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**Supporting Material**

**Solid-state NMR characterization of gas vesicle structure**

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**Supplementary material for  
Solid-state NMR characterization of gas vesicle structure  
by  
Sivertsen, Bayro, Belenky, Griffin, and Herzfeld**

**Table S1. Chemical shifts of the residues in GvpA.**

Res	CO	CA	CB	N	Side-chain
A01	173.7	52.1	20.5	43.4	
V02	177.0	62.7	32.2	125.4	CG1: 23.0, CG2: 22.0
E03	175.5	57.1	31.4	136.7	
S09	174.2	58.6	66.9	118.7	
S10	175.9	57.9	65.8	121.2	
L11	178.4	58.5	41.7	124.0	CG: 27.8, CD1: 27.5, CD2: 27.2
A12	180.1	56.1	18.6	123.9	
E13	180.0	59.9	30.5	120.2	
V14	178.3	67.5	32.3	123.7	CG1: 23.9, CG2: 21.7
I15	178.3	67.6	39.0	122.5	CD1: 14.0, CG1: 31.7, CG2: 18.3
D16	180.2	58.6	41.7	120.2	
R17	180.8	59.9	31.8	120.3	CG: 28.2, CD: 45.1, CZ: 160.5, NE: 88.4
I18	177.9	66.1	39.0	123.3	CG1: 30.5, CG2: 19.8, CD1: 15.1
L19	176.2	55.7	42.1	122.3	CG: 27.7
D20	180.3	57.7	41.5	121.7	
K21	180.0	59.5	34.0	122.4	CG: 26.1
G22	170.9	44.9		115.1	
I23	175.3	62.2	43.1	118.0	CD1: 14.9, CG1: 27.6, CG2: 18.0
V24	175.6	61.6	35.8	128.5	CG1: 22.5, CG2: 21.8
I25	173.8	61.2	43.3	127.9	CD1: 16.2, CG1: 28.4, 19.4
D26	180.4	58.9	41.5	128.4	
A27	175.6	52.5	24.2	128.2	
W28		56.0	32.2	121.6	CG: 111.0, CD1: 129.8
V34	180.0	57.8	32.0	125.6	CG1: 21.1, CG2: 21.0
G35	169.9	45.1		110.8	
I36	175.8	61.3	43.2	117.3	
E37	176.9	55.5	36.1	132.1	CG: 36.4
L38	175.9	56.7	45.5	131.4	CG: 28.2
L39	175.9	54.2	48.2	127.6	CG: 27.9, CD1: 27.3
A40	176.8	52.8	22.2	123.1	
I41	173.9	61.6	42.1	125.2	CG1: 28.3
E42	176.8	55.6	35.8	132.1	
A43	176.0	51.5	24.6	126.6	
R44	179.9	58.9	36.6	126.4	CG: 28.7, NE: 88.7
I45	175.8	60.8	42.8	128.4	CG1: 28.6, CD1: 16.0
V46	175.5	61.4	35.1	129.3	CG1: 21.3, CG2: 19.6
I47	175.5	60.9	42.3	127.6	CG1: 27.8, CG2: 17.5, CD1: 14.8
A48	175.6	52.6	24.3	128.1	

A48x	175.6	52.4	24.3	
S49	175.5	57.3	65.4	116.7
S49x	175.4	57.1	65.9	115.0
V50	178.4	69.3	31.6	121.5
E51	180.1	61.3	30.6	121.1
T52	176.8	67.6	68.3	120.5
T52x	175.8	68.0	69.4	120.9
Y53	178.5	63.8	39.6	127.1
Y53x	178.3	64.1	39.4	127.9
L54	178.6	58.6	41.8	120.4
K55	180.4	60.5	32.9	122.0
Y56	175.9	61.8	38.2	123.2
Y56x		61.3	37.9	
A57	180.2	55.6	20.9	124.3
A57x				124.1
E58	180.1	58.7	30.4	123.9
A59	180.5	55.4	20.9	124.2
V60	176.9	62.9	32.8	107.7
G61	175.5	46.2		110.3
L62	175.4	55.0	48.1	121.4
T63	174.2	60.9	70.0	113.6
Q64	180.4	61.2	30.5	120.9
S65	175.7	58.6	65.9	121.3
A66	180.4	55.3	19.2	124.3
P69	175.5	57.0	31.4	136.7

CG1: 25.3, CG2: 22.5

CG: 37.9, CD: 184.3

CG2: 23.4

CG: 130.4, CD: 133.4, CE: 119.0, CZ: 160.2

CG: 27.3

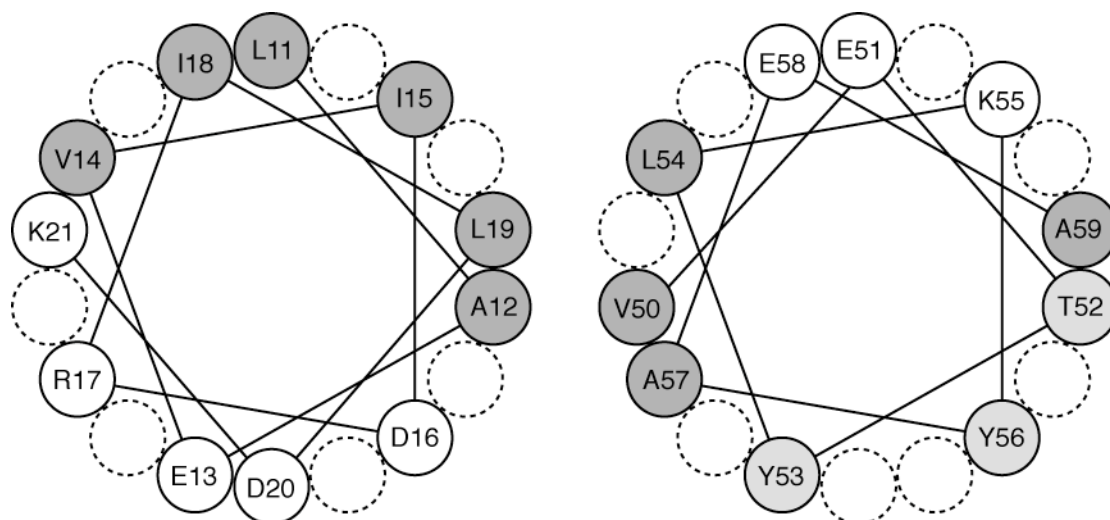
CG: 26.1, CD: 30.5, CE: 43.0, NZ: 36.0

CG: 129.4, CE: 119.6

CG1: 20.9, CG2: 18.0

CG: 27.8, CD1: 24.2, CD2: 23.7

CG2: 23.2



**Figure S1. Helical wheels for the two  $\alpha$ -helices in GvpA. Shading distinguishes between ionizable (white), other polar (light gray), and non-polar (dark gray) residues.**