	0.000	C	140Phe	13C
131.54	0.000	Cd*	140Phe	13C
131.56	0.000	Ce*	140Phe	13C
123.24	0.011	N	141His	15N
7.99	0.009	H	141His	1H
54.17	0.037	Ca	141His	13C
31.26	0.045	Cb	141His	13C
4.05	0.004	Ha	141His	1H
2.19	0.010	Hbb	141His	1H
0.90	0.006	Hba	141His	1H
171.86	0.000	C	141His	13C
6.11	0.000	Hd2	141His	1H
120.38	0.009	N	142Asp	15N
8.01	0.005	H	142Asp	1H
53.25	0.074	Ca	142Asp	13C
42.41	0.016	Cb	142Asp	13C
4.44	0.004	Ha	142Asp	1H
2.75	0.006	Hbb	142Asp	1H
2.35	0.005	Hba	142Asp	1H
175.83	0.001	C	142Asp	13C
122.52	0.045	N	143Ala	15N
8.14	0.005	H	143Ala	1H
18.83	0.054	Cb	143Ala	13C
3.97	0.010	Ha	143Ala	1H
52.73	0.068	Ca	143Ala	13C
1.18	0.005	Hb*	143Ala	1H
176.99	0.000	C	143Ala	13C
120.69	0.007	N	144Asp	15N
8.91	0.011	H	144Asp	1H
41.45	0.070	Cb	144Asp	13C

53.28	0.037	Ca	144Asp	13C
4.59	0.003	Ha	144Asp	1H
3.18	0.006	Hbb	144Asp	1H
2.76	0.007	Hba	144Asp	1H
175.94	0.000	C	144Asp	13C
118.28	0.013	N	145Ala	15N
8.18	0.010	H	145Ala	1H
18.29	0.037	Cb	145Ala	13C
54.80	0.048	Ca	145Ala	13C
178.75	0.000	C	145Ala	13C
4.02	0.009	Ha	145Ala	1H
1.37	0.005	Hb*	145Ala	1H
113.29	0.007	N	146Gln	15N
8.00	0.006	H	146Gln	1H
56.55	0.066	Ca	146Gln	13C
31.04	0.023	Cb	146Gln	13C
34.80	0.020	Cg	146Gln	13C
4.37	0.007	Ha	146Gln	1H
2.29	0.003	Hgb	146Gln	1H
2.27	0.006	Hga	146Gln	1H
1.94	0.005	Hba	146Gln	1H
1.99	0.001	Hbb	146Gln	1H
7.08	0.000	He2a	146Gln	1H
113.11	0.007	Ne2	146Gln	15N
9.77	0.000	He2b	146Gln	1H
174.89	0.001	C	146Gln	13C
119.58	0.027	N	147Asn	15N
8.16	0.005	H	147Asn	1H
52.86	0.028	Ca	147Asn	13C
41.04	0.069	Cb	147Asn	13C
5.26	0.001	Ha	147Asn	1H
2.38	0.002	Hba	147Asn	1H
2.90	0.000	Hbb	147Asn	1H
7.05	0.000	Hd2a	147Asn	1H
116.93	0.008	Nd2	147Asn	15N
8.42	0.000	Hd2b	147Asn	1H
117.34	0.034	N	148Ser	15N
8.94	0.007	H	148Ser	1H
61.29	0.000	Ca	148Ser	13C
63.35	0.000	Cb	148Ser	13C
4.09	0.000	Ha	148Ser	1H
173.07	0.000	C	148Ser	13C

117.86	0.024	N	149His	15N
7.06	0.002	H	149His	1H
54.46	0.024	Ca	149His	13C
34.34	0.059	Cb	149His	13C
173.40	0.000	C	149His	13C
4.90	0.002	Ha	149His	1H
2.88	0.001	Hba	149His	1H
3.13	0.008	Hbb	149His	1H
6.93	0.000	Hd2	149His	1H
113.48	0.030	N	150Ser	15N
8.66	0.008	H	150Ser	1H
58.44	0.032	Ca	150Ser	13C
64.13	0.021	Cb	150Ser	13C
4.32	0.000	Ha	150Ser	1H
4.06	0.000	Hba	150Ser	1H
4.15	0.000	Hbb	150Ser	1H
173.18	0.000	C	150Ser	13C
114.95	0.026	N	151Tyr	15N
7.62	0.013	H	151Tyr	1H
54.72	0.066	Ca	151Tyr	13C
39.00	0.062	Cb	151Tyr	13C
5.22	0.009	Ha	151Tyr	1H
172.01	0.010	C	151Tyr	13C
2.55	0.006	Hbb	151Tyr	1H
1.79	0.003	Hba	151Tyr	1H
118.21	0.021	N	152Cys	15N
8.21	0.011	H	152Cys	1H
54.87	0.035	Ca	152Cys	13C
29.80	0.016	Cb	152Cys	13C
173.33	0.009	C	152Cys	13C
4.89	0.007	Ha	152Cys	1H
3.10	0.000	Hbb	152Cys	1H
2.26	0.000	Hba	152Cys	1H
128.62	0.004	N	153Phe	15N
8.45	0.016	H	153Phe	1H
55.41	0.057	Ca	153Phe	13C
40.20	0.056	Cb	153Phe	13C
5.01	0.000	Ha	153Phe	1H
174.35	0.000	C	153Phe	13C
2.38	0.000	Hbb	153Phe	1H
1.95	0.000	Hba	153Phe	1H
124.24	0.022	N	154Glu	15N

9.78	0.026	H	154Glu	1H
34.26	0.000	Cb	154Glu	13C
54.43	0.029	Ca	154Glu	13C
5.50	0.000	Ha	154Glu	1H
36.74	0.000	Cg	154Glu	13C
1.96	0.000	Hba	154Glu	1H
2.10	0.000	Hbb	154Glu	1H
2.50	0.002	Hgb	154Glu	1H
2.20	0.000	Hga	154Glu	1H
123.26	0.026	N	155Ile	15N
8.50	0.005	H	155Ile	1H
60.14	0.062	Ca	155Ile	13C
40.33	0.057	Cb	155Ile	13C
5.22	0.007	Ha	155Ile	1H
17.16	0.065	Cg2	155Ile	13C
13.35	0.044	Cd1	155Ile	13C
27.56	0.027	Cg1	155Ile	13C
1.60	0.006	Hb	155Ile	1H
1.85	0.004	Hg1b	155Ile	1H
0.91	0.008	Hg1a	155Ile	1H
0.37	0.006	Hg2*	155Ile	1H
0.59	0.005	Hd1*	155Ile	1H
174.97	0.034	C	155Ile	13C
126.35	0.012	N	156Leu	15N
9.32	0.007	H	156Leu	1H
53.23	0.066	Ca	156Leu	13C
45.52	0.073	Cb	156Leu	13C
5.64	0.007	Ha	156Leu	1H
28.16	0.053	Cg	156Leu	13C
26.31	0.056	Cda	156Leu	13C
1.65	0.005	Hbb	156Leu	1H
1.37	0.003	Hba	156Leu	1H
1.46	0.004	Hg	156Leu	1H
0.79	0.004	Hdb*	156Leu	1H
0.57	0.004	Hda*	156Leu	1H
175.85	0.007	C	156Leu	13C
24.97	0.035	Cdb	156Leu	13C
119.98	0.035	N	157Glu	15N
9.35	0.005	H	157Glu	1H
54.61	0.075	Ca	157Glu	13C
33.53	0.039	Cb	157Glu	13C
5.33	0.009	Ha	157Glu	1H

37.33	0.035	Cg	157Glu	13C
1.87	0.004	Hba	157Glu	1H
2.10	0.005	Hbb	157Glu	1H
2.28	0.018	Hgb	157Glu	1H
2.26	0.019	Hga	157Glu	1H
176.15	0.044	C	157Glu	13C
126.80	0.014	N	158Arg	15N
8.24	0.005	H	158Arg	1H
57.36	0.067	Ca	158Arg	13C
30.65	0.047	Cb	158Arg	13C
3.32	0.007	Ha	158Arg	1H
43.06	0.045	Cd	158Arg	13C
27.33	0.016	Cg	158Arg	13C
1.43	0.004	Hbb	158Arg	1H
0.66	0.007	Hga	158Arg	1H
1.20	0.007	Hgb	158Arg	1H
2.73	0.006	Hda	158Arg	1H
2.76	0.017	Hdb	158Arg	1H
176.22	0.019	C	158Arg	13C
6.93	0.000	He	158Arg	1H
84.90	0.000	Ne	158Arg	15N
1.08	0.005	Hba	158Arg	1H
131.59	0.025	N	159Arg	15N
7.99	0.007	H	159Arg	1H
3.95	0.006	Ha	159Arg	1H
58.32	0.035	Ca	159Arg	13C
31.34	0.027	Cb	159Arg	13C
1.68	0.001	Hbb	159Arg	1H
1.37	0.010	Hba	159Arg	1H
28.60	0.024	Cg	159Arg	13C
43.45	0.017	Cd	159Arg	13C
1.50	0.004	Hgb	159Arg	1H
1.39	0.008	Hga	159Arg	1H
181.65	0.000	C	159Arg	13C
3.07	0.012	Hda	159Arg	1H
3.09	0.008	Hdb	159Arg	1H
1.94	0.000	Hga*	160Fol	1H
2.17	0.000	Hgb*	160Fol	1H
7.52	0.000	H16*	160Fol	1H
7.98	0.000	H12*	160Fol	1H
4.22	0.000	Ha*	160Fol	1H
4.36	0.000	H9a*	160Fol	1H

8.10	0.000	H7*	160Fol	1H
6.91	0.000	H2a*	161Nap	1H
6.03	0.000	H1b*	161Nap	1H
8.31	0.000	H8a*	161Nap	1H
8.07	0.000	H5n*	161Nap	1H
8.93	0.000	H4n*	161Nap	1H
4.91	0.000	H2b*	161Nap	1H
5.93	0.000	H1d*	161Nap	1H
9.83	0.000	H2n*	161Nap	1H

8.2 Co-solvent induced Chemical Shift Perturbations by Atom

8.2.1 17% Glycerol Induced Chemical Shift Perturbations in carbon nuclei of the EcDHFR: $NADP^+$: Folate complex

Chemical shift deviations of carbon nuclei of EcDHFR: $NADP^+$: Folate complex in the presence of 17% glycerol co-solvent from chemical shift values of the protein complex in the absence of co-solvent (buffer only) are presented below (**Table 8.2.1)**. To highlight meaningful differences, the values displayed in the cells are the chemical shift difference minus the calculated standard deviation for each atom ($\delta\Delta$ – SD). Nuclei that show perturbations in chemical shift greater than the combined standard deviation of the averaged chemical shift values are coloured green, values showing insignificant or perturbations less than the standard deviation are coloured red and nuclei yielding no data are coloured yellow. Hydrogen bonding status of the residue is listed as Y if the residue is involved in hydrogen bonding and the involvement in secondary structure elements are listed down the left hand side of the table.

H BOND	SECONDARY STRUCTURE 17% GLYCEROL		Residue No	Residue	CA 17% GLY δΔ- SD	CB δΔ- SD	cg (1) δΔ- SD	cg (2) δΔ- SD	CD δΔ-SD	CD δΔ-SD	CE δΔ- SD	C=O δΔ- SD
		Polar	1	1Met	0.024113731							-0.0007
	β	Hydrophobic	2	2Ile	-0.05698993	-0.0500	-0.02818	0.004049	-0.0325			0.1009
Y	β	Polar	3	3Ser		0.0037	0					0.05211
Y	β	Hydrophobic	4	4Leu	-0.04467522	-0.0427	0.03422		0.34644	-0.01111		0.06104
Y	β	Hydrophobic	5	5Ile	-0.05343126	0.0097	0.038379	0.13121	-0.03449			0.17135
Y	β	Hydrophobic	6	6Ala	-0.06523837	0.0461	0					0
	β	Hydrophobic	7	7Ala	-0.07443068	0.0026	0					0.1359
Y	β	Hydrophobic	8	8Leu	0.081788176	0.0463	-0.02398		0.10726			0.24575
Y		Hydrophobic	9	9Ala	-0.03265839	0.1379	0					0.17017
	α	Hydrophobic	10	10Val	-0.08994378	-0.0508	0.048561	0.05421				0.00186
Y	α	Charged	11	11Asp	-0.06922153	-0.0050	0					0.20253
	α	Charged	12	12Arg	-0.02900689	0.0595	-0.06741		0.03134			0.0886
Y	β	Hydrophobic	13	13Val	-0.09470151	-0.0670	0.011442	-0.02055				0
Y	β	Hydrophobic	14	14Ile			0.14113	0	0.08483			
		Hydrophobic	15	15Gly	-0.03623379		0					0.16763
		Polar	16	16Met	-0.05003	0.3302	0				-0.03652	0
	turn	Charged	17	17Glu		0.0800	0.08					0.15031
Y	β bridge	Polar	18	18Asn	-0.05543713	0.0316	0					0.11518

		Hydrophobic	19	19Ala	-0.02694024	0.0149	0					0.00684
		Polar	20	20Met	0.1248		0				-0.011080307	0
Y		Hydrophobic	21	21Pro			0					
Y		Polar	22	22Trp			0					0.02379
Y		Polar	23	23Asn	-0.03384	0.0635	0					0.23783
		Hydrophobic	24	24Leu	0.069735057	-0.0854	0		-0.08853			0
Y	α	Hydrophobic	25	25Pro	0.054109825	-0.0075	0.04524		0.029138			0.09515
	α	Hydrophobic	26	26Ala	0.020427118	0.0422	0					0.0184
Y	α	Charged	27	27Asp	-0.06179063	0.0273	0					0.06063
Y	α	Hydrophobic	28	28Leu	-0.01691025	-0.0025	0.04891		0.0502	-0.07605		0.02352
Y	α	Hydrophobic	29	29Ala	0.067477592	-0.1313	0					0.271
Y	α	Polar	30	30Trp	-0.04037441	-0.0643	0		1.237			0.13921
Y	α	Hydrophobic	31	31Phe	-0.09674959	0.0212	0					0.02979
Y	α	Charged	32	32Lys	-0.09805144	-0.0724	0.07565		0.03766		0.082	0.084531
Y	α	Charged	33	33Arg	-0.00329224	0.0137	0.052574		0.050141			0.2285
Y	α	Polar	34	34Asn	0.036570706	0.0451	0					0.10341
Y	α	Polar	35	35Thr	-0.03366708	0.0610	-0.04952					0.02972
Y	α	Hydrophobic	36	36Leu	0.048521534	-0.0627	0		0.053988	0.10019		0.142828
Y	turn	Charged	37	37Asp	0.021280287	-0.1175	0					0.2311
Y	turn	Charged	38	38Lys	0.11526		0					0
Y	β	Hydrophobic	39	39Pro	-0.05291031		0.04317		0.056044			0.17395
Y	β	Hydrophobic	40	40Val	0.004648249	-0.0005	0.043964	0.025955				0.07527
Y	β	Hydrophobic	41	41Ile	-0.05434177	-0.0284	0.06703	0.05448	0.081881			0.178838
Y	β	Polar	42	42Met	-0.08202775	-0.1976	0.235948				0.0148	0.10762
Y	β	Hydrophobic	43	43Gly	-0.06427297		0					0.17775

	α	Charged	44	44Arg	0.03796		0.06856		0.04511			0.19074
	α	Charged	45	45His	0.03768	0.0198	0					-2.1E-14
Y	α	Polar	46	46Thr	0	0.0771	-0.06794					0.04566
Y	α	Polar	47	47Trp	-0.09336	-0.0419	0					
Y	α	Charged	48	48Glu	-0.1021205	0.2101	0.00218					0.13467
Y	α	Polar	49	49Ser	0.052057787	0.0233	0					0.15988
Y	α	Hydrophobic	50	50Ile	0.089336272	0.2041	0.114764	0.02446	0.080931			0.08958
		Hydrophobic	51	51Gly	-0.07351585		0					0.18239
Y		Charged	52	52Arg	0.005713907	0.0524	0.0736		0.068221			
Y		Hydrophobic	53	53Pro	0.01606		0.07392		0.0442			0.11309
Y		Hydrophobic	54	54Leu	0.019346484	-0.0170	0		0.0406	0.04006		0
Y	turn	Hydrophobic	55	55Pro	0		0					
Y	turn	Hydrophobic	56	56Gly	0.022046105		0					0.2764
		Charged	57	57Arg	-0.02634225	0.0295	0.04982		0.04829			0.05732
		Charged	58	58Lys	-0.0736131	-0.0434	0.08079		0.04607		0.07723	-0.06168
	β	Polar	59	59Asn	0.050932453	0.0648	0					0.148287
Y	β	Hydrophobic	60	60Ile	0.028101844	0.0637	0.026	0.040632	0.046831			0.13035
Y	β	Hydrophobic	61	61Ile	0.037747826	0.2080	0.03495	7.73E-05	0.163463			0.0524
Y	β	Hydrophobic	62	62Leu	-0.01530907	0.0060	0		-0.03249	-0.04517		0.1215
Y		Polar	63	63Ser	-0.13328125	-0.0157	0					0.10638
		Polar	64	64Ser	0.007662656	0.0941	0					0.27791
		Polar	65	65Gln	-0.06411782	0.0034	-0.05996					0
Y		Hydrophobic	66	66Pro	0.036264512	0.0583	0.05279		-0.08244			0.11386
		Hydrophobic	67	67Gly	0.043163256		0					
		Polar	68	68Thr	-0.01400516	-0.0481	0.19725					0.1433
		Charged	69	69Asp	-0.02634678	-0.0283	0					0.08172

	turn	Charged	70	70Asp	0.024146383	0.0542	0					0.20832
	turn	Charged	71	71Arg	-0.04701142	0.0871	0.054112		-0.07189			0.30771
		Hydrophobic	72	72Val	-0.05188479	0.0689	-0.01667	-0.02068				0.11213
Y	β	Polar	73	73Thr	-0.07791625	0.0051	0.05785					0.06588
	β	Polar	74	74Trp	-0.00514433	-0.0104	0					0.172
Y	β	Hydrophobic	75	75Val	0.015786284	0.0543	0.067204	0.097088				0.02017
		Charged	76	76Lys	-0.03432314	-0.0328	-0.07305		0.06738		0.0112	-0.00316
Y		Polar	77	77Ser	-0.02626151	-0.1601	0					0.08546
	α	Hydrophobic	78	78Val	-0.01696808	-0.0250	0.033453	0.097929				0.14887
	α	Charged	79	79Asp	-0.09723194	0.0822	0					0.24837
	α	Charged	80	80Glu	-0.03349753	-0.0112	0.036119					0.24672
Y	α	Hydrophobic	81	81Ala	0.001889081	0.0007	0					0.09165
Y	α	Hydrophobic	82	82Ile	-0.0281468	-0.0498	0.015633	0.087483	0.202586			0.154968
Y	α	Hydrophobic	83	83Ala	-0.02838566		0					0.10123
Y	α	Hydrophobic	84	84Ala	-0.00068879	0.1050	0					0.07789
Y	α	Polar	85	85Cys	-0.05820618	-0.0913	0					0.06882
		Hydrophobic	86	86Gly	0.023277364	0.0000	0					0.14329
		Charged	87	87Asp	-0.02679299	-0.0120	0					-0.16937
		Hydrophobic	88	88Val	0.03024	0.2557	0.00958	0.10388				
Y		Hydrophobic	89	89Pro	-0.05098455	0.0354	0.05799		0.0476			0.1723
		Charged	90	90Glu	-0.05373096	-0.1437	0.04486					0.01074
Y	β	Hydrophobic	91	91Ile	0.000816975	-0.0327	0.05811	0.158885	0.001165			0.158538
Y	β	Polar	92	92Met	-0.16557316	-0.0108	0.00161				-0.0144	0.30997
Y	β	Hydrophobic	93	93Val	0.207630757	0.0852	-0.00827	0.01132				0.08204
Y		Hydrophobic	94	94Ile	0.111452723	0.0755	0.007531	0.05651	0.049262			0.03452
Y		Hydrophobic	95	95Gly	0.024806449	0.0000	0					0.05468

		Hydrophobic	96	96Gly	-0.00364	0.0000	0					
Y	α	Hydrophobic	97	97Gly	-0.01089844	0.0000	0					0.17119
	α	Charged	98	98Arg	-0.12441495	0.1292	0.05348		-0.00569			0.00696
	α	Hydrophobic	99	99Val	-0.028428	0.0693	-0.00093	0.09942				0.09517
Y	α	Polar	100	100Tyr	0.018506274	-0.0206	0					0.03919
	α	Charged	101	101Glu	-0.1146056	0.0547	0.05169					
Y	α	Polar	102	102Gln	0.042772035		0.08					0.16595
Y	3/10 α	Hydrophobic	103	103Phe	-0.04332776	-0.0319	0					
Y	3/10 α	Hydrophobic	104	104Leu	0.02175	0.0193	0		-0.01566	0.11981		
Y	3/10 α	Hydrophobic	105	105Pro	-0.04016		0.05238		0.00359			0.22059
Y	3/10 α	Charged	106	106Lys	0.003673697		0.07718		0.04524		0.04643	0.17285
Y		Hydrophobic	107	107Ala	0.026008962	0.1309	0					0.1268
		Polar	108	108Gln	-0.06024342	0.0193	-0.03821					0.13212
Y	β	Charged	109	109Lys	0.01334901	0.0268	-0.04223		0.044956		-0.082899028	0.13956
Y	β	Hydrophobic	110	110Leu	-0.03130691	-0.0236	0		0.12829			0.13552
Y	β	Polar	111	111Tyr	0.000408983	-0.0321	0					0.20167
Y	β	Hydrophobic	112	112Leu	-0.07841106	-0.0064	0		-0.02883	0.04515		
Y	β	Polar	113	113Thr	0.02687536	0.0802	0					0.30232
Y	β	Charged	114	114His	-0.11492749	-0.1987	0					0.07101
Y	β	Hydrophobic	115	115Ile	-0.04009193	0.2871	0.020514	0.03156	-0.00131			0.03228
Y		Charged	116	116Asp	0.192332062	-0.1023	0					0.04858
		Hydrophobic	117	117Ala	0.008780364	-0.0508	0					0.11065
		Charged	118	118Glu	-0.1451845	0.2233	0.10501					
		Hydrophobic	119	119Val	-0.04419103	0.1040	-0.00734	0.077454				0.09547
		Charged	120	120Glu	0.146741635	0.0530	0.01485					0.25932

		Hydrophobic	121	121Gly	-0.07066215	0.0000	0					0.11776
		Charged	122	122Asp	0.053736599	0.0142	0					
		Polar	123	123Thr	0	0.0000	0					
Y	β	Charged	124	124His	0.080561725	-0.1668	0					
Y	β	Hydrophobic	125	125Phe	0.113485799	-0.0343	0					
Y		Hydrophobic	126	126Pro	-0.05542956	-0.0005	0.015735		0.022603			
		Charged	127	127Asp	-0.06873172	-0.0343	0					
		Polar	128	128Tyr	0.143606105	0.0068	0					
	3/10 α	Charged	129	129Glu	0.007050356		0.0594					
Y	3/10 α	Hydrophobic	130	130Pro	0.057446032	-0.0661	0.21172		-0.00025			0.10381
	1/10 α	Charged	131	131Asp	-0.08417068	-0.0409	0					0.1359
	β	Charged	132	132Asp	-0.05673904	-0.0021	0					0.11394
	β	Polar	133	133Trp	0.073731657	0.0010	0		0.01714			0.09689
Y	β	Charged	134	134Glu	-0.10539153	0.0728	-0.02471					0.03765
Y	β	Polar	135	135Ser	0.157721528	0.0254	0					
	β	Hydrophobic	136	136Val	0.112833072	0.0395	0.073363	0.10475				0.15662
	β	Hydrophobic	137	137Phe	0.014873783	-0.0283	0					0.08556
Y	β	Polar	138	138Ser	0.073460455	0.0970	0					0.03152
Y	β	Charged	139	139Glu	-0.00130597	-0.0061	0.010953					0.16027
	β	Hydrophobic	140	140Phe	-0.02058923	-0.0146	0					0.14716
Y	β	Charged	141	141His	0.022194213	0.0747	0					0.28966
Y		Charged	142	142Asp	-0.10155584	-0.0878	0					0.00409
		Hydrophobic	143	143Ala	-0.06413102	0.0650	0					0.28879
		Charged	144	144Asp	0.070440579	-0.0454	0					0.27165
		Hydrophobic	145	145Ala	0.09862	0.0977	0					0.23829
Y	bend	Polar	146	146Gln	-0.13308334	-0.0017	0.023613					0.24985

	bend	Polar	147	147Asn	-0.1083958	0.0247	0					
Y	bend	Polar	148	148Ser	-0.05271	0.0754	0					0.18427
		Polar	149	149His	0.698619654	0.8962	0					0.09523
		Polar	150	150Ser	0.175999709	0.0588	0					0.08608
Y	β	Polar	151	151Tyr	0.019994351	-0.0128	0					0.06932
Y	β	Polar	152	152Cys	-0.0328		0					0.98358
Y	β	Hydrophobic	153	153Phe	-0.02298	0.1503	0					0.66501
Y	β	Charged	154	154Glu	0.03415	0.7733	0.05					
Y	β	Hydrophobic	155	155Ile	-0.05290956	0.0118	-0.00256	0.01888	0.035743			0.06545
Y	β	Hydrophobic	156	156Leu	0.012294454	-0.0693	0.001362		0.298873	-0.04827		0.14085
Y	β	Charged	157	157Glu	-0.07328994	-0.0275	0.10121					0.17419
Y	β	Charged	158	158Arg	-0.05063821	-0.0233	-0.0373		-0.03498			0.15394
		Charged	159	159Arg	0.148919042	0.0245	0.076051		-0.01006			

Table 8.2.1 Chemical shift deviations of carbon nuclei of EcDHFR: $NADP^+$: Folate complex in the presence of 17% glycerol co-solvent from chemical shift values of the protein complex in the absence of co-solvent (buffer only)

8.2.2 17% Glycerol Induced Chemical Shift Perturbations in carbon nuclei of the EcDHFR: $NADP^+$: Folate complex

Chemical shift deviations of hydrogen nuclei in EcDHFR: $NADP^+$: Folate complex in the presence of 17% glycerol co-solvent from chemical shift values of the protein complex in the absence of co-solvent (buffer only) are shown below (**Table 8.2.2)**. To highlight meaningful differences, the values displayed in the cells are the chemical shift difference minus the calculated standard deviation for each atom ($\delta\Delta$ – SD). Nuclei that show perturbations in chemical shift greater than the combined standard deviation of the averaged chemical shift values are coloured green, values showing insignificant or perturbations less than the standard deviation are coloured red and nuclei yielding no data are coloured yellow. Hydrogen bonding status of the residue is listed as Y if the residue is involved in hydrogen bonding and the involvement in secondary structure elements are listed down the left hand side of the table.

H BOND	SECONDARY STRUCTURE 17% GLYCEROL		Residue	17% GLYCEROL HN δΔ- SD	HA δΔ- SD	HB (1) δΔ- SD	HB (2) δΔ- SD	HG (1) δΔ- SD	HG (2) δΔ- SD	HG(3) δΔ-SD	HD (1) δΔ- SD	HD (2) δΔ- SD	HE δΔ- SD
		Polar	1Met		0.0279								
	β	Hydrophobic	2Ile	-0.033003141	0.0174	0.019092		0.017833	0.031581	0.0119	0.025608		
Y	β	Polar	3Ser	0.009100239	-0.0113	0.026395	0.003186	0			0		
Y	β	Hydrophobic	4Leu	-0.027949274	0.0424	0.024822	0.029749	0.032583			0.029198	0.012533	
Y	β	Hydrophobic	5Ile	-0.028140042	0.0225	0.02723		0.040991	0.066639	0.030908	0.03407		
Y	β	Hydrophobic	6Ala	-0.011410256	0.0245	-0.0057		0			0		
	β	Hydrophobic	7Ala		0.0593	0.018892		0			0		
Y	β	Hydrophobic	8Leu	0.044382816	0.0502	0.038744	-0.0004	0.0456			0.020548	0.044443	
Y		Hydrophobic	9Ala	-0.019111216	0.0802	0.036491		0			0		
	α	Hydrophobic	10Val	0.094811261	0.0151	0.054792		0.012854	0.035461		0		
Y	α	Charged	11Asp	-0.008206808	0.0099	-0.02682	0.028784	0			0		
	α	Charged	12Arg	0.02068256	0.0098	-0.00429	0.001956	0.10704	0.167262		0.02453	0.017041	
Y	β	Hydrophobic	13Val	-0.027759747	0.0237	-0.00869		-0.00817	-0.00076		0		
Y	β	Hydrophobic	14Ile			-0.00669		0.00335			0		
		Hydrophobic	15Gly	0.00322455				0			0		
		Polar	16Met	-0.018350188	0.1327	-0.00261	-0.01029	0			0		
	β bridge	Charged	17Glu					0			0		
Y	β bridge	Polar	18Asn	-0.020090482	0.0312	0.032713	0.004586	0			0		
		Hydrophobic	19Ala	0.014606706	0.0235	0.034544		0			0		
		Polar	20Met	-0.037862091				0			0		

Y		Hydrophobic	21Pro					0			0		
Y		Polar	22Trp	-0.023117887				0			0		
Y		Polar	23Asn	0.000965513	0.0551	-0.0019	0.047491	0			0		
		Hydrophobic	24Leu	0.055369741	0.0562	0.045497	0.009927	0.02731			0.036686	0.01354	
Y	α	Hydrophobic	25Pro		0.0318	0.002386	0.012638	0.022598	0.038691		0.03065	0.05753	
	α	Hydrophobic	26Ala	0.001645178	-0.0012	0.046753		0			0		
Y	α	Charged	27Asp	0.008827035	0.0342	0.028629	0.034253	0			0		
Y	α	Hydrophobic	28Leu	0.016622499	0.0471	0.041713	0.03616	0.035852			0.037071	0.045608	
Y	α	Hydrophobic	29Ala	-0.019017389	0.0252	-0.02979		0			0		
Y	α	Polar	30Trp	0.032046979	0.0142	0.067147	0.037781	0			0.155296		0.00277
Y	α	Hydrophobic	31Phe	-0.003905837	0.0474	0.055183	0.041374	0			0		
Y	α	Charged	32Lys	-0.034474164	0.0497	-0.00396	0.03458	0			0.072076	0.02294	
Y	α	Charged	33Arg	-0.035671049	0.0052	0.028149	0.024727	0.00424	0.012363		0.010215	0.025761	
Y	α	Polar	34Asn	0.036426006	0.0256	0.08493	0.058996	0			0		
Y	α	Polar	35Thr	0.025415944	-0.0024	0.05109		0.05093			0		
Y	α	Hydrophobic	36Leu	0.009495531	0.0114	-0.03124	0.014143	0			0.039612	0.0178	
Y	turn	Charged	37Asp	0.038087717	-0.0101	-0.01353	-0.00292	0			0		
Y	turn	Charged	38Lys	0.087080964	0.0598	-0.00248	0	0			0		
Y	β	Hydrophobic	39Pro		0.0686	-0.00504	-0.00925	0.050976	0.00973		0.044243	0.064091	
Y	β	Hydrophobic	40Val	0.020670037	0.0308	0.039477		0.03697	0.033688		0		
Y	β	Hydrophobic	41Ile	-0.007553934	0.0049	0.008665		0.05108	0.028186	0.026437	0.00694		
Y	β	Polar	42Met	-0.02566764	0.0289	0.01995	0.019432	0.021199	0.050428		0		
Y	β	Hydrophobic	43Gly	-0.003619356				0			0		
	α	Charged	44Arg	0.008951629	0.0000	-0.002	-0.00632	0			-0.00219	-0.00182	
	α	Charged	45His	-0.020535319	0.0787	0	0	0			0		
Y	α	Polar	46Thr	0.131778836		0.00414		0.0526			0		

Y	α	Polar	47Trp	-0.03726836	0.0084	0.074825	0.044496	0			0.03113		0
Y	α	Charged	48Glu		0.0369	0.0279	0.05849	0.00169	0.01239		0		
Y	α	Polar	49Ser	0.05458651	0.0241	0.083818	-0.01078	0			0		
Y	α	Hydrophobic	50Ile	0.040854927	0.0324	0.013266		0.02962	0.031916	0.000781	0.00488		
		Hydrophobic	51Gly	0.029537517	0.0000			0			0		
Y		Charged	52Arg	0.021432388	0.0246	0.024014	0.013665	0.02704	0.029637		0.029325	-0.00653	
Y		Hydrophobic	53Pro		0.0000	-0.00235	-0.00141	-0.00221			-0.00053	0.01672	
Y		Hydrophobic	54Leu	0.029098461	0.0229	0.02521	-0.00715	0			0.033662	0.054121	
Y	turn	Hydrophobic	55Pro					0			0		
Y	turn	Hydrophobic	56Gly	-0.002566798				0			0		
		Charged	57Arg	0.035574594	0.0410	0.02417	0.00315	-0.00101			0.031978	0.024842	
		Charged	58Lys	-0.008942231	0.0404	0.041053	0.006488	0.03526	0.04386		0.020323	0.045973	
	β	Polar	59Asn	0.008584369	0.0110	0.0172	-0.00294	0			0		
Y	β	Hydrophobic	60Ile	-0.008957433	0.0254	0.053156		-0.00971	0.038187	0.015475	0.013049		
Y	β	Hydrophobic	61Ile	-0.007571889	0.0344	0.015536		0.038471	0.074585	0.040694	0.020336		
Y	β	Hydrophobic	62Leu	-0.035646386	0.0171	0.000711	0.016693	0.015307			0.005736	0.006908	
Y		Polar	63Ser	-0.025311661	0.0444	-0.00656	0.02737	0			0		
		Polar	64Ser	0.017274512	-0.0088	-0.00158	-0.00449	0			0		
		Polar	65Gln	0.008632085	0.0047	0.00589	-0.01125	-0.01097	-0.01809		0		
Y		Hydrophobic	66Pro		-0.0021	-0.00534	-0.00187	0.005171	0.025161		0.006396	-0.00561	
		Hydrophobic	67Gly	0.03161673				0			0		
		Polar	68Thr	0.064671097	0.0206	0.00895		-0.01198			0		
		Charged	69Asp	0.002429442	0.0444	0.036532	-0.00601	0			0		
	turn	Charged	70Asp	0.006776137	0.0446	0.017528	0.01068	0			0		
	turn	Charged	71Arg	0.041480558	0.0097	-0.01008	-0.01082	0.038369	0.019404		0.019404	-0.0194	
		Hydrophobic	72Val	0.050098488	0.0167	0.032959		0.02095	0.009664		0		

Y	β	Polar	73Thr	0.037496086	0.0158	0.05424		-0.00411			0		
	β	Polar	74Trp	-0.016092355	0.0207	0.026357	0.031459	0			0.008896		0.06071
Y	β	Hydrophobic	75Val	0.067414778	-0.0040	-0.00605		0.02729	0.003514		0		
		Charged	76Lys	0.000319006	0.0449	0.009903	0.044178	0.041681	0.05907		0.03984	0.037218	
Y		Polar	77Ser	0.015120954	-0.0253	0.045548	0.034475	0			0		
	α	Hydrophobic	78Val	-0.006322106	0.0144	-0.00835		-0.00318	-0.00843		0		
	α	Charged	79Asp	0.046744573	0.0324	-0.01352	0.012839	0			0		
	α	Charged	80Glu	-0.009823336	0.0575	0.015634	-0.00953	0.030097	0.008999		0		
Y	α	Hydrophobic	81Ala	0.081554911	0.0145	-0.00453		0			0		
Y	α	Hydrophobic	82Ile	0.047452681	0.0520	0.028446		0.036987	0.002512	0.009836	0.031608		
Y	α	Hydrophobic	83Ala	-0.00695351	0.0188	0.04964		0			0		
Y	α	Hydrophobic	84Ala	-0.029710048	0.0153	0.03967		0			0		
Y	α	Polar	85Cys	-0.001597861	0.0459	0.035469	0.041238	0			0		
		Hydrophobic	86Gly	0.017526402				0			0		
		Charged	87Asp	0.004612392	0.0338	0.004118	0.00064	0			0		
		Hydrophobic	88Val	-0.027006841	-0.0038	0.016104		0.0346	0.00649		0		
Y		Hydrophobic	89Pro		0.0110	0.011602	0.029445	0.117892	0.1763		0.01141	0.057887	
		Charged	90Glu	0.014946703	0.0257	0.029631	0.067063	0.027801	0.042958		0		
Y	β	Hydrophobic	91Ile	-0.00767348	0.0304	0.029877		0.041337	0.060593	-0.00433	-0.00356		
Y	β	Polar	92Met	-0.027824112	0.0404			0.04707	0.03717		0		
Y	β	Hydrophobic	93Val	-0.016050117	0.0112	0.024564		0.03307	0.011825		0		
Y		Hydrophobic	94Ile	0.023806254	0.0336	0.031453		0.026149	0.039844	0.054471	-0.00904		
Y		Hydrophobic	95Gly	0.02029367				0			0		
		Hydrophobic	96Gly	-0.035099888				0			0		
Y	α	Hydrophobic	97Gly					0			0		
	α	Charged	98Arg	0.036917047	0.0566	0.004689	0.007705	0.064834	0.05754		0.057148	0.01521	

