Table S1. Content of various secondary structural elements of the individual clusters. The number of residues having a given type of secondary structural unit out of total 91 residues.

	2KP5	**1**	**2**	**3**	**4**	**R2**	**R3**	**R4**	**R5**	**R6**	**R7**	**R8**
β-Sheet	34	34	28	26	32	10	15	7	15	12	15	21
Bridge	1	1	1	3	2	0	1	1	1	1	2	2
α-Helix	7	6	12	15	6	14	18	23	7	14	20	5
Turn	27	28	28	20	29	36	32	32	41	29	28	41
3_{10}-helix	0	2	2	2	2	3	3	5	4	3	3	5
Coil	22	20	21	25	20	28	22	23	23	32	23	17

Table S2. The computed radius (C_r) and radius of gyration (R_g) of holo-Hahellin and the REMD clusters (1 to 4 and R2 to R8) in Å.

	2KP5	1	2	3	4	R2	R3	R4	R5	R6	R7	R8
C_r	16.8	17.6±0.7	18.3±0.8	18.4±0.6	17.8±0.7	19.6.±0.7	19.4±0.9	18.5±0.8	19.6±0.6	18.9±0.4	19.6±0.8	18.7±0.4
R_g	12.5	12.8±0.2	13.1±0.3	13.4±0.1	13.0±0.2	13.7.±0.3	13.2±0.2	13.7±0.2	13.3±0.2	13.1±0.3	14.0±0.3	13.0±0.1

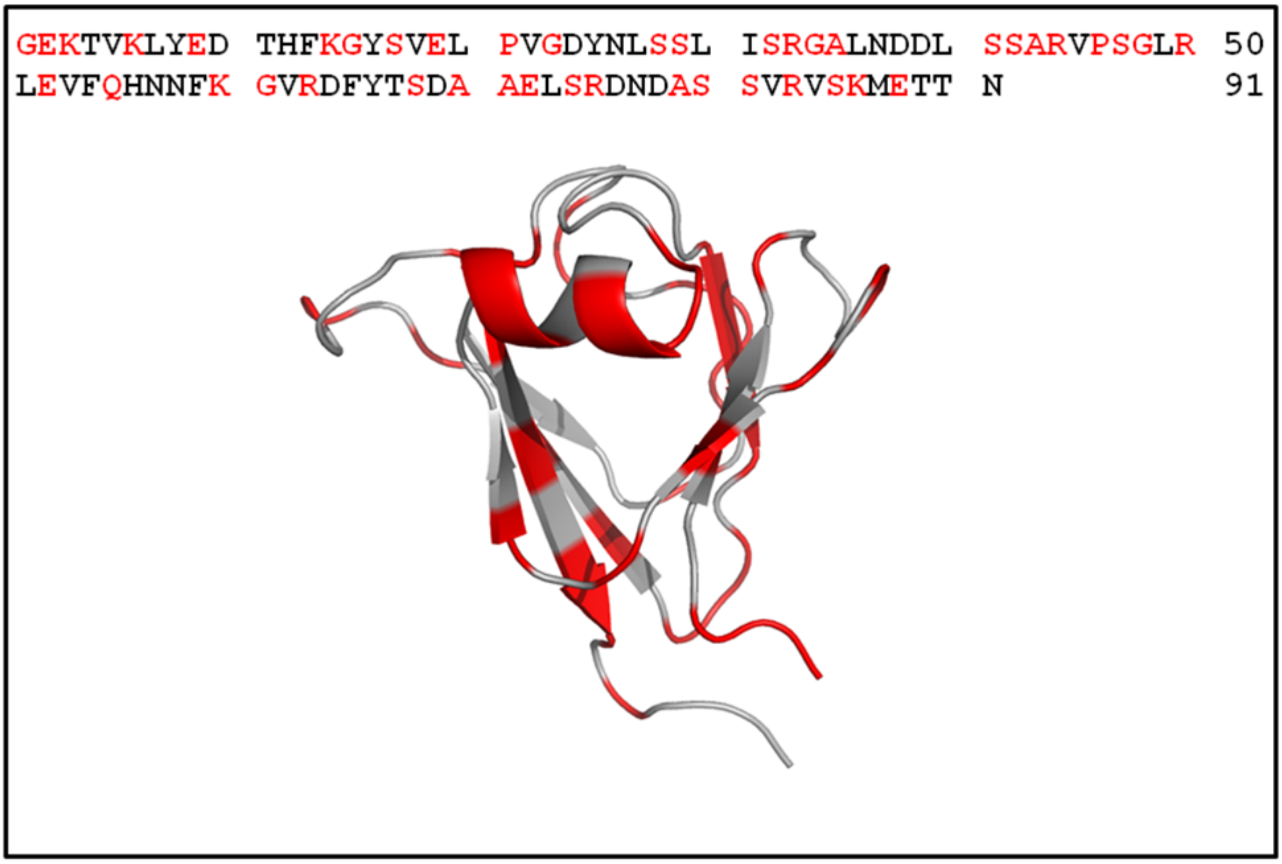

Figure S1. The NMR derived structure of holo-Hahellin highlighting the disorder promoting residues (shown in red). The primary sequence is shown on top of the panel with disorder promoting residues shown again in red.

