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Supporting information for article:

Impact of the crystallization condition on importin-β conformation

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Figure S1 Impß nomenclature of HEAT repeats and helices. A structure of Impβ from *Chaetomium thermophilum* is depicted in cartoon mode. The outer A-helices are coloured in blue and the inner helices in yellow. Connecting residues are coloured in grey. The numbers indicate the number of the respective HEAT repeat, starting from the N-terminus.

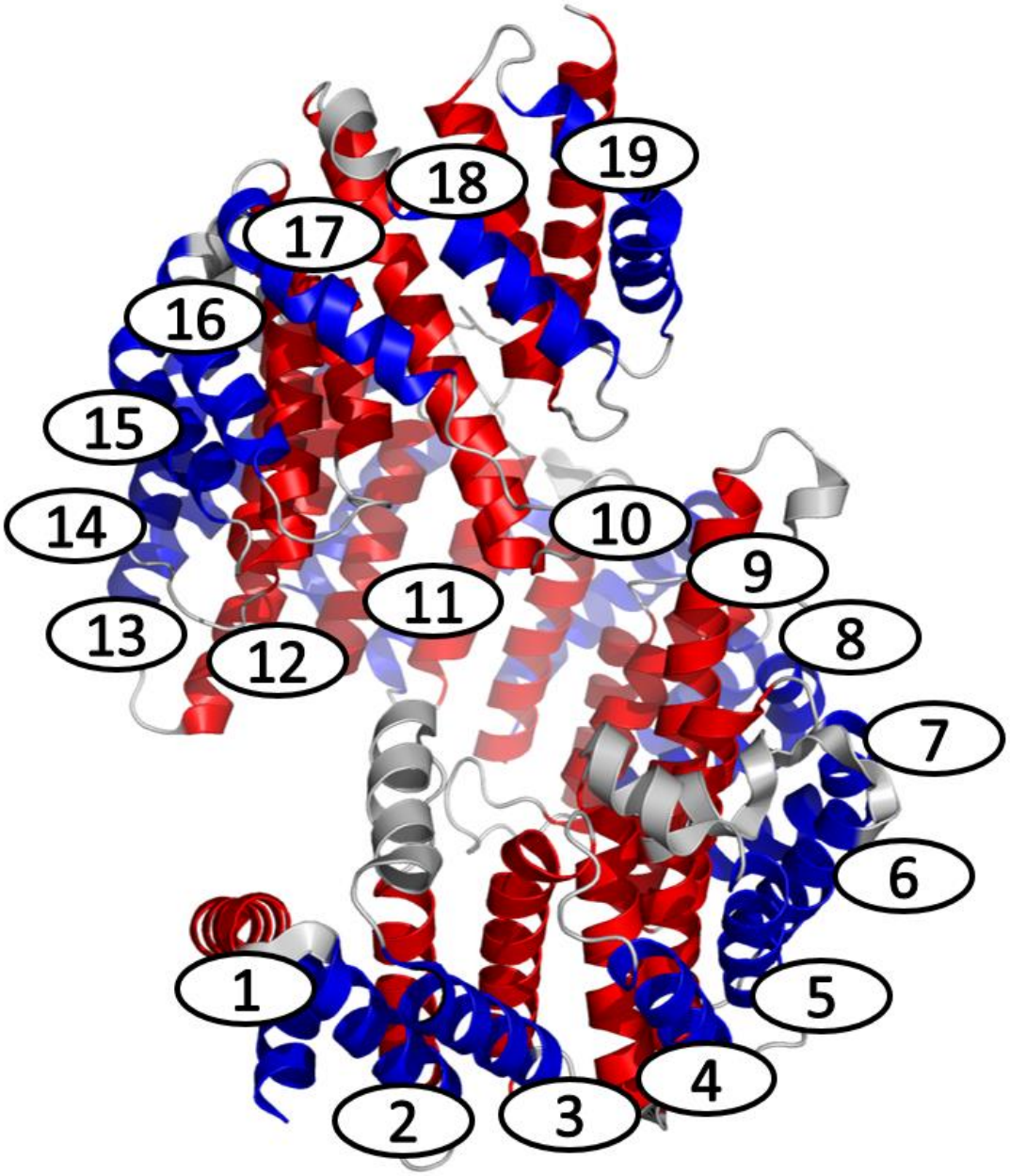


Figure S2 Supplementary figure showing a plot of PEG concentration present in the crystallization condition versus the distance between two common residues of the available Impβ structures suggests a direct correlation of PEG concentration and the distance. Only the structures (respective PDBids are indicated) comprising at least residues 17 to 417 were used.