	α	Hydrophobic	99Val	0.00083996	0.0456	0.025689		0.04731	0.04152		0		
Y	α	Polar	100Tyr	0.010792868	-0.0004	0.028566	0.02888	0			0.04358		0.0061
	α	Charged	101Glu	-0.033447356	0.0304	0.038294	0.024867	0.031997	0.02273		0		
Y	α	Polar	102Gln	0.022515175	0.0555			0			0		
Y	3/10 α	Hydrophobic	103Phe	0.048392178	0.0327	0.027248	0.018218	0			0.02906		0.01403
Y	3/10 α	Hydrophobic	104Leu	-0.035124768	0.0404	0.0432	0.013291	0			0	0.03165	
Y	3/10 α	Hydrophobic	105Pro		0.0000			-0.00036	-0.00036		-0.01697	-0.00422	
Y	3/10 α	Charged	106Lys	0.055638368	-0.0005	0	0	0			-0.00054	-0.00547	
Y		Hydrophobic	107Ala	0.024235716	0.0324	-0.00059		0			0		
		Polar	108Gln	0.010882933	-0.0096	0.020928	0.006867	-0.01305	-0.01253		0		
Y	β	Charged	109Lys	0.078115136	0.0060	0.014129	0.046781	0.0369	0.033366		0.006284	0.06792	
Y	β	Hydrophobic	110Leu	0.046939548	0.0242	0.044283	0.034447				0.036717		0.02919
Y	β	Polar	111Tyr	-0.033973949	0.0344	0.006274	0.045996	0			0		
Y	β	Hydrophobic	112Leu	0.00561351	0.0299	0.024374	0.002381	0.045466			-0.00682	0.040609	
Y	β	Polar	113Thr		-0.0178	-0.00245		0			0.01431		
Y	β	Charged	114His	0.033329399	0.0251			0			0.00655		
Y	β	Hydrophobic	115Ile	0.053316703	0.0615	0.012813		0.044299	0.011395	0.034173	0.004162		
Y		Charged	116Asp	0.026910958	-0.0011	-0.01071	0.013558	0			0		
		Hydrophobic	117Ala	-0.014083851	0.0466	0.058724		0			0		
		Charged	118Glu	0.012642141	0.0517	0.033153	0.041202	0.032525	-0.01669		0		
		Hydrophobic	119Val	0.01279849	0.0230	0.040953		0.061555	0.134944		0		
		Charged	120Glu	0.013914881	0.0358	0.034251	-0.00709	0.020626	0.014067		0		
		Hydrophobic	121Gly	0.115847632				0			0		
		Charged	122Asp	-0.044188608	0.0224	0.01303	-0.00141	0			0		
		Polar	123Thr					0			0		
Y	β	Charged	124His		0.0223	-0.00149	0.011853	0			0.049386		

Y	β	Hydrophobic	125Phe	0.028723531	0.0442	0.028379	0.041877	0			0		
Y		Hydrophobic	126Pro		0.0113	0.0161	0.0313	0.035891	0.040037		0.050679	0.023427	
		Charged	127Asp	-0.002699472	-0.0073	0.005055	0.012504	0					
		Polar	128Tyr	-0.020175392	0.0392	0.017241	0.035122	0			0.01799		0.03339
	3/10 α	Charged	129Glu	0.087407984	0.0512	0		0.019402	0.041828		0		
Y	3/10 α	Hydrophobic	130Pro		0.0434	0.03799	0.021888	0.046748	0.017458		-0.01452		
	1/10 α	Charged	131Asp	0.015213644	0.0320	0.033253	0.013651	0			0		
	β	Charged	132Asp	0.026859195	0.0325	0.004975	-0.00539	0			0		
	β	Polar	133Trp	0.000249923	0.0630	0.013256	0.025198	0			0.01102		0.00393
Y	β	Charged	134Glu	0.084870714	0.0253	0.030238	0.022244	-0.00699	0.0121		0		
Y	β	Polar	135Ser	0.040195133	0.0199	-0.00843	0.03338	0			0		
	β	Hydrophobic	136Val	-0.022615029	0.0093	-0.00973		-0.01114	-0.01411		0		
	β	Hydrophobic	137Phe	0.045846074	0.0350	-0.00298	0.01112	0			0.02367		0.0186
Y	β	Polar	138Ser	0.022244943	0.0455	0.001277	0.079658	0			0		
Y	β	Charged	139Glu	0.152301519	0.0380	0.047786	0.037994	0.048703	0.010644		0		
	β	Hydrophobic	140Phe	-0.028130784	0.0587	0.034851	0.016472	0			0.02465		0.00262
Y	β	Charged	141His	-0.034321606	0.0251	0.030076	0.07947	0			0.02429		
Y		Charged	142Asp	-0.038134168	0.0568	0.007077	0.009567	0			0		
		Hydrophobic	143Ala	-0.044245245	-0.0025	0.040532		0			0		
		Charged	144Asp	0.0806213	0.0078	0.02696	0.008973	0			0		
		Hydrophobic	145Ala	0.143678579	0.0256	-0.01068		0			0		
Y	bend	Polar	146Gln	0.054926655	-0.0059	0.032452	0.019623	0.00363	0.028988		0		
	bend	Polar	147Asn	-0.009358446	0.0067	0.0217	0.00914	0			0		
Y	bend	Polar	148Ser	-0.019881268	0.0573	-0.00229	-0.00514	0			0		
		Polar	149His	0.003515892	-0.0086	0	0.026907	0			0		
		Polar	150Ser	-0.027366716	0.0348	-0.00936	0.00158	0			0		

Y	β	Polar	151Tyr	-0.035573045	0.0419	0.038606	0.010982	0					
Y	β	Polar	152Cys	-0.038128548				0			0		
Y	β	Hydrophobic	153Phe	0.00231488	0.0436	0.03006	0.02773	0			0		
Y	β	Charged	154Glu	-0.049019062	0.0190	0.02996	0.01708	-0.00173	-9.2E-05		0		
Y	β	Hydrophobic	155Ile	0.24301161	0.0581	0.038822		0.057228	0.060446	-0.00115	0.017011		
Y	β	Hydrophobic	156Leu	-0.034250461	0.0407	0.00464	0.017892	0.014918			0.035903	-0.00288	
Y	β	Charged	157Glu	0.010141805	0.0367	0.031618	0.028647	0.04075	-0.01348		0		
Y	β	Charged	158Arg	0.012142358	0.0381	0.049435	0.050218	0.048097	0.081218		-0.00134	-0.01173	
		Charged	159Arg	0.014390442	-0.0045	-0.00707	0.002179	-0.02613	-0.03197		0.033288	-0.00337	

Table 8.2.2 Chemical shift deviations of hydrogen nuclei in EcDHFR: $NADP^+$: Folate complex in the presence of 17% glycerol co-solvent from chemical shift values of the protein complex in the absence of co-solvent (buffer only)

8.2.3 17% Methanol Induced Chemical Shift Perturbations in hydrogen nuclei of the EcDHFR: $NADP^+$: Folate complex

Chemical shift deviations of hydrogen nuclei in EcDHFR: $NADP^+$: Folate complex in the presence of 17% methanol co-solvent from chemical shift values of the protein complex in the absence of co-solvent (buffer only) are shown below **(Table 8.2.3)**. To highlight meaningful differences, the values displayed in the cells are the chemical shift difference minus the calculated standard deviation for each atom ($\delta\Delta$ – SD). Nuclei that show perturbations in chemical shift greater than the combined standard deviation of the averaged chemical shift values are coloured green, values showing insignificant or perturbations less than the standard deviation are coloured red and nuclei yielding no data are coloured yellow. Hydrogen bonding status of the residue is listed as Y if the residue is involved in hydrogen bonding and the involvement in secondary structure elements are listed down the left hand side of the table.

H BOND	SECONDARY STRUCTURE 17% MeOD		Residue No	Residue	HN δΔ-SD	HA δΔ-SD	HB (1) δΔ- SD	HB (2) δΔ- SD	HG(1) δΔ- SD	HG (2) δΔ-SD	HG(3) δΔ-SD	HD (1) δΔ- SD	HD (2) δΔ- SD	HE δΔ- SD
		Polar	1	1Met		-0.0159								
	β	Hydrophobic	2	2Ile	-0.0361	0.0057	-0.003		-0.0085	-0.0015	-0.0026	-0.0108		
Y	β	Polar	3	3Ser	0.00236	-0.0141	-0.0041	0.00484	0			0		
Y	β	Hydrophobic	4	4Leu	-0.0129	-0.0055	-0.0061	-0.0006	-0.0097			-0.001	-0.0117	
Y	β	Hydrophobic	5	5Ile	-0.0152	-0.0105	-0.0144		0.01747	0.04178	0.00315	-0.0038		
Y	β	Hydrophobic	6	6Ala	-0.0257	-0.0101	-0.005		0			0		
	β	Hydrophobic	7	7Ala		-0.0040	-0.0072		0			0		
Y	β	Hydrophobic	8	8Leu	0.00649	0.0297	0.0019	0.00827	0.01976			-0.005	0.01407	
Y		Hydrophobic	9	9Ala	0.03867	0.0192	-0.0068		0			0		
	α	Hydrophobic	10	10Val	0.06867	-0.0093	0.01612		-0.0014	0.02195		0		
Y	α	Charged	11	11Asp	0.00025	-0.0016	-0.0004	-0.004	0			0		
	α	Charged	12	12Arg	0.09897	0.0029	0.0103	-0.0025	0.01974	-0.0102		0.0143	-0.0072	
Y	β	Hydrophobic	13	13Val	0.00599	0.0008	0.00088		0.25747	0.26388		0		
Y	β	Hydrophobic	14	14Ile			0		0			0		
		Hydrophobic	15	15Gly	-0.0135	-0.0135			0			0		
		Polar	16	16Met	-0.0246	0.0270	0	0	0			0		
	turn	Charged	17	17Glu					0			0		
Y	β bridge	Polar	18	18Asn	0.0499	0.0064	0.0003	-0.0074	0			0		
		Hydrophobic	19	19Ala	0.04364	-0.0080	-0.0027		0			0		
		Polar	20	20Met	0.02393				0			0		
Y		Hydrophobic	21	21Pro					0			0		
Y		Polar	22	22Trp	0.02382				0			0		
Y		Polar	23	23Asn	0.03823	0.0045	0.00952	0.01543	0			0		

		Hydrophobic	24	24Leu	0.05819	0.0054	-0.0077	-0.0009	-0.0101			-0.0062	-0.0088	
Y	α	Hydrophobic	25	25Pro		0.0115	-0.0121	-0.0272	-0.0046	0.00062		-0.0052	0.02645	
	α	Hydrophobic	26	26Ala	0.03621	0.0171	0.00778		0			0		
Y	α	Charged	27	27Asp	0.02825	0.0030	0.00174	-0.0046	0			0		
Y	α	Hydrophobic	28	28Leu	0.01213	0.0076	0.006	-0.0013	0.0093			0.00083	0.01139	
Y	α	Hydrophobic	29	29Ala	-0.0162	-0.0164	-0.0426		0					
Y	α	Polar	30	30Trp	0.03529	0.0033	0.01671	0.00379	0			0.0197		0.00613
Y	α	Hydrophobic	31	31Phe	0.01151	0.0076	0.00773	0.00456	0			0		
Y	α	Charged	32	32Lys	-0.0208	0.0062	0.00044	-0.0017	0			0.05006	-0.005	
Y	α	Charged	33	33Arg	-0.0152	0.0091	0.00454	-0.0067	2.9E-06	0.04081		-0.0078	-0.0007	
Y	α	Polar	34	34Asn	0.05123	-0.0126	0.05893	0.03469	0			0		
Y	α	Polar	35	35Thr	-0.0105	0.0330	0.00855		0.01176			0		
Y	α	Hydrophobic	36	36Leu	-0.0201	-0.0044	-0.0059	0.00889	0			0.00351	0.00553	
Y	turn	Charged	37	37Asp	0.00676	0.0137	0.00893	-0.0032	0			0		
Y	turn	Charged	38	38Lys	0.11881	0.0130	0.01607	0.00913	0			0		
Y	β	Hydrophobic	39	39Pro		0.0269	0.01786	-0.0094	0.01402	-0.0143		0.00211	0.01015	
Y	β	Hydrophobic	40	40Val	0.03095	-0.0093	0.00025		-0.0023	0.00414		0		
Y	β	Hydrophobic	41	41Ile	-0.0203	0.0399	0.01453		0.02424	-0.0081	0.01482	0.03967		
Y	β	Polar	42	42Met	-0.0076	-0.0057	-0.0098	-0.0156	-0.0044	0.0069		0		
Y	β	Hydrophobic	43	43Gly	-0.0229				0			0		
	α	Charged	44	44Arg	-0.0213	0.0000	-0.002	-0.0063	0			-0.0022	-0.0018	
	α	Charged	45	45His	0.0759	-0.0044	0	0.01777	0			0		
Y	α	Polar	46	46Thr	0.03727		0.03549		0.01118			0		
Y	α	Polar	47	47Trp	-0.015	0.0387	0.03454	0.01627	0		0.0755	0	0.08676	
Y	α	Charged	48	48Glu		0.0030	4E-05	0.02721	0.0146	0.0096		0		
Y	α	Polar	49	49Ser	0.00525	0.0507	0.05758	0.03454	0			0		

Y	α	Hydrophobic	50	50Ile	0.01471	0.0038	0.00046		0.00499	0.00811	0.00566	0.04713		
		Hydrophobic	51	51Gly	0.02346				0			0		
Y		Charged	52	52Arg	0.02255	-0.0111	0.00049	-0.0002	0.00627	0.00634		0.00559	0.01884	
Y		Hydrophobic	53	53Pro		0.0000	-0.0023	0.00436	-0.0022			-0.0005	-0.0007	
Y		Hydrophobic	54	54Leu	0.09825	-0.0132	-0.0118	-0.0095	0			-0.0035	0.01984	
Y	turn	Hydrophobic	55	55Pro					0			0		
Y	turn	Hydrophobic	56	56Gly	-0.0031				0			0		
		Charged	57	57Arg	0.00913	0.0103	-0.0063	0.00926	0.03474			-0.0047	0.00161	
		Charged	58	58Lys	0.11671	0.0139	0.01546	0.00157	0.00686	0.01309		0.00172	0.01603	
	β	Polar	59	59Asn	-0.0114	0.0853	0.05022	0.04496	0			0		
Y	β	Hydrophobic	60	60Ile	-0.0271	-0.0074	0.01651		-0.0061	0.01117	-0.0201	0.00608		
Y	β	Hydrophobic	61	61Ile	-0.032	-0.0021	-0.0054		0.00681	0.04004	0.00703	-0.0061		
Y	β	Hydrophobic	62	62Leu	-0.0123	0.0040	-0.0041	-0.0103	-0.0174			-0.0082	-0.0067	
Y		Polar	63	63Ser	0.00868	0.0031	0.02432	0.0565	0			0		
		Polar	64	64Ser	-0.017	0.0380	-0.0107	-0.0063	0			0		
		Polar	65	65Gln	-0.0006	0.0021	0.00929	0.00506	0.01023	-0.006		0		
Y		Hydrophobic	66	66Pro		0.0075	-0.0022	0.01113	-0.0055	0.0071		0.01096	-0.0045	
		Hydrophobic	67	67Gly	0.01428				0			0		
		Polar	68	68Thr	0.08423	-0.0023	0.0018		0.03693			0		
		Charged	69	69Asp	0.05247	0.0091	0.00616	0.01217	0			0		
	turn	Charged	70	70Asp	0.03453	-0.0040	-0.008	-0.0021	0			0		
	turn	Charged	71	71Arg	0.05735	-0.0041	-0.0137	-0.0109	-0.0049	-0.0059		0.00199	0.00019	
		Hydrophobic	72	72Val	0.04988	-0.0012	0.00078		0.00609	0.01111		0		
Y	β	Polar	73	73Thr	0.01898	0.0605	0.00685		0.04643			0		
	β	Polar	74	74Trp	-0.0387	-0.0084	-0.0087	-0.0001	0			-0.0174		0.00188
Y	β	Hydrophobic	75	75Val	0.0351	0.0114	0.00064		0.00807	0.01078		0		

		Charged	76	76Lys	-0.018	0.0163	-0.0059	0.00807	0.00823	0.02462		0.01298	0.01121	
Y		Polar	77	77Ser	-0.019	-0.0051	0.00345	-0.008	0			0		
	α	Hydrophobic	78	78Val	0.05712	0.0273	-0.0024		0.0132	0.0287		0		
	α	Charged	79	79Asp	0.0183	-0.0060	-0.0154	0.00515	0			0		
	α	Charged	80	80Glu	0.0215	0.0849	-0.0094	-0.0118	-0.01	-0.0031		0		
Y	α	Hydrophobic	81	81Ala	0.10206	-0.0088	-0.0075		0			0		
Y	α	Hydrophobic	82	82Ile	0.05355	0.0202	0.01748		0.00487	-0.001	0.0065	0.00451		
Y	α	Hydrophobic	83	83Ala	-0.0171	-0.0112	0.0017		0			0		
Y	α	Hydrophobic	84	84Ala	0.0299	0.0006	0.00298		0			0		
Y	α	Polar	85	85Cys	-0.0012	0.0089	-0.0082	0.0025	0			0		
		Hydrophobic	86	86Gly	0.06303				0			0		
		Charged	87	87Asp	0.04162	0.0422	0.00186	-0.0042	0			0		
		Hydrophobic	88	88Val	0.00233	0.0004	-0.0005		0.00024	0.01453		0		
Y		Hydrophobic	89	89Pro		-0.0004	-0.0041	0.01603	0.14794	0.15924		0.00218	0.02812	
		Charged	90	90Glu	0.0094	-0.0016	-0.0001	0.04094	0.00111	0.0018		0		
Y	β	Hydrophobic	91	91Ile	0.03019	0.0043	-0.0082		0.01538	0.03403	0.03797	-0.0015		
Y	β	Polar	92	92Met	0.0012	-0.0134			0.02019	-0.0032		0		
Y	β	Hydrophobic	93	93Val	-0.0222	0.0404	-0.0048		0.01191	0.0034		0		
Y		Hydrophobic	94	94Ile	0.0008	-0.0045	-0.0051		-0.0077	0.01058	0.01986	0.00034		
Y		Hydrophobic	95	95Gly	-0.0205				0			0		
		Hydrophobic	96	96Gly	-0.021				0			0		
Y	α	Hydrophobic	97	97Gly					0			0		
	α	Charged	98	98Arg	0.02466	0.0236	-0.0056	-0.0133	0.0304	0.02586		0.03015	-0.0089	
	α	Hydrophobic	99	99Val	-0.0257	0.0194	0.0169		0.00913	-0.0045		0		
Y	α	Polar	100	100Tyr	-0.0249	0.0108	-0.0049	0.00973	0		0.06891	0		0.00892
	α	Charged	101	101Glu	-0.0071	-0.0068	0.0129	-0.0005	0.00476	-0.0046		0		

Y	α	Polar	102	102Gln	0.09919	0.0555			0			0		
Y	3/10 α	Hydrophobic	103	103Phe	0.02352	-0.0046	-0.0135	-0.0119	0		0.00852	0		-0.0134
Y	3/10 α	Hydrophobic	104	104Leu	-0.0033	0.0115	0.0159	0.00367	0				0.01431	
Y	3/10 α	Hydrophobic	105	105Pro					-0.0111	-0.0004		-0.017	-0.0041	
Y	3/10 α	Charged	106	106Lys	0.05929	0.0166	0.00401	-0.0033	0.01734			0.00551	0.01687	
Y		Hydrophobic	107	107Ala	-0.0118	0.0047	0.0064		0			0		
		Polar	108	108Gln	-0.0145	0.0065	0.00373	0.00146	0.0094	-0.001		0		
Y	β	Charged	109	109Lys	0.05939	-0.0064	0.00483	0.01031	0.01249	0.00722		0.0107	0.04208	
Y	β	Hydrophobic	110	110Leu	-0.0042	-0.0182	-0.0028	0.00398				0.02336		
Y	β	Polar	111	111Tyr	-0.0122	-0.0086	-0.02	0.00277	0		0.05372	0	0	
Y	β	Hydrophobic	112	112Leu	-0.0105	-0.0108	-0.0017	-0.015	0.00656			-0.0124		0.00944
Y	β	Polar	113	113Thr			-0.0112		0			0		
Y	β	Charged	114	114His	-0.0287	0.0012			0		-0.0013	0		
Y	β	Hydrophobic	115	115Ile	0.19059	0.0090	-0.0112		-0.0042	-0.0081	-0.0008	-0.0042		
Y		Charged	116	116Asp	0.11013	-0.0078	0.03199	0.03628	0			0		
		Hydrophobic	117	117Ala	-0.0032	-0.0018	0.01198		0			0		
		Charged	118	118Glu	-0.0161	0.0131	-0.0003	0.00806	-0.0129	-0.003		0		
		Hydrophobic	119	119Val	0.0296	-0.0052	0.01142		0.09005	0.1068		0		
		Charged	120	120Glu	0.0077	0.0082	0.0083	-0.0158	-0.0056	0.00317		0		
		Hydrophobic	121	121Gly	0.10065				0			0		
		Charged	122	122Asp	0.00332	-0.0052	-0.0001	-0.0072	0			0		
		Polar	123	123Thr					0			0		
Y	β	Charged	124	124His		0.0003	-0.0049	-0.0074	0		0.03522	0		
Y	β	Hydrophobic	125	125Phe	0.02187	0.0061	-0.0116	-0.0021	0			0		
Y		Hydrophobic	126	126Pro		0.0008	0.0171	0.0118	0.00918	0.01227		0.00083	-0.005	
		Charged	127	127Asp	-0.0175	0.0021	-0.0006	-0.0054	0					

		Polar	128	128Tyr	0.07065	-0.0038	-0.0072	-0.0017	0		-0.0168	0		-0.0072
	3/10 α	Charged	129	129Glu	0.05702	0.0255	0		-0.0136	-0.0045		0		
Y	3/10 α	Hydrophobic	130	130Pro		-0.0013	0.01011	-0.0073	0.01792	-0.0091		-0.0316		
	1/10 α	Charged	131	131Asp	0.02431	0.0003	-0.0004	0.00126	0			0		
	β	Charged	132	132Asp	0.00736	0.0075	0.00242	0.00473	0			0		
	β	Polar	133	133Trp	0.03131	0.0286	-0.0121	-0.0122	0		-0.0236	0		0.0071
Y	β	Charged	134	134Glu	0.06691	0.0069	0.00509	-0.0026	0.01701	-0.0068		0		
Y	β	Polar	135	135Ser	-0.0038	-0.0039	-0.015	0.01483	0			0		
	β	Hydrophobic	136	136Val	0.03056	0.0034	0.00049		-0.0016	0.00166		0		
	β	Hydrophobic	137	137Phe	0.09692	-0.0064	0.01175	0.00784	0		0.00896	0		0.02252
Y	β	Polar	138	138Ser	0.04057	-0.0015	0.01534	0.03781	0			0		
Y	β	Charged	139	139Glu	0.25072	-0.0023	0.00225	0.00409	0.02013	-0.0031		0		
	β	Hydrophobic	140	140Phe	-0.0108	0.0343	0.01	-0.0011	0		0.00722	0		0.00335
Y	β	Charged	141	141His	0.0599	-0.0083	-0.0134	-0.0031	0		-0.0256	0		
Y		Charged	142	142Asp	-0.0089	0.0144	-0.0061	0.00711	0			0		
		Hydrophobic	143	143Ala	-0.0137	0.0069	0.00068		0			0		
		Charged	144	144Asp	0.10273	0.0059	0.00211	-0.0014	0			0		
		Hydrophobic	145	145Ala	0.23254	-0.0018	-0.0047		0			0		
Y	bend	Polar	146	146Gln	-0.0014	-0.0119	0.0221	0.00359	0.0038	0.00333		0		
	bend	Polar	147	147Asn	0.00444	0.0153	0.01426	0.00464	0			0		
Y	bend	Polar	148	148Ser	0.0091	0.0826	-0.0025	-0.0133	0			0		
		Polar	149	149His	0.04825	0.0171	0	-0.0119	0		0.01837	0		
		Polar	150	150Ser	-0.0034	-0.0125	0.03515	0.01646	0			0		
Y	β	Polar	151	151Tyr	0.04379	0.0153	0.01186	-0.009	0					
Y	β	Polar	152	152Cys	0.10459				0			0		
Y	β	Hydrophobic	153	153Phe	-0.0256	0.0096	0.00641	-0.0021	0			0		

Y	β	Charged	154	154Glu	-0.0064	0.0011	0.00224	0.00154	-0.0017	-9E-05		0		
Y	β	Hydrophobic	155	155Ile	0.22467	0.0100	0.00924		0.00974	0.02744	0.00181	0.01401		
Y	β	Hydrophobic	156	156Leu	-0.0153	-0.0021	-0.0126	-0.0132	0.00226			0.00178	-0.0044	
Y	β	Charged	157	157Glu	0.00726	0.0031	-0.0033	-0.0016	0.00354	-0.0187		0		
Y	β	Charged	158	158Arg	0.02607	0.0315	0.02134	0.02202	0.01875	0.05469		0.00464	0.02945	
		Charged	159	159Arg	0.03964		-0.0093	-0.0054	0.00275	0.02648		0.00786	-0.0046	

Table 8.2.3 Chemical shift deviations of hydrogen nuclei in EcDHFR: $NADP^+$: Folate complex in the presence of 17% methanol co-solvent from chemical shift values of the protein complex in the absence of co-solvent (buffer only)

8.2.4 17% Methanol Induced Chemical Shift Perturbations in carbon nuclei of the EcDHFR: $NADP^+$: Folate complex

Chemical shift deviations of carbon nuclei in EcDHFR: $NADP^+$: Folate complex in the presence of 17% methanol co-solvent from chemical shift values of the protein complex in the absence of co-solvent (buffer only) are shown below **(Table 8.2.4)**. To highlight meaningful differences, the values displayed in the cells are the chemical shift difference minus the calculated standard deviation for each atom ($\delta\Delta$ – SD). Nuclei that show perturbations in chemical shift greater than the combined standard deviation of the averaged chemical shift values are coloured green, values showing insignificant or perturbations less than the standard deviation are coloured red and nuclei yielding no data are coloured yellow. Hydrogen bonding status of the residue is listed as Y if the residue is involved in hydrogen bonding and the involvement in secondary structure elements are listed down the left hand side of the table.

H BOND	SECONDARY STRUCTURE 17% MEOD		Residue No	Residue	CA δΔ-SD	CB 17% δΔ-SD	cg (1) δΔ- SD	cg (2) δΔ-SD	CD (1) δΔ-SD	CD (2) δΔ- SD	CE 17% δΔ- SD	C=O δΔ-SD
		Polar	1	1Met	-0.007508747							0.4125
	β	Hydrophobic	2	2Ile	0.077761293	-0.06	-0.05599	0.030258	0.096442			-0.01511
Y	β	Polar	3	3Ser	0.026183038	0.00	0					-0.01644
Y	β	Hydrophobic	4	4Leu	-0.013364999	-0.01	-0.02178		0.55881	0.653732		0.01266
Y	β	Hydrophobic	5	5Ile	-0.015168206	-0.04	0.012117	0.23121	0.070728			0.17135
Y	β	Hydrophobic	6	6Ala	0.001020011	-0.07	0					0
	β	Hydrophobic	7	7Ala	0.071067838	0.00	0					0.00821
Y	β	Hydrophobic	8	8Leu	-0.01337273	0.00	-0.06442		0.015542	0.099316		0.24575
Y		Hydrophobic	9	9Ala	0.066453956	-0.05	0					0.01415
	α	Hydrophobic	10	10Val	-0.045027431	0.05	-0.03863	0.029242				0.00186
Y	α	Charged	11	11Asp	0.000399382	0.07	0					0.22534
	α	Charged	12	12Arg	-0.029929004	0.25	0.01875		-0.01229			0.10612
Y	β	Hydrophobic	13	13Val	0.124851067	0.00	0.033535	-0.05517				0
Y	β	Hydrophobic	14	14Ile		0.21	0.189177	0	0.545057			
		Hydrophobic	15	15Gly	-0.051618725		0					0.11308
		Polar	16	16Met	0.04419	0.00	0				0.08714	0
	turn	Charged	17	17Glu		0.08	0.08					0.20686
Y	β bridge	Polar	18	18Asn	0.027284497	-0.09	0					0.10867
		Hydrophobic	19	19Ala	0.008643813	0.02	0					0.00684
		Polar	20	20Met	0.222	0.26	0				-0.04725	0
Y		Hydrophobic	21	21Pro			0					
Y		Polar	22	22Trp			0					0.11436
Y		Polar	23	23Asn	0.031989893	-0.02	0					0.21095

		Hydrophobic	24	24Leu	-0.073684857	-0.11	0		0.001358			0
Y	α	Hydrophobic	25	25Pro	-0.078371316	-0.03	0.03572		-0.00212			0.10286
	α	Hydrophobic	26	26Ala	-0.078400032	-0.03	0					0.14096
Y	α	Charged	27	27Asp	-0.024153024	-0.10	0					0.01223
Y	α	Hydrophobic	28	28Leu	-0.059785168	-0.10	0.02905		0.0037	0.0004		0.02352
Y	α	Hydrophobic	29	29Ala	-0.021181444	0.00	0					0.271
Y	α	Polar	30	30Trp	-0.036556718	0.01	0		0			0.11622
Y	α	Hydrophobic	31	31Phe	-0.029415453	-0.10	0					0.02979
Y	α	Charged	32	32Lys	-0.062800658	-0.09	0.02435		-0.02188		0.018	0.046421
Y	α	Charged	33	33Arg	-0.067300788	-0.02	0.04179		0.020801			0.2285
Y	α	Polar	34	34Asn	0.262827654	-0.02	0					0.02243
Y	α	Polar	35	35Thr	-0.047421906	-0.09	-0.02207					0.02972
Y	α	Hydrophobic	36	36Leu	0.004018529	-0.03	0		-0.01337	0.010213		0.142778
Y	turn	Charged	37	37Asp	-0.016217455	-0.22	0					0.19089
Y	turn	Charged	38	38Lys	0.06059	0.08	0					0
Y	β	Hydrophobic	39	39Pro	-0.017555806	0.00	0.04717		-0.04381			0.14551
Y	β	Hydrophobic	40	40Val	0.03718182	-0.09	0.000894	0.018073				0.07527
Y	β	Hydrophobic	41	41Ile	-0.086694703	-0.08	0.01383	0.01156	0.019666			0.084878
Y	β	Polar	42	42Met	0.029393764	-0.07	0.135948				0.10728	0.10762
Y	β	Hydrophobic	43	43Gly	0.028723662		0					0.17775
	α	Charged	44	44Arg	0.04368	0.21	0.06856		0.04511			0.05641
	α	Charged	45	45His	0.03768		0					-2.1E-14
Y	α	Polar	46	46Thr	0	0.03	-0.09163					0.04566
Y	α	Polar	47	47Trp	-0.06255	0.00	0					
Y	α	Charged	48	48Glu	0.008329241	0.09	-0.06507					0.07434
Y	α	Polar	49	49Ser	0.059510851	-0.05	0					0.2868

Y	α	Hydrophobic	50	50Ile	0.152739329	-0.01	0.036426	-0.00827	-0.04377			0.11439
		Hydrophobic	51	51Gly	0.02848813		0					0.18239
Y		Charged	52	52Arg	-0.012674588	-0.01	0.0264		-0.03178			
Y		Hydrophobic	53	53Pro	0.3122	-0.09	0.07392		0.0442			0.14967
Y		Hydrophobic	54	54Leu	0.100326734	-0.07	0		-0.01082	-0.0189		0
Y	turn	Hydrophobic	55	55Pro	0		0					
Y	turn	Hydrophobic	56	56Gly	0.057247693		0					0.2764
		Charged	57	57Arg	0.07859212	0.01	0.04982		0.02505			0.01147
		Charged	58	58Lys	0.121530277	-0.06	0.01921		0.02713		0.02277	-0.00795
	β	Polar	59	59Asn	-0.029429148	-0.11	0					0.148287
Y	β	Hydrophobic	60	60Ile	-0.118559891	-0.14	0.015161	-0.04821	0.052274			0.08753
Y	β	Hydrophobic	61	61Ile	-0.048113073	0.02	-0.04143	-0.00732	0.018911			0.04018
Y	β	Hydrophobic	62	62Leu	-0.047208192	-0.04	0		0.057145	-0.03136		0.10809
Y		Polar	63	63Ser	-0.118181168	-0.06	0					0.00887
		Polar	64	64Ser	0.023010374	-0.14	0					0.09872
		Polar	65	65Gln	-0.079486962	0.00	-0.01317					0
Y		Hydrophobic	66	66Pro	-0.071328662	-0.09	0.01609		0.001418			0.21736
		Hydrophobic	67	67Gly	-0.122635517		0					
		Polar	68	68Thr	-0.140617087	-0.02	0.09725					0.14676
		Charged	69	69Asp	0.060716579	0.07	0					0.06664
	turn	Charged	70	70Asp	0.14131054	0.00	0					0.22075
	turn	Charged	71	71Arg	0.042067521	-0.01	-0.04037		-0.02468			0.0151
		Hydrophobic	72	72Val	-0.025217177	-0.13	-0.05425	-0.0113				0.14618
Y	β	Polar	73	73Thr	0.063115676	0.06	0.15785					0.01444
	β	Polar	74	74Trp	0.114622072	-0.08	0					0.14212
Y	β	Hydrophobic	75	75Val	-0.030188334	-0.02	0.001264	-0.00791				0.02017

		Charged	76	76Lys	0.03747	-0.13	0.005333		-0.00832		-0.08034	-0.01307
Y		Polar	77	77Ser	0.10901647	-0.11	0					0.02107
	α	Hydrophobic	78	78Val	0.056907995	-0.15	0.063218	0.011119				0.13612
	α	Charged	79	79Asp	0.071016211	0.01	0					0.24887
	α	Charged	80	80Glu	0.130256699	-0.12	-0.02674					0.30835
Y	α	Hydrophobic	81	81Ala	0.13760429	-0.03	0					0.01144
Y	α	Hydrophobic	82	82Ile	0.150742732	-0.03	0.168037	-0.065	0.265296			0.154968
Y	α	Hydrophobic	83	83Ala	0.005000339	0.09	0					0.09492
Y	α	Hydrophobic	84	84Ala	0.046814138	-0.09	0					0.07789
Y	α	Polar	85	85Cys	-0.013823483	-0.13	0					0.06882
		Hydrophobic	86	86Gly	-0.037158339		0					0.14329
		Charged	87	87Asp	0.080042327	-0.09	0					-0.18169
		Hydrophobic	88	88Val	-0.000970053	0.16	0.07872	-0.03982				
Y		Hydrophobic	89	89Pro	-0.002546264	0.02	0.02675		0.00486			0.25573
		Charged	90	90Glu	-0.016896328	0.00	0.03026					0.071228
Y	β	Hydrophobic	91	91Ile	0.053650973	0.05	0.00127	0.028443	0.065287			0.1282
Y	β	Polar	92	92Met	-0.02846666	-0.10	0.00161				0.088	0.02162
Y	β	Hydrophobic	93	93Val	0.0398984	-0.02	0.061123	0.025462				0.06796
Y		Hydrophobic	94	94Ile	-0.062489289	-0.02	-0.10537	0.00505	-0.04465			0.02831
Y		Hydrophobic	95	95Gly	-0.068318259		0					0.07192
		Hydrophobic	96	96Gly	0.17682		0					
Y	α	Hydrophobic	97	97Gly	-0.085155468		0					0.07846
	α	Charged	98	98Arg	-0.047702449	-0.01	-0.02352		0.018327			-0.06513
	α	Hydrophobic	99	99Val	0.083493896	-0.01	0.36333	0.12259				0.01075
Y	α	Polar	100	100Tyr	-0.042010928	-0.09	0					0.02204
	α	Charged	101	101Glu	0.068331591	-0.01	0.03699					0

Y	α	Polar	102	102Gln	-0.082293708	0.18	0.08					0.13385
Y	3/10 α	Hydrophobic	103	103Phe	0.010303425	-0.09	0					
Y	3/10 α	Hydrophobic	104	104Leu	-0.05352	-0.08	0		0.084342	0.01981		0.30973
Y	3/10 α	Hydrophobic	105	105Pro	0.04835	0.07	0.05238		0.00359			0.32884
Y	3/10 α	Charged	106	106Lys	0.196770757	-0.11	-0.05186		0.064751		0.020169	0.25462
Y		Hydrophobic	107	107Ala	-0.008691835	-0.10	0					0.11209
		Polar	108	108Gln	-0.006147671	-0.11	-0.10228					0.15808
Y	β	Charged	109	109Lys	0.154684677	-0.02	0.041209		0.005236		0.027108	0.01389
Y	β	Hydrophobic	110	110Leu	0.014551542	-0.04	0		-0.06453			0.04738
Y	β	Polar	111	111Tyr	0.054456409	0.23	0					0.06356
Y	β	Hydrophobic	112	112Leu	-0.037645816	-0.03	0		-0.00566	0.158192		
Y	β	Polar	113	113Thr	0.136035271	0.01	0					0.32584
Y	β	Charged	114	114His	-0.01429	0.71	0					0.15295
Y	β	Hydrophobic	115	115Ile	0.036478141	0.08	-0.05442	0.03924	0.133873			0.02577
Y		Charged	116	116Asp	0.42595429	-0.03	0					0.02101
		Hydrophobic	117	117Ala	-0.116203816	-0.08	0					0.024
		Charged	118	118Glu	-0.063964319	0.11	0.00501					0
		Hydrophobic	119	119Val	-0.081847328	-0.04	-0.01024	-0.04303				0.09547
		Charged	120	120Glu	0.243065629	0.02	0.11485					0.25979
		Hydrophobic	121	121Gly	0.037752113	0.00	0					0.17921
		Charged	122	122Asp	-0.051442227	0.03	0					0
		Polar	123	123Thr	0		0					0
Y	β	Charged	124	124His	0.03729346	-0.05	0					0
Y	β	Hydrophobic	125	125Phe	0.18944652	0.03	0					0
Y		Hydrophobic	126	126Pro	0.050250199	0.03	-0.00699		0.031642			0
		Charged	127	127Asp	0.002849605	0.03	0					0

		Polar	128	128Tyr	0.14067	0.03	0					0
	3/10 α	Charged	129	129Glu	0.107185543	0.25	0.01106					0
Y	3/10 α	Hydrophobic	130	130Pro	0.169311278	0.03	0.31172		0.09975			0.18634
	1/10 α	Charged	131	131Asp	0.005357568	-0.06	0					-0.00809
	β	Charged	132	132Asp	-0.050351015	-0.10	0					0.01862
	β	Polar	133	133Trp	0.178829552	-0.09	0					0.1161
Y	β	Charged	134	134Glu	-0.018881038	-0.02	0.01489					0.08012
Y	β	Polar	135	135Ser	0.025058268	-0.06	0					
	β	Hydrophobic	136	136Val	0.060308049	-0.05	-0.05371	-0.07392				0.18171
	β	Hydrophobic	137	137Phe	-0.007260349	0.08	0					0.02778
Y	β	Polar	138	138Ser	-0.001150378	-0.03	0					0.03543
Y	β	Charged	139	139Glu	-0.073399677	-0.04	-0.07927					0.16027
	β	Hydrophobic	140	140Phe	0.116096824	-0.04	0					0.15125
Y	β	Charged	141	141His	-0.07439678	-0.05	0					0.28966
Y		Charged	142	142Asp	-0.002412898	-0.05	0					0.0027
		Hydrophobic	143	143Ala	0.037979132	-0.04	0					0.29018
		Charged	144	144Asp	0.172979341	0.06	0					0.32684
		Hydrophobic	145	145Ala	0.016406572	-0.06	0					0.2917
Y	bend	Polar	146	146Gln	0.110130703	0.10	-0.06411					0.24841
	bend	Polar	147	147Asn	0.002345062	-0.03	0					
Y	bend	Polar	148	148Ser	0.01158	0.00	0					0.18427
		Polar	149	149His	0.531565995	0.44	0					0.10009
		Polar	150	150Ser	0.165501636	0.14	0					0.08608
Y	β	Polar	151	151Tyr	-0.048600477	-0.10	0					0.03992
Y	β	Polar	152	152Cys	0.12666	0.00	0					0.98358
Y	β	Hydrophobic	153	153Phe	0.04586	0.05	0					0.66501

Y	β	Charged	154	154Glu	0.00881	0.67	0.05					0
Y	β	Hydrophobic	155	155Ile	-0.10938953	-0.09	-0.00256	-0.06602	-0.00332			0.03225
Y	β	Hydrophobic	156	156Leu	-0.090861083	-0.03	-0.09864		0.198873	0.051695		0.08839
Y	β	Charged	157	157Glu	-0.012930616	-0.05	0.20121					0.17419
Y	β	Charged	158	158Arg	0.175456942	0.08	0.062695		0.065023			0.15394
		Charged	159	159Arg	-0.047458929	0.10	0.10721		0.06736			

Table 8.2.4 Chemical shift deviations of carbon nuclei in EcDHFR: $NADP^+$: Folate complex in the presence of 17% methanol co-solvent from chemical shift values of the protein complex in the absence of co-solvent (buffer only).

