

Supporting Information for the manuscript

Manual and automatic assignment of two different A β 40 amyloid fibril polymorphs using MAS solid-state NMR spectroscopy

Natalia Rodina^{1,2}, Riddhiman Sarkar^{1,2}, Dimitrios Tsakalos¹, Saba Suladze¹, Zheng Niu⁴, and Bernd Reif^{1,2}

¹Department of Bioscience, TUM School of Natural Sciences, Technical University of Munich, Munich, Germany

²Institute of Structural Biology, Helmholtz Zentrum Munich or German Research Center for Environmental Health, Munich, Germany

⁴School of Pharmacy, Henan University, Kaifeng, China

For submission to: Biomolecular NMR Assignments

To whom correspondence should be addressed: reif@tum.de

SI Table 1. Chemical shifts in ppm obtained for P1 with automated assignment by ARTINA

	RESIDUE	N	Nδ	Nε	C	Cα	Cβ	Cγ	Cδ	Cε	Cζ
1	Asp	123.36	-	-	171.54	51.28	42.34	171.55	-	-	-
2	Ala	122.56	-	-	174.04	48.34	20.59	-	-	-	-
3	Glu	120.64	-	-	171.72	52.72	32.01	34.21	171.75	-	-
4	Phe	124.06	-	-	171.74	54.69	41.61	134.96	128.81	129.66	129.66
5	Arg	128.12	-	-	171.73	52.43	25.39	25.41	41.67	-	-
6	His	126.07	-	-	173.86	52.15	30.11	128.72	118.47	134.26	-
7	Asp	126.21	-	-	175.81	54.56	36.81	175.81	-	-	-
8	Ser	121.18	-	-	170.52	55.8	63.29	-	-	-	-
9	Gly	112.7	-	-	171.55	43.26	-	-	-	-	-
10	Tyr	128.05	-	-	171.64	52.32	41.64	120.92	128.79	118.54	169.68
11	Glu	126.03	-	-	173.46	52.55	30.22	34.34	180.95	-	-
12	Val	123.52	-	-	172.68	58.25	33.88	18.77. 18.75	-	-	-
13	His	124.48	-	-	172.96	58.31	34.15	134.41	119.86	134.41	-
14	His	124.34	-	-	173.01	58.31	31.01	134.41	119.86	134.41	-
15	Gln	113.59	-	-	173.02	51.37	31	34.22	174.42	-	-
16	Lys	123.37	-	-	172.9	52.62	34.18	24	28.07	40.33	-
17	Leu	124.39	-	-	172.78	53.88	36.92	25.29	24.57. 23.20	-	-
18	Val	116.14	-	-	171.74	58.09	36.06	22.25. 18.77	-	-	-
19	Phe	125.28	-	-	169.86	54.88	40.98	134.96	129.59	129.66	128.77
20	Phe	130.38	-	-	171.13	53.82	40.99	134.96	134.96	129.31	128.77
21	Ala	124.83	-	-	174.91	47.7	20.89	-	-	-	-
22	Glu	111.92	-	-	174.87	57.33	26.53	32.93	182.27	-	-
23	Asp	115.68	-	-	173.15	50.54	41.88	180.01	-	-	-
24	Val	124.35	-	-	173.08	58.25	31	20.38. 18.73	-	-	-
25	Gly	112.58	-	-	171.49	43.41	-	-	-	-	-
26	Ser	111.33	-	-	172.01	57.57	61.76	-	-	-	-
27	Asn	117.75	-	-	173.97	52.18	38.43	173.9	-	-	-
28	Lys	117.73	-	-	174.03	52.44	36.08	24.87	27.48	42.41	-
29	Gly	115.74	-	-	171.57	47.09	-	-	-	-	-
30	Ala	115.33	-	-	172.48	47.7	20.87	-	-	-	-
31	Ile	120.52	-	-	172.41	58.69	38.74	15.88. 26.77	12.33	-	-
32	Ile	123.84	-	-	172.28	56.44	41.5	15.86. 25.24	12.47	-	-
33	Gly	109.5	-	-	167.83	42.67	-	-	-	-	-
34	Leu	125.91	-	-	171.73	51.48	42.81	26.25	26.28. 26.23	-	-
35	Met	120.62	-	-	171.74	52.75	34.09	31.99	-	17.61	-
36	Val	124.03	-	-	172.75	57.78	33.75	18.78. 18.78	-	-	-
37	Gly	116.07	-	-	170.51	45.9	-	-	-	-	-
38	Gly	112.75	-	-	170.54	42.82	-	-	-	-	-
39	Val	116.07	-	-	172.72	57.97	33.76	18.77. 18.77	-	-	-
40	Val	116.09	-	-	171.69	58.09	36.05	18.77. 22.24	-	-	-

SI Table 2. Chemical shifts in ppm obtained for P2 with automated assignment by ARTINA.

