

Supplemental Data

Conformational Heterogeneity of Karyopherin β 2

Is Segmental

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Table S1. Summary of Refinement Using NCS to Constrain Kap β 2 Chains A to D and Chains B to C

<i>Refinement #</i>	<i>Number of NCS Groups</i>	<i>NCS Groups</i>	<i>NCS Restraints</i>	<i>R_{free} (%)</i>	<i>R_{factor} (%)</i>
1	0	None	None	28.4	24.6
2	2	A,D*(H1-20) [§] B,C*(H1-20)	Tight Tight	31.4	29.1
3	8	A,D(H1-4,H5-12,H14-17, H19-20) B,C(H1-4,H5-12,H14-17, H19-20)	Tight, Tight, Tight, Tight Tight, Tight, Tight, Tight	28.4	25.9
4	6	A,D(H1-12,H14-17, H19-20) B,C(H1-12,H14-17, H19-20)	Tight, Tight, Tight Tight, Tight, Tight	29.2	26.5
5	6	A,D(H1-4,H5-17, H19-20) B,C(H1-4,H5-17, H19-20)	Tight, Tight, Tight Tight, Tight, Tight	29.1	26.8
6	6	A,D(H1-4,H5-12,H14-20) B,C(H1-4,H5-12,H14-20)	Tight, Tight, Tight Tight, Tight, Tight	28.6 [†]	26.1 [†]

[‡] G.N. Murshudov, A.A.Vagin and E.J.Dodson, Refinement of Macromolecular Structures by the Maximum-Likelihood Method. (1997) Acta Cryst. **D53**, 240-255.

* A, D indicates that Kap β 2 chains A and D are constrained by NCS; B, C denotes Kap β 2 chains B and C are constrained by NCS.

[§] (H1-20) denotes Kap β 2 HEAT repeats 1 through 20.

[†] Reported in Table 1.

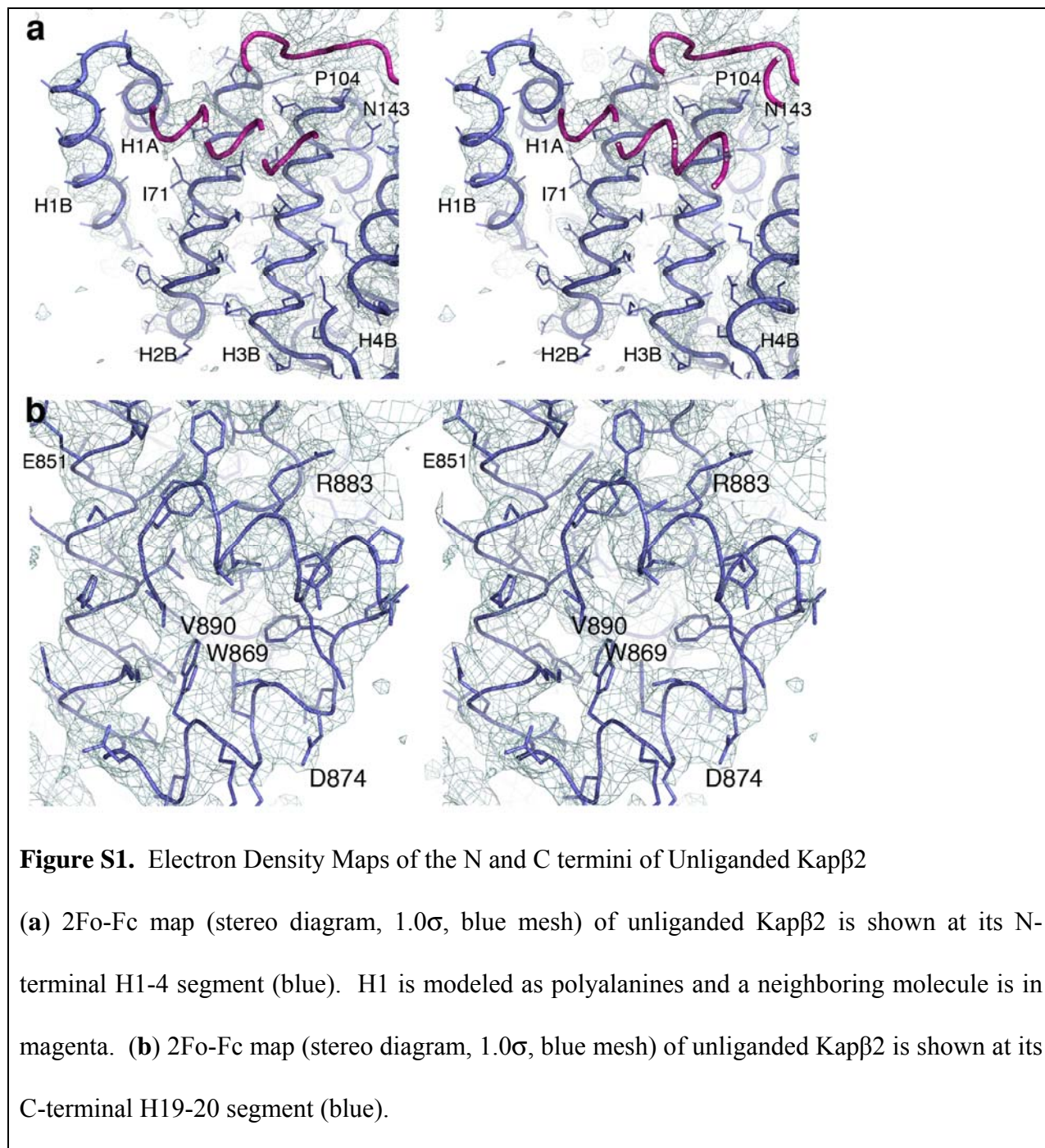
Table S2. Summary of Refinement Using NCS to Constrain Kap β 2 Chains A, B, C, and D