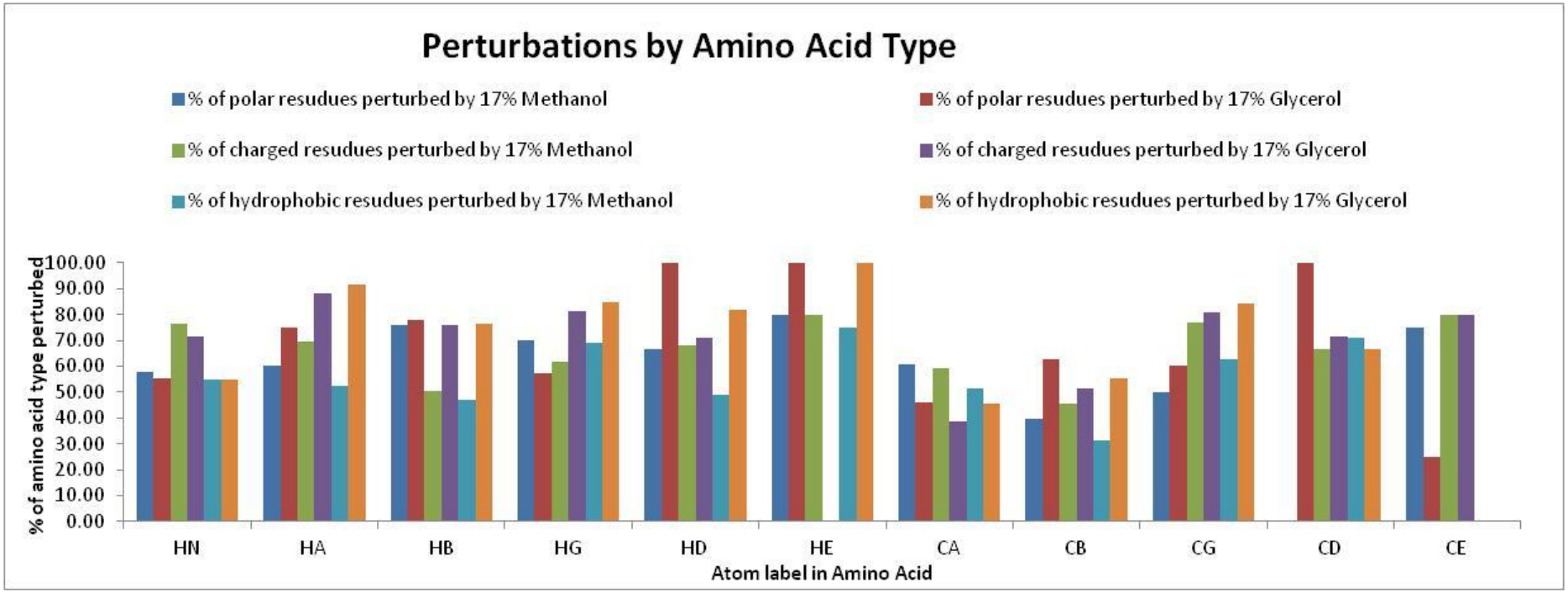

Figure 8.2.1 Chemical shift perturbations by amino acid type. The amino acid residues in EcDHFR: $NADP^+$: folate complex were categorised according to whether they are hydrophobic, charged or polar. The percentage of atoms perturbed by the addition of 17% methanol and 17% glycerol in each residue type is reported above.

8.3 T1 and T2 Relaxation of the EcDHFR: $NADP^+$: Folate complex under standard buffer conditions

8.3.1 T1 Relaxation of the EcDHFR: NADP+: Folate complex under standard buffer conditions at 600 MHz

The T1 values at 600MHz of the EcDHFR: NADP+: folate complex under standard buffer conditions are shown below **(Table 8.3.1)**. Values for which the SD of the error is greater than 10% of the T1 value are highlighted red and were excluded from the T1 analysis. T1 values for a total of 109 residues were calculated, 10 of these are discounted due to large errors. The average T2 value of the resulting data was calculated (742.02 ms, *s* =48.82 ms, *n* = 99).

600 MHz T1	Residue	T1 (ms) at 600 MHz Buffer	T1 Error	Fit Error	Num Peaks	Comments
1	1Met	no peak				
2	2Ile	845.42	66.79	4.26	12	large doubling
3	3Ser	760.31	38.83	1.33	12	Some ambiguity
4	4Leu	806.83	22.07	1.28	12	overlapped
5	5Ile	834.44	73.41	1.18	12	
6	6Ala	745.49	28.58	1.65	12	
7	7Ala	no peak				
8	8Leu	742.02	24.50	1.03	12	
9	9Ala	803.66	31.58	1.09	12	
10	10Val	846.65	44.99	2.22	12	
11	11Asp	866.84	14.47	0.57	12	broadening
12	12Arg	doubling				
13	13Val	878.49	32.75	1.14	12	slight doubling
14	14Ile	no peak				
15	15Gly	No peak				
16	16Met	886.65	147.77	5.68	12	SD error > 10%
17	17Glu	no peak				
18	18Asn	no peak				

19	19Ala	801.16	24.46	1.35	12	
20	20Met	870.69	30.92	0.60	12	
21	21Pro	proline				
22	22Trp	no peak				
23	23Asn	overlapped with 148				
24	24Leu	Large movement/no peak				
25	25Pro	proline				
26	26Ala	803.14	11.83	0.89	12	
27	27Asp	821.44	29.84	1.39	12	
28	28Leu	837.35	8.48	0.73	12	
29	29Ala	842.61	30.44	1.73	12	
30	30Trp	823.22	17.72	1.11	12	
31	31Phe	751.46	28.21	1.14	12	
32	32Lys	717.84	153.68	9.84	12	SD error > 10%
33	33Arg	788.38	32.27	1.48	12	
34	34Asn	784.91	31.94	1.46	12	
35	35Thr	813.42	61.48	2.88	12	
36	36Leu	874.94	64.40	3.56	12	
37	37Asp	902.88	43.53	2.79	12	
38	38Lys	816.63	16.92	1.53	12	
39	39Pro	proline				
40	40Val	No peak				
41	41Ile	876.13	42.48	0.53	12	
42	42Met	no peak				
43	43Gly	842.74	52.18	0.85	12	
44	44Arg	doubled				
45	45His	overlapped with 106				
46	46Thr	653.02	341.20	19.53	12	SD error > 10%
47	47Trp	818.63	26.70	0.84	12	
48	48Glu					
49	49Ser	809.35	34.23	1.79	12	
50	50Ile	812.18	47.61	1.73	12	
51	51Gly	799.84	39.55	2.14	12	doubled
52	52Arg	809.83	28.85	1.61	12	doubled
53	53Pro	proline				
54	54Leu	1156.84	526.90	12.54	12	SD error > 10%
55	55Pro	proline				
56	56Gly	no peak				
57	57Arg	784.79	10.05	1.42	12	
58	58Lys	928.41	10.53	1.14	12	slight movement

59	59Asn	819.73	24.71	1.53	12	
60	60Ile	407.65	368.70	32.19	12	l SD error > 10%
61	61Ile	846.37	45.94	0.48	12	
62	62Leu	863.60	40.10	0.55	12	
63	63Ser	819.85	9.07	0.94	12	
64	64Ser	796.97	21.85	1.20	12	
65	65Gln	806.29	13.80	1.58	12	
66	66Pro	proline				
67	67Gly	766.54	13.91	0.98	12	large movement
68	68Thr	large movement				
69	69Asp	759.03	13.62	1.85	12	slight doubling
70	70Asp	820.58	22.84	2.34	12	slight movement
71	71Arg	753.57	21.86	1.79	12	
72	72Val	807.19	19.01	2.30	12	
73	73Thr	864.98	14.71	1.48	12	
74	74Trp	930.79	12.18	1.10	12	slight movement
75	75Val	881.64	49.11	0.81	12	
76	76Lys	870.71	11.50	1.34	12	
77	77Ser	792.35	11.33	1.40	12	
78	78Val	790.18	6.66	0.72	12	
79	79Asp	769.51	12.28	1.77	12	
80	80Glu	784.31	14.26	1.95	12	
81	81Ala	796.65	17.29	0.71	12	
82	82Ile	845.27	6.84	0.86	12	
83	83Ala	808.24	7.46	1.01	12	
84	84Ala	830.16	5.82	0.74	12	
85	85Cys	848.22	8.35	0.93	12	
86	86Gly	875.50	14.79	1.52	12	
87	87Asp	859.64	29.88	3.77	12	
88	88Val	851.68	35.02	1.32	12	
89	89Pro	proline				
90	90Glu	doubling				
91	91Ile	819.97	23.51	0.71	12	
92	92Met	no peak				
93	93Val	892.76	28.59	0.61	12	
94	94Ile	no peak				
95	95Gly	doubled				
96	96Gly	820.14	41.28	1.97	12	
97	97Gly	no peak				

98	98Arg	797.85	38.55	1.29	12	
99	99Val	823.58	21.20	1.03	12	
100	100Tyr	815.38	36.40	1.60	12	slight doubling
101	101Glu	808.94	12.64	1.15	12	
102	102Gln	1001.23	14.51	2.31	12	
103	103Phe	overlapped with 146				
104	104Leu	934.50	7.61	0.96	12	
105	105Pro	proline				
106	106Lys	overlapped with 45				
107	107Ala	814.01	44.52	1.65	12	
108	108Gln	868.96	12.55	0.92	12	
109	109Lys	833.54	7.92	0.59	12	
110	110Leu	529.12	477.42	37.23	12	SD error > 10%
111	111Tyr	785.96	48.78	0.62	12	
112	112Leu	1499.33	1519.49	18.71	12	doubled + SD error > 10%
113	113Thr	no peak				
114	114His	835.25	36.17	2.11	12	
115	115Ile	doubled				
116	116Asp	828.41	16.66	1.17	12	
117	117Ala	doubled				
118	118Glu	overlapped with 155				
119	119Val	ambiguous				
120	120Glu	893.19	32.66	2.22	12	
121	121Gly	doubled				
122	122Asp	795.68	31.27	0.88	12	
123	123Thr	no peak				
124	124His	no peak				
125	125Phe	831.50	27.06	1.46	12	
126	126Pro	proline				
127	127Asp	128.69	-21.02	88.58	12	SD error > 10%
128	128Tyr	overlapped				
129	129Glu	926.65	11.45	0.75	12	
130	130Pro	proline				
131	131Asp	doubled and moved				
132	132Asp	930.73	166.46	14.59	12	SD error > 10%
133	133Trp	915.91	88.63	3.74	12	
134	134Glu	963.01	59.57	2.58	12	
135	135Ser	831.26	10.89	1.44	12	

136	136Val	1122.80	506.41	35.51	12	SD error > 10%
137	137Phe	804.57	9.59	0.86	12	
138	138Ser	859.94	10.90	1.14	12	
139	139Glu	839.44	12.98	1.08	12	
140	140Phe	doubled				
141	141His	831.56	8.34	0.83	12	
142	142Asp	864.96	9.64	1.41	12	
143	143Ala	947.15	23.34	2.88	12	
144	144Asp	835.35	25.38	0.96	12	
145	145Ala	835.80	29.67	1.67	12	
146	146Gln	overlapped with 103				
147	147Asn	871.27	26.65	1.69	12	
148	148Ser	overlapped with 23				
149	149His	876.92	15.04	1.55	12	
150	150Ser	841.56	11.26	1.20	12	
151	151Tyr	doubled				
152	152Cys	783.34	12.86	1.13	12	overlapped
153	153Phe	810.41	9.99	0.64	12	
154	154Glu	813.16	21.64	0.75	12	
155	155Ile	overlapped with 118				
156	156Leu	doubled				
157	157Glu	898.54	12.62	0.57	12	
158	158Arg	905.74	38.71	2.57	12	
159	159Arg	796.75	12.24	1.86	12	

Table 8.3.1 T1 at 600MHz of the EcDHFR: NADP+: folate complex under standard buffer conditions.

8.3.2 T1 Relaxation of the EcDHFR: NADP+: Folate complex under standard buffer conditions at 900 MHz

The T1 values at 900MHz of the EcDHFR: NADP+: folate complex under standard buffer conditions are presented below **(Table 8.3.2)**. Values for which the SD of the error is greater than 10% of the T1 value are highlighted red and were excluded from the T1 analysis. T1 values for a total of 113 residues were calculated, 12 of these are discounted due to large errors. The average T1 value of the resulting data was calculated (997.01 ms, *s* =75.78 ms, *n* = 101).

900 MHz T1	Residue	T1 900 MHz (buffer)	T1 Error	Fit Error	Num Peaks	notes
1	1Met					no peak
2	2Ile	977.23	48.12	18.48	12	drifting
3	3Ser	926.59	58.06	15.53	12	ambiguity
4	4Leu	142.76	-36.72	271.75	12	SD error > 10%
5	5Ile	987.04	79.92	6.57	12	
6	6Ala	904.97	88.75	21.16	12	
7	7Ala					no peak
8	8Leu	958.00	67.40	12.57	12	
9	9Ala	1082.70	161.78	12.15	12	SD error > 10%
10	10Val	1037.29	78.12	16.57	12	
11	11Asp	1092.49	124.75	10.28	12	Broadening + SD error > 10%
12	12Arg	1052.23	89.91	14.13	12	
13	13Val	1064.06	96.93	14.46	12	slight doubling
14	14Ile					no peak
15	15Gly					
16	16Met	934.58	77.32	21.81	12	
17	17Glu					no peak
18	18Asn					no peak
19	19Ala	922.65	60.38	22.54	12	
20	20Met	943.25	56.62	3.46	12	
21	21Pro					proline
22	22Trp					no peak
23	23Asn					overlapped with 148
24	24Leu					
25	25Pro					proline
26	26Ala	941.69	55.60	10.09	12	

27	27Asp	943.34	79.32	22.16	12	
28	28Leu	984.07	78.05	22.28	12	
29	29Ala	1015.58	86.82	17.84	12	
30	30Trp	974.05	50.11	9.88	12	
31	31Phe	965.06	59.57	12.61	12	
32	32Lys	1025.53	93.40	23.29	12	
33	33Arg	1031.69	79.12	17.86	12	
34	34Asn	1019.70	74.32	19.29	12	
35	35Thr	1018.72	59.01	15.15	12	
36	36Leu	1059.16	71.34	17.80	12	
37	37Asp	1193.09	93.04	23.12	12	
38	38Lys	1064.05	63.39	21.23	12	
39	39Pro					proline
40	40Val					
41	41Ile	974.72	66.64	2.27	12	
42	42Met					no peak
43	43Gly	1060.75	61.36	4.18	12	
44	44Arg					doubled
45	45His					overlapped with 106
46	46Thr	1037.60	82.19	9.34	12	
47	47Trp	1866.19	772.54	31.54	12	l SD error > 10%
48	48Glu					
49	49Ser	988.49	52.18	18.99	12	
50	50Ile	966.98	73.55	13.35	12	
51	51Gly	1040.67	84.90	23.70	12	
52	52Arg	936.92	65.37	15.75	12	slight doubling
53	53Pro					proline
54	54Leu	1008.91	80.41	24.48	12	
55	55Pro					proline
56	56Gly					no peak
57	57Arg	933.88	39.51	25.24	12	
58	58Lys	681.54	-180.62	376.88	12	SD error > 10%
59	59Asn	996.67	88.08	23.46	12	
60	60Ile	1216.25	56.86	1.82	12	
61	61Ile	1007.64	75.31	2.20	12	
62	62Leu	1074.36	48.93	2.50	12	
63	63Ser	1026.79	95.54	38.76	12	
64	64Ser	973.17	51.50	11.04	12	
65	65Gln	901.11	38.75	16.86	12	
66	66Pro					proline

67	67Gly	835.97	63.62	14.34	12	
68	68Thr	746.36	45.15	7.08	12	small movement
69	69Asp	752.46	42.81	26.24	12	slight doubling
70	70Asp	899.34	98.25	38.84	12	SD error > 10%
71	71Arg	437.93	-250.86	325.51	12	SD error > 10%
72	72Val	894.82	38.50	21.35	12	
73	73Thr	1065.52	48.10	15.62	12	
74	74Trp	1119.16	52.92	19.71	12	
75	75Val	1064.11	92.07	5.38	12	
76	76Lys	1020.35	41.68	19.96	12	
77	77Ser	902.87	30.58	16.42	12	
78	78Val	933.11	39.59	23.22	12	
79	79Asp	890.34	37.07	21.85	12	
80	80Glu	921.00	39.60	24.20	12	
81	81Ala	888.09	71.54	9.42	12	
82	82Ile	1073.48	38.58	13.94	12	
83	83Ala	974.42	34.36	14.89	12	
84	84Ala	1021.65	40.86	17.61	12	
85	85Cys	1004.12	31.16	12.10	12	
86	86Gly	1071.71	36.69	16.07	12	
87	87Asp	950.30	149.74	66.04	12	SD error > 10%
88	88Val	1133.78	80.35	16.67	12	
89	89Pro					proline
90	90Glu					doubling
91	91Ile	920.91	79.29	5.65	12	
92	92Met					no peak
93	93Val	864.65	39.69	2.22	12	
94	94Ile					no peak
95	95Gly	1111.60	54.03	12.00	12	
96	96Gly	1071.82	83.98	21.73	12	
97	97Gly					no peak
98	98Arg	1089.69	123.69	19.50	12	SD error > 10%
99	99Val	1093.93	80.85	24.49	12	
100	100Tyr	1062.35	59.65	11.73	12	slight doubling?
101	101Glu	1005.32	34.09	9.84	12	
102	102Gln	1141.07	39.23	31.63	12	
103	103Phe					overlapped with 146

104	104Leu	1048.06	29.54	5.27	12	
105	105Pro					proline
106	106Lys					overlapped with 45
107	107Ala	1033.70	55.85	12.82	12	
108	108Gln	988.49	44.44	12.81	12	
109	109Lys	943.77	35.54	10.25	12	
110	110Leu	970.27	78.24	9.84	12	
111	111Tyr	987.93	87.86	7.70	12	
112	112Leu	1552.52	376.31	15.78	12	SD error > 10%
113	113Thr					no peak
114	114His	966.41	66.11	8.90	12	
115	115Ile					doubled
116	116Asp	966.93	66.13	17.22	12	
117	117Ala					doubled
118	118Glu					overlapped with 155
119	119Val					ambiguous
120	120Glu	1079.13	109.69	34.74	12	SD error > 10%
121	121Gly					doubled
122	122Asp	961.74	66.68	5.94	12	
123	123Thr					no peak
124	124His					no peak
125	125Phe	990.17	87.17	20.08	12	
126	126Pro					proline
127	127Asp	1147.49	45.33	21.42	12	
128	128Tyr					overlapped
129	129Glu	1025.58	49.01	8.71	12	
130	130Pro					proline
131	131Asp	1100.65	81.54	10.74	12	slight doubling
132	132Asp	882.62	93.79	47.03	12	SD error > 10%
133	133Trp	1047.44	84.84	11.74	12	
134	134Glu	1134.64	49.29	5.41	12	
135	135Ser	987.25	44.89	15.57	12	
136	136Val	977.08	34.08	7.16	12	
137	137Phe	919.87	48.17	8.87	12	
138	138Ser	969.79	60.94	12.16	12	
139	139Glu	920.32	67.39	14.43	12	
140	140Phe					doubled
141	141His	970.59	56.15	12.87	12	

142	142Asp	1023.64	45.65	25.07	12	
143	143Ala	1037.78	42.51	24.24	12	
144	144Asp	1000.27	45.89	9.82	12	
145	145Ala	1012.52	45.64	12.40	12	
146	146Gln					overlapped with 103
147	147Asn	1020.20	59.54	15.22	12	
148	148Ser					overlapped with 23
149	149His	876.60	91.83	33.03	12	
150	150Ser	1015.92	46.02	15.86	12	
151	151Tyr					doubled
152	152Cys	963.05	38.91	9.56	12	overlapped
153	153Phe	886.59	75.51	9.81	12	
154	154Glu	834.26	60.88	5.64	12	
155	155Ile					overlapped with 118
156	156Leu					doubled
157	157Glu	1136.22	62.56	7.86	12	
158	158Arg	1110.25	50.87	9.61	12	
159	159Arg	966.59	27.50	12.45	12	

Table 8.3.2 T1 values at 900MHz of the EcDHFR: NADP+: folate complex under standard buffer conditions.

8.3.3 T2 Relaxation of the EcDHFR: NADP+: Folate complex under standard buffer conditions at 600 MHz

The T2 values at 600MHz of the EcDHFR: NADP+: folate complex under standard buffer conditions are presented below **(Table 8.3.3)**. Values for which the SD of the error is greater than 10% of the T2 value are highlighted red and were excluded from the T2 analysis. T2 values for a total of 105 residues were calculated, 9 of these are discounted due to large errors. The average T2 value of the resulting data was calculated (78.59 ms, s =12.64, n = 96).

600 MHz T2	Residue	T2 600 MHz Buffer	T2 Error	Fit Error	Num Peaks	notes
1	1Met					no peak
2	2Ile					large doubling
3	3Ser	70.40196	2.374	0.69252	12	ambiguity
4	4Leu	71.75533	2.70184	1.22836	12	overlapped
5	5Ile	60.09066	3.11744	0.49075	12	
6	6Ala	70.88202	2.12032	0.89202	12	
7	7Ala					no peak
8	8Leu	63.64281	2.70246	0.88634	12	
9	9Ala	71.45869	2.93761	0.76142	12	
10	10Val	70.38923	1.65978	0.71168	12	
11	11Asp	61.13032	1.74626	0.54821	12	broadening
12	12Arg	74.11928	4.05725	1.35976	12	slight doubling
13	13Val	69.34516	2.12575	0.67469	12	slight doubling
14	14Ile					no peak
15	15Gly					
16	16Met	73.29217	1.80015	0.71348	12	
17	17Glu					no peak
18	18Asn					no peak
19	19Ala	80.59828	2.05511	0.82691	12	
20	20Met	133.0567	28.19724	1.80222	12	SD error > 10%
21	21Pro					proline
22	22Trp					no peak
23	23Asn					overlapped with 148
24	24Leu					

25	25Pro					proline
26	26Ala	70.8506	2.1637	1.16282	12	
27	27Asp	70.59895	1.76796	0.68689	12	
28	28Leu	76.34994	1.95688	1.22736	12	
29	29Ala	78.90357	2.70154	1.1029	12	
30	30Trp	75.52527	2.66611	1.20622	12	
31	31Phe	66.63014	2.52121	0.80091	12	
32	32Lys	70.16208	2.98076	1.31413	12	
33	33Arg	72.47675	3.08955	1.11947	12	
34	34Asn	78.41323	2.61203	0.8661	12	
35	35Thr	80.32535	5.02179	1.52984	12	
36	36Leu	70.66565	3.39008	1.57881	12	
37	37Asp	78.99033	3.46275	1.79432	12	
38	38Lys	76.80906	2.60029	1.69234	12	
39	39Pro					proline
40	40Val					
41	41Ile	85.82047	4.3582	0.39519	12	
42	42Met					no peak
43	43Gly	71.89997	3.96503	0.51486	12	
44	44Arg					doubled
45	45His					overlapped with 106
46	46Thr	138.7359	39.57791	5.30214	12	SD error > 10%
47	47Trp	80.25583	3.00223	0.67952	12	
48	48Glu					
49	49Ser	91.6188	10.66564	2.94763	12	SD error > 10%
50	50Ile	73.8976	2.70647	0.7706	12	
51	51Gly					doubled
52	52Arg					doubled
53	53Pro					proline
54	54Leu	77.64982	1.96136	0.72683	12	
55	55Pro					proline
56	56Gly					no peak
57	57Arg	74.9479	2.27848	2.10787	12	
58	58Lys	86.35614	2.54062	1.99303	12	slight movement
59	59Asn	77.94605	2.51169	1.18503	12	
60	60Ile	128.4238	66.65199	11.74584	12	SD error > 10%
61	61Ile	67.70943	7.36323	0.65395	12	SD error > 10%
62	62Leu	105.717	5.68226	0.44948	12	

63	63Ser	75.91762	2.36944	1.68451	12	
64	64Ser	75.17336	2.28338	0.86597	12	
65	65Gln	72.87533	1.98826	1.59089	12	
66	66Pro					proline
67	67Gly					large movement
68	68Thr					large movement
69	69Asp	105.5755	2.74036	1.95546	12	slight doubling
70	70Asp	83.27757	2.53293	1.67029	12	slight movement
71	71Arg	74.4701	2.73925	1.49308	12	
72	72Val	76.80342	1.95619	1.67409	12	
73	73Thr	73.23965	2.13076	1.67395	12	
74	74Trp	76.55291	3.03629	2.13047	12	slight movement
75	75Val	65.38223	3.27167	0.4818	12	
76	76Lys	77.08613	2.17514	1.97583	12	
77	77Ser	77.57672	2.09872	1.85296	12	
78	78Val	76.98015	2.64037	1.9404	12	
79	79Asp	77.16587	2.04708	1.90614	12	
80	80Glu	95.04345	10.00607	7.47791	12	SD error > 10%
81	81Ala	84.02026	3.53532	0.90326	12	
82	82Ile	81.2625	2.4636	2.15603	12	
83	83Ala	77.12286	2.24705	2.10722	12	
84	84Ala	82.03405	2.62149	2.09534	12	
85	85Cys	75.54037	2.13493	1.74547	12	
86	86Gly	81.85855	2.90212	2.31554	12	
87	87Asp	86.65031	2.43486	2.1027	12	
88	88Val	146.8798	773.7213	33.677	12	SD error > 10%
89	89Pro					proline
90	90Glu					doubling
91	91Ile	80.74108	4.89609	0.95553	12	
92	92Met					no peak
93	93Val	165.8232	12.40559	0.9005	12	
94	94Ile					no peak
95	95Gly					doubled
96	96Gly	72.02879	2.4936	0.97621	12	
97	97Gly					no peak
98	98Arg	68.53831	2.2396	0.63636	12	
99	99Val	75.13418	2.41253	0.94293	12	
100	100Tyr	70.70113	2.32214	0.84867	12	slight

						doubling?
101	101Glu	78.46705	2.48963	1.66149	12	
102	102Gln	113.2939	2.57442	2.77115	12	
103	103Phe					overplapped with 146
104	104Leu	90.82428	2.97225	2.27071	12	
105	105Pro					proline
106	106Lys					overlapped with 45
107	107Ala	88.7565	3.1357	0.99747	12	
108	108Gln	75.15355	2.03377	1.14977	12	
109	109Lys	74.76572	2.05132	1.11466	12	
110	110Leu	113.4814	41.74094	9.93104	12	SD error > 10%
111	111Tyr	64.70862	4.65302	0.53274	12	
112	112Leu					doubled
113	113Thr					no peak
114	114His	75.83654	2.45314	1.08868	12	
115	115Ile					doubled
116	116Asp	76.09596	2.69178	1.44143	12	
117	117Ala					doubled
118	118Glu					overlapped with 155
119	119Val					ambiguous
120	120Glu	84.90261	2.02398	1.25206	12	
121	121Gly					doubled
122	122Asp	73.99821	3.29108	0.72894	12	
123	123Thr					no peak
124	124His					no peak
125	125Phe	70.56557	1.97046	0.87975	12	
126	126Pro					proline
127	127Asp	82.09955	1.91228	1.10549	12	
128	128Tyr					overlapped
129	129Glu	80.42019	2.72359	1.3408	12	
130	130Pro					proline
131	131Asp					doubled and moved
132	132Asp	106.1934	16.06027	8.34164	12	SD error > 10%
133	133Trp	84.34749	6.47869	1.84117	12	
134	134Glu	76.0654	2.62036	0.97186	12	
135	135Ser	75.6838	3.51339	3.35013	12	
136	136Val	121.0943	49.54012	16.26571	12	SD error > 10%

137	137Phe	84.84216	2.93612	1.6157	12	
138	138Ser	79.1879	1.89246	1.35291	12	
139	139Glu	80.76193	2.72565	1.55198	12	
140	140Phe					doubled
141	141His	89.43658	2.88176	1.74372	12	
142	142Asp	117.8127	22.54417	12.02656	12	SD error > 10%
143	143Ala	104.4392	3.3599	2.57461	12	
144	144Asp	68.26737	2.50225	0.81525	12	
145	145Ala	79.07323	3.83871	1.53047	12	
146	146Gln					overlapped with 103
147	147Asn	76.94165	1.94452	0.93783	12	
148	148Ser					overlapped with 23
149	149His	84.73707	8.91851	5.47071	12	SD error > 10%
150	150Ser	76.96499	2.40041	1.81321	12	
151	151Tyr					doubled
152	152Cys	77.04752	2.03614	1.07788	12	overlapped
153	153Phe	79.59833	3.11795	1.24685	12	
154	154Glu	76.38599	3.07439	0.72593	12	
155	155Ile					overlapped with 118
156	156Leu					doubled
157	157Glu	74.04556	2.35657	0.83027	12	
158	158Arg	77.48968	3.36945	1.75883	12	
159	159Arg	91.20611	2.6088	2.23185	12	

Table 8.3.3 T2 values at 600MHz of the EcDHFR: NADP+: folate complex under standard buffer conditions.

8.3.4 T2 Relaxation of the EcDHFR: NADP+: Folate complex under standard buffer conditions at 900 MHz

The T2 values at 900MHz of the EcDHFR: NADP+: folate complex under standard buffer conditions are presented below **(Table 8.3.4)**. Values for which the SD of the error is greater than 10% of the T2 value are highlighted red and were excluded from the T2 analysis. T2 values for a total of 103 residues were calculated, 10 of these are discounted due to large errors. The average T2 value of the resulting data was calculated (63.62 ms, s =9.06, n = 93).