	RESIDUE	N	N δ	N ϵ	C	C α	C β	C γ	C δ	C ϵ	C ζ
1	Asp	122.33	-	-	173.72	55.24	37.93	182.75	-	-	-
2	Ala	119.08	-	-	173.53	48.42	21.16	-	-	-	-
3	Glu	120.43	-	-	173.27	52.11	30.25	34.61	172.03	-	-
4	Phe	125.47	-	-	173.65	56.67	40.19	-	-	-	-
5	Arg	123.45	-	91.83	172.62	53.18	31.75	26.17	40.69	-	-
6	His	124.22	-	-	172.96	57.82	33.29	116.45	116.45	-	-
7	Asp	126.86	-	-	174.54	51.98	42.07	179.15	-	-	-
8	Ser	117.24	-	-	172.09	55.48	65.53	-	-	-	-
9	Gly	110.18	-	-	170.34	43.32	-	-	-	-	-
10	Tyr	128.31	-	-	172.88	59.38	38.41	116.45	-	-	168.11
11	Glu	124.32	-	-	172	52.74	29.26	37.16	180.97	-	-
12	Val	121.03	-	-	174.36	57.62	33.41	17.97. 17.97	-	-	-
13	His	113.93	-	-	172.98	54.24	30.27	132.8	116.43	135.65	-
14	His	125.28	-	-	172.88	54.24	30.32	132.8	116.43	135.65	-
15	Gln	125.33	-	110.61	173.11	54.23	30.37	34.8	181.39	-	-
16	Lys	125.27	-	-	173.09	54.13	34.66	24.98	28.21	39.27	-
17	Leu	126.97	-	-	173.57	53.14	44.78	29.98	26.17. 22.08	-	-
18	Val	119.5	-	-	173.21	58.79	34.5	20.95. 19.24	-	-	-
19	Phe	126.95	-	-	170.76	55.09	42.14	-	-	-	-
20	Phe	128.23	-	-	170.65	53.22	42.16	-	-	-	-
21	Ala	127.9	-	-	173.33	48.2	21.27	-	-	-	-
22	Glu	120.59	-	-	172.99	54.22	33.42	34.58	174.45	-	-
23	Asp	128.01	-	-	173.11	51.41	40.9	173	-	-	-
24	Val	117.22	-	-	175.03	59.1	34.38	20.32. 19.44	-	-	-
25	Gly	110.76	-	-	170.52	44.71	-	-	-	-	-
26	Ser	108.26	-	-	172.79	54.25	63.92	-	-	-	-
27	Asn	113.79	115.12	-	175.11	51.27	37.2	175.15	-	-	-
28	Lys	115.12	-	-	173.33	54.67	33.96	24.54	28.38	40.34	-
29	Gly	107.69	-	-	169.92	42.33	-	-	-	-	-
30	Ala	126.52	-	-	173.58	47.96	19.38	-	-	-	-
31	Ile	123.35	-	-	172.78	59.4	38.45	17.93. 26.84	12.46	-	-
32	Ile	124.69	-	-	174.7	56.52	40.95	25.63. 16.15	12.55	-	-
33	Gly	114.11	-	-	171.82	47.15	-	-	-	-	-
34	Leu	122.98	-	-	174.15	52.04	44.37	26.94	23.80. 23.21	-	-
35	Met	119.35	-	-	172.1	52.91	34.54	31.72	-	18.99	-
36	Val	125.4	-	-	173.22	58.87	31.49	18.91	-	-	-
37	Gly	111	-	-	172.06	44.38	-	-	-	-	-
38	Gly	106.07	-	-	169.92	42.39	-	-	-	-	-
39	Val	124.01	-	-	173.09	59.4	33.15	19.40. 19.31	-	-	-
40	Val	125.95	-	-	173.16	59.57	33.11	19.12. 21.83	-	-	-