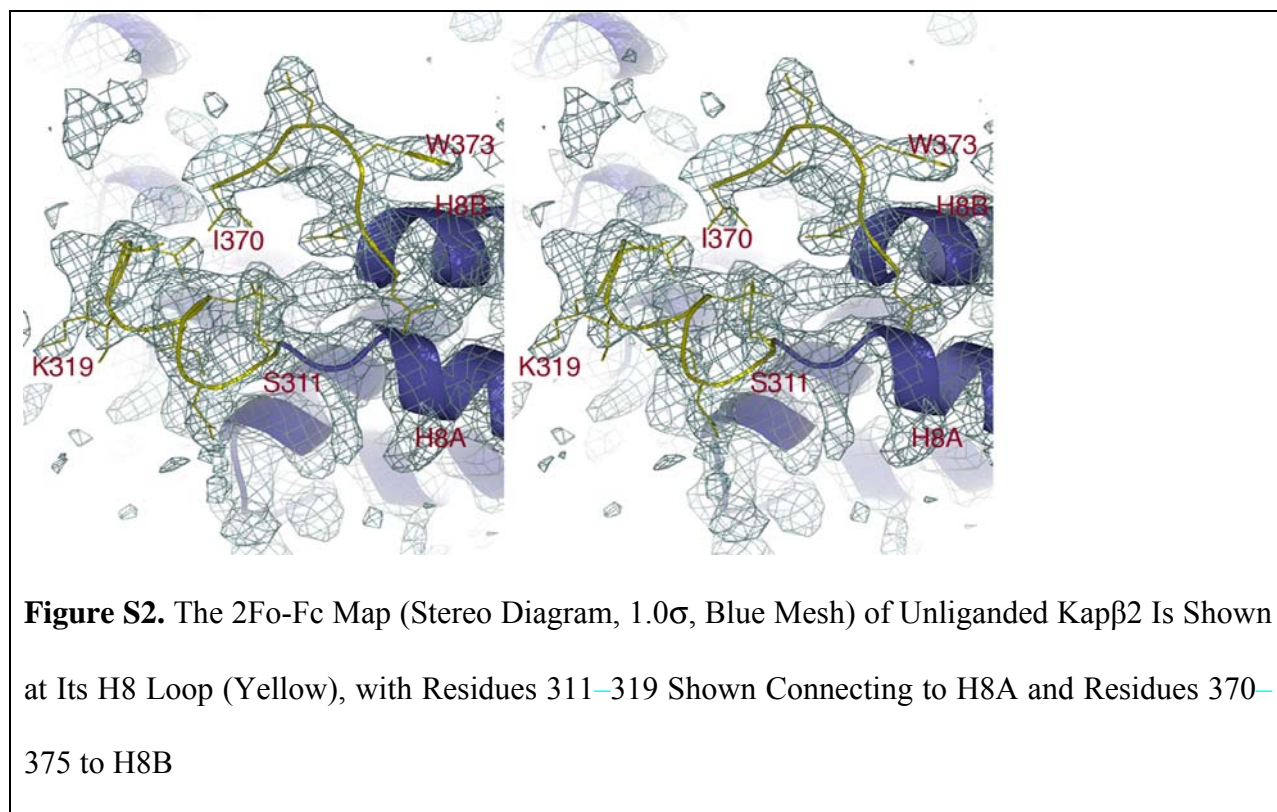
<i>Refinement #</i>	<i>Number of NCS Groups</i>	<i>NCS Groups</i>	<i>NCS Restraints</i>	<i>R_{free} (%)</i>	<i>R_{factor} (%)</i>
7	1	A-D*(H1-20) [§]	Tight	42.6	40.5
8	4	A-D(H1-4,H5-12,H14-17, H19-20)	Tight, Tight, Tight, Tight	32.3	30.4
9	4	A-D(H1-4,H5-12,H14-17, H19-20)	Medium, Tight, Tight, Tight	32.4	30.0
10	4	A-D(H1-4,H5-12,H14-17, H19-20)	Tight, Medium, Tight, Tight	30.6	27.8
11	4	A-D(H1-4,H5-12,H14-17, H19-20)	Tight, Tight, Medium, Tight	32.8	30.0
12	4	A-D(H1-4,H5-12,H14-17, H19-20)	Tight, Tight, Tight, Medium	30.7	28.8
13	4	A-D(H1-4,H5-12,H14-17, H19-20)	Tight, Medium, Tight, Medium	28.7	26.0
14	4	A-D(H1-4,H5-12,H14-17, H19-20)	Tight, Loose, Tight, Medium	28.5	25.7
15	4	A-D(H1-4,H5-12,H14-17, H19-20)	Tight, Medium, Tight, Loose	28.5	25.9
16	4	A-D(H1-4,H5-12,H14-17, H19-20)	Tight, Loose, Tight, Loose	28.3	25.6