900 MHz T2	Residue	T2 900 MHz Buffer	T2 Error	Fit Error	Num Peaks	notes
1	1Met					no peak
2	2Ile	72.77347	6.21978	32.01526	12	
3	3Ser	61.41105	2.65598	10.87016	12	ambiguity
4	4Leu	64.79606	2.70133	10.0273	12	overlapped
5	5Ile	61.50478	2.20528	2.97955	12	
6	6Ala	56.00811	2.27307	9.63246	12	
7	7Ala					no peak
8	8Leu	53.71056	5.16721	16.87185	12	
9	9Ala	45.01988	3.00121	5.01258	12	
10	10Val	56.04656	1.599	5.87803	12	
11	11Asp	45.9261	1.78087	2.59074	12	broadening
12	12Arg	55.70879	2.35476	6.4308	12	
13	13Val	60.64604	3.29276	9.07847	12	slight doubling
14	14Ile					no peak
15	15Gly					
16	16Met	63.77448	2.34494	10.55921	12	
17	17Glu					no peak
18	18Asn					no peak
19	19Ala					
20	20Met	67.89017	3.4863	16.2437	12	
21	21Pro	69.67612	2.53112	2.46657	12	proline
22	22Trp					no peak
23	23Asn					overlapped with 148
24	24Leu					

25	25Pro					proline
26	26Ala	58.59879	2.34627	6.51711	12	
27	27Asp	56.25715	1.77588	8.62957	12	
28	28Leu	61.79602	2.59256	11.05004	12	
29	29Ala	56.51554	1.77521	6.63807	12	
30	30Trp	70.2828	5.45674	15.08216	12	
31	31Phe	54.11871	2.45673	10.28716	12	
32	32Lys	61.30549	4.32171	19.01454	12	
33	33Arg	59.30647	1.87396	8.60227	12	
34	34Asn	63.01916	2.18023	10.19671	12	
35	35Thr	60.17178	2.55251	10.9815	12	
36	36Leu	63.27976	2.88152	10.65765	12	
37	37Asp	71.3039	3.01976	15.73688	12	
38	38Lys	63.58657	1.96455	12.81656	12	
39	39Pro					proline
40	40Val					
41	41Ile	84.00016	4.99789	1.66356	12	
42	42Met					no peak
43	43Gly	61.64014	2.33237	2.61147	12	
44	44Arg					doubled
45	45His					overlapped with 106
46	46Thr	58.74161	5.80198	11.39086	12	
47	47Trp	91.52715	67.19463	72.69101	12	SD error > 10%
48	48Glu					
49	49Ser	67.26126	2.88461	14.89511	12	
50	50Ile	67.74697	2.35212	7.17116	12	
51	51Gly	73.91369	2.96656	13.78059	12	
52	52Arg	61.70724	2.39871	9.41434	12	slight doubling
53	53Pro					proline
54	54Leu	61.56499	2.15982	11.59329	12	
55	55Pro					proline
56	56Gly					no peak
57	57Arg	59.47005	2.31952	21.31268	12	
58	58Lys	71.39802	2.30376	14.09218	12	
59	59Asn	64.66727	2.60887	10.86564	12	
60	60Ile	59.00089	3.10629	2.14391	12	
61	61Ile	56.91693	2.14069	1.20475	12	
62	62Leu	67.61362	3.60406	2.81583	12	
63	63Ser	66.74098	2.97775	18.89596	12	
64	64Ser	66.32406	2.39739	7.27215	12	

65	65Gln	65.12347	2.84167	15.59984	12	
66	66Pro					proline
67	67Gly	76.92265	3.76554	10.13427	12	
68	68Thr	67.52809	3.92606	5.43597	12	small movement
69	69Asp	81.39671	2.70203	15.5819	12	slight doubling
70	70Asp	62.73865	2.31723	10.06844	12	
71	71Arg	60.80412	2.31622	14.62372	12	
72	72Val	57.98634	2.12007	17.83277	12	
73	73Thr	60.90121	2.28231	13.28554	12	
74	74Trp	59.56056	2.60882	16.20851	12	
75	75Val	56.91893	3.70046	3.86391	12	
76	76Lys	69.89855	2.72885	17.61115	12	
77	77Ser	58.75462	2.16004	19.19287	12	
78	78Val	68.93628	2.30479	17.36205	12	
79	79Asp	62.36835	2.06844	15.19519	12	
80	80Glu	79.60031	7.62937	50.99543	12	
81	81Ala	84.21931	5.64615	5.57695	12	
82	82Ile	85.13977	9.2158	30.62057	12	SD error > 10%
83	83Ala	69.11194	4.02413	25.59255	12	
84	84Ala	65.37537	2.67067	19.43865	12	
85	85Cys	68.86507	2.55249	12.41742	12	
86	86Gly	72.56907	2.30458	14.3036	12	
87	87Asp	76.36309	2.44113	8.8573	12	
88	88Val	68.01813	2.14468	8.46451	12	
89	89Pro					proline
90	90Glu					doubling
91	91Ile	72.95493	12.40461	5.40333	12	SD error > 10%
92	92Met					no peak
93	93Val	220.9264	12.57633	1.97508	12	SD error > 10%
94	94Ile					no peak
95	95Gly	45.47207	1.53201	6.45012	12	
96	96Gly	65.65021	4.05761	16.66225	12	
97	97Gly					no peak
98	98Arg	61.10027	4.92491	14.09393	12	
99	99Val	67.68855	2.48791	11.35697	12	
100	100Tyr	59.95533	2.10021	8.39315	12	slight doubling?
101	101Glu	68.53378	2.51258	10.31771	12	
102	102Gln	96.62941	3.19045	30.80429	12	

103	103Phe					overplapped with 146
104	104Leu	80.58412	10.41865	17.95407	12	SD error > 10%
105	105Pro					proline
106	106Lys					overlapped with 45
107	107Ala	105.953	28.45348	31.82742	12	SD error > 10%
108	108Gln	60.80263	2.2324	10.89205	12	
109	109Lys	61.75418	2.88454	9.50316	12	
110	110Leu	56.85888	3.95408	9.00128	12	
111	111Tyr	58.56662	2.04839	3.12621	12	
112	112Leu	66.18671	12.49408	18.08658	12	SD error > 10%
113	113Thr					no peak
114	114His	44.80363	3.3617	13.71604	12	
115	115Ile					doubled
116	116Asp	59.59972	2.1485	8.66805	12	
117	117Ala					doubled
118	118Glu					overlapped with 155
119	119Val					ambiguous
120	120Glu	70.96137	3.5845	20.02562	12	
121	121Gly					doubled
122	122Asp	61.41726	2.74434	3.83608	12	
123	123Thr					no peak
124	124His					no peak
125	125Phe	57.31754	4.06563	16.57116	12	
126	126Pro					proline
127	127Asp	68.96454	2.78871	19.80201	12	
128	128Tyr					overlapped
129	129Glu	64.86777	2.91689	8.11389	12	
130	130Pro					proline
131	131Asp	70.40984	3.01102	5.75448	12	slight doubling
132	132Asp	68.04617	3.23883	15.10217	12	
133	133Trp	55.76754	1.83995	4.80704	12	
134	134Glu	75.11788	4.3799	6.6974	12	
135	135Ser	68.75661	2.60145	11.99384	12	
136	136Val	84.06015	12.11634	18.01564	12	SD error > 10%
137	137Phe	54.1732	4.27402	21.59625	12	
138	138Ser	49.79402	3.16308	20.0132	12	
139	139Glu	47.69746	3.90853	22.9614	12	

140	140Phe					doubled
141	141His	57.32642	4.01068	24.72892	12	
142	142Asp	77.85537	3.2213	21.45692	12	
143	143Ala	82.25336	2.56117	17.77846	12	
144	144Asp	62.21103	2.75922	8.78595	12	
145	145Ala	56.78294	2.95017	14.59042	12	
146	146Gln					overlapped with 103
147	147Asn	64.5571	2.19945	9.26232	12	
148	148Ser					overlapped with 23
149	149His	43.34043	1.23896	5.20656	12	
150	150Ser	66.4226	2.63035	14.53689	12	
151	151Tyr					doubled
152	152Cys	82.65815	13.38887	18.7287	12	SD error > 10%
153	153Phe	45.04465	3.23759	12.91567	12	
154	154Glu	47.46808	5.56872	13.7051	12	SD error > 10%
155	155Ile					overlapped with 118
156	156Leu					doubled
157	157Glu	62.40237	2.20325	5.78371	12	
158	158Arg	61.42325	2.73332	9.11665	12	
159	159Arg	76.07782	2.54281	14.7495	12	

Table 8.3.4 The T2 values at 900MHz of the EcDHFR: NADP+: folate complex under standard buffer conditions.

8.4 T1 and T2 Relaxation of the EcDHFR: $NADP^+$: Folate complex in the presence of 17 % glycerol co-solvent

8.4.1 T2 Relaxation values of the EcDHFR: $NADP^+$: Folate complex in the presence of 17 % glycerol co-solvent at 900 MHZ

The T2 900MHz of the EcDHFR: NADP+: folate complex in the presence of 17% glycerol are presented below **(Table 8.4.1)**. Values for which the SD of the error is greater than 10% of the T2 value are highlighted red and were excluded from the T2 analysis. T2 values for a total of 130 residues were calculated, 24 of these are discounted due to large errors. The average T2 value of the resulting data was calculated (40.96 ms, *s* = 6.47 ms, n = 106).

No.	Residue	T2 at 900 MHz 17% Glycerol	T2 Error	Fit Error	Number of Peaks
1	1Met				
2	2Ile	44.54	3.93	2711.50	7
3	3Ser	37.50	1.52	736.92	7
4	4Leu	38.56	1.79	735.69	7
5	5Ile	34.39	2.36	337.65	7
6	6Ala	34.84	1.45	760.67	7
7	7Ala				
8	8Leu	41.83	3.04	1316.69	7
9	9Ala	42.13	2.15	490.48	7
10	10Val	36.92	2.59	1488.75	7
11	11Asp	30.87	0.93	341.72	7
12	12Arg	34.32	2.08	836.08	7
13	13Val	34.04	0.94	391.07	7
14	14Ile				
15	15Gly				
16	16Met	38.88	2.55	1415.12	7
17	17Glu				
18	18Asn	37.62	8.55	318.08	7
19	19Ala	40.74	2.15	1342.07	7
20	20Met	48.70	1.71	408.58	7
21	21Pro				
22	22Trp				
23	23Asn				

24	24Leu	28.32	3.57	1153.71	7
25	25Pro				
26	26Ala	33.43	1.88	684.44	7
27	27Asp	38.39	1.85	807.00	7
28	28Leu	38.11	2.32	1160.15	7
29	29Ala	42.22	1.73	694.50	7
30	30Trp	44.95	2.58	1027.68	7
31	31Phe	36.12	1.50	826.11	7
32	32Lys	41.88	5.59	2703.39	7
33	33Arg	35.37	1.14	665.69	7
34	34Asn	29.88	3.97	2545.32	7
35	35Thr	36.45	1.27	508.11	7
36	36Leu	38.03	1.97	950.95	7
37	37Asp	44.57	1.55	1469.68	7
38	38Lys	39.46	1.38	1348.98	7
39	39Pro				
40	40Val	34.82	8.62	388.80	7
41	41Ile	57.62	15.47	410.59	7
42	42Met	30.75	4.84	548.73	7
43	43Gly	34.17	1.14	199.62	7
44	44Arg	35.31	1.49	1364.75	7
45	45His				
46	46Thr				
47	47Trp				
48	48Glu				
49	49Ser	42.29	1.66	999.84	7
50	50Ile	38.92	1.84	750.59	7
51	51Gly	45.87	1.64	1291.75	7
52	52Arg	38.56	2.36	1554.18	7
53	53Pro				
54	54Leu	38.06	2.05	1509.80	7
55	55Pro				
56	56Gly				
57	57Arg	34.85	1.07	1594.51	7
58	58Lys	43.72	1.71	1998.40	7
59	59Asn	37.15	2.24	1594.28	7
60	60Ile	43.46	6.27	512.69	7
61	61Ile	35.35	10.44	475.99	7
62	62Leu	66.39	5.41	475.66	7
63	63Ser	41.23	2.42	2013.28	7
64	64Ser	37.60	1.21	655.74	7
65	65Gln	37.07	1.98	1222.96	7
66	66Pro				
67	67Gly	50.34	2.77	1030.68	7

68	68Thr	47.00	2.57	455.86	7
69	69Asp	52.23	2.42	2301.82	7
70	70Asp	40.70	1.88	1418.25	7
71	71Arg	36.46	1.55	1089.66	7
72	72Val	37.38	1.60	1843.15	7
73	73Thr	36.64	1.22	1187.44	7
74	74Trp	36.45	1.88	1778.19	7
75	75Val	36.05	2.67	327.95	7
76	76Lys	42.43	1.73	1745.78	7
77	77Ser	37.68	1.30	1722.70	7
78	78Val	43.46	2.20	1651.88	7
79	79Asp	37.21	1.46	1539.21	7
80	80Glu	44.40	1.27	1107.57	7
81	81Ala	61.68	3.93	440.01	7
82	82Ile	48.80	4.70	2471.23	7
83	83Ala	41.08	2.99	2838.18	7
84	84Ala	39.44	1.40	1459.50	7
85	85Cys	38.84	1.78	1065.09	7
86	86Gly	43.30	2.22	1923.81	7
87	87Asp	48.04	2.20	2219.95	7
88	88Val	61.53	3.39	6595.77	7
89	89Pro				
90	90Glu	37.22	1.49	1716.13	7
91	91Ile	28.94	10.98	654.69	7
92	92Met				
93	93Val	54.17	31.47	334.60	7
94	94Ile	63.33	8.96	582.07	7
95	95Gly	31.74	0.94	722.35	7
96	96Gly	30.77	7.36	3876.24	7
97	97Gly				
98	98Arg	37.84	1.91	741.56	7
99	99Val	41.79	2.42	1361.70	7
100	100Tyr	35.91	1.84	1152.19	7
101	101Glu	42.43	1.90	1031.14	7
102	102Gln	40.72	2.30	1330.22	7
103	103Phe	44.03	1.47	1107.64	7
104	104Leu	41.18	5.08	3183.42	7
105	105Pro				
106	106Lys				
107	107Ala	48.20	2.29	713.92	7
108	108Gln	36.49	1.57	1064.69	7
109	109Lys	39.05	2.30	873.44	7
110	110Leu	37.17	4.73	1991.54	7
111	111Tyr	42.79	8.43	886.57	7

112	112Leu	27.44	3.11	427.14	7
113	113Thr				
114	114His	29.97	2.48	1032.36	7
115	115Ile	45.50	4.61	1495.49	7
116	116Asp	36.13	1.15	835.13	7
117	117Ala	45.21	2.18	729.72	7
118	118Glu	42.50	2.53	2030.78	7
119	119Val				
120	120Glu	43.22	2.44	3433.29	7
121	121Gly	30.96	0.79	295.49	7
122	122Asp	37.02	3.78	757.10	7
123	123Thr				
124	124His				
125	125Phe	38.34	2.27	1442.74	7
126	126Pro				
127	127Asp	40.09	1.64	1991.34	7
128	128Tyr	40.60	1.68	1948.38	7
129	129Glu	41.57	2.26	1410.28	7
130	130Pro				
131	131Asp	43.98	2.59	1199.94	7
132	132Asp	41.06	1.61	1754.29	7
133	133Trp	39.46	1.82	733.41	7
134	134Glu	40.63	4.28	693.59	7
135	135Ser	41.01	3.41	2932.25	7
136	136Val	46.84	6.59	1457.98	7
137	137Phe	40.13	2.40	1334.65	7
138	138Ser	34.80	1.63	1344.87	7
139	139Glu	35.89	2.24	1355.88	7
140	140Phe	43.63	4.08	1715.73	7
141	141His	46.92	3.15	2093.93	7
142	142Asp	63.17	3.46	3593.84	7
143	143Ala	46.16	1.53	1937.27	7
144	144Asp	36.88	0.90	332.38	7
145	145Ala	38.11	1.54	912.28	7
146	146Gln	45.17	1.75	1357.88	7
147	147Asn	43.50	2.05	940.18	7
148	148Ser	38.31	1.15	772.17	7
149	149His	55.03	4.65	2258.87	7
150	150Ser	40.88	2.16	1832.43	7
151	151Tyr	47.83	5.67	1805.62	7
152	152Cys	40.81	2.69	1479.76	7
153	153Phe	34.70	2.58	798.38	7
154	154Glu	28.53	4.51	746.46	7
155	155Ile	48.09	6.49	2333.08	7

156	156Leu	43.98	3.86	1088.96	7
157	157Glu	32.06	2.92	698.46	7
158	158Arg	45.19	1.16	628.15	7
159	159Arg	48.91	2.08	1770.78	7

Table 8.4.1 T2 900MHz of the EcDHFR: NADP+: folate complex in the presence of 17% glycerol.

8.4.2 T1 Relaxation values of the EcDHFR: $NADP^+$: Folate complex in the presence of 17 % glycerol co-solvent at 900 MHZ

The T1 values of the EcDHFR: NADP+: folate complex in the presence of 17% glycerol at 900MHz are presented below **(Table 8.4.2)**. Values for which the SD of the error is greater than 10% of the T1 value are highlighted red and were excluded from the T1 analysis. T1 values for a total of 129 residues were calculated, 20 of these are discounted due to large errors. The average T1 value of the resulting data was calculated (2416.10 ms, *s* =263.81 ms, *n* = 109).

No.	Residue	T1 (ms) 900MHz 17% glycerol	T1 error	Fit Error	Number of Peaks
1	1Met				
2	2Ile	2268.21	42.50	1013.07	13
3	3Ser	2576.61	84.13	848.89	13
4	4Leu	2656.99	94.19	878.98	13
5	5Ile	2523.24	123.03	430.33	13
6	6Ala	2529.68	44.71	512.68	13
7	7Ala				
8	8Leu	2511.65	48.05	649.25	13
9	9Ala	2442.82	87.90	516.66	13
10	10Val	2475.14	43.78	577.13	13
11	11Asp	2360.75	81.60	779.02	13
12	12Arg	2510.26	43.56	375.52	13
13	13Val	2647.05	84.07	696.23	13
14	14Ile				
15	15Gly				
16	16Met	2441.55	58.72	821.57	13
17	17Glu				
18	18Asn	2205.31	205.63	435.52	13
19	19Ala	2237.85	128.56	2209.29	13
20	20Met	2070.17	51.79	455.40	13
21	21Pro				
22	22Trp				
23	23Asn				
24	24Leu	2641.40	163.65	983.40	13
25	25Pro				
26	26Ala	2368.01	57.51	516.56	13
27	27Asp	2557.92	944.76	21575.80	13
28	28Leu	2618.57	62.24	723.79	13
29	29Ala	2724.64	264.79	2835.55	13
30	30Trp	2520.09	90.09	880.91	13
31	31Phe	2554.83	61.53	737.64	13

32	32Lys	2420.95	55.01	873.49	13
33	33Arg	2418.63	69.62	888.01	13
34	34Asn	2401.30	48.16	682.80	13
35	35Thr	2351.36	52.92	564.46	13
36	36Leu	2524.50	64.11	785.95	13
37	37Asp	2569.40	50.59	909.11	13
38	38Lys	2474.82	65.93	1527.61	13
39	39Pro				
40	40Val	2474.47	278.16	508.91	13
41	41Ile	1284.92	227.99	544.57	13
42	42Met	2580.89	127.25	254.30	13
43	43Gly	2603.75	123.29	413.92	13
44	44Arg	2391.94	79.68	1831.04	13
45	45His				
46	46Thr				
47	47Trp				
48	48Glu				
49	49Ser	2439.72	60.71	895.42	13
50	50Ile	2228.23	61.40	649.90	13
51	51Gly	2362.07	51.60	1036.81	13
52	52Arg	2214.11	70.11	1400.77	13
53	53Pro				
54	54Leu	2507.12	43.49	742.81	13
55	55Pro				
56	56Gly				
57	57Arg	2265.33	40.87	1264.43	13
58	58Lys	2596.68	74.11	2055.80	13
59	59Asn	2408.68	75.47	1329.73	13
60	60Ile	2838.90	151.76	347.62	13
61	61Ile	-341.77	-73.80	4534.92	13
62	62Leu	2139.93	207.51	803.87	13
63	63Ser	2705.93	74.08	1565.90	13
64	64Ser	2690.61	121.61	708.76	13
65	65Gln	2344.80	20.58	347.09	13
66	66Pro				
67	67Gly	1411.99	33.44	605.62	13
68	68Thr	1375.63	74.30	641.61	13
69	69Asp	1385.52	28.64	1337.59	13
70	70Asp	2331.53	78.67	1703.37	13
71	71Arg	2331.81	38.28	669.72	13
72	72Val	2330.83	52.87	1379.73	13
73	73Thr	2573.46	60.38	982.19	13
74	74Trp	2793.90	44.41	721.91	13
75	75Val	2601.53	156.06	551.04	13

76	76Lys	2607.70	32.40	860.05	13
77	77Ser	2611.51	35.97	776.70	13
78	78Val	2358.56	19.99	467.33	13
79	79Asp	2318.12	27.11	677.32	13
80	80Glu	2374.18	31.28	851.87	13
81	81Ala	624.24	1032.67	8639.12	13
82	82Ile	2603.35	117.01	2452.34	13
83	83Ala	2246.25	43.58	1177.54	13
84	84Ala	2393.18	183.03	4919.21	13
85	85Cys	2545.36	43.81	570.17	13
86	86Gly	2651.42	38.51	709.88	13
87	87Asp	2455.76	81.99	2368.72	13
88	88Val	2311.90	30.01	1920.45	13
89	89Pro				
90	90Glu	2437.92	37.61	945.51	13
91	91Ile	2423.44	426.94	997.25	13
92	92Met				
93	93Val	1333.33	238.41	400.29	13
94	94Ile	1483.94	88.82	408.31	13
95	95Gly	2479.76	60.63	874.25	13
96	96Gly	2831.83	116.95	1260.96	13
97	97Gly				
98	98Arg	2496.45	236.23	1992.39	13
99	99Val	2514.93	76.66	1135.90	13
100	100Tyr	2291.82	94.18	1646.11	13
101	101Glu	2391.14	53.48	911.44	13
102	102Gln	2553.09	71.03	861.48	13
103	103Phe	2461.24	60.46	914.49	13
104	104Leu	2615.13	480.63	14024.60	13
105	105Pro				
106	106Lys				
107	107Ala	2150.35	46.91	525.54	13
108	108Gln	2423.84	87.19	1336.38	13
109	109Lys	2421.35	128.51	1324.86	13
110	110Leu	2659.45	1104.05	14639.80	13
111	111Tyr	2590.88	85.62	374.61	13
112	112Leu	2916.81	606.21	966.59	13
113	113Thr				
114	114His	2135.95	469.95	2716.97	13
115	115Ile	2721.58	164.00	1950.14	13
116	116Asp	2536.49	54.68	854.10	13
117	117Ala	2721.22	81.71	663.14	13
118	118Glu	3014.79	651.45	9531.96	13
119	119Val				

120	120Glu	2278.54	29.21	1129.65	13
121	121Gly	2110.95	47.05	497.80	13
122	122Asp	2344.83	105.11	559.28	13
123	123Thr				
124	124His				
125	125Phe	2551.38	53.04	797.46	13
126	126Pro				
127	127Asp	2462.96	46.93	1306.80	13
128	128Tyr	2040.70	58.32	2241.63	13
129	129Glu				
130	130Pro	2253.79	48.87	910.46	13
131	131Asp	2211.25	48.00	807.27	13
132	132Asp	2365.83	64.06	1662.78	13
133	133Trp	2340.36	115.74	1378.66	13
134	134Glu	2704.56	163.40	848.77	13
135	135Ser	2441.02	163.04	3096.75	13
136	136Val	2654.51	195.52	2067.50	13
137	137Phe	2299.82	310.48	2819.53	13
138	138Ser	2040.13	369.11	5182.52	13
139	139Glu	2142.83	359.08	3177.54	13
140	140Phe	2613.39	187.26	2806.74	13
141	141His	1991.48	360.56	4981.53	13
142	142Asp	2214.22	115.40	5610.31	13
143	143Ala	2286.05	35.47	1223.30	13
144	144Asp	2600.00	55.16	449.68	13
145	145Ala	2246.78	76.04	1115.47	13
146	146Gln	2353.44	27.92	483.66	13
147	147Asn	2716.47	47.24	545.25	13
148	148Ser	2514.23	51.84	603.21	13
149	149His	2250.77	47.72	850.16	13
150	150Ser	2568.79	45.58	768.46	13
151	151Tyr	2381.08	145.97	2615.14	13
152	152Cys	2138.99	311.47	3112.90	13
153	153Phe	2058.37	428.82	1789.51	13
154	154Glu	2515.62	579.58	1023.18	13
155	155Ile	3364.19	1515.03	16046.50	13
156	156Leu	2641.51	203.21	2153.53	13
157	157Glu	2865.65	98.24	479.27	13
158	158Arg	2448.49	62.73	1082.80	13
159	159Arg	1930.35	23.98	955.21	13

Table 8.4.2 T1 900MHz of the EcDHFR: NADP+: folate complex in the presence of 17% glycerol.

8.4.3 T2 Relaxation values of the EcDHFR: NADP^{+}: Folate complex in the presence of 17 % glycerol co-solvent at 600 MHz with ^{15}N only labelling

The T1 values at 600MHz of the EcDHFR: NADP+: folate complex in the presence of 17% glycerol are presented below **(Table 8.4.3)**. Values for which the SD of the error is greater than 10% of the T1 value are highlighted red and were excluded from the T1 analysis. T1 values for a total of 131 residues were calculated, 15 of these are discounted due to large errors. The average T1 value of the resulting data was calculated (972.44 ms, *s* =97.08 ms, *n* = 116).

No.	Residue	T1_600MHz_17 % Glycerol ^{15}N only	T1 Erorr	Fit Error	Number of Peaks
1	1Met				
2	2Ile	953.50	68.16	28.66	11
3	3Ser	977.94	60.30	20.86	11
4	4Leu	1024.24	54.17	19.25	11
5	5Ile	984.75	54.48	19.62	11
6	6Ala	992.01	95.27	24.46	11
7	7Ala				
8	8Leu	950.64	62.25	18.41	11
9	9Ala	1036.85	62.74	15.38	11
10	10Val	1020.60	91.35	26.47	11
11	11Asp	892.35	94.01	17.98	11
12	12Arg	1065.35	77.01	21.57	11
13	13Val	1732.93	242.99	54.23	11
14	14Ile				
15	15Gly				
16	16Met	890.60	58.75	25.20	11
17	17Glu				
18	18Asn	668.32	165.43	16.76	11
19	19Ala	1034.23	37.80	23.45	11
20	20Met	921.07	83.13	20.29	11
21	21Pro				
22	22Trp				
23	23Asn				
24	24Leu	997.03	66.13	15.09	11
25	25Pro				
26	26Ala	1002.33	45.47	19.01	11
27	27Asp	880.74	22.69	8.19	11
28	28Leu	1035.29	41.56	14.84	11

29	29Ala	934.16	24.77	12.82	11
30	30Trp	955.12	59.65	23.25	11
31	31Phe	943.29	88.13	26.81	11
32	32Lys	472.70	-153.99	388.93	11
33	33Arg	973.69	37.31	19.36	11
34	34Asn	926.46	53.16	23.76	11
35	35Thr	988.01	51.54	15.82	11
36	36Leu	1016.55	55.76	23.43	11
37	37Asp	928.42	72.07	18.45	11
38	38Lys	1001.68	27.51	16.60	11
39	39Pro				
40	40Val	989.61	60.78	22.10	11
41	41Ile	1026.12	80.59	22.27	11
42	42Met	825.49	49.79	18.56	11
43	43Gly	1178.30	92.29	19.40	11
44	44Arg	898.84	60.10	19.79	11
45	45His				
46	46Thr				
47	47Trp				
48	48Glu				
49	49Ser	897.13	59.82	33.68	11
50	50Ile	886.02	50.70	19.61	11
51	51Gly	1010.54	58.96	24.83	11
52	52Arg	1003.09	27.36	16.18	11
53	53Pro				
54	54Leu	450.46	196.70	91.46	11
55	55Pro				
56	56Gly				
57	57Arg	951.73	31.64	25.62	11
58	58Lys	1196.38	38.15	12.89	11
59	59Asn	925.87	40.83	13.67	11
60	60Ile	1082.49	73.97	21.12	11
61	61Ile	998.86	89.41	26.01	11
62	62Leu	899.92	41.95	16.95	11
63	63Ser	974.93	37.33	22.21	11
64	64Ser	963.64	57.22	12.27	11
65	65Gln	969.96	36.78	20.22	11
66	66Pro				
67	67Gly	731.42	43.86	25.90	11
68	68Thr	776.96	72.78	21.58	11
69	69Asp	830.88	20.88	22.90	11
70	70Asp	1049.21	45.27	19.75	11
71	71Arg	903.19	52.82	22.31	11
72	72Val	966.61	25.64	18.51	11
73	73Thr	919.00	80.32	27.67	11

74	74Trp	1175.54	52.07	22.93	11
75	75Val	936.93	52.60	21.45	11
76	76Lys	1082.65	47.48	15.21	11
77	77Ser	850.73	35.89	29.79	11
78	78Val	908.05	80.08	28.46	11
79	79Asp	990.87	34.09	25.68	11
80	80Glu	972.42	33.77	19.77	11
81	81Ala	935.77	37.01	27.00	11
82	82Ile	959.70	42.70	21.58	11
83	83Ala	955.67	27.10	18.38	11
84	84Ala	940.13	46.30	48.08	11
85	85Cys	945.93	51.39	30.32	11
86	86Gly	948.41	25.55	16.59	11
87	87Asp	1088.11	52.87	34.60	11
88	88Val	1188.50	24.38	24.45	11
89	89Pro				
90	90Glu	1048.01	54.76	29.59	11
91	91Ile	886.04	69.24	19.91	11
92	92Met	1051.22	58.54	21.45	11
93	93Val	1088.81	81.30	17.32	11
94	94Ile	985.33	105.92	15.99	11
95	95Gly	958.49	60.49	19.43	11
96	96Gly	875.99	31.46	9.84	11
97	97Gly				
98	98Arg	881.03	33.96	15.84	11
99	99Val	875.96	51.93	23.53	11
100	100Tyr	943.05	45.69	22.75	11
101	101Glu	938.91	36.31	20.61	11
102	102Gln	1002.34	54.40	16.87	11
103	103Phe	1042.29	115.87	72.88	11
104	104Leu	948.07	46.37	20.86	11
105	105Pro				
106	106Lys				
107	107Ala	979.67	22.01	16.25	11
108	108Gln	918.36	67.79	15.09	11
109	109Lys	988.88	69.57	28.26	11
110	110Leu	904.49	79.88	26.10	11
111	111Tyr	955.69	98.30	20.83	11
112	112Leu	871.25	74.68	16.33	11
113	113Thr				
114	114His	818.44	94.22	23.38	11
115	115Ile	822.91	131.93	25.22	11
116	116Asp	853.70	125.84	41.45	11
117	117Ala	1020.30	48.26	18.86	11
118	118Glu	1079.37	40.41	23.16	11

119	119Val				
120	120Glu	1065.96	16.39	11.77	11
121	121Gly	1087.79	47.47	16.16	11
122	122Asp	856.52	69.40	14.14	11
123	123Thr				
124	124His				
125	125Phe	834.95	72.97	17.02	11
126	126Pro				
127	127Asp	1079.73	33.69	23.76	11
128	128Tyr	1406.15	49.60	20.01	11
129	129Glu	1022.50	52.10	16.46	11
130	130Pro				
131	131Asp	1006.47	50.04	21.64	11
132	132Asp	910.60	57.45	26.34	11
133	133Trp	936.27	49.00	19.25	11
134	134Glu	1069.48	40.24	15.25	11
135	135Ser	1036.91	50.80	20.86	11
136	136Val	1192.32	291.68	36.69	11
137	137Phe	891.22	86.47	38.56	11
138	138Ser	811.12	60.99	31.38	11
139	139Glu	970.96	69.67	18.97	11
140	140Phe	713.50	71.05	29.67	11
141	141His	871.35	82.29	29.32	11
142	142Asp	1225.89	13.58	11.69	11
143	143Ala	971.73	28.85	20.14	11
144	144Asp	1000.05	87.10	30.33	11
145	145Ala	901.89	54.82	28.71	11
146	146Gln	1023.82	62.03	39.62	11
147	147Asn	1074.38	57.82	24.05	11
148	148Ser	1020.20	58.75	24.10	11
149	149His	944.69	25.82	13.24	11
150	150Ser	968.56	39.04	21.19	11
151	151Tyr	869.45	61.08	13.16	11
152	152Cys	901.25	90.06	22.94	11
153	153Phe	853.65	108.58	26.18	11
154	154Glu	918.61	98.22	23.75	11
155	155Ile	946.65	60.19	19.82	11
156	156Leu	401.85	-0.96	305.20	11
157	157Glu	1082.42	109.04	25.91	11
158	158Arg	1073.49	80.27	23.51	11
159	159Arg	986.51	50.30	21.74	11

Table 8.4.3 T1 values at 600MHz of the EcDHFR: NADP+: folate complex in the presence of 17% glycerol.

8.4.4 T1 Relaxation values of the EcDHFR: $NADP^+$: Folate complex in the presence of 17 % glycerol co-solvent at 600 MHz with ^{15}N only labelling

The T2 values at 600MHz of the EcDHFR: NADP+: folate complex in the presence of 17% glycerol are presented below (**Table 8.4.4)**. Values for which the SD of the error is greater than 10% of the T2 value are highlighted red and were excluded from the T2 analysis. T2 values for a total of 131 residues were calculated, 5 of these are discounted due to large errors. The average T2 value of the resulting data was calculated (57.59 ms, *s* = 7.57 ms, n = 126).

600 MHz T2 17% glycerol ^{15}N labelled	Residue	T2	T2 Error	Fit Error	Num Peaks
1	1Met				
2	2Ile	61.53	1.94	279.18	12
3	3Ser	55.90	2.80	356.48	12
4	4Leu	56.94	0.79	131.96	12
5	5Ile	50.94	1.44	210.97	12
6	6Ala	57.24	2.43	282.22	12
7	7Ala				
8	8Leu	50.89	2.30	271.49	12
9	9Ala	67.45	2.49	213.34	12
10	10Val	52.20	1.86	206.71	12
11	11Asp	50.05	1.96	135.04	12
12	12Arg	52.45	1.73	195.19	12
13	13Val	92.61	9.17	1106.75	12
14	14Ile				
15	15Gly				
16	16Met	56.88	1.44	209.67	12
17	17Glu				
18	18Asn	59.90	6.94	163.51	12
19	19Ala	56.41	1.33	324.02	12
20	20Met	66.36	1.50	137.90	12
21	21Pro				
22	22Trp				
23	23Asn				
24	24Leu	50.45	2.90	277.79	12
25	25Pro				
26	26Ala	50.96	1.70	274.75	12
27	27Asp	50.73	3.82	667.91	12
28	28Leu	51.37	1.81	228.17	12

29	29Ala	49.45	1.67	277.32	12
30	30Trp	57.43	1.27	173.64	12
31	31Phe	52.67	1.73	244.34	12
32	32Lys	54.75	1.24	215.77	12
33	33Arg	54.05	1.51	293.14	12
34	34Asn	57.53	1.82	256.65	12
35	35Thr	53.67	1.74	199.31	12
36	36Leu	51.97	1.19	205.35	12
37	37Asp	57.21	6.20	543.54	12
38	38Lys	56.92	0.96	240.78	12
39	39Pro				
40	40Val	54.47	1.58	220.08	12
41	41Ile	64.69	1.80	176.45	12
42	42Met	52.22	1.41	176.06	12
43	43Gly	50.20	1.47	143.72	12
44	44Arg	50.47	1.17	165.22	12
45	45His				
46	46Thr				
47	47Trp				
48	48Glu				
49	49Ser	57.77	1.52	274.07	12
50	50Ile	54.60	1.19	155.71	12
51	51Gly	54.64	1.55	252.02	12
52	52Arg	55.12	1.28	272.49	12
53	53Pro				
54	54Leu	58.02	2.62	284.53	12
55	55Pro				
56	56Gly				
57	57Arg	57.17	1.05	279.71	12
58	58Lys	61.86	1.84	279.44	12
59	59Asn	59.53	1.32	168.14	12
60	60Ile	56.41	1.63	217.62	12
61	61Ile	50.60	1.35	176.62	12
62	62Leu	59.28	1.03	128.19	12
63	63Ser	54.12	1.61	319.26	12
64	64Ser	51.94	0.91	74.50	12
65	65Gln	56.30	1.77	337.49	12
66	66Pro				
67	67Gly	68.28	1.46	255.18	12
68	68Thr	70.44	3.57	238.31	12
69	69Asp	83.42	2.51	632.78	12
70	70Asp	65.49	2.00	300.80	12
71	71Arg	54.14	1.79	305.64	12
72	72Val	54.60	1.43	336.86	12
73	73Thr	55.74	2.05	230.63	12

74	74Trp	53.50	1.57	299.35	12
75	75Val	51.76	1.82	258.15	12
76	76Lys	57.76	1.56	215.34	12
77	77Ser	53.01	0.96	227.61	12
78	78Val	59.49	2.09	233.67	12
79	79Asp	55.86	0.78	245.08	12
80	80Glu	266.63	-5572.91	8184.04	12
81	81Ala	58.01	0.87	231.54	12
82	82Ile	62.81	1.47	247.39	12
83	83Ala	56.97	0.71	177.16	12
84	84Ala	55.74	1.04	372.56	12
85	85Cys	58.58	1.45	306.99	12
86	86Gly	57.71	1.19	296.11	12
87	87Asp	67.49	1.04	259.40	12
88	88Val	86.93	1.95	615.87	12
89	89Pro				
90	90Glu	56.68	1.58	326.43	12
91	91Ile	54.51	2.87	305.63	12
92	92Met	56.09	1.97	270.71	12
93	93Val	58.85	2.68	235.37	12
94	94Ile	49.18	3.49	209.05	12
95	95Gly	49.52	1.61	180.45	12
96	96Gly	55.96	3.08	308.09	12
97	97Gly				
98	98Arg	55.63	1.77	247.77	12
99	99Val	57.49	1.90	223.90	12
100	100Tyr	53.48	1.53	278.54	12
101	101Glu	55.74	0.99	235.51	12
102	102Gln	58.70	2.42	251.54	12
103	103Phe	62.76	1.32	274.70	12
104	104Leu	56.44	1.43	259.34	12
105	105Pro				
106	106Lys				
107	107Ala	58.66	1.12	261.76	12
108	108Gln	55.41	1.64	145.14	12
109	109Lys	51.09	1.40	274.45	12
110	110Leu	56.83	1.75	251.49	12
111	111Tyr	53.04	1.94	172.40	12
112	112Leu	49.31	3.98	258.40	12
113	113Thr				
114	114His	52.88	1.50	110.52	12
115	115Ile	48.88	2.93	293.06	12
116	116Asp	56.53	1.88	230.09	12
117	117Ala	58.62	2.17	312.78	12
118	118Glu	59.03	1.19	286.21	12

119	119Val				
120	120Glu	64.78	1.73	441.22	12
121	121Gly	47.70	1.52	224.60	12
122	122Asp	61.94	2.71	172.32	12
123	123Thr				
124	124His				
125	125Phe	60.15	3.29	230.38	12
126	126Pro				
127	127Asp	59.70	1.38	385.10	12
128	128Tyr	62.57	1.16	227.46	12
129	129Glu	60.27	2.59	305.52	12
130	130Pro				
131	131Asp	60.74	1.27	236.36	12
132	132Asp	59.95	1.26	283.47	12
133	133Trp	52.87	1.77	269.26	12
134	134Glu	58.12	2.13	312.59	12
135	135Ser	58.31	1.95	356.54	12
136	136Val	57.50	3.84	327.10	12
137	137Phe	53.72	1.83	221.48	12
138	138Ser	50.11	2.10	252.86	12
139	139Glu	57.84	3.43	272.25	12
140	140Phe	57.84	2.85	384.65	12
141	141His	96.43	7.89	530.23	12
142	142Asp	177.58	10.83	1558.21	12
143	143Ala	63.11	1.07	230.03	12
144	144Asp	53.17	1.20	168.31	12
145	145Ala	57.80	2.03	323.95	12
146	146Gln	63.05	1.17	317.10	12
147	147Asn	58.17	1.80	373.18	12
148	148Ser	54.84	1.90	304.18	12
149	149His	51.22	0.96	150.07	12
150	150Ser	59.98	1.62	301.98	12
151	151Tyr	48.39	2.04	199.10	12
152	152Cys	55.60	1.91	164.10	12
153	153Phe	59.04	3.26	201.60	12
154	154Glu	51.30	2.48	160.43	12
155	155Ile	63.80	2.61	311.93	12
156	156Leu	52.89	10.53	1024.83	12
157	157Glu	55.43	2.43	291.59	12
158	158Arg	64.35	1.51	168.60	12
159	159Arg	68.76	1.22	185.79	12

Table 8.4.4 The T2 values at 600MHz of the EcDHFR: NADP+: folate complex in the presence of 17% glycerol.