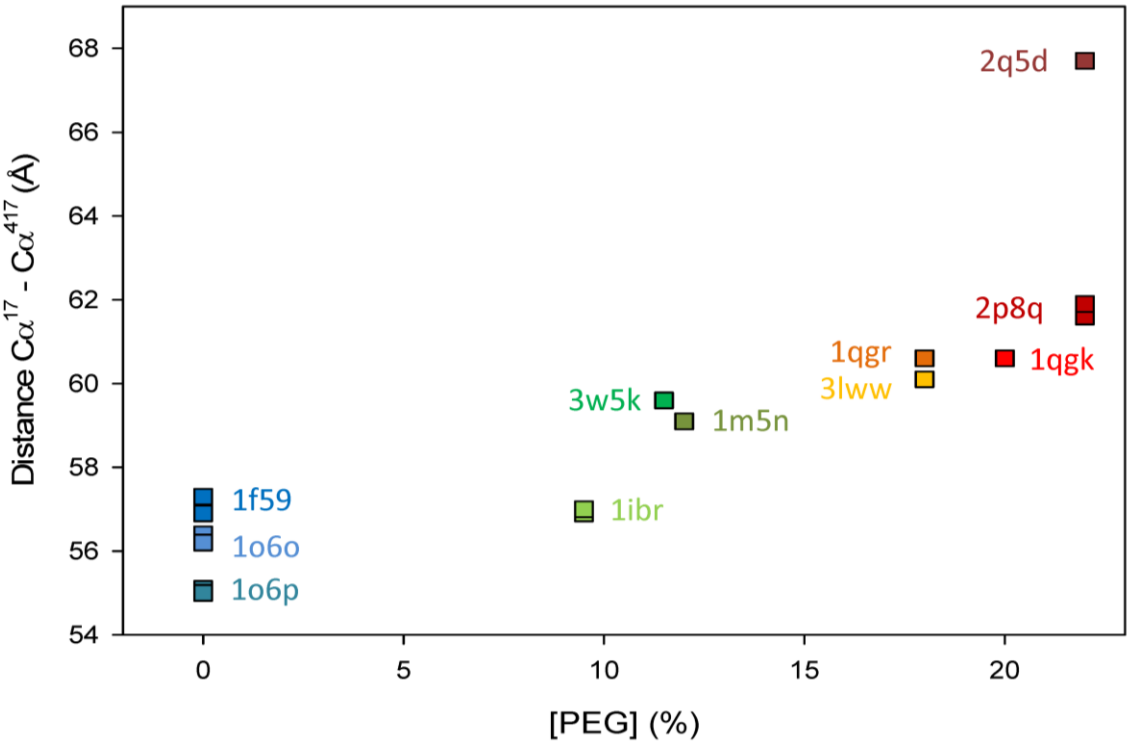


Figure S3 The point mutation S107P in ctImpβ is involved in crystal contacts in the $NH_4)_2SO_4$ crystallization conditions, but not in the PEG condition. **(a)**The 2.05 Å ctImpβ structure in $NH_4)_2SO_4$ is depicted in yellow and a symmetry related molecule in green. The mutated P107 is in close spatial proximity to this symmetry partner and possible hydrophobic interactions are marked by dashed lines (black) also stating the according distances. It is assumed that the increased rigidity of proline compared to serine enables the formation of this crystal contact. Due to this, crystallization of original unmutated ctImpβ in $NH_4)_2SO_4$ was not possible. **(b)** In the 3.25 Å structure of ctImpβ no symmetry related molecules are in spatial proximity to residue 107, as a result, alterations of this amino acid do not influence crystallization outcome and crystals are obtained with the original and mutated ctImpβ. **(c)** Structure of the region of ctImpβ encompassing the V134A mutation and **(d)** Structure of the region of wt ctImpβ encompassing the V134. Both regions exhibit highly similar structural properties. **(e)** Overlay of both molecules using the complete structures. **(f)** Overlay of both structures using only HEAT repeats 2-4 of the individual superposition. Both superpositions were performed using PyMol.