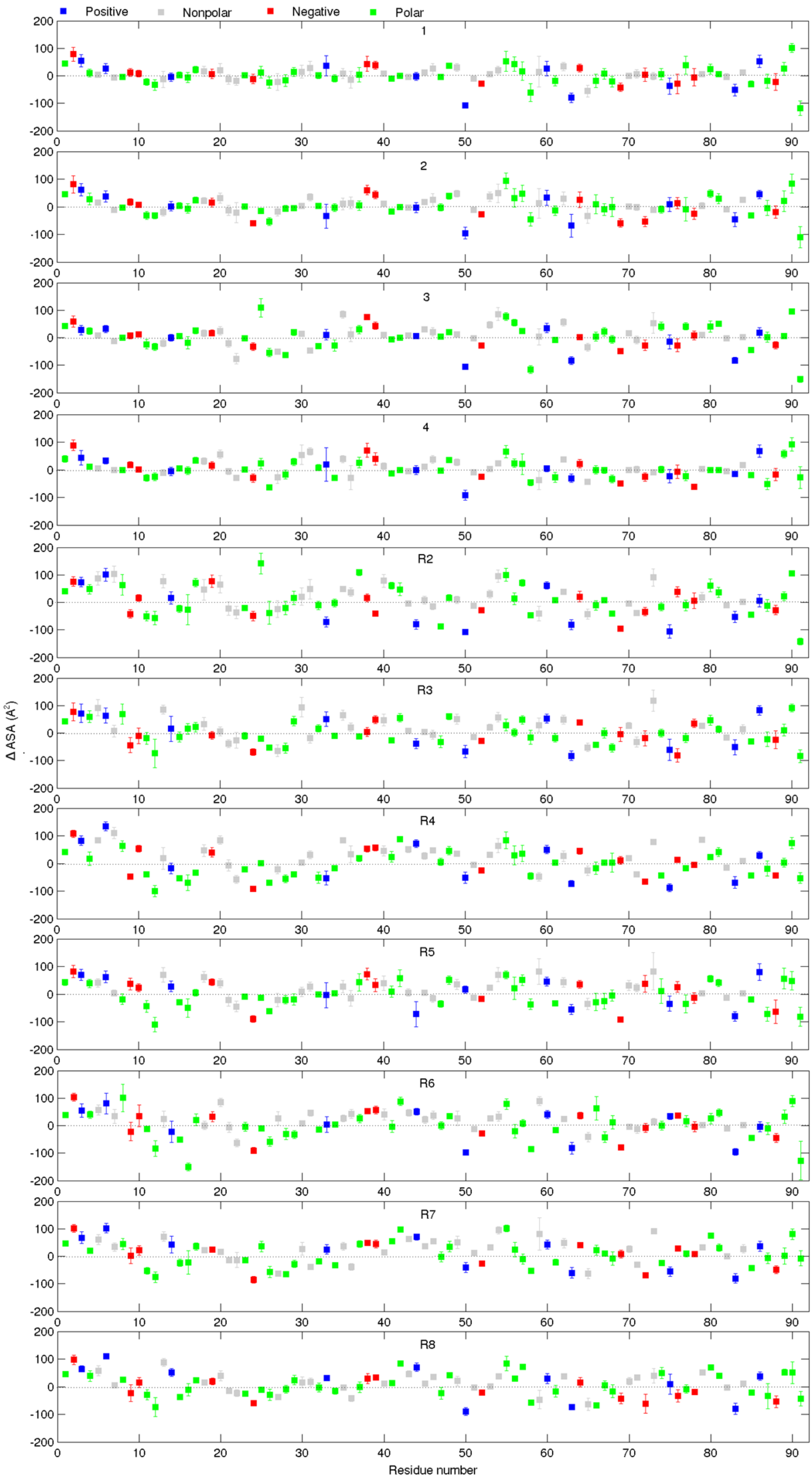
Positive
Nonpolar
Negative
Polar
1
2
3
4
R2
R3
R4
R5
R6
R7
R8
200
100
0
-100
-200
0
10
20
30
40
50
60
70
80
90
Δ ASA (Å²)
Residue number

Figure S2. The change in residue-wise solvent accessible surface area (ΔASA) for each of the eleven clusters (see main text). The negative value indicates that the residue in holo-Hahellin is more exposed, while positive values indicate the opposite and zero values indicate that cluster member and holo-Hahellin have similar ASA. The standard deviation seen in ΔASA for individual cluster members is indicated with an error bar.