8.5 T1 and T2 Relaxation values of the EcDHFR: $NADP^+$: Folate complex in the presence of 17 % methanol co-solvent

8.5.1 T1 Relaxation values of the EcDHFR: $NADP^+$: Folate complex in the presence of 17 % methanol co-solvent at 900 MHz

The T1 values at 900MHz data for EcDHFR: $NADP^{|+}$: folate in the presence of 17% methanol are presented below **(Table 8.5.1)**. Values for which the SD of the error is greater than 10% of the T1 value are highlighted red and were excluded from the T1 analysis. T1 values were calculated for a total of 116 residues, 17 of these were discounted due to large errors. The average T1 value of the resulting data was calculated (1401.82 ms, *s* =140.99 ms, *n* = 99).

No.	Residue	T1 900MHz 17% MeOD	T1 Error	Fit Error	Number of Peaks
1	1Met				
2	2Ile	1325.98	96.62	6.23	12
3	3Ser	186.70	-45.90	37.86	12
4	4Leu	1311.87	99.63	2.69	12
5	5Ile				
6	6Ala	1318.19	113.10	3.41	12
7	7Ala				
8	8Leu	1422.83	113.10	3.87	12
9	9Ala	1199.54	198.22	6.55	12
10	10Val	1593.23	124.39	3.60	12
11	11Asp	1372.18	98.65	1.91	12
12	12Arg	1483.99	105.51	2.36	12
13	13Val	1610.25	167.23	3.50	12
14	14Ile				
15	15Gly				
16	16Met	159.00	-116.71	67.03	12
17	17Glu				
18	18Asn				
19	19Ala	1275.49	102.71	5.86	12
20	20Met	1091.69	79.08	1.42	12

21	21Pro				
22	22Trp				
23	23Asn				
24	24Leu	1257.08	113.52	6.58	12
25	25Pro				
26	26Ala	1429.30	95.98	2.49	12
27	27Asp	1530.31	139.59	8.46	12
28	28Leu	1449.02	120.72	5.59	12
29	29Ala	1415.75	127.43	4.19	12
30	30Trp	1445.19	99.22	3.58	12
31	31Phe	1418.63	122.60	4.66	12
32	32Lys	1380.95	126.12	5.78	12
33	33Arg	1262.27	112.23	15.08	12
34	34Asn	1417.48	117.43	5.33	12
35	35Thr	1467.14	81.77	3.75	12
36	36Leu	1511.55	148.18	4.90	12
37	37Asp	1620.71	124.50	6.47	12
38	38Lys	1431.45	104.64	6.36	12
39	39Pro				
40	40Val				
41	41Ile				
42	42Met				
43	43Gly	1737.83	243.04	1.25	12
44	44Arg	1580.33	79.89	5.39	12
45	45His				
46	46Thr	1254.36	95.21	3.09	12
47	47Trp	1222.15	71.45	2.03	12
48	48Glu				
49	49Ser	577.59	7639.44	61.46	12
50	50Ile	1404.71	113.28	2.60	12
51	51Gly	1467.16	147.55	5.86	12
52	52Arg	1366.48	130.31	5.28	12
53	53Pro				
54	54Leu	1472.62	95.77	5.54	12
55	55Pro				
56	56Gly				
57	57Arg	1368.41	71.70	9.16	12
58	58Lys	1473.35	127.72	9.14	12
59	59Asn	1276.70	116.13	6.77	12
60	60Ile				
61	61Ile				
62	62Leu				

63	63Ser	1610.46	144.58	9.09	12
64	64Ser	1498.87	125.14	3.86	12
65	65Gln	1325.14	79.23	6.61	12
66	66Pro				
67	67Gly	1068.67	90.95	3.21	12
68	68Thr	826.52	79.97	2.04	12
69	69Asp	889.48	56.61	9.43	12
70	70Asp	1200.57	111.18	8.86	12
71	71Arg	1284.55	90.99	8.33	12
72	72Val	1435.81	103.05	10.12	12
73	73Thr	1522.32	115.73	6.27	12
74	74Trp	1616.09	94.07	7.07	12
75	75Val				
76	76Lys	1161.78	231.21	1.94	12
77	77Ser	1509.05	85.32	7.99	12
78	78Val	1327.94	74.01	10.06	12
79	79Asp	1303.11	77.51	10.93	12
80	80Glu	1312.81	73.63	9.93	12
81	81Ala	1573.04	23.61	7.61	12
82	82Ile	1505.03	74.12	7.05	12
83	83Ala	1305.64	63.51	7.93	12
84	84Ala	1394.20	58.71	7.42	12
85	85Cys	1410.58	77.73	7.29	12
86	86Gly	1486.95	81.84	7.75	12
87	87Asp	1303.73	137.54	20.07	12
88	88Val	1575.72	87.20	17.80	12
89	89Pro				
90	90Glu	1461.73	119.42	9.45	12
91	91Ile	1366.69	140.55	1.83	12
92	92Met				
93	93Val				
94	94Ile				
95	95Gly	1533.06	112.47	3.89	12
96	96Gly	1533.75	132.70	5.44	12
97	97Gly				
98	98Arg	657.80	-31.59	48.39	12
99	99Val	1548.41	127.29	5.50	12
100	100Tyr	1376.51	108.35	4.57	12
101	101Glu	1419.22	69.95	4.77	12
102	102Gln	1605.36	113.57	4.31	12
103	103Phe	1487.85	102.52	7.26	12
104	104Leu	1385.29	69.12	3.85	12

105	105Pro				
106	106Lys	1453.65	71.28	8.01	12
107	107Ala	1383.54	76.97	1.71	12
108	108Gln	1458.27	105.80	5.16	12
109	109Lys	1411.23	88.08	3.23	12
110	110Leu				
111	111Tyr				
112	112Leu	1190.02	155.31	1.35	12
113	113Thr				
114	114His	172.61	-58.11	42.14	12
115	115Ile	1508.66	199.95	4.41	12
116	116Asp	1388.59	99.67	4.05	12
117	117Ala	1590.29	107.63	2.39	12
118	118Glu	1462.17	111.45	6.86	12
119	119Val				
120	120Glu	1284.77	95.62	6.39	12
121	121Gly	1512.12	112.89	1.91	12
122	122Asp	1146.66	115.63	2.28	12
123	123Thr				
124	124His				
125	125Phe	1576.07	298.02	3.16	12
126	126Pro	1507.20	128.28	5.37	12
127	127Asp				
128	128Tyr	1527.27	76.03	7.47	12
129	129Glu	1345.30	85.14	6.25	12
130	130Pro	1355.50	91.60	3.43	12
131	131Asp				
132	132Asp	1417.69	96.98	2.24	12
133	133Trp	1425.77	79.74	2.70	12
134	134Glu	1739.65	166.57	2.26	12
135	135Ser	1388.34	86.41	8.36	12
136	136Val	1322.76	76.97	4.04	12
137	137Phe	1384.46	60.75	2.84	12
138	138Ser	1406.43	91.94	4.55	12
139	139Glu	1321.00	105.94	5.03	12
140	140Phe	1431.78	78.42	5.14	12
141	141His	1399.49	90.10	4.32	12
142	142Asp	1395.27	87.17	6.90	12
143	143Ala	1346.29	93.97	10.48	12
144	144Asp	1506.08	115.31	2.60	12
145	145Ala				
146	146Gln	1615.14	109.96	3.18	12

147	147Asn	1394.31	102.12	5.74	12
148	148Ser	1394.86	126.26	6.38	12
149	149His	1363.29	96.79	4.74	12
150	150Ser	1502.54	109.82	6.78	12
151	151Tyr	1309.45	99.95	4.99	12
152	152Cys				
153	153Phe	215.10	-33.28	17.32	12
154	154Glu	1252.30	133.62	0.99	12
155	155Ile				
156	156Leu	1324.23	109.06	3.80	12
157	157Glu				
158	158Arg	1414.80	79.17	3.13	12
159	159Arg	1269.39	66.35	8.14	12

Table 8.5.1 T1 values at 900MHz data for EcDHFR: $NADP^{|+}$: folate in the presence of 17% methanol.

8.5.2 T2 Relaxation values of the EcDHFR: $NADP^+$: Folate complex in the presence of 17 % methanol co-solvent at 900 MHz

The T2 values at 900MHz data for EcDHFR: $NADP^{|+}$: folate in the presence of 17% methanol are presented below **(Table 8.5.2)**. Values for which the SD of the error is greater than 10% of the T2 value are highlighted red and were excluded from the T2 analysis. T2 values for a total of 116 residues were calculated, 4 of these are discounted due to large errors. The average T2 value of the resulting data was calculated (52.90 ms, *s* = 10.46 ms, n = 112).

No.	Residue	T2 900 MHz 17% MeOD	T2 Error	Fit Error	Number of Peaks
1	1Met				
2	2Ile	51.30	2.09	5.12	12
3	3Ser	23.14	2.55	8.63	12
4	4Leu	67.62	4.27	2.50	12
5	5Ile				
6	6Ala	47.12	2.28	2.31	12
7	7Ala				
8	8Leu	44.10	2.22	2.91	12
9	9Ala	54.87	3.25	1.67	12
10	10Val	44.41	1.92	2.71	12
11	11Asp	34.27	1.23	1.01	12
12	12Arg	47.83	1.80	1.64	12
13	13Val	39.53	2.02	2.13	12
14	14Ile				
15	15Gly				
16	16Met	51.59	1.81	3.33	12
17	17Glu				
18	18Asn				
19	19Ala	48.60	2.03	4.08	12
20	20Met	101.73	9.10	2.36	12
21	21Pro				
22	22Trp				
23	23Asn				
24	24Leu	56.64	2.50	3.00	12
25	25Pro				
26	26Ala	45.39	1.56	1.60	12

27	27Asp	45.88	1.65	4.32	12
28	28Leu	43.75	1.51	2.87	12
29	29Ala	49.98	9.72	7.82	12
30	30Trp	45.97	1.48	2.22	12
31	31Phe	43.94	0.80	1.34	12
32	32Lys	43.50	1.67	3.13	12
33	33Arg	52.50	1.53	6.36	12
34	34Asn	46.47	0.78	2.82	12
35	35Thr	46.80	1.54	2.65	12
36	36Leu	46.40	2.19	3.09	12
37	37Asp	57.11	1.60	3.48	12
38	38Lys	56.95	2.19	4.60	12
39	39Pro				
40	40Val				
41	41Ile				
42	42Met				
43	43Gly	48.59	6.17	1.44	12
44	44Arg	50.47	2.78	6.59	12
45	45His				
46	46Thr	76.86	6.95	4.29	12
47	47Trp	90.81	7.99	3.91	12
48	48Glu				
49	49Ser	50.67	1.61	4.07	12
50	50Ile	45.47	2.26	2.24	12
51	51Gly	53.61	2.29	4.00	12
52	52Arg	48.10	2.00	2.99	12
53	53Pro				
54	54Leu	49.56	1.73	3.87	12
55	55Pro				
56	56Gly				
57	57Arg	45.61	1.51	6.67	12
58	58Lys	53.31	2.10	6.04	12
59	59Asn	48.73	1.53	3.17	12
60	60Ile				
61	61Ile				
62	62Leu				
63	63Ser	49.18	1.72	4.66	12
64	64Ser	49.82	3.22	3.58	12
65	65Gln	48.27	1.47	3.80	12
66	66Pro				
67	67Gly	58.60	2.85	2.73	12
68	68Thr	54.00	4.19	1.99	12

69	69Asp	61.22	1.88	6.11	12
70	70Asp	51.40	1.76	4.04	12
71	71Arg	48.50	1.73	4.84	12
72	72Val	45.85	1.63	6.26	12
73	73Thr	54.80	2.50	4.90	12
74	74Trp	47.07	1.75	5.36	12
75	75Val	40.23	4.09	1.25	12
76	76Lys	52.73	1.69	5.91	12
77	77Ser	47.81	1.63	6.76	12
78	78Val	51.24	1.76	7.11	12
79	79Asp	51.29	1.71	6.70	12
80	80Glu	398.63	38.69	42.72	12
81	81Ala				
82	82Ile	57.48	1.90	5.55	12
83	83Ala	58.40	3.25	10.54	12
84	84Ala	53.72	1.63	6.35	12
85	85Cys	50.95	1.86	5.65	12
86	86Gly	56.57	2.35	6.96	12
87	87Asp	58.77	1.93	7.76	12
88	88Val	70.97	2.41	16.67	12
89	89Pro				
90	90Glu	51.42	2.84	8.33	12
91	91Ile	59.92	3.94	1.22	12
92	92Met				
93	93Val				
94	94Ile				
95	95Gly	39.10	4.34	4.52	12
96	96Gly	48.76	1.57	2.71	12
97	97Gly				
98	98Arg	47.78	3.30	3.17	12
99	99Val	48.83	2.17	3.88	12
100	100Tyr	46.41	1.40	2.34	12
101	101Glu	53.48	1.74	3.93	12
102	102Gln	52.66	1.47	2.67	12
103	103Phe	53.98	1.71	4.72	12
104	104Leu	61.74	2.15	3.07	12
105	105Pro				
106	106Lys	52.43	2.05	8.06	12
107	107Ala	91.21	8.36	3.86	12
108	108Gln	48.05	1.88	3.91	12
109	109Lys	44.81	2.65	3.02	12
110	110Leu				

111	111Tyr				
112	112Leu	43.75	3.45	0.88	12
113	113Thr				
114	114His	46.10	1.75	1.86	12
115	115Ile	51.62	3.36	2.69	12
116	116Asp	49.90	2.01	2.97	12
117	117Ala	56.31	2.59	2.29	12
118	118Glu	48.19	1.35	3.23	12
119	119Val				
120	120Glu	63.87	3.08	5.57	12
121	121Gly	44.96	3.51	1.91	12
122	122Asp	64.36	4.39	1.83	12
123	123Thr				
124	124His	63.35	4.27	1.63	12
125	125Phe	44.31	1.30	2.47	12
126	126Pro				
127	127Asp	54.19	1.74	6.27	12
128	128Tyr	50.14	1.72	3.99	12
129	129Glu	50.58	1.66	2.24	12
130	130Pro				
131	131Asp	51.34	2.19	1.99	12
132	132Asp				
133	133Trp	51.62	2.32	2.42	12
134	134Glu	51.39	1.97	1.16	12
135	135Ser	51.68	1.68	5.48	12
136	136Val	50.09	1.60	2.71	12
137	137Phe	128.37	19.07	10.69	12
138	138Ser	48.78	1.50	2.59	12
139	139Glu	51.30	1.61	2.62	12
140	140Phe	47.89	1.86	4.44	12
141	141His	66.18	3.03	4.00	12
142	142Asp	69.29	2.65	5.93	12
143	143Ala	56.31	1.76	6.38	12
144	144Asp	48.98	1.92	1.67	12
145	145Ala				
146	146Gln	68.92	5.03	4.48	12
147	147Asn	58.78	2.40	4.35	12
148	148Ser	48.37	1.78	3.50	12
149	149His	61.39	3.48	3.97	12
150	150Ser	49.18	1.61	4.22	12
151	151Tyr	49.83	2.18	3.02	12
152	152Cys				

153	153Phe	76.37	7.33	2.04	12
154	154Glu	38.49	2.83	0.78	12
155	155Ile				
156	156Leu	49.05	1.59	1.82	12
157	157Glu				
158	158Arg	57.60	2.09	2.63	12
159	159Arg	59.76	1.48	4.95	12

Table 8.5.2 The T2 values at 900MHz data for EcDHFR: $NADP^{|+}$: folate in the presence of 17% methanol.

8.5.3 T1 Relaxation values of the EcDHFR: $NADP^{+}$: Folate complex in the presence of 17 % methanol co-solvent at 600 MHz

The T1 values at 600MHz for EcDHFR: $NADP^{|+}$: folate in the presence of 17% methanol are presented below **(Table 8.5.3)**. Values for which the SD of the error is greater than 10% of the T1 value are highlighted red and were excluded from the T1 analysis. T1 values were calculated for a total of 120 residues, 13 of these were discounted due to large errors. The average T1 value of the resulting data was calculated (999.94 ms, *s* =79.46 ms, *n* = 107).

No.	Residue	T1 600 MHz 17% MeOD	T1 Error	Fit Error	Number of Peaks
1	1Met				
2	2Ile	874.14	73.95	7.98	12
3	3Ser	944.72	53.60	1.65	12
4	4Leu	1059.47	84.66	1.96	12
5	5Ile				
6	6Ala	972.28	81.06	3.62	12
7	7Ala				
8	8Leu	969.64	68.82	3.80	12
9	9Ala	993.36	92.12	3.41	12
10	10Val	978.90	65.63	4.00	12
11	11Asp	1062.93	51.27	1.50	12
12	12Arg	1018.98	70.40	3.26	12
13	13Val	1037.81	71.87	3.39	12
14	14Ile				
15	15Gly				
16	16Met	888.62	77.24	6.21	12
17	17Glu				
18	18Asn				
19	19Ala	957.46	64.09	4.34	12
20	20Met	923.73	86.20	1.92	12
21	21Pro				
22	22Trp	909.77	79.40	2.73	12
23	23Asn				
24	24Leu	1114.10	46.81	2.03	12
25	25Pro				
26	26Ala	945.95	68.46	3.29	12

27	27Asp	1073.91	86.65	7.63	12
28	28Leu	961.68	51.48	3.31	12
29	29Ala	1088.58	40.31	2.55	12
30	30Trp	1000.83	76.60	4.09	12
31	31Phe	956.13	55.53	3.07	12
32	32Lys	921.90	74.26	5.72	12
33	33Arg	908.75	57.50	5.05	12
34	34Asn	985.81	82.50	4.20	12
35	35Thr	1001.36	46.64	2.20	12
36	36Leu	1033.04	66.85	3.36	12
37	37Asp	1052.60	63.89	5.02	12
38	38Lys	1020.09	64.68	5.54	12
39	39Pro				
40	40Val				
41	41Ile				
42	42Met				
43	43Gly	989.88	126.47	1.24	12
44	44Arg	1056.34	63.02	5.38	12
45	45His				
46	46Thr	979.07	71.11	3.24	12
47	47Trp	985.07	62.04	2.53	12
48	48Glu				
49	49Ser	1002.14	54.44	3.80	12
50	50Ile	970.66	69.90	2.99	12
51	51Gly	1054.55	80.45	4.18	12
52	52Arg	950.90	67.65	4.37	12
53	53Pro				
54	54Leu	1062.71	53.70	3.12	12
55	55Pro				
56	56Gly				
57	57Arg	979.22	55.28	5.70	12
58	58Lys	1083.31	72.51	5.74	12
59	59Asn	935.43	71.91	5.19	12
60	60Ile				
61	61Ile				
62	62Leu				
63	63Ser	1002.75	77.99	7.51	12
64	64Ser	1001.51	73.59	2.28	12
65	65Gln	991.74	51.81	4.18	12
66	66Pro				
67	67Gly	748.25	42.97	3.34	12
68	68Thr	699.07	55.40	1.81	12

69	69Asp	757.06	50.75	6.49	12
70	70Asp	924.79	78.60	6.31	12
71	71Arg	916.28	45.63	3.44	12
72	72Val	983.22	65.79	6.44	12
73	73Thr	1033.37	63.34	4.94	12
74	74Trp	1122.96	61.54	4.75	12
75	75Val	931.85	91.40	0.99	12
76	76Lys	1057.20	55.62	4.95	12
77	77Ser	940.81	48.17	5.27	12
78	78Val	956.66	36.70	2.82	12
79	79Asp	918.92	52.33	6.13	12
80	80Glu	1327.28	55.00	9.48	12
81	81Ala				
82	82Ile	1092.22	31.36	1.86	12
83	83Ala	944.28	42.45	4.30	12
84	84Ala	1017.36	51.19	5.45	12
85	85Cys	1043.39	43.86	2.94	12
86	86Gly	1006.96	36.76	3.32	12
87	87Asp	961.91	71.50	7.70	12
88	88Val	1139.25	52.57	7.99	12
89	89Pro				
90	90Glu	987.04	62.05	5.66	12
91	91Ile	832.94	95.49	0.69	12
92	92Met				
93	93Val				
94	94Ile				
95	95Gly	1016.40	75.48	3.21	12
96	96Gly	1031.73	83.20	4.27	12
97	97Gly				
98	98Arg	1005.95	86.76	3.42	12
99	99Val	1015.86	74.04	3.65	12
100	100Tyr	983.94	78.15	5.51	12
101	101Glu	969.25	54.79	3.91	12
102	102Gln	1073.76	72.02	4.17	12
103	103Phe	989.62	67.32	5.13	12
104	104Leu	1072.83	47.74	1.55	12
105	105Pro				
106	106Lys	1043.05	52.38	5.24	12
107	107Ala	999.04	39.19	1.23	12
108	108Gln	992.01	76.45	5.44	12
109	109Lys	1137.38	22.04	0.68	12
110	110Leu				

111	111Tyr				
112	112Leu	981.68	178.97	1.31	12
113	113Thr				
114	114His	831.48	105.19	5.04	12
115	115Ile	985.02	106.75	5.04	12
116	116Asp	955.09	66.17	4.40	12
117	117Ala	1097.58	63.57	2.72	12
118	118Glu	1212.93	191.86	13.15	12
119	119Val	1007.63	93.55	2.10	12
120	120Glu	1025.99	63.31	5.44	12
121	121Gly	1062.01	64.36	2.31	12
122	122Asp	950.00	79.87	2.23	12
123	123Thr				
124	124His	993.85	111.42	2.73	12
125	125Phe	1012.43	76.75	5.12	12
126	126Pro				
127	127Asp	1106.24	33.01	3.16	12
128	128Tyr	1044.24	14.53	0.98	12
129	129Glu	1001.15	64.91	2.92	12
130	130Pro				
131	131Asp	995.74	61.92	2.56	12
132	132Asp	955.93	68.26	3.72	12
133	133Trp	1062.25	44.34	1.97	12
134	134Glu	1112.28	83.30	1.01	12
135	135Ser	1128.90	94.21	8.71	12
136	136Val	881.77	148.73	8.44	12
137	137Phe	929.66	57.51	3.01	12
138	138Ser	923.89	88.51	6.78	12
139	139Glu	931.83	122.11	7.88	12
140	140Phe	996.26	59.54	5.32	12
141	141His	922.46	95.99	5.86	12
142	142Asp	1006.95	35.29	4.31	12
143	143Ala	996.20	59.76	6.07	12
144	144Asp	1048.72	82.37	3.25	12
145	145Ala				
146	146Gln	1029.18	54.20	2.74	12
147	147Asn	977.68	81.04	4.98	12
148	148Ser	972.07	60.73	3.44	12
149	149His	1041.63	58.40	2.86	12
150	150Ser	979.70	79.22	7.16	12
151	151Tyr	890.55	90.57	5.14	12
152	152Cys				

153	153Phe	888.63	103.96	2.09	12
154	154Glu	749.96	115.88	1.19	12
155	155Ile				
156	156Leu	985.81	33.29	0.93	12
157	157Glu				
158	158Arg	1059.43	15.71	0.65	12
159	159Arg	976.53	28.81	3.08	12

Table 8.5.3 The T1 values at 600MHz for EcDHFR: $NADP^{|+}$: folate in the presence of 17% methanol.

8.5.4 T2 Relaxation values of the EcDHFR: $NADP^+$: Folate complex in the presence of 17 % methanol co-solvent at 600 MHz

The T2 relaxation values at 600MHz for EcDHFR: $NADP^{|+}$: folate in the presence of 17% methanol are presented below **(Table 8.5.4)**. Values for which the SD of the error is greater than 10% of the T2 value are highlighted red and were excluded from the T2 analysis. T2 values for a total of 116 residues were calculated, 5 of these are discounted due to large errors. The average T2 value of the resulting data was calculated (66.39 ms, *s* = 1.40 ms, n = 111).

No.	Residue	T2 600 MHz 17% Methanol	T2 Error	Fit Error	Number of Peaks
1	1Met				
2	2Ile	67.61	2.29	2.54	12
3	3Ser	65.82	3.05	1.14	12
4	4Leu	66.77	3.17	0.86	12
5	5Ile				
6	6Ala	62.61	2.76	1.54	12
7	7Ala				
8	8Leu	60.70	1.90	1.29	12
9	9Ala	58.08	2.75	1.36	12
10	10Val	61.90	1.51	1.13	12
11	11Asp	50.18	2.80	1.20	12
12	12Arg	58.93	1.92	1.06	12
13	13Val	61.87	2.50	1.47	12
14	14Ile				
15	15Gly				
16	16Met	63.50	1.53	1.27	12
17	17Glu				
18	18Asn				
19	19Ala	66.95	1.71	1.31	12
20	20Met	75.19	3.49	0.87	12
21	21Pro				
22	22Trp				
23	23Asn				
24	24Leu	65.79	2.10	1.02	12
25	25Pro				

26	26Ala	57.12	1.81	1.00	12
27	27Asp	63.57	1.72	2.08	12
28	28Leu	61.85	2.05	1.53	12
29	29Ala	78.58	4.86	3.03	12
30	30Trp	61.97	2.40	1.72	12
31	31Phe	57.27	1.61	1.18	12
32	32Lys	57.89	2.11	1.98	12
33	33Arg	66.49	1.41	1.56	12
34	34Asn	64.01	3.18	2.36	12
35	35Thr	63.92	1.59	0.81	12
36	36Leu	59.35	2.36	1.60	12
37	37Asp	74.43	2.22	1.94	12
38	38Lys	69.67	1.97	1.81	12
39	39Pro				
40	40Val				
41	41Ile				
42	42Met				
43	43Gly	50.44	3.38	0.51	12
44	44Arg	59.48	1.90	2.10	12
45	45His				
46	46Thr	67.35	2.58	1.22	12
47	47Trp	76.11	2.89	1.16	12
48	48Glu				
49	49Ser	69.52	2.76	1.92	12
50	50Ile	66.34	2.55	1.29	12
51	51Gly	67.80	2.02	1.50	12
52	52Arg	62.96	1.84	1.45	12
53	53Pro				
54	54Leu	65.49	1.94	1.77	12
55	55Pro				
56	56Gly				
57	57Arg	59.55	1.25	1.53	12
58	58Lys	75.24	2.53	2.41	12
59	59Asn	68.06	2.09	1.72	12
60	60Ile				
61	61Ile				
62	62Leu				
63	63Ser	63.01	2.14	2.57	12
64	64Ser	60.93	1.76	0.77	12
65	65Gln	62.53	1.66	1.48	12
66	66Pro				
67	67Gly	77.10	3.32	2.09	12

68	68Thr	77.35	5.35	1.37	12
69	69Asp	84.96	2.34	2.26	12
70	70Asp	67.60	2.42	2.10	12
71	71Arg	62.27	1.73	1.39	12
72	72Val	59.90	1.76	2.13	12
73	73Thr	64.14	1.94	2.00	12
74	74Trp	61.47	2.01	2.09	12
75	75Val	63.35	4.54	0.48	12
76	76Lys	66.52	1.48	1.63	12
77	77Ser	59.71	2.51	3.35	12
78	78Val	67.06	2.76	2.30	12
79	79Asp	63.42	1.33	1.70	12
80	80Glu	351.24	38.67	13.86	12
81	81Ala				
82	82Ile	75.90	4.46	2.76	12
83	83Ala	66.43	1.22	1.33	12
84	84Ala	67.13	1.70	1.92	12
85	85Cys	69.75	2.42	1.68	12
86	86Gly	59.86	1.51	1.70	12
87	87Asp	71.77	1.79	2.01	12
88	88Val	100.80	3.39	4.64	12
89	89Pro				
90	90Glu	62.05	1.98	2.33	12
91	91Ile	70.86	20.56	0.73	12
92	92Met				
93	93Val				
94	94Ile				
95	95Gly	44.05	1.74	1.40	12
96	96Gly	63.57	1.51	1.06	12
97	97Gly				
98	98Arg	61.31	3.34	1.73	12
99	99Val	64.60	3.07	1.81	12
100	100Tyr	58.32	1.57	1.36	12
101	101Glu	66.38	1.72	1.39	12
102	102Gln	61.05	4.13	3.27	12
103	103Phe	72.62	2.06	1.70	12
104	104Leu	90.63	8.93	2.04	12
105	105Pro				
106	106Lys	68.25	1.45	1.75	12
107	107Ala	113.59	9.41	1.88	12
108	108Gln	61.31	1.94	1.74	12
109	109Lys	76.43	3.31	0.97	12

110	110Leu				
111	111Tyr				
112	112Leu	62.67	6.28	0.76	12
113	113Thr				
114	114His	56.30	4.38	3.00	12
115	115Ile	58.85	4.86	3.77	12
116	116Asp	63.33	2.95	2.27	12
117	117Ala	71.68	2.74	1.41	12
118	118Glu	61.49	2.03	2.39	12
119	119Val				
120	120Glu	74.55	2.06	2.04	12
121	121Gly	50.15	1.93	0.88	12
122	122Asp	65.17	1.75	0.57	12
123	123Thr				
124	124His	64.82	3.76	1.18	12
125	125Phe	62.51	1.71	1.40	12
126	126Pro				
127	127Asp	67.30	1.62	2.27	12
128	128Tyr	73.84	6.09	3.14	12
129	129Glu	66.44	3.24	1.85	12
130	130Pro				
131	131Asp	72.53	1.52	0.63	12
132	132Asp				
133	133Trp	64.37	2.21	1.09	12
134	134Glu	59.76	5.64	0.84	12
135	135Ser	65.35	2.19	2.99	12
136	136Val	67.22	2.69	1.63	12
137	137Phe	66.59	6.61	5.18	12
138	138Ser	57.76	3.79	4.11	12
139	139Glu	60.46	5.02	5.24	12
140	140Phe	65.07	2.75	2.96	12
141	141His	63.66	4.63	4.40	12
142	142Asp	84.40	2.32	2.24	12
143	143Ala	69.14	2.49	3.07	12
144	144Asp	60.15	2.32	1.20	12
145	145Ala				
146	146Gln	89.53	2.79	1.24	12
147	147Asn	67.15	2.02	1.36	12
148	148Ser	60.65	1.93	1.43	12
149	149His	51.04	1.40	0.77	12
150	150Ser	65.51	1.96	2.06	12
151	151Tyr	56.72	3.33	2.53	12

152	152Cys				
153	153Phe	68.09	6.84	1.75	12
154	154Glu	53.35	6.04	1.00	12
155	155Ile				
156	156Leu	83.31	12.04	1.96	12
157	157Glu				
158	158Arg	90.18	3.71	1.15	12
159	159Arg	81.89	2.22	2.20	12

Table 8.5.4 The T2 relaxation values at 600MHz for EcDHFR: $NADP^{|+}$: folate in the presence of 17% methanol.

8.6 Heteronuclear NOE values and comparison of the EcDHFR: $NADP^+$: Folate complex in the presence of buffer and co-solvents

8.6.1 Heteronuclear NOE values for EcDHFR:folate:$NADP^+$ complex in buffer at 600 MHz and 900 MHz

Resonances	600 MHz hetNOE Buffer	SD	900 MHz hetNOE Buffer	SD
2IleN 2IleH	0.78624	0.01337	0.86473	0.00777
3SerN 3SerH	0.74826	0.02472	0.82719	0.01092
4LeuN 4LeuH	0.83366	0.01342	0.8778	0.01092
5IleN 5IleH	0.82409	0.04819	0.87697	0.03181
6AlaN 6AlaH	0.85987	0.01747	0.85043	0.01478
8LeuN 8LeuH	0.8034	0.02072	0.83213	0.01314
9AlaN 9AlaH	0.79733	0.02248	0.78153	0.02691
10ValN 10ValH	0.79098	0.01625	0.86776	0.01369
11AspN 11AspH	0.77596	0.01504	0.8137	0.02451
12ArgN 12ArgH			0.83205	0.01609
13ValN 13ValH	0.78386	0.01953	0.84519	0.01504
16MetN 16MetH	0.79941	0.01924	0.85007	0.0116
19AlaN 19AlaH	0.69198	0.01519	0.81459	0.00975
20MetN 20MetH	0.55263	0.03061	0.67127	0.03315
26AlaN 26AlaH	0.82183	0.01064	0.86016	0.01167
27AspN 27AspH	0.78187	0.01643	0.84152	0.01013
28LeuN 28LeuH	0.79883	0.0086	0.8828	0.01017
29AlaN 29AlaH	0.79604	0.01378	0.90723	0.01292
30TrpN 30TrpH	0.81998	0.01183	0.83039	0.01154
31PheN 31PheH	0.79905	0.02036	0.89993	0.01217
32LysN 32LysH	0.8355	0.01606	0.82491	0.00915
33ArgN 33ArgH	0.79349	0.01822	0.85068	0.01077
34AsnN 34AsnH	0.79709	0.01727	0.81346	0.00953
35ThrN 35ThrH	0.81223	0.01216	0.83026	0.00876
36LeuN 36LeuH	0.81572	0.01269	0.85999	0.00986
37AspN 37AspH	0.8105	0.01118	0.87481	0.00875

38LysN 38LysH	0.79553	0.00869	0.83346	0.00626
41IleN 41IleH	0.68559	0.05742	0.65712	0.0673
43GlyN 43GlyH	0.90942	0.05752	0.85958	0.03755
46ThrN 46ThrH	0.85116	0.0354	0.82304	0.01991
47TrpN 47TrpH	0.7571	0.02636	0.81735	0.02087
49SerN 49SerH	0.7982	0.01675	0.83447	0.00909
50IleN 50IleH	0.78105	0.02121	0.8432	0.01559
51GlyN 51GlyH	0.74678	0.01468	0.83246	0.00921
52ArgN 52ArgH	0.75703	0.01464	0.80946	0.01127
54LeuN 54LeuH	0.80802	0.01802	0.86822	0.00926
57ArgN 57ArgH	0.82192	0.00613	0.87876	0.00542
58LysN 58LysH	0.79767	0.0068	0.87183	0.0078
59AsnN 59AsnH	0.84123	0.01422	0.82338	0.0117
60IleN 60IleH	0.85036	0.04251	0.9648	0.05202
61IleN 61IleH	0.84254	0.06383	0.93419	0.07481
62LeuN 62LeuH	0.61632	0.05168	0.78232	0.04851
63SerN 63SerH	0.80524	0.00783	0.90079	0.00766
64SerN 64SerH	0.81929	0.01354	0.89561	0.0121
65GlnN 65GlnH	0.79772	0.00743	0.8498	0.00698
67GlyN 67GlyH	0.66316	0.01104	0.70473	0.01423
68ThrH 68ThrN			0.52839	0.01867
69AspN 69AspH	0.41496	0.00514	0.52762	0.00548
70AspN 70AspH	0.77726	0.00758	0.8122	0.00703
71ArgN 71ArgH	0.82382	0.01121	0.84984	0.00856
72ValN 72ValH	0.77461	0.0064	0.84874	0.00531
73ThrN 73ThrH	0.8055	0.0077	0.8928	0.00758
74TrpN 74TrpH	0.82931	0.00801	0.87314	0.00615
75ValN 75ValH	0.84385	0.04318	0.84998	0.03868
76LysN 76LysH	0.77754	0.00654	0.80784	0.00522
77SerN 77SerH	0.83202	0.00668	0.89169	0.00544
78ValN 78ValH	0.85941	0.00813	0.8717	0.00546
79AspN 79AspH	0.82427	0.00668	0.85858	0.00583
80GluN 80GluH	0.78385	0.00655	0.84139	0.00512
81AlaN 81AlaH	0.79696	0.01985	0.82944	0.0193
82IleN 82IleH	0.81292	0.0058	0.86212	0.00534
83AlaN 83AlaH	0.77884	0.00496	0.92168	0.00474

84AlaN 84AlaH	0.77914	0.00587	0.85234	0.00521
85CysN 85CysH	0.8188	0.00593	0.87459	0.00588
86GlyN 86GlyH	0.8266	0.00615	0.88641	0.00553
87AspN 87AspH	0.78754	0.00644	0.77454	0.00601
88ValN 88ValH	0.78613	0.01752	0.82925	0.01016
91IleN 91IleH	0.87519	0.02677	0.88301	0.03283
93ValN 93ValH	0.24781	0.02938	0.05673	0.05575
			0.93533	0.01052
96GlyN 96GlyH	0.85051	0.01995	0.84576	0.01079
98ArgN 98ArgH	0.79835	0.02468	0.90488	0.0171
99ValN 99ValH	0.82592	0.01636	0.92753	0.00976
100TyrN 100TyrH	0.88708	0.01991	0.89653	0.01128
101GluN 101GluH	0.81547	0.00785	0.84978	0.00655
102GlnN 102GlnH	0.61577	0.00381	0.66824	0.00339
104LeuN 104LeuH	0.69408	0.00576	0.92493	0.01115
107AlaN 107AlaH	0.77798	0.02257	0.85453	0.01239
108GlnN 108GlnH	0.83084	0.01029	0.8855	0.00964
109LysN 109LysH	0.79943	0.00944	0.89737	0.00971
110LeuN 110LeuH	0.81477	0.01662	0.84944	0.01674
111TyrN 111TyrH	0.85806	0.0671	0.90754	0.02983
112LeuN 112LeuH	0.69938	0.05958	0.88047	0.03511
114HisN 114HisH	0.81897	0.0126	0.91112	0.0188
116AspN 116AspH	0.80879	0.01217	0.84898	0.011
120GluN 120GluH	0.60416	0.01209	0.71852	0.00869
122AspN 122AspH	0.79692	0.02634	0.84548	0.02721
125PheN 125PheH	0.82159	0.01464	0.91886	0.01222
127AspN 127AspH	0.7936	0.00981	0.79756	0.00533