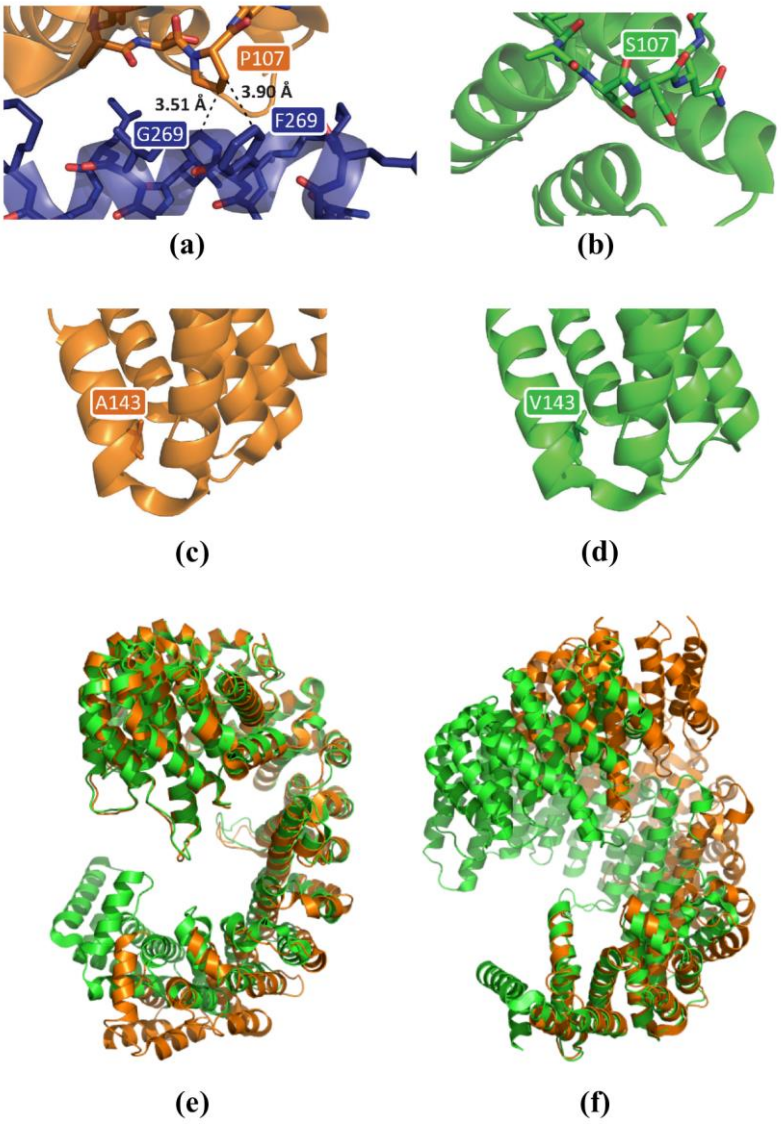
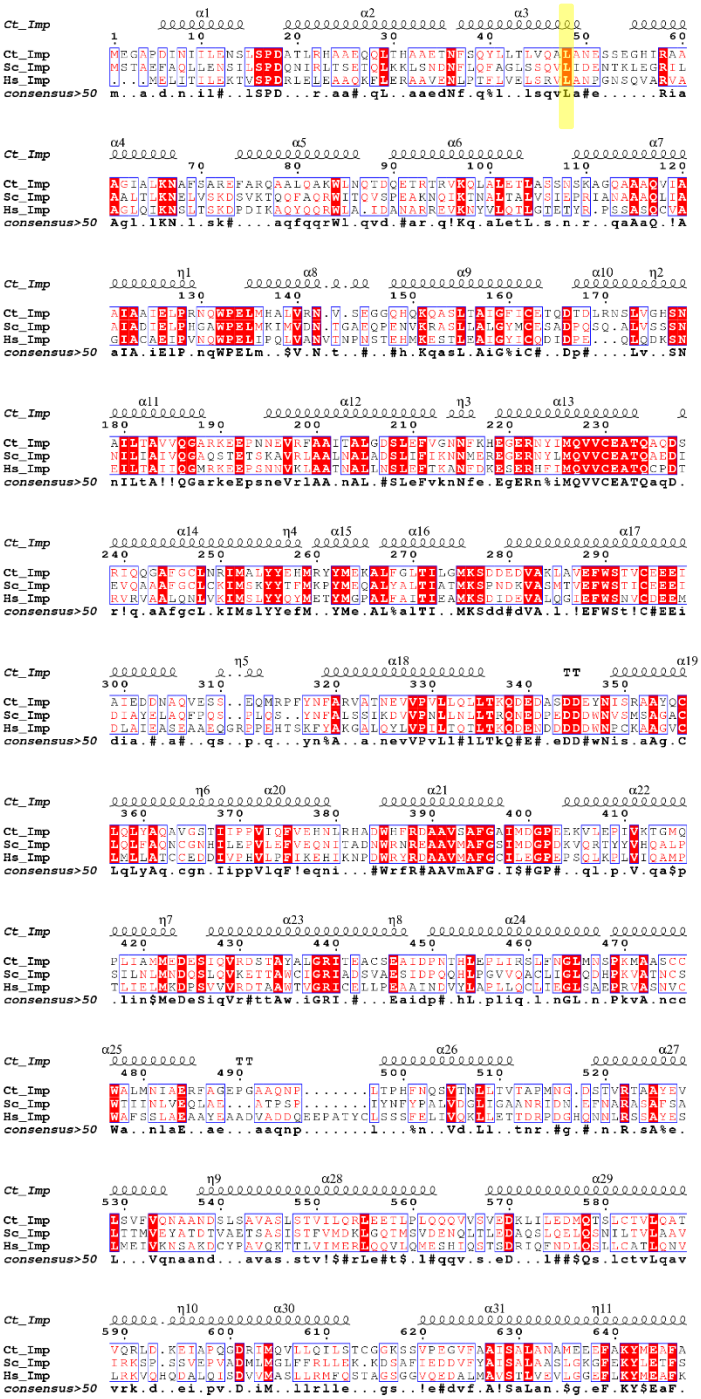