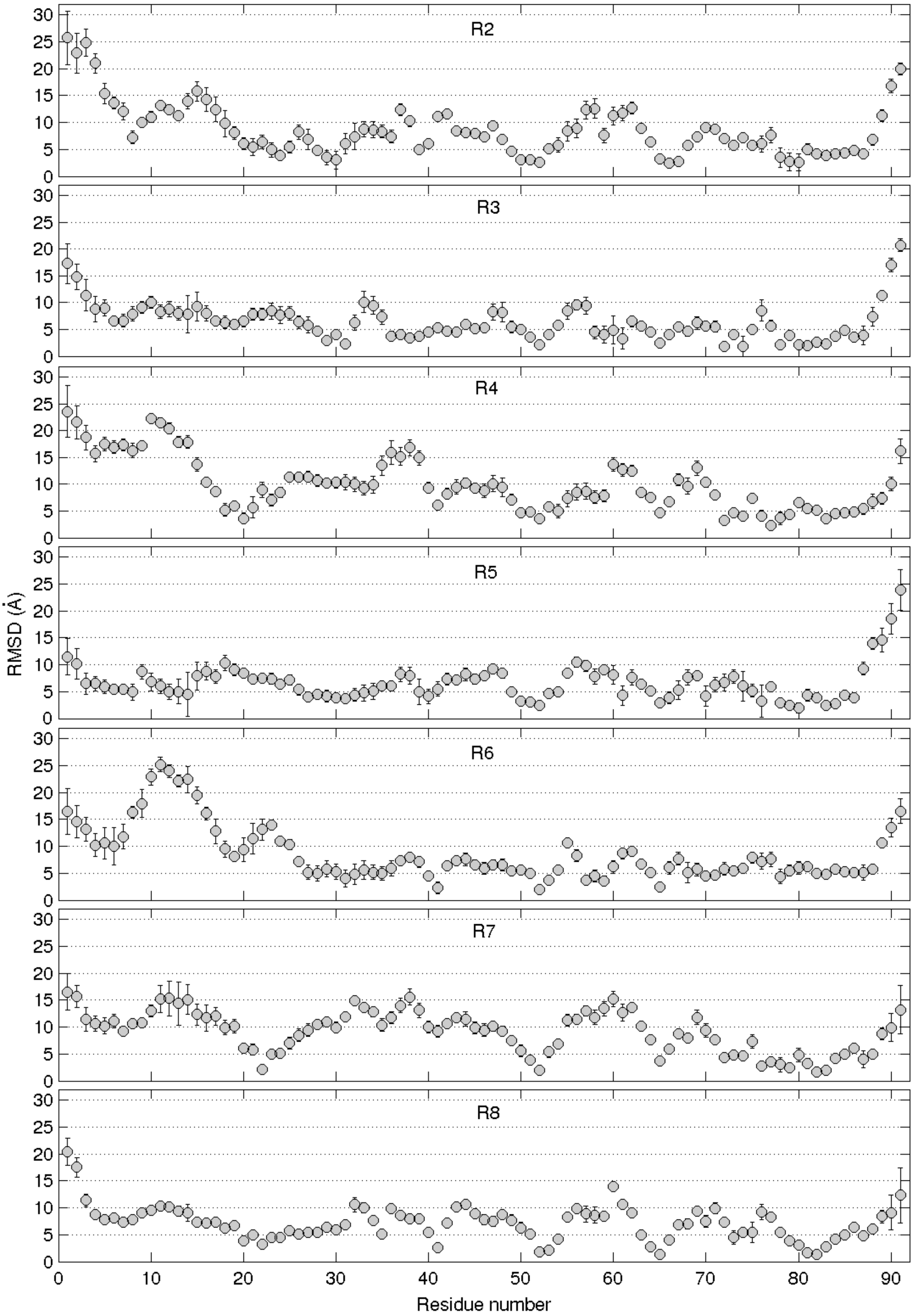

Figure S3. Residue wise RMSD values w.r.t. the holo-Hahellin for the far-native clusters (R2 to R8), which show large structural deviation all along the polypeptide sequence.

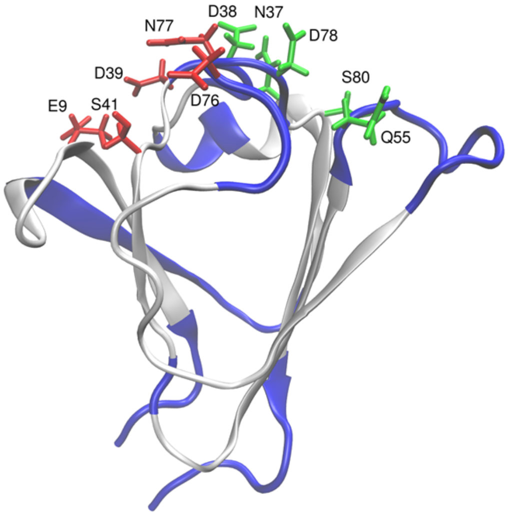

Figure S4. Residues showing higher values of RMSD (> 4 Å) were mapped on to the NMR derived holo-Hahellin structure and were shown in blue. The calcium binding residues of the N- and C-terminal Greek key motives are indicated in red and green stick models, respectively.