129GluN 129GluH	0.71026	0.00971	0.75763	0.01132
131AspH 131AspN			0.7733	0.01699
132AspN 132AspH	0.83091	0.00768	0.83694	0.00591
133TrpN 133TrpH	0.7827	0.00658	0.79761	0.01529
134GluN 134GluH	0.7885	0.01302	0.88163	0.01644
135SerN 135SerH	0.75655	0.00554	0.83666	0.00853
136ValN 136ValH	0.80181	0.01988	0.81869	0.0132
137PheN 137PheH	0.7758	0.0083	0.84848	0.01076
138SerN 138SerH	0.80145	0.00768	0.82477	0.0107
139GluN 139GluH	0.80269	0.00957	0.85424	0.01117
141HisN 141HisH	0.7478	0.0078	0.85507	0.00963
142AspN 142AspH	0.71665	0.00556	0.7809	0.00474
143AlaN 143AlaH	0.66403	0.00571	0.79725	0.00494
144AspN 144AspH	0.81384	0.02077	0.87898	0.01254
145AlaN 145AlaH	0.77752	0.0141	0.88314	0.01093
147AsnN 147AsnH	0.7888	0.01182	0.81393	0.00958
149HisN 149HisH	0.62114	0.00633	0.67566	0.00673
150SerN 150SerH	0.8071	0.00829	0.80797	0.00742
152CysN 152CysH	0.72817	0.00852	0.86493	0.01266
153PheN 153PheH	0.7718	0.01164	0.85194	0.01825
154GluN 154GluH	0.80054	0.02139	0.85316	0.02612
157GluN 157GluH	0.81427	0.01486	0.84778	0.01407
158ArgN 158ArgH	0.80156	0.00959	0.85081	0.01015
159ArgN 159ArgH	0.65554	0.00543	0.76387	0.00499

Table 8.6.1 Heteronuclear NOE values for EcDHFR:folate:$NADP^+$ complex in buffer only

8.6.2 Heteronuclear NOE values for EcDHFR:folate:NADP$^+$ complex in 17 % methanol at 600 MHz and 900 MHz

Resonances	900 MHz hetNOE 17% Methanol	SD	600 MHz hetNOE 17% Methanol	SD
2IleH 2IleN	0.81155	0.00771	0.76836	0.01126
3SerH 3SerN	0.84208	0.04529	0.85785	0.02062
4LeuH 4LeuN	0.83282	0.0312	0.82011	0.044
5IleH 5IleN			0.59611	0.0897
6AlaH 6AlaN	0.86288	0.021	0.79618	0.02663
8LeuH 8LeuN	0.88609	0.01525	0.79695	0.01805
9AlaH 9AlaN	0.85845	0.02999	0.75128	0.02725
10ValH 10ValN	0.82653	0.01394	0.79682	0.01879
11AspH 11AspN	0.78187	0.02152	0.77532	0.02539
12ArgH 12ArgN	0.82353	0.01866	0.74201	0.02133
13ValH 13ValN	0.92847	0.01901	0.78576	0.02087
15GlyH 15GlyN	0.8274	0.09035	0.63941	0.09929
16MetH 16MetN	0.80217	0.0118	0.75075	0.01578
18AsnH 18AsnN				
19AlaH 19AlaN	0.81175	0.01103	0.74543	0.01763
20MetH 20MetN	0.71759	0.04419	0.66878	0.04047
22TrpH 22TrpN	0.43001	0.05245	0.5919	0.06384
23AsnH 23AsnN	0.89818	0.04391	0.89884	0.05434
24LeuH 24LeuN	0.83029	0.01919	0.72691	0.01999
26AlaH 26AlaN	0.88028	0.0188	0.83839	0.02464
27AspH 27AspN	0.83757	0.01037	0.49929	0.00761
28LeuH 28LeuN	0.82594	0.01007	0.80994	0.01803
29AlaH 29AlaN	0.94132	0.01451	0.73513	0.01525
30TrpH 30TrpN	0.85279	0.01294	0.82605	0.0214
31PheH 31PheN	0.85793	0.01154	0.85271	0.01889
32LysH 32LysN	0.8658	0.0094	0.8275	0.01634
33ArgH 33ArgN	0.95484	0.00833	0.80376	0.01066
34AsnH 34AsnN	0.86446	0.00973	0.8226	0.0193
35ThrH 35ThrN	0.88305	0.01115	0.82973	0.01988
36LeuH 36LeuN	0.8865	0.01248	0.82446	0.01966
37AspH 37AspN	0.83199	0.00864	0.77702	0.0136
38LysH 38LysN	0.84004	0.0085	0.79212	0.01291

43GlyH 43GlyN				
44ArgH 44ArgN	0.86953	0.0082	0.78453	0.01329
46ThrH 46ThrN	0.81099	0.0221	0.73273	0.02472
47TrpH 47TrpN	0.81525	0.02173	0.67266	0.024
49SerH 49SerN	0.80119	0.00891	0.77657	0.01581
50IleH 50IleN	0.84467	0.01852	0.82507	0.02652
51GlyH 51GlyN	0.80102	0.01102	0.76867	0.01705
52ArgH 52ArgN	0.81617	0.01175	0.7173	0.01561
54LeuH 54LeuN	0.867	0.00994	0.85673	0.01484
56GlyH 56GlyN	0.8188	0.01356	0.92574	0.04048
57ArgH 57ArgN	0.84884	0.00654	0.80944	0.01036
58LysH 58LysN	0.76826	0.00737	0.73657	0.0113
59AsnH 59AsnN	0.84703	0.01098	0.82929	0.01624
63SerH 63SerN	0.8923	0.00813	0.82056	0.01287
64SerH 64SerN	0.88543	0.01662	0.88859	0.0286
65GlnH 65GlnN	0.8312	0.00972	0.7659	0.0124
67GlyH 67GlyN	0.69137	0.01742	0.62134	0.01709
68ThrH 68ThrN	0.50845	0.01807	0.41559	0.02093
69AspH 69AspN	0.50077	0.00507	0.38551	0.00703
70AspH 70AspN	0.76196	0.00871	0.7732	0.01344
71ArgH 71ArgN	0.84625	0.00986	0.81761	0.01513
72ValH 72ValN	0.81647	0.00676	0.8272	0.01214
73ThrH 73ThrN	0.84852	0.00975	0.80155	0.01399
74TrpH 74TrpN	0.84094	0.00802	0.80668	0.01129
75ValH 75ValN				
76LysH 76LysN	0.82121	0.00713	0.789	0.01111
77SerH 77SerN	0.84863	0.00623	0.86375	0.01194
78ValH 78ValN	0.87814	0.00754	0.84366	0.01246
79AspH 79AspN	0.85694	0.0071	0.802	0.00921
80GluH 80GluN			0.20565	0.00241
82IleH 82IleN	0.95276	0.01296	0.80983	0.01179
83AlaH 83AlaN	0.89531	0.00699	0.8341	0.01052
84AlaH 84AlaN	0.84215	0.00612	0.82512	0.00979
85CysH 85CysN	0.81241	0.00763	0.85489	0.01457

86GlyH 86GlyN	0.82639	0.00681	0.80659	0.01058
87AspH 87AspN	0.70441	0.00622	0.72586	0.00862
88ValH 88ValN	0.50649	0.00271	0.51355	0.00476
90GluH 90GluN	0.84182	0.0076	0.78294	0.0127
91IleH 91IleN				
95GlyH 95GlyN	0.87073	0.01105	0.86917	0.01918
96GlyH 96GlyN	0.8469	0.0121	0.84321	0.02124
98ArgH 98ArgN	0.86054	0.01934	0.8942	0.0288
99ValH 99ValN	0.90043	0.01177	0.7382	0.01751
100TyrH 100TyrN	0.88523	0.0098	0.85558	0.01683
101GluH 101GluN	0.88119	0.0097	0.8193	0.01493
102GlnH 102GlnN	0.847	0.01056	0.80255	0.01803
103PheH 103PheN	0.78382	0.00784	0.80292	0.01516
104LeuH 104LeuN	0.88105	0.02926	0.8158	0.02422
106LysH 106LysN	0.78692	0.0058	0.77747	0.00869
107AlaH 107AlaN	0.80116	0.03792	0.68514	0.03553
108GlnH 108GlnN	0.86835	0.01036	0.81205	0.01605
109LysH 109LysN	0.90101	0.03104	0.68305	0.02766
111TyrH 111TyrN	0.51668	0.07427		
112LeuH 112LeuN				
114HisH 114HisN	0.87344	0.0178	0.84542	0.033
115IleH 115IleN	0.7448	0.01412	0.86027	0.02467
116AspH 116AspN	0.86632	0.01295	0.80049	0.01723
117AlaH 117AlaN	0.83256	0.02022	0.75269	0.02197
118GluH 118GluN	0.77607	0.00843	0.73296	0.01158
119ValH 119ValN	0.71163	0.04401	0.63272	0.03923
120GluH 120GluN	0.74569	0.00945	0.56301	0.01062
121GlyH 121GlyN	0.53642	0.01894	0.38964	0.01625
122AspH 122AspN	0.85149	0.0339	0.74264	0.03691
123ThrH 123ThrN	0.72228	0.04698	0.89818	0.08147
124HisH 124HisN	0.71828	0.03559	0.85431	0.06559
125PheH 125PheN	0.83983	0.01053	0.83822	0.01631
127AspH 127AspN	0.7837	0.01135	0.38418	0.0055
128TyrH 128TyrN	0.42553	0.00444	0.71949	0.01486
129GluH 129GluN	0.69017	0.01166	0.64254	0.01751
131AspH 131AspN	0.7372	0.01613	0.63211	0.01987

132AspH 132AspN	0.74212	0.01065	0.78897	0.02042
133TrpH 133TrpN	0.77417	0.01411	0.72662	0.02156
134GluH 134GluN	0.836	0.05475	0.83439	0.06686
135SerH 135SerN	0.7723	0.00547	0.70389	0.00852
136ValH 136ValN	0.94637	0.02833	0.82092	0.02744
137PheH 137PheN	0.83084	0.01126	0.74665	0.02295
138SerH 138SerN	0.85477	0.01032	0.78607	0.01849
139GluH 139GluN	0.84334	0.01094	0.7593	0.02128
140PheH 140PheN	0.85871	0.00983	0.7996	0.01271
141HisH 141HisN	0.87366	0.0102	0.35858	0.01135
142AspH 142AspN	0.84153	0.00843	0.71247	0.00929
143AlaH 143AlaN	0.79817	0.00711	0.6676	0.00959
144AspH 144AspN	0.85977	0.02072	0.8547	0.02695
146GlnH 146GlnN	0.89839	0.01786	0.85616	0.02419
147AsnH 147AsnN	0.80529	0.01076	0.73603	0.01668
148SerH 148SerN	0.79227	0.01022	0.77398	0.01713
149HisH 149HisN	0.7583	0.01123	0.78719	0.01977
150SerH 150SerN	0.86562	0.00888	0.81615	0.01455
151TyrH 151TyrN	0.87574	0.01242	0.83465	0.02165
152CysH 152CysN			0.46137	0.08107
153PheH 153PheN	0.76018	0.03542	0.68606	0.06682
154GluH 154GluN	0.76387	0.08493		
156LeuH 156LeuN	0.92181	0.04852	0.78646	0.03108
157GluH 157GluN	0.83063	0.05715	0.83616	0.0886
158ArgH 158ArgN	0.77673	0.01968	0.80242	0.02127
159ArgH 159ArgN	0.7685	0.00668	0.66397	0.00895

Table 8.6.2 Heteronuclear NOE values for EcDHFR:folate:$NADP^+$ complex in the presence of 17% methanol measuredat 600 and 900 MHZ.

8.6.3 Heteronuclear NOE values for EcDHFR:folate:$NADP^+$ complex in 17 % glycerol at 600 MHz and 900 MHz

Resonances	600 MHz hetNOE 17% glycerol co-solvent	SD	900 MHz hetNOE 17% glycerol co-solvent	SD
2IleN 2IleH	0.79663	0.00724	0.88374	0.02446
3SerN 3SerH	0.82481	0.01768	0.84434	0.03713
4LeuN 4LeuH	0.89208	0.01855	0.89161	0.04115
5IleN 5IleH	0.802	0.05321		
6AlaN 6AlaH	0.79965	0.02526	0.90772	0.05071
8LeuN 8LeuH	0.85087	0.01163	0.89444	0.04289
9AlaN 9AlaH	0.81924	0.01296	0.83538	0.07475
10ValN 10ValH	0.79906	0.009	0.87724	0.03843
11AspN 11AspH	0.80169	0.02034	0.8139	0.05432
12ArgN 12ArgH	0.7953	0.0136	0.81282	0.05791
13ValN 13ValH	0.81825	0.01174	0.90266	0.05337
16MetN 16MetH	0.77829	0.01007	0.81763	0.04224
18AsnN 18AsnH	0.69207	0.07984		
19AlaN 19AlaH	0.7247	0.00861	0.77658	0.02987
20MetN 20MetH	0.64979	0.01632	0.70124	0.07254
22TrpN 22TrpH	-0.0768	0.00992	0.22882	0.04873
24LeuN 24LeuH	0.69212	0.01227	0.82575	0.07275
26AlaN 26AlaH	0.83508	0.01384	0.86798	0.05202
27AspN 27AspH	0.73674	0.00916	0.5488	0.01918
28LeuN 28LeuH	0.84525	0.00991	0.85592	0.03336
29AlaN 29AlaH	0.81811	0.01052	0.88997	0.03949
30TrpN 30TrpH	0.79352	0.01131	0.91192	0.05085
31PheN 31PheH	0.83722	0.01391	0.86128	0.03919
32LysN 32LysH	0.83203	0.00976	0.85531	0.03137
33ArgN 33ArgH	0.81325	0.00979	0.88198	0.03791
34AsnN 34AsnH	0.81381	0.01092	0.91508	0.04135
35ThrN 35ThrH	0.77594	0.01384	0.88174	0.04735
36LeuN 36LeuH	0.83103	0.01061	0.89974	0.03662
37AspN 37AspH	0.78596	0.00879	0.81129	0.0257
38LysN 38LysH	0.79	0.00751	0.87044	0.02596

41IleN 41IleH				
42MetN 42MetH	0.80601	0.0703		
43GlyN 43GlyH	0.80318	0.05317		
44ArgN 44ArgH	0.82439	0.00801	0.81575	0.02616
45HisN 45HisH	0.76407	0.00699	0.85188	0.01411
46ThrN 46ThrH				
47TrpN 47TrpH			0.87401	0.07506
49SerN 49SerH	0.78507	0.01143	0.7816	0.03213
50IleN 50IleH	0.80023	0.01161	0.84136	0.05252
51GlyN 51GlyH	0.72753	0.00829	0.82252	0.03114
52ArgN 52ArgH	0.71013	0.00892	0.73408	0.02782
54LeuN 54LeuH	0.80394	0.00868	0.84928	0.03401
56GlyN 56GlyH				
57ArgN 57ArgH	0.81017	0.00719	0.80718	0.0187
58LysN 58LysH	0.74828	0.00612	0.72502	0.01714
59AsnN 59AsnH	0.79775	0.01063	0.74063	0.09514
60IleN 60IleH				
61IleN 61IleH				
62LeuN 62LeuH	0.72538	0.05553		
63SerN 63SerH	0.81211	0.00676	0.86575	0.02508
64SerN 64SerH	0.84832	0.02332	0.87646	0.07309
65GlnN 65GlnH	0.76539	0.0091	0.80973	0.03475
67GlyN 67GlyH	0.62095	0.00941	0.65492	0.04695
68ThrN 68ThrH	0.3535	0.0143	0.53571	0.06598
69AspN 69AspH	0.36506	0.00506	0.54296	0.02039
70AspN 70AspH	0.74813	0.00824	0.71156	0.02536
71ArgN 71ArgH	0.78111	0.00999	0.82099	0.02877
72ValN 72ValH	0.78874	0.00729	0.82573	0.02262
73ThrN 73ThrH	0.81443	0.00817	0.85111	0.02849
74TrpN 74TrpH	0.78447	0.00849	0.83515	0.02342
75ValN 75ValH				
76LysN 76LysH	0.77095	0.00745	0.76541	0.01738
77SerN 77SerH	0.84463	0.0072	0.8578	0.02213
78ValN 78ValH	0.84473	0.00973	0.87157	0.02268
79AspN 79AspH	0.82607	0.00723	0.82343	0.02257
80GluN 80GluH	0.76139	0.00684	0.87885	0.02117
81AlaN 81AlaH	0.65237	0.08512	0.76867	0.07651
82IleN 82IleH	0.83734	0.01394	0.92306	0.02007
83AlaN 83AlaH	0.84773	0.00733	0.91428	0.01951
84AlaN 84AlaH	0.80334	0.00657	0.88044	0.0189
85CysN 85CysH	0.80769	0.00947	0.8668	0.02918
86GlyN 86GlyH	0.81479	0.00734	0.84379	0.02164

87AspN 87AspH	0.71603	0.00599	0.62077	0.01481
88ValN 88ValH	0.461	0.0031	0.40726	0.00822
90GluN 90GluH	0.79922	0.00758	0.83697	0.0205
91IleN 91IleH	0.45456	0.09946	0.81007	0.02663
92MetN 92MetH	0.61569	0.07185	0.84696	0.0531
93ValN 93ValH			0.9151	0.05169
94IleN 94IleH				
95GlyN 95GlyH	0.85817	0.00903	0.9572	0.03232
96GlyN 96GlyH	0.81587	0.01269	0.85489	0.04197
98ArgN 98ArgH	0.81782	0.01487	0.90905	0.05671
99ValN 99ValH	0.80658	0.01012	0.8948	0.03222
100TyrN 100TyrH	0.82471	0.00866	0.94729	0.03536
101GluN 101GluH	0.82507	0.00966	0.91794	0.0333
102GlnN 102GlnH	0.82714	0.00968	0.89205	0.03437
103PheN 103PheH	0.7803	0.00897	0.81204	0.03072
104LeuN 104LeuH	0.62688	0.0071		
106LysN 106LysH	0.80349	0.00442		
107AlaN 107AlaH	0.77629	0.02165	0.93786	0.02504
108GlnN 108GlnH	0.79733	0.00946	0.93491	0.03891
109LysN 109LysH	0.82616	0.01974	0.85293	0.04657
110LeuN 110LeuH	0.83387	0.02506	0.87763	0.05291
111TyrN 111TyrH	0.92496	0.06705		
112LeuN 112LeuH	0.89567	0.04539		
113ThrN 113ThrH	0.81223	0.01662		
114HisN 114HisH	0.74445	0.01003	0.80104	0.03004
115IleN 115IleH	0.85474	0.01119	0.87597	0.03713
116AspN 116AspH	0.79505	0.00816	0.88929	0.03218
117AlaN 117AlaH	0.73468	0.01095	0.82833	0.04853
118GluN 118GluH	0.74736	0.00634	0.72278	0.0228
119ValN 119ValH	0.68556	0.01863	0.59739	0.08849
120GluN 120GluH	0.56819	0.00505	0.66193	0.01595
121GlyN 121GlyH	0.4755	0.00883	0.4975	0.04518
122AspN 122AspH	0.78135	0.01855	0.69987	0.08777
123ThrN 123ThrH				
124HisN 124HisH			0.8102	0.03092
125PheN 125PheH	0.82918	0.00981	0.82983	0.02637
127AspN 127AspH	0.70835	0.00596	0.68997	0.0173
128TyrN 128TyrH	0.28372	0.00459	0.83797	0.02205
129GluN 129GluH	0.64117	0.01065	0.64095	0.02877
131AspN 131AspH	0.67643	0.01362	0.69497	0.03317
132AspN 132AspH	0.80435	0.00827	0.75676	0.03493

133TrpN 133TrpH	0.72125	0.01251	0.72371	0.03892
134GluN 134GluH	0.71609	0.04468		
135SerN 135SerH	0.71804	0.0061	0.71403	0.02292
136ValN 136ValH	0.72712	0.04606	0.82337	0.03926
137PheN 137PheH	0.74852	0.00895	0.87138	0.02812
138SerN 138SerH	0.8134	0.00689	0.81812	0.0769
139GluN 139GluH	0.78961	0.00763	0.79467	0.09114
140PheN 140PheH	0.76848	0.00698	0.80116	0.08273
141HisN 141HisH	0.80982	0.00785	0.72125	0.06703
142AspN 142AspH	0.6432	0.00502	0.72006	0.01324
143AlaN 143AlaH	0.72462	0.00683	0.77322	0.01795
144AspN 144AspH	0.80733	0.01181	0.78419	0.05041
145AlaN 145AlaH	0.80665	0.00934	0.7771	0.01869
146GlnN 146GlnH	0.75625	0.00946	0.76049	0.03034
147AsnN 147AsnH	0.7547	0.0123	0.79061	0.03958
148SerN 148SerH	0.75526	0.01149	0.77147	0.03589
149HisN 149HisH	0.69171	0.00935	0.51943	0.0228
150SerN 150SerH	0.78878	0.00837	0.81439	0.02995
151TyrN 151TyrH	0.82638	0.00824	0.82066	0.02684
152CysN 152CysH	0.81961	0.00933	0.81788	0.08825
153PheN 153PheH	0.83607	0.01597		
154GluN 154GluH	0.85218	0.03565		
155IleN 155IleH	0.63432	0.03003		
156LeuN 156LeuH				
157GluN 157GluH	0.78087	0.0288	0.88582	0.08008
158ArgN 158ArgH	0.76507	0.01515	0.79681	0.02807
159ArgN 159ArgH	0.65804	0.00601	0.67847	0.01452

Table 8.6.3 Heteronuclear NOE values for EcDHFR:folate:$NADP^+$ complex in the presence of 17% glycerol co-solvent at 600 and 900 MHz

8.6.4 Comaprison of the heteronuclear NOE values for EcDHFR:folate:NADP$^+$ complex in buffer only and the presence of co-solvents 600 MHz and 900 MHz

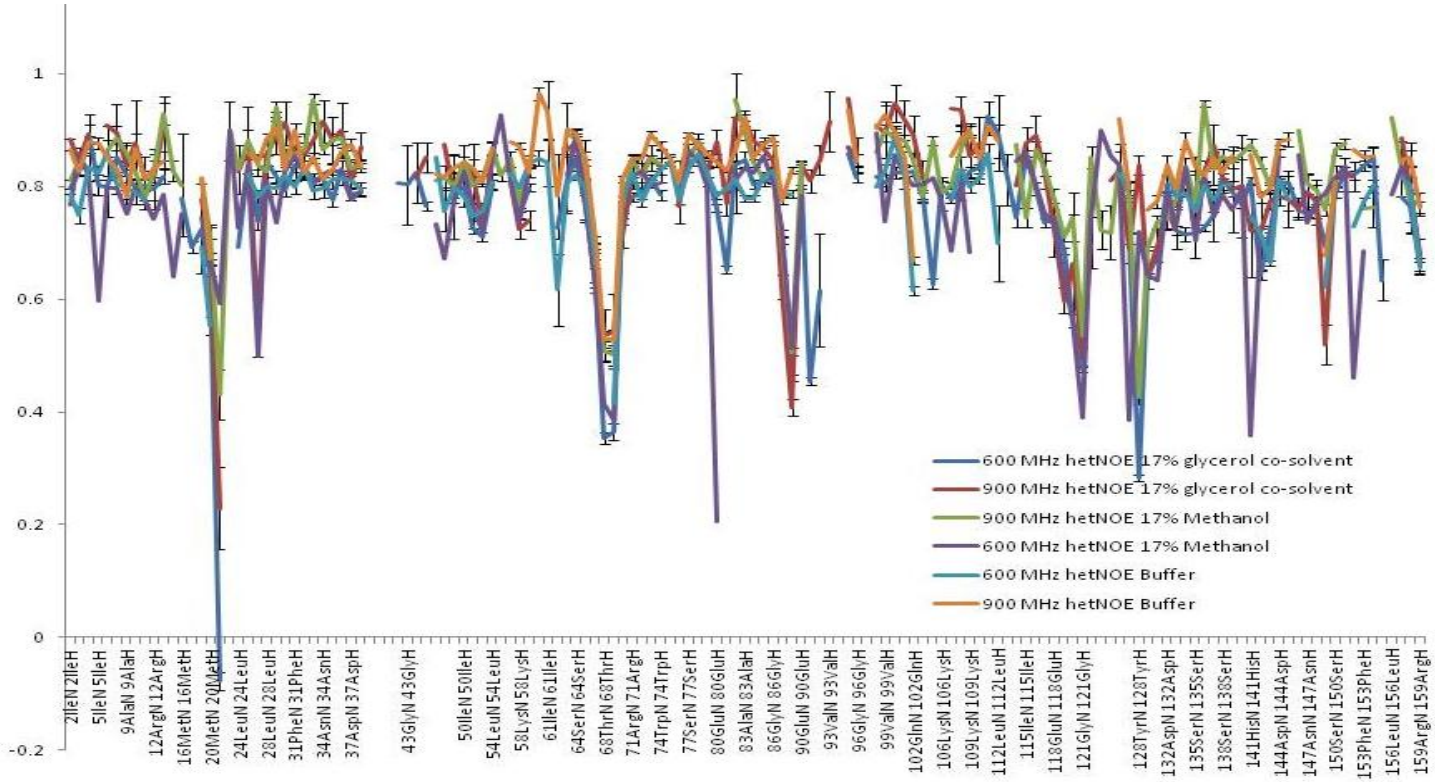

Figure 6.1 Graph to show heteronuclear NOE values at 600 MHz and 900 MHz for all backbone amide residues of EcDHFR: NADP$^+$: Folate complex in the presence of 17% glycerol and 17% methanol co-solvents and in the absence of co-solvent (buffer only).

8.7 T1/T2 values for EcDHFR:folate:$NADP^+$ complex in buffer only and the presence of co-solvents 600 MHz and 900 MHz

8.7.1 T1/T2 values for EcDHFR:folate:$NADP^+$ complex in the presence of 17% methanol co-solvent at 600 MHz

The T1/T2 values for EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 600 MHz are presented below (**Table 8.7.1.1)**. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below **(Table 8.7.1.2**). The residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 600 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio are presented in **Table 8.7.1.3** and residues which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio are showed in **Table 8.7.1.4**.

17% MeOD	T1 600 MHz	T1 Error	T1 % error	T2	T2 Error	T2 % error	T1/T2	T1/T2
1Met								
2Ile	874.14	73.95	8.46	67.61	2.29	3.38	12.93	12.93
3Ser	944.72	53.60	5.67	65.82	3.05	4.64	14.35	14.35
4Leu	1059.47	84.66	7.99	66.77	3.17	4.74	15.87	15.87
5Ile								
6Ala	972.28	81.06	8.34	62.61	2.76	4.40	15.53	15.53
7Ala								
8Leu	969.64	68.82	7.10	60.70	1.90	3.14	15.97	15.97
9Ala	993.36	92.12	9.27	58.08	2.75	4.73	17.10	17.10
10Val	978.90	65.63	6.70	61.90	1.51	2.44	15.81	15.81
11Asp	1062.93	51.27	4.82	50.18	2.80	5.58	21.18	21.18
12Arg	1018.98	70.40	6.91	58.93	1.92	3.25	17.29	17.29
13Val	1037.81	71.87	6.93	61.87	2.50	4.05	16.77	16.77

14Ile								
15Gly								
16Met	888.62	77.24	8.69	63.50	1.53	2.41	13.99	13.99
17Glu								
18Asn								
19Ala	957.46	64.09	6.69	66.95	1.71	2.55	14.30	14.30
20Met	923.73	86.20	9.33	75.19	3.49	4.65	12.29	12.29
21Pro								
22Trp	909.77	79.40	8.73					
23Asn								
24Leu	1114.10	46.81	4.20	65.79	2.10	3.19	16.94	16.94
25Pro								
26Ala	945.95	68.46	7.24	57.12	1.81	3.17	16.56	16.56
27Asp	1073.91	86.65	8.07	63.57	1.72	2.70	16.89	16.89
28Leu	961.68	51.48	5.35	61.85	2.05	3.32	15.55	15.55
29Ala	1088.58	40.31	3.70	78.58	4.86	6.19	13.85	13.85
30Trp	1000.83	76.60	7.65	61.97	2.40	3.88	16.15	16.15
31Phe	956.13	55.53	5.81	57.27	1.61	2.82	16.70	16.70
32Lys	921.90	74.26	8.05	57.89	2.11	3.64	15.92	15.92
33Arg	908.75	57.50	6.33	66.49	1.41	2.13	13.67	13.67
34Asn	985.81	82.50	8.37	64.01	3.18	4.96	15.40	15.40
35Thr	1001.36	46.64	4.66	63.92	1.59	2.48	15.67	15.67
36Leu	1033.04	66.85	6.47	59.35	2.36	3.98	17.40	17.40
37Asp	1052.60	63.89	6.07	74.43	2.22	2.98	14.14	14.14
38Lys	1020.09	64.68	6.34	69.67	1.97	2.82	14.64	14.64
39Pro								
40Val								
41Ile								
42Met								
43Gly	989.88	126.47	12.78	50.44	3.38	6.70	19.62	
44Arg	1056.34	63.02	5.97	59.48	1.90	3.19	17.76	17.76

45His								
46Thr	979.07	71.11	7.26	67.35	2.58	3.82	14.54	14.54
47Trp	985.07	62.04	6.30	76.11	2.89	3.80	12.94	12.94
48Glu								
49Ser	1002.14	54.44	5.43	69.52	2.76	3.97	14.42	14.42
50Ile	970.66	69.90	7.20	66.34	2.55	3.84	14.63	14.63
51Gly	1054.55	80.45	7.63	67.80	2.02	2.98	15.55	15.55
52Arg	950.90	67.65	7.11	62.96	1.84	2.92	15.10	15.10
53Pro								
54Leu	1062.71	53.70	5.05	65.49	1.94	2.96	16.23	16.23
55Pro								
56Gly								
57Arg	979.22	55.28	5.65	59.55	1.25	2.10	16.44	16.44
58Lys	1083.31	72.51	6.69	75.24	2.53	3.37	14.40	14.40
59Asn	935.43	71.91	7.69	68.06	2.09	3.08	13.75	13.75
60Ile								
61Ile								
62Leu								
63Ser	1002.75	77.99	7.78	63.01	2.14	3.40	15.92	15.92
64Ser	1001.51	73.59	7.35	60.93	1.76	2.89	16.44	16.44
65Gln	991.74	51.81	5.22	62.53	1.66	2.65	15.86	15.86
66Pro								
67Gly	748.25	42.97	5.74	77.10	3.32	4.31	9.70	9.70
68Thr	699.07	55.40	7.93	77.35	5.35	6.92	9.04	9.04
69Asp	757.06	50.75	6.70	84.96	2.34	2.76	8.91	8.91
70Asp	924.79	78.60	8.50	67.60	2.42	3.59	13.68	13.68
71Arg	916.28	45.63	4.98	62.27	1.73	2.78	14.71	14.71
72Val	983.22	65.79	6.69	59.90	1.76	2.95	16.42	16.42
73Thr	1033.37	63.34	6.13	64.14	1.94	3.02	16.11	16.11
74Trp	1122.96	61.54	5.48	61.47	2.01	3.27	18.27	18.27
75Val	931.85	91.40	9.81	63.35	4.54	7.16	14.71	14.71

76Lys	1057.20	55.62	5.26	66.52	1.48	2.23	15.89	15.89
77Ser	940.81	48.17	5.12	59.71	2.51	4.21	15.76	15.76
78Val	956.66	36.70	3.84	67.06	2.76	4.11	14.27	14.27
79Asp	918.92	52.33	5.69	63.42	1.33	2.10	14.49	14.49
80Glu	1327.28	55.00	4.14	351.24	38.67	11.01	3.78	
81Ala								
82Ile	1092.22	31.36	2.87	75.90	4.46	5.88	14.39	14.39
83Ala	944.28	42.45	4.50	66.43	1.22	1.84	14.21	14.21
84Ala	1017.36	51.19	5.03	67.13	1.70	2.53	15.16	15.16
85Cys	1043.39	43.86	4.20	69.75	2.42	3.47	14.96	14.96
86Gly	1006.96	36.76	3.65	59.86	1.51	2.53	16.82	16.82
87Asp	961.91	71.50	7.43	71.77	1.79	2.50	13.40	13.40
88Val	1139.25	52.57	4.61	100.80	3.39	3.36	11.30	11.30
89Pro								
90Glu	987.04	62.05	6.29	62.05	1.98	3.19	15.91	15.91
91Ile	832.94	95.49	11.46	70.86	20.56	29.02	11.75	
92Met								
93Val								
94Ile								
95Gly	1016.40	75.48	7.43	44.05	1.74	3.95	23.07	23.07
96Gly	1031.73	83.20	8.06	63.57	1.51	2.38	16.23	16.23
97Gly								
98Arg	1005.95	86.76	8.62	61.31	3.34	5.45	16.41	16.41
99Val	1015.86	74.04	7.29	64.60	3.07	4.76	15.73	15.73
100Tyr	983.94	78.15	7.94	58.32	1.57	2.68	16.87	16.87
101Glu	969.25	54.79	5.65	66.38	1.72	2.59	14.60	14.60
102Gln	1073.76	72.02	6.71	61.05	4.13	6.76	17.59	17.59
103Phe	989.62	67.32	6.80	72.62	2.06	2.84	13.63	13.63
104Leu	1072.83	47.74	4.45	90.63	8.93	9.85	11.84	11.84
105Pro								
106Lys	1043.05	52.38	5.02	68.25	1.45	2.12	15.28	15.28

107Ala	999.04	39.19	3.92	113.59	9.41	8.28	8.80	8.80
108Gln	992.01	76.45	7.71	61.31	1.94	3.16	16.18	16.18
109Lys	1137.38	22.04	1.94	76.43	3.31	4.33	14.88	14.88
110Leu								
111Tyr								
112Leu	981.68	178.97	18.23	62.67	6.28	10.03	15.66	15.66
113Thr								
114His	831.48	105.19	12.65	56.30	4.38	7.77	14.77	14.77
115Ile	985.02	106.75	10.84	58.85	4.86	8.26	16.74	16.74
116Asp	955.09	66.17	6.93	63.33	2.95	4.66	15.08	15.08
117Ala	1097.58	63.57	5.79	71.68	2.74	3.83	15.31	15.31
118Glu	1212.93	191.86	15.82	61.49	2.03	3.30	19.73	
119Val	1007.63	93.55	9.28					
120Glu	1025.99	63.31	6.17	74.55	2.06	2.77	13.76	13.76
121Gly	1062.01	64.36	6.06	50.15	1.93	3.86	21.18	21.18
122Asp	950.00	79.87	8.41	65.17	1.75	2.68	14.58	14.58
123Thr								
124His	993.85	111.42	11.21	64.82	3.76	5.80	15.33	
125Phe	1012.43	76.75	7.58	62.51	1.71	2.73	16.20	16.20
126Pro								
127Asp	1106.24	33.01	2.98	67.30	1.62	2.40	16.44	16.44
128Tyr	1044.24	14.53	1.39	73.84	6.09	8.24	14.14	14.14
129Glu	1001.15	64.91	6.48	66.44	3.24	4.88	15.07	15.07
130Pro								
131Asp	995.74	61.92	6.22	72.53	1.52	2.09	13.73	13.73
132Asp	955.93	68.26	7.14					
133Trp	1062.25	44.34	4.17	64.37	2.21	3.43	16.50	16.50
134Glu	1112.28	83.30	7.49	59.76	5.64	9.44	18.61	18.61
135Ser	1128.90	94.21	8.35	65.35	2.19	3.35	17.27	17.27
136Val	881.77	148.73	16.87	67.22	2.69	4.00	13.12	
137Phe	929.66	57.51	6.19	66.59	6.61	9.92	13.96	13.96

138Ser	923.89	88.51	9.58	57.76	3.79	6.57	16.00	16.00
139Glu	931.83	122.11	13.10	60.46	5.02	8.31	15.41	
140Phe	996.26	59.54	5.98	65.07	2.75	4.23	15.31	15.31
141His	922.46	95.99	10.41	63.66	4.63	7.27	14.49	
142Asp	1006.95	35.29	3.50	84.40	2.32	2.75	11.93	11.93
143Ala	996.20	59.76	6.00	69.14	2.49	3.61	14.41	14.41
144Asp	1048.72	82.37	7.85	60.15	2.32	3.85	17.44	17.44
145Ala								
146Gln	1029.18	54.20	5.27	89.53	2.79	3.11	11.50	11.50
147Asn	977.68	81.04	8.29	67.15	2.02	3.01	14.56	14.56
148Ser	972.07	60.73	6.25	60.65	1.93	3.17	16.03	16.03
149His	1041.63	58.40	5.61	51.04	1.40	2.75	20.41	20.41
150Ser	979.70	79.22	8.09	65.51	1.96	2.99	14.95	14.95
151Tyr	890.55	90.57	10.17	56.72	3.33	5.87	15.70	
152Cys								
153Phe	888.63	103.96	11.70	68.09	6.84	10.05	13.05	
154Glu	749.96	115.88	15.45	53.35	6.04	11.31	14.06	
155Ile								
156Leu	985.81	33.29	3.38	83.31	12.04	14.45	11.83	
157Glu								
158Arg	1059.43	15.71	1.48	90.18	3.71	4.12	11.75	11.75
159Arg	976.53	28.81	2.95	81.89	2.22	2.71	11.92	11.92

Table 8.7.1.1 T1/T2 values for EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 600 MHz. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below **(Table 8.7.2)**.