Figure S4 Supplementary figure with an alignment of the Impβ sequences of the structures used, indicating the residues (L48 and W858 for ctImpβ) chosen for determination of Dd (highlighted in yellow. See also Figure S5 for definition.



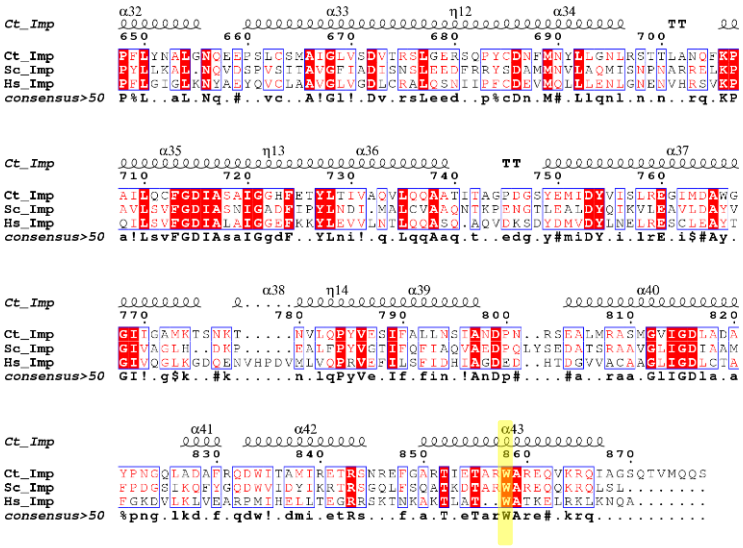

Ct_Imp
Sc_Imp
Hs_Imp
consensus>50
α32
α33
η12
α34
α35
η13
α36
α37
α38
η14
α39
α40
α41
α42
α43

Figure S5 Supplementary figure illustrating the definition of the distances used for structural comparison of Impβ. The distances are the following: "Distance N-C" (Dd) describing the distance between two common residues at the distal ends (darkgreen) present in all structures. The helical pitch describing the distance between two residues one turn apart in the superhelix (with similar positioning with respect to the central axis of Impβ, in red) and the distances measured between two residues orthogonal to the central axis in both, the N- and C-terminal regions (Diameter N (purple) and C (orange), respectively). The respective distances are measured between the Cα-atoms of the residues. Coloring is identical in Figures 2-5.