[‡] G.N. Murshudov, A.A.Vagin and E.J.Dodson, Refinement of Macromolecular Structures by the

* A-D indicates that Kap β 2 chains A, B, C and D are all subjected to NCS restraints.

[§] (H1-20) represents HEAT repeats 1 through 20.





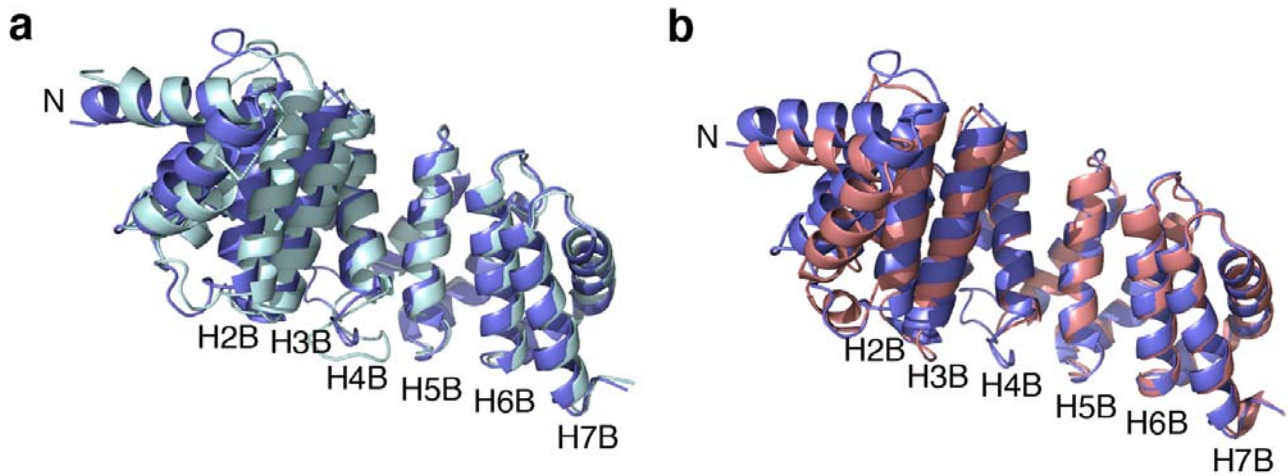


Figure S3. Conformational Flexibility at the N-Terminal H1-H4 Segment of Kap β 2

(a) Ribbon diagram showing H1-H7 of chains A (blue) and C (light blue) of unliganded Kap β 2, superimposed at H5-H13. (b) same as (a), except chain A of unliganded Kap β 2 is superimposed with substrate-bound Kap β 2 (pink).