(1) EcDHFR complex in 17% MeOD 600 MHz	(2) Raw Values for 116 residues	(3) Average of 103 residues	(4) Average of 84 residues
Mean T1/T2 Ratio	15.08	15.20	15.34
Standard Deviation (SD) of T1/T2	2.53	2.27	1.13
Mean T1/T2 + SD	17.61	17.48	
Mean T1/T2 – SD	12.55	12.93	

Table 8.7.1.2 Values in column **(2)** represent the average T1/T2 ratio over all of the 116 amino acid residues in the EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 600 MHz for which both T1 and T2 values were calculated (**Table 8.7.1.1)**. Values in column **(3)** represent the average T1/T2 ratio of the 103 residues for which the T1 and T2 errors were less than 10% of the values themselves, a total of 13 residues were discounted due to large errors. The overall correlation time for the molecule can be calculated from the average of T1/T2 for residues, which display T1/T2 ratios that fall within 1 standard deviation of the mean value. Column **(4)** represents the T1/T2 ratio for the 84 residues that fall within 1SD of the mean, along with the standard deviation of these values. The 19 residues with T1/T2 values outside the mean ± 1SD were discounted.

Residue	600 MHz 17% MethanolT1/T2
20Met	12.29
67Gly	9.70
68Thr	9.04
69Asp	8.91
88Val	11.30
104Leu	11.84
107Ala	8.80
142Asp	11.93
146Gln	11.50
158Arg	11.75
159Arg	11.92

Table 8.7.1.3 List of residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 600 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio.

Residue	600 MHz 17% Methanol T1/T2
11Asp	21.18
44Arg	17.76
74Trp	18.27
95Gly	23.07
102Gln	17.59
121Gly	21.18
134Glu	18.61
149His	20.41

Table 8.7.1.4 List of residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 600 MHz which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio.

8.7.2 T1/T2 values for EcDHFR:folate:$NADP^+$ complex in the presence of 17% methanol co-solvent at 900 MHz

The T1/T2 values for EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 900 MHz are presented below (**Table 8.7.2.1)**. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below **(Table 8.7.2.2**). The residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 900 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio are presented in **Table 8.7.2.3** and residues which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio are showed in **Table 8.7.2.4**.

900 MHz 17% MeOD	T1	T1 Error	T1 % Error	T2	T2 Error	T2 % Error	T1/T2	T1/T2
1Met								
2Ile	1325.98	96.62	7.29	51.30	2.09	4.07	25.85	25.85
3Ser	186.70	-45.90	-24.59	23.14	2.55	11.03	8.07	
4Leu	1311.87	99.63	7.59	67.62	4.27	6.31	19.40	19.40
5Ile								
6Ala	1318.19	113.10	8.58	47.12	2.28	4.83	27.97	27.97
7Ala								
8Leu	1422.83	113.10	7.95	44.10	2.22	5.04	32.27	32.27
9Ala	1199.54	198.22	16.52	54.87	3.25	5.92	21.86	
10Val	1593.23	124.39	7.81	44.41	1.92	4.32	35.88	35.88
11Asp	1372.18	98.65	7.19	34.27	1.23	3.57	40.04	40.04
12Arg	1483.99	105.51	7.11	47.83	1.80	3.76	31.02	31.02
13Val	1610.25	167.23	10.39	39.53	2.02	5.11	40.73	
14Ile								
15Gly								
16Met	159.00	-116.71	-73.40	51.59	1.81	3.50	3.08	
17Glu								

18Asn								
19Ala	1275.49	102.71	8.05	48.60	2.03	4.19	26.25	26.25
20Met	1091.69	79.08	7.24	101.73	9.10	8.95	10.73	10.73
21Pro								
22Trp								
23Asn								
24Leu	1257.08	113.52	9.03	56.64	2.50	4.41	22.19	22.19
25Pro								
26Ala	1429.30	95.98	6.71	45.39	1.56	3.43	31.49	31.49
27Asp	1530.31	139.59	9.12	45.88	1.65	3.61	33.35	33.35
28Leu	1449.02	120.72	8.33	43.75	1.51	3.45	33.12	33.12
29Ala	1415.75	127.43	9.00	49.98	9.72	19.45	28.32	
30Trp	1445.19	99.22	6.87	45.97	1.48	3.22	31.44	31.44
31Phe	1418.63	122.60	8.64	43.94	0.80	1.82	32.28	32.28
32Lys	1380.95	126.12	9.13	43.50	1.67	3.83	31.75	31.75
33Arg	1262.27	112.23	8.89	52.50	1.53	2.92	24.04	24.04
34Asn	1417.48	117.43	8.28	46.47	0.78	1.69	30.50	30.50
35Thr	1467.14	81.77	5.57	46.80	1.54	3.28	31.35	31.35
36Leu	1511.55	148.18	9.80	46.40	2.19	4.71	32.58	32.58
37Asp	1620.71	124.50	7.68	57.11	1.60	2.80	28.38	28.38
38Lys	1431.45	104.64	7.31	56.95	2.19	3.84	25.14	25.14
39Pro								
40Val								
41Ile								
42Met								
43Gly	1737.83	243.04	13.99	48.59	6.17	12.69	35.76	
44Arg	1580.33	79.89	5.06	50.47	2.78	5.51	31.31	31.31
45His								
46Thr	1254.36	95.21	7.59	76.86	6.95	9.04	16.32	16.32
47Trp	1222.15	71.45	5.85	90.81	7.99	8.80	13.46	13.46

48Glu								
49Ser				50.67	1.61	3.18		
50Ile	1404.71	113.28	8.06	45.47	2.26	4.97	30.89	30.89
51Gly	1467.16	147.55	10.06	53.61	2.29	4.27	27.37	
52Arg	1366.48	130.31	9.54	48.10	2.00	4.16	28.41	28.41
53Pro								
54Leu	1472.62	95.77	6.50	49.56	1.73	3.50	29.71	29.71
55Pro								
56Gly								
57Arg	1368.41	71.70	5.24	45.61	1.51	3.32	30.00	30.00
58Lys	1473.35	127.72	8.67	53.31	2.10	3.93	27.64	27.64
59Asn	1276.70	116.13	9.10	48.73	1.53	3.14	26.20	26.20
60Ile								
61Ile								
62Leu								
63Ser	1610.46	144.58	8.98	49.18	1.72	3.49	32.75	32.75
64Ser	1498.87	125.14	8.35	49.82	3.22	6.46	30.09	30.09
65Gln	1325.14	79.23	5.98	48.27	1.47	3.05	27.45	27.45
66Pro								
67Gly	1068.67	90.95	8.51	58.60	2.85	4.86	18.24	18.24
68Thr	826.52	79.97	9.68	54.00	4.19	7.76	15.31	15.31
69Asp	889.48	56.61	6.36	61.22	1.88	3.07	14.53	14.53
70Asp	1200.57	111.18	9.26	51.40	1.76	3.43	23.36	23.36
71Arg	1284.55	90.99	7.08	48.50	1.73	3.57	26.49	26.49
72Val	1435.81	103.05	7.18	45.85	1.63	3.55	31.32	31.32
73Thr	1522.32	115.73	7.60	54.80	2.50	4.56	27.78	27.78
74Trp	1616.09	94.07	5.82	47.07	1.75	3.71	34.33	34.33
75Val				40.23	4.09	10.18		
76Lys	1161.78	231.21	19.90	52.73	1.69	3.20	22.03	
77Ser	1509.05	85.32	5.65	47.81	1.63	3.42	31.56	31.56
78Val	1327.94	74.01	5.57	51.24	1.76	3.44	25.92	25.92

79Asp	1303.11	77.51	5.95	51.29	1.71	3.34	25.41	25.41
80Glu	1312.81	73.63	5.61	398.63	38.69	9.71	3.29	3.29
81Ala	1573.04	23.61	1.50					
82Ile	1505.03	74.12	4.92	57.48	1.90	3.30	26.18	26.18
83Ala	1305.64	63.51	4.86	58.40	3.25	5.57	22.36	22.36
84Ala	1394.20	58.71	4.21	53.72	1.63	3.03	25.95	25.95
85Cys	1410.58	77.73	5.51	50.95	1.86	3.65	27.69	27.69
86Gly	1486.95	81.84	5.50	56.57	2.35	4.16	26.28	26.28
87Asp	1303.73	137.54	10.55	58.77	1.93	3.29	22.18	
88Val	1575.72	87.20	5.53	70.97	2.41	3.39	22.20	22.20
89Pro								
90Glu	1461.73	119.42	8.17	51.42	2.84	5.52	28.42	28.42
91Ile	1366.69	140.55	10.28	59.92	3.94	6.58	22.81	
92Met								
93Val								
94Ile								
95Gly	1533.06	112.47	7.34	39.10	4.34	11.11	39.21	39.21
96Gly	1533.75	132.70	8.65	48.76	1.57	3.23	31.45	31.45
97Gly								
98Arg	657.80	-31.59	-4.80	47.78	3.30	6.90	13.77	
99Val	1548.41	127.29	8.22	48.83	2.17	4.44	31.71	31.71
100Tyr	1376.51	108.35	7.87	46.41	1.40	3.02	29.66	29.66
101Glu	1419.22	69.95	4.93	53.48	1.74	3.24	26.54	26.54
102Gln	1605.36	113.57	7.07	52.66	1.47	2.80	30.49	30.49
103Phe	1487.85	102.52	6.89	53.98	1.71	3.17	27.56	27.56
104Leu	1385.29	69.12	4.99	61.74	2.15	3.49	22.44	22.44
105Pro								
106Lys	1453.65	71.28	4.90	52.43	2.05	3.91	27.73	27.73
107Ala	1383.54	76.97	5.56	91.21	8.36	9.16	15.17	15.17
108Gln	1458.27	105.80	7.26	48.05	1.88	3.90	30.35	30.35

109Lys	1411.23	88.08	6.24	44.81	2.65	5.91	31.49	31.49
110Leu								
111Tyr								
112Leu	1190.02	155.31	13.05	43.75	3.45	7.90	27.20	
113Thr								
114His	172.61	-58.11	-33.66	46.10	1.75	3.79	3.74	
115Ile	1508.66	199.95	13.25	51.62	3.36	6.52	29.23	
116Asp	1388.59	99.67	7.18	49.90	2.01	4.03	27.83	27.83
117Ala	1590.29	107.63	6.77	56.31	2.59	4.60	28.24	28.24
118Glu	1462.17	111.45	7.62	48.19	1.35	2.80	30.34	30.34
119Val								
120Glu	1284.77	95.62	7.44	63.87	3.08	4.82	20.11	20.11
121Gly	1512.12	112.89	7.47	44.96	3.51	7.81	33.63	33.63
122Asp	1146.66	115.63	10.08	64.36	4.39	6.82	17.82	
123Thr								
124His				63.35	4.27	6.75		
125Phe	1576.07	298.02	18.91	44.31	1.30	2.93	35.57	
126Pro	1507.20	128.28	8.51					
127Asp				54.19	1.74	3.21	0.00	
128Tyr	1527.27	76.03	4.98	50.14	1.72	3.43	30.46	30.46
129Glu	1345.30	85.14	6.33	50.58	1.66	3.27	26.60	26.60
130Pro	1355.50	91.60	6.76					
131Asp				51.34	2.19	4.27		
132Asp	1417.69	96.98	6.84					
133Trp	1425.77	79.74	5.59	51.62	2.32	4.49	27.62	27.62
134Glu	1739.65	166.57	9.57	51.39	1.97	3.84	33.85	33.85
135Ser	1388.34	86.41	6.22	51.68	1.68	3.24	26.86	26.86
136Val	1322.76	76.97	5.82	50.09	1.60	3.19	26.41	
137Phe	1384.46	60.75	4.39	128.37	19.07	14.86	10.79	
138Ser	1406.43	91.94	6.54	48.78	1.50	3.06	28.83	28.83

139Glu	1321.00	105.94	8.02	51.30	1.61	3.14	25.75	
140Phe	1431.78	78.42	5.48	47.89	1.86	3.89	29.90	29.90
141His	1399.49	90.10	6.44	66.18	3.03	4.57	21.15	
142Asp	1395.27	87.17	6.25	69.29	2.65	3.83	20.14	20.14
143Ala	1346.29	93.97	6.98	56.31	1.76	3.13	23.91	23.91
144Asp	1506.08	115.31	7.66	48.98	1.92	3.92	30.75	30.75
145Ala								
146Gln	1615.14	109.96	6.81	68.92	5.03	7.29	23.43	23.43
147Asn	1394.31	102.12	7.32	58.78	2.40	4.08	23.72	23.72
148Ser	1394.86	126.26	9.05	48.37	1.78	3.67	28.84	28.84
149His	1363.29	96.79	7.10	61.39	3.48	5.67	22.21	22.21
150Ser	1502.54	109.82	7.31	49.18	1.61	3.27	30.55	30.55
151Tyr	1309.45	99.95	7.63	49.83	2.18	4.38	26.28	26.28
152Cys								
153Phe	215.10	-33.28	-15.47	76.37	7.33	9.60	2.82	
154Glu	1252.30	133.62	10.67	38.49	2.83	7.36	32.54	
155Ile								
156Leu	1324.23	109.06	8.24	49.05	1.59	3.24	27.00	27.00
157Glu								
158Arg	1414.80	79.17	5.60	57.60	2.09	3.64	24.56	24.56
159Arg	1269.39	66.35	5.23	59.76	1.48	2.48	21.24	21.24

Table 8.7.2.1 T1/T2 values for EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 900 MHz. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below (**Table 8.7.2.2)**.

EcDHFR complex in 17% MeOD 900 MHz	**Raw Values for 111 residues**	**Values for 90 residues within error**
Average T1/T2 Ratio	25.78	27.06
Standard Deviation (SD) of T1/T2	7.81	5.96
Average T1/T2 + SD	33.59	33.02
Average T1/T2 – SD	17.97	21.11

Table 8.7.2.2 Raw values represent the average T1/T2 ratio over all of the 111 amino acid residues in the EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 900 MHz for which both T1 and T2 values were calculated (**Table 8.7.2.1**).Values within error represent the average T1/T2 ratio of the 90 residues for which the T1 and T2 errors were less than 10% of the values themselves, a total of 21 residues were discounted due to large errors.

Residue	900 MHz 17% MethanolT1/T2
4Leu	19.40
20Met	10.73
46Thr	16.32
47Trp	13.46
67Gly	18.24
68Thr	15.31
69Asp	14.53
80Glu	3.29
107Ala	15.17
120Glu	20.11
142Asp	20.14

Table 8.7.2.3 List of residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 900 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio.

Residue	900 MHz 17% MethanolT1/T2
10Val	35.88
11Asp	40.04
27Asp	33.35
28Leu	33.12
74Trp	34.33
95Gly	39.21
121Gly	33.63
134Glu	33.85

Table 8.7.2.4 List of residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 900 MHz which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio.

8.7.3 T1/T2 values for EcDHFR:folate:$NADP^+$ complex with no co-solvent at 600 MHz

The T1/T2 values for EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 600 MHz are presented below (**Table 8.7.3.1)**. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below **(Table 8.7.3.2**). The residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 600 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio are presented in **Table 8.7.3.3** and residues which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio are showed in **Table 8.7.3.4**.

600 MHz Buffer only	T1	T1 Error	T1 %error	T2	T2 Error	T2 % error	T1/T2	T1/T2
1Met								
2Ile	845.42	66.79	7.90					
3Ser	760.31	38.83	5.11	70.40	2.37	3.37	10.80	10.80
4Leu	806.83	22.07	2.74	71.76	2.70	3.77	11.24	11.24
5Ile	834.44	73.41	8.80	60.09	3.12	5.19	13.89	13.89
6Ala	745.49	28.58	3.83	70.88	2.12	2.99	10.52	10.52
7Ala								
8Leu	742.02	24.50	3.30	63.64	2.70	4.25	11.66	11.66
9Ala	803.66	31.58	3.93	71.46	2.94	4.11	11.25	11.25
10Val	846.65	44.99	5.31	70.39	1.66	2.36	12.03	12.03
11Asp	866.84	14.47	1.67	61.13	1.75	2.86	14.18	14.18
12Arg				74.12	4.06	5.47		
13Val	878.49	32.75	3.73	69.35	2.13	3.07	12.67	12.67
14Ile								

15Gly								
16Met	886.65	147.77	16.67	73.29	1.80	2.46	12.10	
17Glu								
18Asn								
19Ala	801.16	24.46	3.05	80.60	2.06	2.55	9.94	9.94
20Met	870.69	30.92	3.55	133.06	28.20	21.19	6.54	
21Pro								
22Trp								
23Asn								
24Leu								
25Pro								
26Ala	803.14	11.83	1.47	70.85	2.16	3.05	11.34	11.34
27Asp	821.44	29.84	3.63	70.60	1.77	2.50	11.64	11.64
28Leu	837.35	8.48	1.01	76.35	1.96	2.56	10.97	10.97
29Ala	842.61	30.44	3.61	78.90	2.70	3.42	10.68	10.68
30Trp	823.22	17.72	2.15	75.53	2.67	3.53	10.90	10.90
31Phe	751.46	28.21	3.75	66.63	2.52	3.78	11.28	11.28
32Lys	717.84	153.68	21.41	70.16	2.98	4.25	10.23	
33Arg	788.38	32.27	4.09	72.48	3.09	4.26	10.88	10.88
34Asn	784.91	31.94	4.07	78.41	2.61	3.33	10.01	10.01
35Thr	813.42	61.48	7.56	80.33	5.02	6.25	10.13	10.13
36Leu	874.94	64.40	7.36	70.67	3.39	4.80	12.38	12.38
37Asp	902.88	43.53	4.82	78.99	3.46	4.38	11.43	11.43
38Lys	816.63	16.92	2.07	76.81	2.60	3.39	10.63	10.63
39Pro								
40Val								
41Ile	876.13	42.48	4.85	85.82	4.36	5.08	10.21	10.21
42Met								

43Gly	842.74	52.18	6.19	71.90	3.97	5.51	11.72	11.72
44Arg								
45His								
46Thr	653.02	341.20	52.25	138.74	39.58	28.53	4.71	
47Trp	818.63	26.70	3.26	80.26	3.00	3.74	10.20	10.20
48Glu								
49Ser	809.35	34.23	4.23	91.62	10.67	11.64	8.83	
50Ile	812.18	47.61	5.86	73.90	2.71	3.66	10.99	10.99
51Gly	799.84	39.55	4.94					
52Arg	809.83	28.85	3.56					
53Pro								
54Leu	1156.84	526.90	45.55	77.65	1.96	2.53	14.90	
55Pro								
56Gly								
57Arg	784.79	10.05	1.28	74.95	2.28	3.04	10.47	10.47
58Lys	928.41	10.53	1.13	86.36	2.54	2.94	10.75	10.75
59Asn	819.73	24.71	3.01	77.95	2.51	3.22	10.52	10.52
60Ile	407.65	368.70	90.45	128.42	66.65	51.90	3.17	
61Ile	846.37	45.94	5.43	67.71	7.36	10.87	12.50	
62Leu	863.60	40.10	4.64	105.72	5.68	5.37	8.17	8.17
63Ser	819.85	9.07	1.11	75.92	2.37	3.12	10.80	10.80
64Ser	796.97	21.85	2.74	75.17	2.28	3.04	10.60	10.60
65Gln	806.29	13.80	1.71	72.88	1.99	2.73	11.06	11.06
66Pro								
67Gly	766.54	13.91	1.81					
68Thr								
69Asp	759.03	13.62	1.79	105.5	2.74	2.60	7.19	7.19

				8				
70Asp	820.58	22.84	2.78	83.28	2.53	3.04	9.85	9.85
71Arg	753.57	21.86	2.90	74.47	2.74	3.68	10.12	10.12
72Val	807.19	19.01	2.36	76.80	1.96	2.55	10.51	10.51
73Thr	864.98	14.71	1.70	73.24	2.13	2.91	11.81	11.81
74Trp	930.79	12.18	1.31	76.55	3.04	3.97	12.16	12.16
75Val	881.64	49.11	5.57	65.38	3.27	5.00	13.48	13.48
76Lys	870.71	11.50	1.32	77.09	2.18	2.82	11.30	11.30
77Ser	792.35	11.33	1.43	77.58	2.10	2.71	10.21	10.21
78Val	790.18	6.66	0.84	76.98	2.64	3.43	10.26	10.26
79Asp	769.51	12.28	1.60	77.17	2.05	2.65	9.97	9.97
80Glu	784.31	14.26	1.82	95.04	10.01	10.53	8.25	
81Ala	796.65	17.29	2.17	84.02	3.54	4.21	9.48	9.48
82Ile	845.27	6.84	0.81	81.26	2.46	3.03	10.40	10.40
83Ala	808.24	7.46	0.92	77.12	2.25	2.91	10.48	10.48
84Ala	830.16	5.82	0.70	82.03	2.62	3.20	10.12	10.12
85Cys	848.22	8.35	0.98	75.54	2.13	2.83	11.23	11.23
86Gly	875.50	14.79	1.69	81.86	2.90	3.55	10.70	10.70
87Asp	859.64	29.88	3.48	86.65	2.43	2.81	9.92	9.92
88Val	851.68	35.02	4.11	146.88	773.72	526.77	5.80	
89Pro								
90Glu								
91Ile	819.97	23.51	2.87	80.74	4.90	6.06	10.16	10.16
92Met								
93Val	892.76	28.59	3.20	165.82	12.41	7.48	5.38	5.38
94Ile								
95Gly								
96Gly	820.14	41.28	5.03	72.03	2.49	3.46	11.39	11.39
97Gly								

98Arg	797.85	38.55	4.83	68.54	2.24	3.27	11.64	11.64
99Val	823.58	21.20	2.57	75.13	2.41	3.21	10.96	10.96
100Tyr	815.38	36.40	4.46	70.70	2.32	3.28	11.53	11.53
101Glu	808.94	12.64	1.56	78.47	2.49	3.17	10.31	10.31
102Gln	1001.23	14.51	1.45	113.29	2.57	2.27	8.84	8.84
103Phe								
104Leu	934.50	7.61	0.81	90.82	2.97	3.27	10.29	10.29
105Pro								
106Lys								
107Ala	814.01	44.52	5.47	88.76	3.14	3.53	9.17	9.17
108Gln	868.96	12.55	1.44	75.15	2.03	2.71	11.56	11.56
109Lys	833.54	7.92	0.95	74.77	2.05	2.74	11.15	11.15
110Leu	529.12	477.42	90.23	113.48	41.74	36.78	4.66	
111Tyr	785.96	48.78	6.21	64.71	4.65	7.19	12.15	12.15
112Leu	1499.33	1519.49	101.34					
113Thr								
114His	835.25	36.17	4.33	75.84	2.45	3.23	11.01	11.01
115Ile								
116Asp	828.41	16.66	2.01	76.10	2.69	3.54	10.89	10.89
117Ala								
118Glu								
119Val								
120Glu	893.19	32.66	3.66	84.90	2.02	2.38	10.52	10.52
121Gly								
122Asp	795.68	31.27	3.93	74.00	3.29	4.45	10.75	10.75
123Thr								
124His								
125Phe	831.50	27.06	3.25	70.57	1.97	2.79	11.78	11.78

126Pro								
127Asp	128.69	-21.02	-16.33	82.10	1.91	2.33	1.57	
128Tyr								
129Glu	926.65	11.45	1.24	80.42	2.72	3.39	11.52	11.52
130Pro								
131Asp								
132Asp	930.73	166.46	17.89	106.19	16.06	15.12	8.76	
133Trp	915.91	88.63	9.68	84.35	6.48	7.68	10.86	10.86
134Glu	963.01	59.57	6.19	76.07	2.62	3.44	12.66	12.66
135Ser	831.26	10.89	1.31	75.68	3.51	4.64	10.98	10.98
136Val	1122.80	506.41	45.10	121.09	49.54	40.91	9.27	
137Phe	804.57	9.59	1.19	84.84	2.94	3.46	9.48	9.48
138Ser	859.94	10.90	1.27	79.19	1.89	2.39	10.86	10.86
139Glu	839.44	12.98	1.55	80.76	2.73	3.37	10.39	10.39
140Phe								
141His	831.56	8.34	1.00	89.44	2.88	3.22	9.30	9.30
142Asp	864.96	9.64	1.11	117.81	22.54	19.14	7.34	
143Ala	947.15	23.34	2.46	104.44	3.36	3.22	9.07	9.07
144Asp	835.35	25.38	3.04	68.27	2.50	3.67	12.24	12.24
145Ala	835.80	29.67	3.55	79.07	3.84	4.85	10.57	10.57
146Gln								
147Asn	871.27	26.65	3.06	76.94	1.94	2.53	11.32	11.32
148Ser								
149His	876.92	15.04	1.72	84.74	8.92	10.52	10.35	
150Ser	841.56	11.26	1.34	76.96	2.40	3.12	10.93	10.93
151Tyr								
152Cys	783.34	12.86	1.64	77.05	2.04	2.64	10.17	10.17

153Phe	810.41	9.99	1.23	79.60	3.12	3.92	10.18	10.18
154Glu	813.16	21.64	2.66	76.39	3.07	4.02	10.65	10.65
155Ile								
156Leu								
157Glu	898.54	12.62	1.40	74.05	2.36	3.18	12.13	12.13
158Arg	905.74	38.71	4.27	77.49	3.37	4.35	11.69	11.69
159Arg	796.75	12.24	1.54	91.21	2.61	2.86	8.74	8.74

Table 8.7.3.1 T1/T2 values for EcDHFR: $NADP^+$: folate complex under standard buffer conditions at 600 MHz. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below (**Table 8.7.3.2)**.

EcDHFR complex under standard buffer conditions at 600 MHz	**Raw Values for 105 residues**	**Values for 88 residues within error**
Average T1/T2 Ratio	10.36	10.78
Standard Deviation (SD) of T1/T2	2.03	1.24
Average T1/T2 + SD	12.39	12.02
Average T1/T2 – SD	8.32	9.53

Table 8.7.3.2 Raw values represent the average T1/T2 ratio over all of the 105 amino acid residues in the EcDHFR: $NADP^+$: folate complex under standard buffer conditions at 600 MHz for which both T1 and T2 values were calculated (**Table 8.7.3.1**).Values within error represent the average T1/T2 ratio of the 88 residues for which the T1 and T2 errors were less than 10% of the values themselves, a total of 17 residues were discounted due to large errors.

Residue	600 MHz Buffer T1/T2
93Val	5.38
69Asp	7.19
62Leu	8.17
159Arg	8.74
102Gln	8.84
143Ala	9.07
107Ala	9.17
141His	9.30
81Ala	9.48
137Phe	9.48

Table 8.7.3.3 List of residues in EcDHFR: $NADP^{|+}$: Folate complex under standard buffer conditions at 600 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio.

Field	600 MHz Buffer T1/T2
5Ile	13.89
10Val	12.03
11Asp	14.18
13Val	12.67
36Leu	12.38
74Trp	12.16
75Val	13.48
111Tyr	12.15
134Glu	12.66
144Asp	12.24
157Glu	12.13

Table 8.7.3.4 List of residues in EcDHFR: $NADP^{|+}$: Folate complex under standard buffer conditions at 600 MHz which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio.

8.7.4 T1/T2 values for EcDHFR:folate:$NADP^+$ complex with no co-solvent at 900 MHz

The T1/T2 values for EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 600 MHz are presented below (**Table 8.7.4.1)**. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below **(Table 8.7.4.2**). The residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 600 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio are presented in **Table 8.7.4.3** and residues which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio are showed in **Table 8.7.4.4**.

900MHz Buffer	T1	T1 Error	T1 %error	T2	T2 Error	T1 % error	T1/T2	T1/T2
1Met								
2Ile	977.23	48.12	4.92	72.77	6.22	8.55	13.43	13.43
3Ser	926.59	58.06	6.27	61.41	2.66	4.32	15.09	15.09
4Leu	142.76	-36.72	-25.73	64.80	2.70	4.17	2.20	
5Ile	987.04	79.92	8.10	61.50	2.21	3.59	16.05	16.05
6Ala	904.97	88.75	9.81	56.01	2.27	4.06	16.16	16.16
7Ala								
8Leu	958.00	67.40	7.04	53.71	5.17	9.62	17.84	17.84
9Ala	1082.70	161.78	14.94	45.02	3.00	6.67	24.05	
10Val	1037.29	78.12	7.53	56.05	1.60	2.85	18.51	18.51
11Asp	1092.49	124.75	11.42	45.93	1.78	3.88	23.79	
12Arg	1052.23	89.91	8.55	55.71	2.35	4.23	18.89	18.89
13Val	1064.06	96.93	9.11	60.65	3.29	5.43	17.55	17.55
14Ile								
15Gly								
16Met	934.58	77.32	8.27	63.77	2.34	3.68	14.65	14.65
17Glu								
18Asn								

19Ala	922.65	60.38	6.54					
20Met	943.25	56.62	6.00	67.89	3.49	5.14	13.89	13.89
21Pro				69.68	2.53	3.63		
22Trp								
23Asn								
24Leu								
25Pro								
26Ala	941.69	55.60	5.90	58.60	2.35	4.00	16.07	16.07
27Asp	943.34	79.32	8.41	56.26	1.78	3.16	16.77	16.77
28Leu	984.07	78.05	7.93	61.80	2.59	4.20	15.92	15.92
29Ala	1015.58	86.82	8.55	56.52	1.78	3.14	17.97	17.97
30Trp	974.05	50.11	5.14	70.28	5.46	7.76	13.86	13.86
31Phe	965.06	59.57	6.17	54.12	2.46	4.54	17.83	17.83
32Lys	1025.53	93.40	9.11	61.31	4.32	7.05	16.73	16.73
33Arg	1031.69	79.12	7.67	59.31	1.87	3.16	17.40	17.40
34Asn	1019.70	74.32	7.29	63.02	2.18	3.46	16.18	16.18
35Thr	1018.72	59.01	5.79	60.17	2.55	4.24	16.93	16.93
36Leu	1059.16	71.34	6.74	63.28	2.88	4.55	16.74	16.74
37Asp	1193.09	93.04	7.80	71.30	3.02	4.24	16.73	16.73
38Lys	1064.05	63.39	5.96	63.59	1.96	3.09	16.73	16.73
39Pro								
40Val								
41Ile	974.72	66.64	6.84	84.00	5.00	5.95	11.60	
42Met								
43Gly	1060.75	61.36	5.78	61.64	2.33	3.78	17.21	17.21
44Arg								
45His								
46Thr	1037.60	82.19	7.92	58.74	5.80	9.88	17.66	17.66
47Trp	1866.19	772.54	41.40	91.53	67.19	73.41	20.39	
48Glu								
49Ser	988.49	52.18	5.28	67.26	2.88	4.29	14.70	14.70
50Ile	966.98	73.55	7.61	67.75	2.35	3.47	14.27	14.27
51Gly	1040.67	84.90	8.16	73.91	2.97	4.01	14.08	14.08

52Arg	936.92	65.37	6.98	61.71	2.40	3.89	15.18	15.18
53Pro								
54Leu	1008.91	80.41	7.97	61.56	2.16	3.51	16.39	16.39
55Pro								
56Gly								
57Arg	933.88	39.51	4.23	59.47	2.32	3.90	15.70	15.70
58Lys	681.54	-180.62	-26.50	71.40	2.30	3.23	9.55	
59Asn	996.67	88.08	8.84	64.67	2.61	4.03	15.41	15.41
60Ile	1216.25	56.86	4.68	59.00	3.11	5.26	20.61	20.61
61Ile	1007.64	75.31	7.47	56.92	2.14	3.76	17.70	17.70
62Leu	1074.36	48.93	4.55	67.61	3.60	5.33	15.89	15.89
63Ser	1026.79	95.54	9.30	66.74	2.98	4.46	15.38	15.38
64Ser	973.17	51.50	5.29	66.32	2.40	3.61	14.67	14.67
65Gln	901.11	38.75	4.30	65.12	2.84	4.36	13.84	13.84
66Pro								
67Gly	835.97	63.62	7.61	76.92	3.77	4.90	10.87	10.87
68Thr	746.36	45.15	6.05	67.53	3.93	5.81	11.05	11.05
69Asp	752.46	42.81	5.69	81.40	2.70	3.32	9.24	9.24
70Asp	899.34	98.25	10.92	62.74	2.32	3.69	14.33	
71Arg	437.93	-250.86	-57.28	60.80	2.32	3.81	7.20	
72Val	894.82	38.50	4.30	57.99	2.12	3.66	15.43	15.43
73Thr	1065.52	48.10	4.51	60.90	2.28	3.75	17.50	17.50
74Trp	1119.16	52.92	4.73	59.56	2.61	4.38	18.79	18.79
75Val	1064.11	92.07	8.65	56.92	3.70	6.50	18.70	18.70
76Lys	1020.35	41.68	4.08	69.90	2.73	3.90	14.60	14.60
77Ser	902.87	30.58	3.39	58.75	2.16	3.68	15.37	15.37
78Val	933.11	39.59	4.24	68.94	2.30	3.34	13.54	13.54
79Asp	890.34	37.07	4.16	62.37	2.07	3.32	14.28	14.28
80Glu	921.00	39.60	4.30	79.60	7.63	9.58	11.57	11.57
81Ala	888.09	71.54	8.06	84.22	5.65	6.70	10.54	10.54
82Ile	1073.48	38.58	3.59	85.14	9.22	10.82	12.61	12.61
83Ala	974.42	34.36	3.53	69.11	4.02	5.82	14.10	14.10
84Ala	1021.65	40.86	4.00	65.38	2.67	4.09	15.63	15.63

85Cys	1004.12	31.16	3.10	68.87	2.55	3.71	14.58	14.58
86Gly	1071.71	36.69	3.42	72.57	2.30	3.18	14.77	14.77
87Asp	950.30	149.74	15.76	76.36	2.44	3.20	12.44	
88Val	1133.78	80.35	7.09	68.02	2.14	3.15	16.67	16.67
89Pro								
90Glu								
91Ile	920.91	79.29	8.61	72.95	12.40	17.00	12.62	
92Met								
93Val	864.65	39.69	4.59	220.93	12.58	5.69	3.91	
94Ile								
95Gly	1111.60	54.03	4.86	45.47	1.53	3.37	24.45	24.45
96Gly	1071.82	83.98	7.83	65.65	4.06	6.18	16.33	16.33
97Gly								
98Arg	1089.69	123.69	11.35	61.10	4.92	8.06	17.83	
99Val	1093.93	80.85	7.39	67.69	2.49	3.68	16.16	16.16
100Tyr	1062.35	59.65	5.62	59.96	2.10	3.50	17.72	17.72
101Glu	1005.32	34.09	3.39	68.53	2.51	3.67	14.67	14.67
102Gln	1141.07	39.23	3.44	96.63	3.19	3.30	11.81	11.81
103Phe								
104Leu	1048.06	29.54	2.82	80.58	10.42	12.93	13.01	
105Pro								
106Lys								
107Ala	1033.70	55.85	5.40	105.95	28.45	26.85	9.76	
108Gln	988.49	44.44	4.50	60.80	2.23	3.67	16.26	16.26
109Lys	943.77	35.54	3.77	61.75	2.88	4.67	15.28	15.28
110Leu	970.27	78.24	8.06	56.86	3.95	6.95	17.06	17.06
111Tyr	987.93	87.86	8.89	58.57	2.05	3.50	16.87	16.87
112Leu	1552.52	376.31	24.24	66.19	12.49	18.88	23.46	
113Thr								
114His	966.41	66.11	6.84	44.80	3.36	7.50	21.57	21.57
115Ile								
116Asp	966.93	66.13	6.84	59.60	2.15	3.60	16.22	16.22
117Ala								

118Glu								
119Val								
120Glu	1079.13	109.69	10.16	70.96	3.58	5.05	15.21	
121Gly								
122Asp	961.74	66.68	6.93	61.42	2.74	4.47	15.66	15.66
123Thr								
124His								
125Phe	990.17	87.17	8.80	57.32	4.07	7.09	17.28	17.28
126Pro								
127Asp	1147.49	45.33	3.95	68.96	2.79	4.04	16.64	16.64
128Tyr								
129Glu	1025.58	49.01	4.78	64.87	2.92	4.50	15.81	15.81
130Pro								
131Asp	1100.65	81.54	7.41	70.41	3.01	4.28	15.63	15.63
132Asp	882.62	93.79	10.63	68.05	3.24	4.76	12.97	
133Trp	1047.44	84.84	8.10	55.77	1.84	3.30	18.78	18.78
134Glu	1134.64	49.29	4.34	75.12	4.38	5.83	15.10	15.10
135Ser	987.25	44.89	4.55	68.76	2.60	3.78	14.36	14.36
136Val	977.08	34.08	3.49	84.06	12.12	14.41	11.62	
137Phe	919.87	48.17	5.24	54.17	4.27	7.89	16.98	16.98
138Ser	969.79	60.94	6.28	49.79	3.16	6.35	19.48	19.48
139Glu	920.32	67.39	7.32	47.70	3.91	8.19	19.30	19.30
140Phe								
141His	970.59	56.15	5.79	57.33	4.01	7.00	16.93	16.93
142Asp	1023.64	45.65	4.46	77.86	3.22	4.14	13.15	13.15
143Ala	1037.78	42.51	4.10	82.25	2.56	3.11	12.62	12.62
144Asp	1000.27	45.89	4.59	62.21	2.76	4.44	16.08	16.08
145Ala	1012.52	45.64	4.51	56.78	2.95	5.20	17.83	17.83
146Gln								
147Asn	1020.20	59.54	5.84	64.56	2.20	3.41	15.80	15.80
148Ser								
149His	876.60	91.83	10.48	43.34	1.24	2.86	20.23	
150Ser	1015.92	46.02	4.53	66.42	2.63	3.96	15.29	15.29

151Tyr								
152Cys	963.05	38.91	4.04	82.66	13.39	16.20	11.65	
153Phe	886.59	75.51	8.52	45.04	3.24	7.19	19.68	19.68
154Glu	834.26	60.88	7.30	47.47	5.57	11.73	17.58	17.58
155Ile								
156Leu								
157Glu	1136.22	62.56	5.51	62.40	2.20	3.53	18.21	18.21
158Arg	1110.25	50.87	4.58	61.42	2.73	4.45	18.08	18.08
159Arg	966.59	27.50	2.84	76.08	2.54	3.34	12.71	12.71

Table 8.7.4.1 T1/T2 values for EcDHFR: $NADP^+$: folate complex under standard buffer conditions at 900 MHz. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below (**Table 8.7.4.2)**.