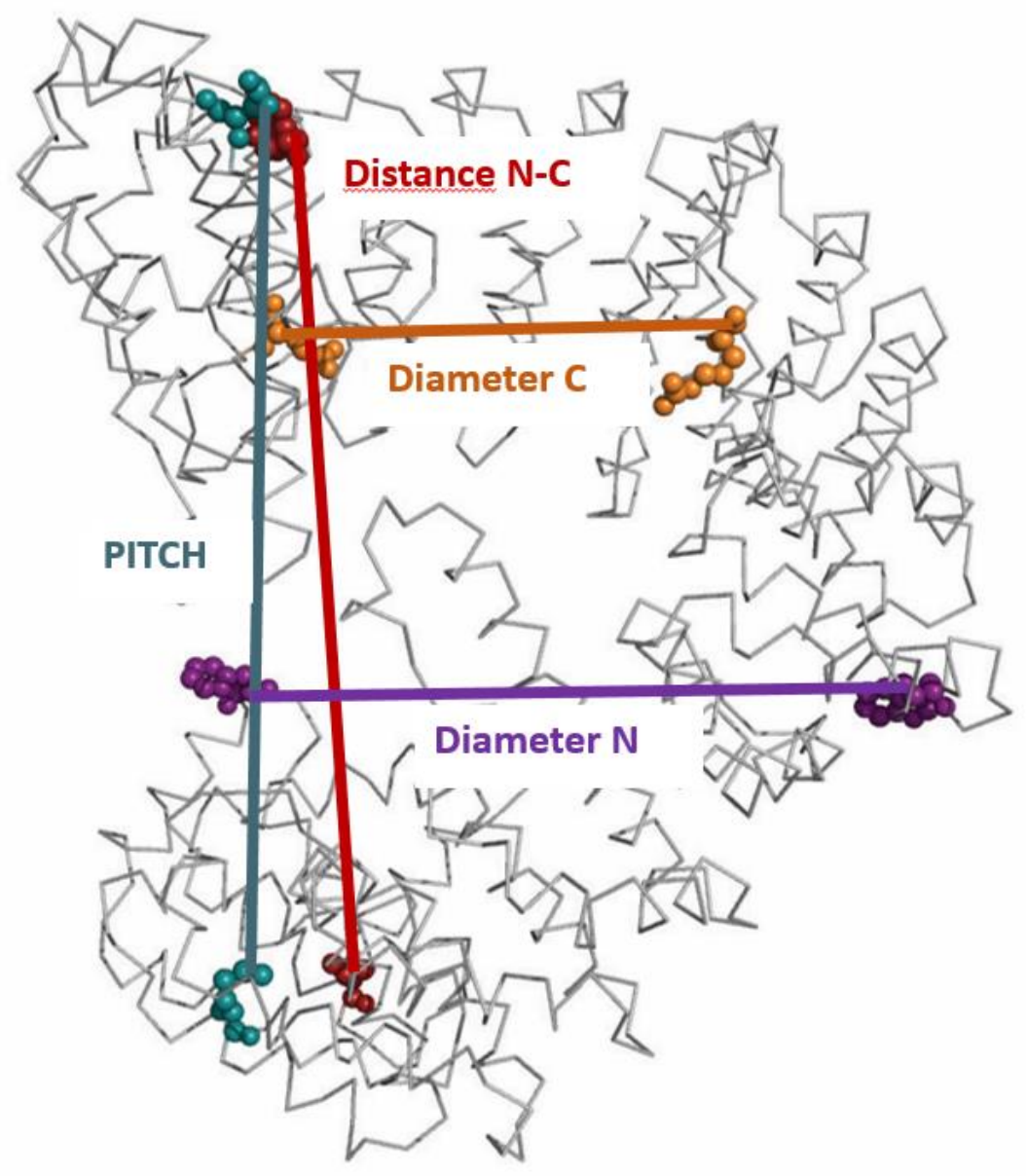
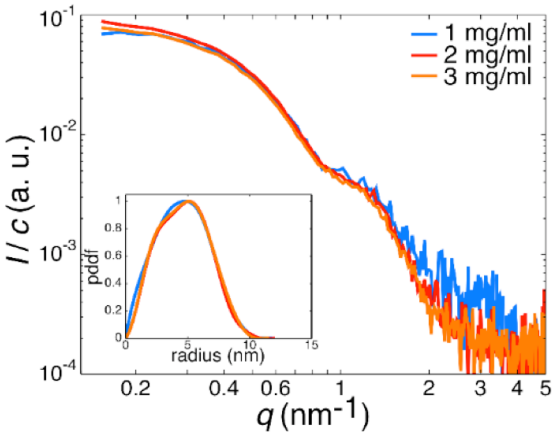
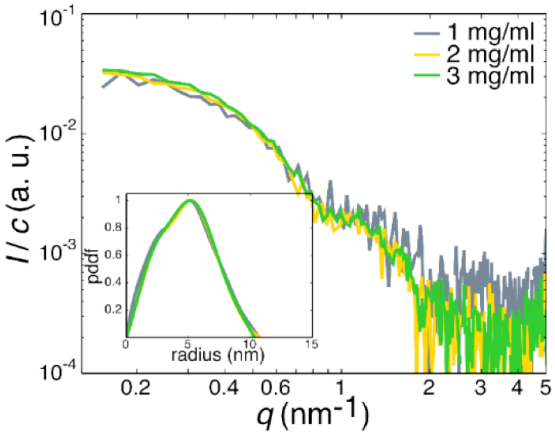