SI Table 3. Random coil chemical shifts predicted for A β 40 peptide

Predicted random coil chemical shifts		by tab2bmr tool https://bmr.io/tab2bmr/				by the SBiNLab online tool https://www1.bio.ku.dk/english/research/bms/sbinlab/randomchemicalshifts/			
Residue		C α	C β	C	N	C α	C β	C	N
1	Asp	54.45	40.995	176.166	121.86	54.464	41.028	176.166	121.86
2	Ala	52.955	18.833	177.889	124.587	52.944	18.857	177.889	124.587
3	Glu	56.86	30.183	176.427	119.045	56.865	30.206	176.427	119.045
4	Phe	57.54	39.52	175.471	120.931	57.516	39.532	175.471	120.931
5	Arg	55.912	30.857	175.674	122.849	55.906	30.875	175.674	122.849
6	His	56.64	30.745	175.128	121.289	56.679	30.823	175.128	121.289
7	Asp	54.556	41.075	176.328	121.994	54.57	41.108	176.328	121.994
8	Ser	59.027	63.427	175.269	116.257	59.018	63.449	175.269	116.257
9	Gly	45.315	**.*	173.242	112.29	45.332	**.*	173.242	112.29
10	Tyr	57.865	38.705	175.709	118.727	57.84	38.719	175.709	118.727
11	Glu	56.262	30.279	175.981	122.987	56.267	30.302	175.981	122.987
12	Val	62.542	32.728	175.915	121.655	62.528	32.741	175.915	121.655
13	His	56.293	30.995	175.126	123.62	56.332	31.073	175.126	123.62
14	His	56.46	31.208	175.133	121.81	56.499	31.286	175.133	121.81
15	Gln	56.035	29.398	175.615	122.2	56.046	29.416	175.615	122.2
16	Lys	56.321	32.884	176.313	123.133	56.317	32.896	176.313	123.133
17	Leu	55.229	42.232	177.144	124.695	55.238	42.256	177.144	124.695
18	Val	62.591	32.587	175.518	121.891	62.577	32.6	175.518	121.891
19	Phe	57.465	39.537	175.019	123.736	57.441	39.549	175.019	123.736
20	Phe	57.241	39.658	174.753	122.448	57.217	39.67	174.753	122.448
21	Ala	52.486	19.103	177.38	125.921	52.475	19.127	177.38	125.921
22	Glu	56.812	30.349	176.205	120.334	56.817	30.372	176.205	120.334
23	Asp	54.301	41.108	176.37	121.354	54.315	41.141	176.37	121.354
24	Val	62.76	32.342	176.958	121.016	62.746	32.355	176.958	121.016
25	Gly	45.355	**.*	173.709	114.145	45.372	**.*	173.709	114.145
26	Ser	58.62	63.776	174.615	115.809	58.611	63.798	174.615	115.809
27	Asn	53.343	38.536	175.316	119.712	53.357	38.562	175.316	119.712
28	Lys	56.886	32.886	177.145	121.509	56.882	32.898	177.145	121.509
29	Gly	45.12	0	173.107	111.372	45.137	**.*	173.107	111.372
30	Ala	52.423	19.243	177.635	124.081	52.412	19.267	177.635	124.081
31	Ile	60.905	38.622	176.286	120.784	60.895	38.645	176.286	120.784
32	Ile	61.255	38.697	176.463	126.207	61.245	38.72	176.463	126.207
33	Gly	45.25	**.*	173.535	114.388	45.267	**.*	173.535	114.388
34	Leu	55.198	42.379	177.401	122.453	55.207	42.403	177.401	122.453
35	Met	55.247	32.621	176.152	121.511	55.268	32.667	176.152	121.511
36	Val	62.535	32.77	176.565	122.356	62.521	32.783	176.565	122.356
37	Gly	45.359	**.*	173.889	114.064	45.376	**.*	173.889	114.064
38	Gly	45.166	**.*	173.517	110.229	45.183	**.*	173.517	110.229
39	Val	62.358	32.746	176.389	120.383	62.344	32.759	176.389	120.383
40	Val	62.381	32.788	176.091	124.981	62.367	32.801	176.091	124.981