EcDHFR complex under standard buffer conditions at 900 MHz	**Raw Values for 112 residues**	**Values for 92 residues within error**
Average T1/T2 Ratio	15.60	15.98
Standard Deviation (SD) of T1/T2	3.44	2.38
Average T1/T2 + SD	19.05	18.36
Average T1/T2 – SD	12.16	13.60

Table 8.7.4.2 Raw values represent the average T1/T2 ratio over all of the 112 amino acid residues in the EcDHFR: $NADP^+$: folate complex under standard buffer conditions at 900 MHz for which both T1 and T2 values were calculated (**Table 8.7.4.1**).Values within error represent the average T1/T2 ratio of the 92 residues for which the T1 and T2 errors were less than 10% of the values themselves, a total of 20 residues were discounted due to large errors.

Field	900 MHz Buffer T1/T2
2Ile	13.43
67Gly	10.87
68Thr	11.05
69Asp	9.24
78Val	13.54
80Glu	11.57
81Ala	10.54
82Ile	12.61
102Gln	11.81
142Asp	13.15
143Ala	12.62
159Arg	12.71

Table 8.7.4.3 List of residues in EcDHFR: $NADP^{|+}$: Folate complex under standard buffer conditions at 900 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio.

Field	900 MHz Buffer T1/T2
12Arg	18.89
60Ile	20.61
74Trp	18.79
75Val	18.70
95Gly	24.45
114His	21.57
133Trp	18.78
138Ser	19.48
139Glu	19.30
153Phe	19.68

Table 8.7.4.4 List of residues in EcDHFR: $NADP^{|+}$: Folate complex under standard buffer conditions at 900 MHz which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio.

8.7.5 T1/T2 values for EcDHFR:folate:$NADP^+$ complex in the presence of 17% glycerol co-solvent at 900 MHz

The T1/T2 values for EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 600 MHz are presented below (**Table 8.7.5.1)**. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below **(Table 8.7.5.2**). The residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 600 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio are presented in **Table 8.7.5.3** and residues which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio are showed in **Table 8.7.5.4**.

900 MHz 17% Glycerol	T1	T1 Error	T1 % error	T2	T2 Error	T2 % error	T1/T2	T1/T2
1Met								
2Ile	2268.21	42.50	1.87	44.54	3.93	8.83	50.93	50.93
3Ser	2576.61	84.13	3.27	37.50	1.52	4.06	68.72	68.72
4Leu	2656.99	94.19	3.54	38.56	1.79	4.64	68.90	68.90
5Ile	2523.24	123.03	4.88	34.39	2.36	6.86	73.38	73.38
6Ala	2529.68	44.71	1.77	34.84	1.45	4.16	72.60	72.60
7Ala								
8Leu	2511.65	48.05	1.91	41.83	3.04	7.26	60.04	60.04
9Ala	2442.82	87.90	3.60	42.13	2.15	5.11	57.98	57.98
10Val	2475.14	43.78	1.77	36.92	2.59	7.00	67.04	67.04
11Asp	2360.75	81.60	3.46	30.87	0.93	3.02	76.46	76.46
12Arg	2510.26	43.56	1.74	34.32	2.08	6.06	73.14	73.14
13Val	2647.05	84.07	3.18	34.04	0.94	2.75	77.75	77.75
14Ile								

15Gly								
16Met	2441.55	58.72	2.40	38.88	2.55	6.55	62.80	62.80
17Glu								
18Asn	2205.31	205.63	9.32	37.62	8.55	22.73	58.62	
19Ala	2237.85	128.56	5.74	40.74	2.15	5.28	54.92	54.92
20Met	2070.17	51.79	2.50	48.70	1.71	3.51	42.51	42.51
21Pro								
22Trp								
23Asn								
24Leu	2641.40	163.65	6.20	28.32	3.57	12.62	93.26	
25Pro								
26Ala	2368.01	57.51	2.43	33.43	1.88	5.63	70.83	70.83
27Asp	2557.92	944.76	36.93	38.39	1.85	4.81	66.63	
28Leu	2618.57	62.24	2.38	38.11	2.32	6.08	68.71	68.71
29Ala	2724.64	264.79	9.72	42.22	1.73	4.09	64.53	64.53
30Trp	2520.09	90.09	3.57	44.95	2.58	5.75	56.07	56.07
31Phe	2554.83	61.53	2.41	36.12	1.50	4.15	70.74	70.74
32Lys	2420.95	55.01	2.27	41.88	5.59	13.34	57.81	
33Arg	2418.63	69.62	2.88	35.37	1.14	3.22	68.38	68.38
34Asn	2401.30	48.16	2.01	29.88	3.97	13.29	80.37	
35Thr	2351.36	52.92	2.25	36.45	1.27	3.47	64.52	64.52
36Leu	2524.50	64.11	2.54	38.03	1.97	5.18	66.38	66.38
37Asp	2569.40	50.59	1.97	44.57	1.55	3.48	57.65	57.65
38Lys	2474.82	65.93	2.66	39.46	1.38	3.50	62.72	62.72
39Pro								
40Val	2474.47	278.16	11.24	34.82	8.62	24.76	71.06	
41Ile	1284.92	227.99	17.74	57.62	15.47	26.85	22.30	
42Met	2580.89	127.25	4.93	30.75	4.84	15.76	83.94	
43Gly	2603.75	123.29	4.74	34.17	1.14	3.35	76.19	76.19
44Arg	2391.94	79.68	3.33	35.31	1.49	4.21	67.74	67.74
45His								
46Thr								
47Trp								

48Glu								
49Ser	2439.72	60.71	2.49	42.29	1.66	3.92	57.69	57.69
50Ile	2228.23	61.40	2.76	38.92	1.84	4.72	57.25	57.25
51Gly	2362.07	51.60	2.18	45.87	1.64	3.56	51.49	51.49
52Arg	2214.11	70.11	3.17	38.56	2.36	6.13	57.42	57.42
53Pro								
54Leu	2507.12	43.49	1.73	38.06	2.05	5.39	65.87	65.87
55Pro								
56Gly								
57Arg	2265.33	40.87	1.80	34.85	1.07	3.08	65.01	65.01
58Lys	2596.68	74.11	2.85	43.72	1.71	3.90	59.40	59.40
59Asn	2408.68	75.47	3.13	37.15	2.24	6.02	64.84	64.84
60Ile	2838.90	151.76	5.35	43.46	6.27	14.43	65.32	
61Ile	-341.77	-73.80	21.59	35.35	10.44	29.52	-9.67	
62Leu	2139.93	207.51	9.70	66.39	5.41	8.15	32.23	32.23
63Ser	2705.93	74.08	2.74	41.23	2.42	5.88	65.62	65.62
64Ser	2690.61	121.61	4.52	37.60	1.21	3.21	71.56	71.56
65Gln	2344.80	20.58	0.88	37.07	1.98	5.33	63.25	63.25
66Pro								
67Gly	1411.99	33.44	2.37	50.34	2.77	5.49	28.05	28.05
68Thr	1375.63	74.30	5.40	47.00	2.57	5.47	29.27	29.27
69Asp	1385.52	28.64	2.07	52.23	2.42	4.63	26.53	26.53
70Asp	2331.53	78.67	3.37	40.70	1.88	4.61	57.29	57.29
71Arg	2331.81	38.28	1.64	36.46	1.55	4.24	63.95	63.95
72Val	2330.83	52.87	2.27	37.38	1.60	4.27	62.35	62.35
73Thr	2573.46	60.38	2.35	36.64	1.22	3.33	70.25	70.25
74Trp	2793.90	44.41	1.59	36.45	1.88	5.15	76.65	76.65
75Val	2601.53	156.06	6.00	36.05	2.67	7.41	72.16	72.16
76Lys	2607.70	32.40	1.24	42.43	1.73	4.07	61.46	61.46
77Ser	2611.51	35.97	1.38	37.68	1.30	3.44	69.30	69.30
78Val	2358.56	19.99	0.85	43.46	2.20	5.05	54.27	54.27
79Asp	2318.12	27.11	1.17	37.21	1.46	3.93	62.29	62.29
80Glu	2374.18	31.28	1.32	44.40	1.27	2.86	53.47	53.47

81Ala	624.24	1032.67	165.43	61.68	3.93	6.37	10.12	
82Ile	2603.35	117.01	4.49	48.80	4.70	9.64	53.35	53.35
83Ala	2246.25	43.58	1.94	41.08	2.99	7.28	54.68	54.68
84Ala	2393.18	183.03	7.65	39.44	1.40	3.54	60.68	60.68
85Cys	2545.36	43.81	1.72	38.84	1.78	4.59	65.53	65.53
86Gly	2651.42	38.51	1.45	43.30	2.22	5.13	61.24	61.24
87Asp	2455.76	81.99	3.34	48.04	2.20	4.58	51.12	51.12
88Val	2311.90	30.01	1.30	61.53	3.39	5.51	37.57	37.57
89Pro								
90Glu	2437.92	37.61	1.54	37.22	1.49	3.99	65.50	65.50
91Ile	2423.44	426.94	17.62	28.94	10.98	37.92	83.73	
92Met								
93Val	1333.33	238.41	17.88	54.17	31.47	58.09	24.61	
94Ile	1483.94	88.82	5.99	63.33	8.96	14.15	23.43	
95Gly	2479.76	60.63	2.45	31.74	0.94	2.96	78.13	78.13
96Gly	2831.83	116.95	4.13	30.77	7.36	23.91	92.03	
97Gly								
98Arg	2496.45	236.23	9.46	37.84	1.91	5.05	65.97	65.97
99Val	2514.93	76.66	3.05	41.79	2.42	5.79	60.19	60.19
100Tyr	2291.82	94.18	4.11	35.91	1.84	5.14	63.81	63.81
101Glu	2391.14	53.48	2.24	42.43	1.90	4.48	56.36	56.36
102Gln	2553.09	71.03	2.78	40.72	2.30	5.66	62.69	62.69
103Phe	2461.24	60.46	2.46	44.03	1.47	3.35	55.90	55.90
104Leu	2615.13	480.63	18.38	41.18	5.08	12.33	63.51	
105Pro								
106Lys								
107Ala	2150.35	46.91	2.18	48.20	2.29	4.75	44.61	44.61
108Gln	2423.84	87.19	3.60	36.49	1.57	4.30	66.42	66.42
109Lys	2421.35	128.51	5.31	39.05	2.30	5.90	62.01	62.01
110Leu	2659.45	1104.05	41.51	37.17	4.73	12.72	71.54	
111Tyr	2590.88	85.62	3.30	42.79	8.43	19.71	60.55	
112Leu	2916.81	606.21	20.78	27.44	3.11	11.35	106.29	
113Thr								

114His	2135.95	469.95	22.00	29.97	2.48	8.29	71.26	
115Ile	2721.58	164.00	6.03	45.50	4.61	10.12	59.81	
116Asp	2536.49	54.68	2.16	36.13	1.15	3.20	70.21	70.21
117Ala	2721.22	81.71	3.00	45.21	2.18	4.83	60.19	60.19
118Glu	3014.79	651.45	21.61	42.50	2.53	5.96	70.94	
119Val								
120Glu	2278.54	29.21	1.28	43.22	2.44	5.65	52.72	52.72
121Gly	2110.95	47.05	2.23	30.96	0.79	2.56	68.18	68.18
122Asp	2344.83	105.11	4.48	37.02	3.78	10.22	63.35	
123Thr								
124His								
125Phe	2551.38	53.04	2.08	38.34	2.27	5.93	66.54	66.54
126Pro								
127Asp	2462.96	46.93	1.91	40.09	1.64	4.08	61.44	61.44
128Tyr	2040.70	58.32	2.86	40.60	1.68	4.14	50.26	50.26
129Glu				41.57	2.26	5.42		
130Pro	2253.79	48.87	2.17					
131Asp	2211.25	48.00	2.17	43.98	2.59	5.88	50.28	50.28
132Asp	2365.83	64.06	2.71	41.06	1.61	3.92	57.62	57.62
133Trp	2340.36	115.74	4.95	39.46	1.82	4.62	59.32	59.32
134Glu	2704.56	163.40	6.04	40.63	4.28	10.53	66.57	
135Ser	2441.02	163.04	6.68	41.01	3.41	8.31	59.52	59.52
136Val	2654.51	195.52	7.37	46.84	6.59	14.07	56.68	
137Phe	2299.82	310.48	13.50	40.13	2.40	5.97	57.31	
138Ser	2040.13	369.11	18.09	34.80	1.63	4.67	58.63	
139Glu	2142.83	359.08	16.76	35.89	2.24	6.25	59.71	
140Phe	2613.39	187.26	7.17	43.63	4.08	9.34	59.89	59.89
141His	1991.48	360.56	18.11	46.92	3.15	6.71	42.44	
142Asp	2214.22	115.40	5.21	63.17	3.46	5.47	35.05	35.05
143Ala	2286.05	35.47	1.55	46.16	1.53	3.31	49.53	49.53
144Asp	2600.00	55.16	2.12	36.88	0.90	2.45	70.51	70.51
145Ala	2246.78	76.04	3.38	38.11	1.54	4.04	58.96	58.96
146Gln	2353.44	27.92	1.19	45.17	1.75	3.88	52.11	52.11

147Asn	2716.47	47.24	1.74	43.50	2.05	4.70	62.45	62.45
148Ser	2514.23	51.84	2.06	38.31	1.15	2.99	65.62	65.62
149His	2250.77	47.72	2.12	55.03	4.65	8.46	40.90	40.90
150Ser	2568.79	45.58	1.77	40.88	2.16	5.28	62.83	62.83
151Tyr	2381.08	145.97	6.13	47.83	5.67	11.85	49.78	
152Cys	2138.99	311.47	14.56	40.81	2.69	6.60	52.41	
153Phe	2058.37	428.82	20.83	34.70	2.58	7.44	59.33	
154Glu	2515.62	579.58	23.04	28.53	4.51	15.80	88.18	
155Ile	3364.19	1515.03	45.03	48.09	6.49	13.50	69.95	
156Leu	2641.51	203.21	7.69	43.98	3.86	8.77	60.07	60.07
157Glu	2865.65	98.24	3.43	32.06	2.92	9.12	89.38	89.38
158Arg	2448.49	62.73	2.56	45.19	1.16	2.57	54.19	54.19
159Arg	1930.35	23.98	1.24	48.91	2.08	4.25	39.47	39.47

Table 8.7.5.1 T1/T2 values for EcDHFR: $NADP^+$: folate complex in the presence of 17% glycerol at 900 MHz. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below (**Table 8.7.5.2).**

EcDHFR complex in the presence of 17% glycerol at 900 MHz	**Raw Values for 129 residues**	**Values for 95 residues within error**
Average T1/T2 Ratio	60.27	60.25
Standard Deviation (SD) of T1/T2	11.58	11.29
Average T1/T2 + SD	71.86	71.54
Average T1/T2 – SD	48.69	48.96

Table 8.7.5.2 Raw values represent the average T1/T2 ratio over all of the 129 amino acid residues in the EcDHFR: $NADP^+$: folate complex in the presence of 17% glycerol at 900 MHz for which both T1 and T2 values were calculated (**Table 8.7.5.1**). Values within error represent the average T1/T2 ratio of the 95 residues for which the T1 and T2 errors were less than 10% of the values themselves, a total of 34 residues were discounted due to large errors.

Residue	900 MHz 17% Glycerol T1/T2
20Met	42.51
62Leu	32.23
67Gly	28.05
68Thr	29.27
69Asp	26.53
88Val	37.57
107Ala	44.61
142Asp	35.05
149His	40.90
159Arg	39.47

Table 8.7.5.3 List of residues in EcDHFR: $NADP^{|+}$: Folate complex in 17% glycerol conditions at 900 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio.

Residue	900 MHz 17% Glycerol T1/T2
5Ile	73.38
6Ala	72.60
11Asp	76.46
12Arg	73.14
13Val	77.75
43Gly	76.19
64Ser	71.56
74Trp	76.65
75Val	72.16
95Gly	78.13
157Glu	89.38

Table 8.7.5.4 List of residues in EcDHFR: $NADP^{|+}$: Folate complex in 17% glycerol conditions at 900 MHz which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio.

8.7.6 T1/T2 values for ^{15}N only EcDHFR:folate:$NADP^+$ complex in the presence of 17% glycerol co-solvent at 600 MHz

The T1/T2 values for EcDHFR: $NADP^+$: folate complex in the presence of 17% methanol (MeOD) at 600 MHz are presented below (**Table 8.7.6.1)**. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below **(Table 8.7.6.2**). The residues in EcDHFR: $NADP^{|+}$: Folate complex in the presence of 17% methanol at 600 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio are presented in **Table 8.7.6.3** and residues which display T1/T2 ratios that are 1 standard deviation above the mean T1/T2 ratio are showed in **Table 8.7.6.4**.

600 MHz N15 17% Glycerol	T1	T1 Error	T1 % Error	T2	T2 Error	T2% Error	T1/T2	T1/T2
1Met								
2Ile	953.50	68.16	7.15	61.53	1.94	3.15	15.50	15.50
3Ser	977.94	60.30	6.17	55.90	2.80	5.02	17.49	17.49
4Leu	1024.24	54.17	5.29	56.94	0.79	1.38	17.99	17.99
5Ile	984.75	54.48	5.53	50.94	1.44	2.83	19.33	19.33
6Ala	992.01	95.27	9.60	57.24	2.43	4.25	17.33	17.33
7Ala								
8Leu	950.64	62.25	6.55	50.89	2.30	4.51	18.68	18.68
9Ala	1036.85	62.74	6.05	67.45	2.49	3.69	15.37	15.37
10Val	1020.60	91.35	8.95	52.20	1.86	3.56	19.55	19.55
11Asp	892.35	94.01	10.53	50.05	1.96	3.93	17.83	
12Arg	1065.35	77.01	7.23	52.45	1.73	3.30	20.31	20.31
13Val	1732.93	242.99	14.02	92.61	9.17	9.91	18.71	
14Ile								
15Gly								
16Met	890.60	58.75	6.60	56.88	1.44	2.54	15.66	15.66

17Glu								
18Asn	668.32	165.43	24.75	59.90	6.94	11.58	11.16	
19Ala	1034.23	37.80	3.66	56.41	1.33	2.36	18.33	18.33
20Met	921.07	83.13	9.03	66.36	1.50	2.25	13.88	13.88
21Pro								
22Trp								
23Asn								
24Leu	997.03	66.13	6.63	50.45	2.90	5.75	19.76	19.76
25Pro								
26Ala	1002.33	45.47	4.54	50.96	1.70	3.34	19.67	19.67
27Asp	880.74	22.69	2.58	50.73	3.82	7.53	17.36	17.36
28Leu	1035.29	41.56	4.01	51.37	1.81	3.52	20.15	20.15
29Ala	934.16	24.77	2.65	49.45	1.67	3.38	18.89	18.89
30Trp	955.12	59.65	6.25	57.43	1.27	2.21	16.63	16.63
31Phe	943.29	88.13	9.34	52.67	1.73	3.28	17.91	17.91
32Lys	472.70	-153.99	-32.58	54.75	1.24	2.27	8.63	
33Arg	973.69	37.31	3.83	54.05	1.51	2.80	18.01	18.01
34Asn	926.46	53.16	5.74	57.53	1.82	3.16	16.10	16.10
35Thr	988.01	51.54	5.22	53.67	1.74	3.24	18.41	18.41
36Leu	1016.55	55.76	5.48	51.97	1.19	2.30	19.56	19.56
37Asp	928.42	72.07	7.76	57.21	6.20	10.83	16.23	16.23
38Lys	1001.68	27.51	2.75	56.92	0.96	1.69	17.60	17.60
39Pro								
40Val	989.61	60.78	6.14	54.47	1.58	2.91	18.17	18.17
41Ile	1026.12	80.59	7.85	64.69	1.80	2.78	15.86	15.86
42Met	825.49	49.79	6.03	52.22	1.41	2.70	15.81	15.81
43Gly	1178.30	92.29	7.83	50.20	1.47	2.93	23.47	23.47
44Arg	898.84	60.10	6.69	50.47	1.17	2.32	17.81	17.81
45His								
46Thr								
47Trp								
48Glu								
49Ser	897.13	59.82	6.67	57.77	1.52	2.64	15.53	15.53

50Ile	886.02	50.70	5.72	54.60	1.19	2.18	16.23	16.23
51Gly	1010.54	58.96	5.83	54.64	1.55	2.84	18.49	18.49
52Arg	1003.09	27.36	2.73	55.12	1.28	2.32	18.20	18.20
53Pro								
54Leu	450.46	196.70	43.67	58.02	2.62	4.52	7.76	
55Pro								
56Gly								
57Arg	951.73	31.64	3.32	57.17	1.05	1.83	16.65	16.65
58Lys	1196.38	38.15	3.19	61.86	1.84	2.97	19.34	19.34
59Asn	925.87	40.83	4.41	59.53	1.32	2.22	15.55	15.55
60Ile	1082.49	73.97	6.83	56.41	1.63	2.88	19.19	19.19
61Ile	998.86	89.41	8.95	50.60	1.35	2.67	19.74	19.74
62Leu	899.92	41.95	4.66	59.28	1.03	1.74	15.18	15.18
63Ser	974.93	37.33	3.83	54.12	1.61	2.98	18.01	18.01
64Ser	963.64	57.22	5.94	51.94	0.91	1.76	18.55	18.55
65Gln	969.96	36.78	3.79	56.30	1.77	3.14	17.23	17.23
66Pro								
67Gly	731.42	43.86	6.00	68.28	1.46	2.13	10.71	10.71
68Thr	776.96	72.78	9.37	70.44	3.57	5.07	11.03	11.03
69Asp	830.88	20.88	2.51	83.42	2.51	3.00	9.96	9.96
70Asp	1049.21	45.27	4.31	65.49	2.00	3.05	16.02	16.02
71Arg	903.19	52.82	5.85	54.14	1.79	3.31	16.68	16.68
72Val	966.61	25.64	2.65	54.60	1.43	2.62	17.70	17.70
73Thr	919.00	80.32	8.74	55.74	2.05	3.67	16.49	16.49
74Trp	1175.54	52.07	4.43	53.50	1.57	2.93	21.97	21.97
75Val	936.93	52.60	5.61	51.76	1.82	3.51	18.10	18.10
76Lys	1082.65	47.48	4.39	57.76	1.56	2.70	18.74	18.74
77Ser	850.73	35.89	4.22	53.01	0.96	1.82	16.05	16.05
78Val	908.05	80.08	8.82	59.49	2.09	3.51	15.26	15.26
79Asp	990.87	34.09	3.44	55.86	0.78	1.39	17.74	17.74
80Glu	972.42	33.77	3.47	266.63	-5572.91	-2090.11	3.65	

81Ala	935.77	37.01	3.96	58.01	0.87	1.50	16.13	16.13
82Ile	959.70	42.70	4.45	62.81	1.47	2.34	15.28	15.28
83Ala	955.67	27.10	2.84	56.97	0.71	1.25	16.77	16.77
84Ala	940.13	46.30	4.92	55.74	1.04	1.87	16.87	16.87
85Cys	945.93	51.39	5.43	58.58	1.45	2.48	16.15	16.15
86Gly	948.41	25.55	2.69	57.71	1.19	2.05	16.44	16.44
87Asp	1088.11	52.87	4.86	67.49	1.04	1.54	16.12	16.12
88Val	1188.50	24.38	2.05	86.93	1.95	2.24	13.67	13.67
89Pro								
90Glu	1048.01	54.76	5.22	56.68	1.58	2.79	18.49	18.49
91Ile	886.04	69.24	7.81	54.51	2.87	5.26	16.25	16.25
92Met	1051.22	58.54	5.57	56.09	1.97	3.52	18.74	18.74
93Val	1088.81	81.30	7.47	58.85	2.68	4.55	18.50	18.50
94Ile	985.33	105.92	10.75	49.18	3.49	7.10	20.03	
95Gly	958.49	60.49	6.31	49.52	1.61	3.25	19.36	19.36
96Gly	875.99	31.46	3.59	55.96	3.08	5.50	15.65	15.65
97Gly								
98Arg	881.03	33.96	3.85	55.63	1.77	3.19	15.84	15.84
99Val	875.96	51.93	5.93	57.49	1.90	3.31	15.24	15.24
100Tyr	943.05	45.69	4.85	53.48	1.53	2.85	17.64	17.64
101Glu	938.91	36.31	3.87	55.74	0.99	1.78	16.85	16.85
102Gln	1002.34	54.40	5.43	58.70	2.42	4.11	17.07	17.07
103Phe	1042.29	115.87	11.12	62.76	1.32	2.10	16.61	
104Leu	948.07	46.37	4.89	56.44	1.43	2.54	16.80	16.80
105Pro								
106Lys								
107Ala	979.67	22.01	2.25	58.66	1.12	1.90	16.70	16.70
108Gln	918.36	67.79	7.38	55.41	1.64	2.97	16.57	16.57
109Lys	988.88	69.57	7.03	51.09	1.40	2.74	19.35	19.35
110Leu	904.49	79.88	8.83	56.83	1.75	3.07	15.91	15.91
111Tyr	955.69	98.30	10.29	53.04	1.94	3.65	18.02	
112Leu	871.25	74.68	8.57	49.31	3.98	8.07	17.67	17.67
113Thr								

114His	818.44	94.22	11.51	52.88	1.50	2.84	15.48	
115Ile	822.91	131.93	16.03	48.88	2.93	5.99	16.84	
116Asp	853.70	125.84	14.74	56.53	1.88	3.33	15.10	
117Ala	1020.30	48.26	4.73	58.62	2.17	3.70	17.41	17.41
118Glu	1079.37	40.41	3.74	59.03	1.19	2.02	18.29	18.29
119Val								
120Glu	1065.96	16.39	1.54	64.78	1.73	2.67	16.46	16.46
121Gly	1087.79	47.47	4.36	47.70	1.52	3.18	22.80	22.80
122Asp	856.52	69.40	8.10	61.94	2.71	4.37	13.83	13.83
123Thr								
124His								
125Phe	834.95	72.97	8.74	60.15	3.29	5.47	13.88	13.88
126Pro								
127Asp	1079.73	33.69	3.12	59.70	1.38	2.31	18.08	18.08
128Tyr	1406.15	49.60	3.53	62.57	1.16	1.86	22.47	22.47
129Glu	1022.50	52.10	5.10	60.27	2.59	4.30	16.97	16.97
130Pro								
131Asp	1006.47	50.04	4.97	60.74	1.27	2.09	16.57	16.57
132Asp	910.60	57.45	6.31	59.95	1.26	2.10	15.19	15.19
133Trp	936.27	49.00	5.23	52.87	1.77	3.35	17.71	17.71
134Glu	1069.48	40.24	3.76	58.12	2.13	3.67	18.40	18.40
135Ser	1036.91	50.80	4.90	58.31	1.95	3.34	17.78	17.78
136Val	1192.32	291.68	24.46	57.50	3.84	6.67	20.74	
137Phe	891.22	86.47	9.70	53.72	1.83	3.41	16.59	16.59
138Ser	811.12	60.99	7.52	50.11	2.10	4.19	16.19	16.19
139Glu	970.96	69.67	7.17	57.84	3.43	5.93	16.79	16.79
140Phe	713.50	71.05	9.96	57.84	2.85	4.93	12.34	12.34
141His	871.35	82.29	9.44	96.43	7.89	8.18	9.04	9.04
142Asp	1225.89	13.58	1.11	177.58	10.83	6.10	6.90	
143Ala	971.73	28.85	2.97	63.11	1.07	1.69	15.40	15.40
144Asp	1000.05	87.10	8.71	53.17	1.20	2.26	18.81	18.81
145Ala	901.89	54.82	6.08	57.80	2.03	3.51	15.60	15.60
146Gln	1023.82	62.03	6.06	63.05	1.17	1.85	16.24	16.24

147Asn	1074.38	57.82	5.38	58.17	1.80	3.10	18.47	18.47
148Ser	1020.20	58.75	5.76	54.84	1.90	3.47	18.60	18.60
149His	944.69	25.82	2.73	51.22	0.96	1.88	18.44	18.44
150Ser	968.56	39.04	4.03	59.98	1.62	2.70	16.15	16.15
151Tyr	869.45	61.08	7.02	48.39	2.04	4.21	17.97	17.97
152Cys	901.25	90.06	9.99	55.60	1.91	3.44	16.21	16.21
153Phe	853.65	108.58	12.72	59.04	3.26	5.53	14.46	
154Glu	918.61	98.22	10.69	51.30	2.48	4.83	17.91	
155Ile	946.65	60.19	6.36	63.80	2.61	4.10	14.84	14.84
156Leu	401.85	-0.96	-0.24	52.89	10.53	19.92	7.60	
157Glu	1082.42	109.04	10.07	55.43	2.43	4.38	19.53	
158Arg	1073.49	80.27	7.48	64.35	1.51	2.34	16.68	16.68
159Arg	986.51	50.30	5.10	68.76	1.22	1.77	14.35	14.35

Table 8.7.6.1 T1/T2 values for ^{15}N only labelled EcDHFR: $NADP^+$: folate complex in the presence of 17% glycerol at 600 MHz. Rows coloured red represent T1 or T2 values for which the error is greater than 10% of the value itself. Rows coloured yellow represent T1/T2 values that fall outside the average T1/T2 value ± standard deviation, as displayed below (**Table 8.7.6.2)**.

^{15}N labelled EcDHFR complex in the presence of 17% glycerol at 600 MHz	**Raw Values for 131 residues**	**Values for 113 residues within error**
Average T1/T2 Ratio	16.66	17.04
Standard Deviation (SD) of T1/T2	3.00	2.27
Average T1/T2 + SD	19.66	19.32
Average T1/T2 – SD	13.66	14.77

Table 8.7.6.2 Raw values represent the average T1/T2 ratio over all of the 131 amino acid residues in the ^{15}N only labelled EcDHFR: NADP^{+}: folate complex in the presence of 17% glycerol at 600 MHz for which both T1 and T2 values were calculated (**Table 8.7.6.1**).Values within error represent the average T1/T2 ratio of the 113 residues for which the T1 and T2 errors were less than 10% of the values themselves, a total of 18 residues were discounted due to large errors.

Residue	**600 MHz ^{15}N 17% Glycerol T1/T2**
20Met	13.88
67Gly	10.71
68Thr	11.03
69Asp	9.96
88Val	13.67
122Asp	13.83
125Phe	13.88
140Phe	12.34
141His	9.04
159Arg	14.35

Table 8.7.6.3 List of residues in solely ^{15}N labelled EcDHFR: NADP$^{|+}$: Folate complex in 17% glycerol conditions at 600 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio.

Residue	600 MHz ^{15}N 17% Glycerol T1/T2
5Ile	19.33
10Val	19.55
12Arg	20.31
24Leu	19.76
26Ala	19.67
28Leu	20.15
36Leu	19.56
43Gly	23.47
58Lys	19.34
61Ile	19.74
74Trp	21.97
95Gly	19.36
109Lys	19.35
121Gly	22.80
128Tyr	22.47

Table 8.7.6.4 List of residues in solely ^{15}N labelled EcDHFR: $NADP^{|+}$: Folate complex in 17% glycerol conditions at 600 MHz which display T1/T2 ratios that are 1 standard deviation below the mean T1/T2 ratio.

8.7.7 Comparison of the T1/T2 values for EcDHFR:folate:NADP$^+$ complex in buffer only and the presence of co-solvent at 600 MHz and 900 MHz.

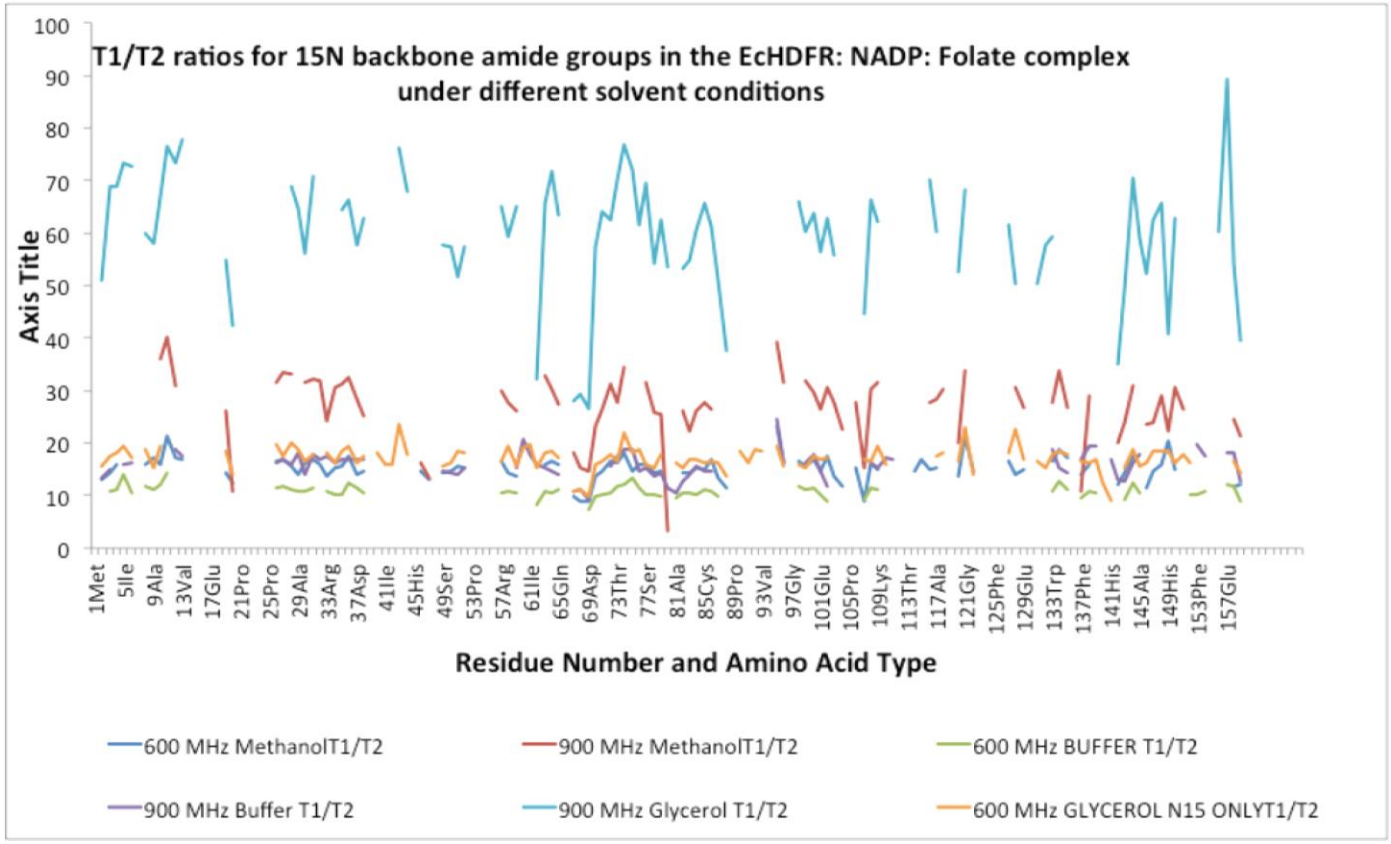

Figure 8.7.7.1 T1/T2 for all residues in the EcDHFR: NADP$^+$: Folate complex inthe presneeand absence of co-solvents for which the T1 and T2 errors were less than 10% of the total values.