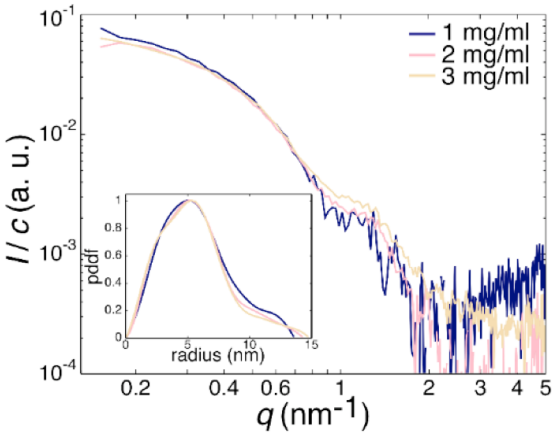
Figure S6 Supplementary figure showing the SAXS curves of the individual measurements for Impβ in the three environments tested. **(a)** Impβ in buffer only, **(b)** in buffer with $(NH_4)_2SO_4$ added. **(c)** in buffer with PEG added. For details of the experimental setup, please refer to the Methods section in the main text. See also Table S1 for results.



(a)



(b)



(c)

Table S1 SAXS data of the individual experiments used for averaging. All samples of Impβ were diluted in buffer containing 100 mM NaCl and 10 mM Tris and the respective compound indicated under "system condition". For methodological and computational details, see the Methods section in the main text.

System condition	***c*** **(mg/ml)**	R_g **(nm)**	D_{max} **(nm)**	I_0 **/** ***c*** **(cm^{-1} mg^{-1} ml) x10^{-2}**	***q*-range[#] (nm^{-1})**	**Total estimate (max = 1)**
-	3	3.62 ± 0.01	10.8	8.6 ± 0.1	[0.15; 3.43]	0.93
	2	3.61 ± 0.02	10.7	9.5 ± 0.1	[0.15; 3.43]	0.90
	1	3.53 ± 0.02	10.3	8.5 ± 0.1	[0.15; 3.43]	0.91
+ 1 M $(NH_4)_2SO_4$	3	3.72± 0.05	11.0	3.8 ± 0.2	[0.15; 3.43]	0.98
	2	3.73 ± 0.05	11.1	3.6 ± 0.1	[0.15; 3.43]	0.93
	1	3.74 ± 0.07	10.7	3.3 ± 0.1	[0.15; 3.43]	0.82
+ 14% w/v PEG 4000 + 8% w/v PEG 200	3	3.71 ± 0.03	11.0	6.0 ± 0.1	[0.28; 3.43]	0.85
	2	3.62 ± 0.02	10.0	5.5 ± 01	[0.28; 3.43]	0.85
	1	3.76 ± 0.05	10.6	6.5 ± 0.2	[0.28; 3.43]	0.85

[#] *q*-range used to perform the analysis with GNOM.