Structure 15

Supplemental Data

Conformational Heterogeneity of Karyopherinβ2

Is Segmental

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Refinement	Number	NCS	NCS	Rfree	R_{factor}
#	of NCS	Groups	Restraints	(%)	(%)
	Ğroups	•		. ,	. ,
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 [†]

T-11- S1 Server of D-Green and H-in- NGS to Constrain K-nO2 Chains A to D and Chains D to C

[¥]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 Kapβ2 chains A and D are constrained by NCS; B, C denotes Kapβ2 chains

B and C are constrained by NCS.

[§] (H1-20) denotes Kapβ2 HEAT repeats 1 through 20.

[†] Reported in Table 1.

Refinement	Number	NCS	NCS	<i>R</i> _{free}	R _{factor}
#	of NCS	Groups	Restraints	(%)	(%)
	Groups				
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

Table S2. Summary of Refinement Using NCS to Constrain Kapβ2 Chains A, B, C, and D

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

* A-D indicates that Kapβ2 chains A, B, C and D are all subjected to NCS restraints.

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



(a) 2Fo-Fc map (stereo diagram, 1.0σ , blue mesh) of unliganded Kap β 2 is shown at its N-terminal H1-4 segment (blue). H1 is modeled as polyalanines and a neighboring molecule is in magenta. (b) 2Fo-Fc map (stereo diagram, 1.0σ , blue mesh) of unliganded Kap β 2 is shown at its C-terminal H19-20 segment (blue).







Figure S4. Conformational Flexibility at the C-Terminal H19-H20 Segment of Kapβ2
(a) Ribbon diagram showing H18-H20 of chains A (blue) and C (light blue) of unliganded
Kapβ2, superimposed at H14-H18. (b) same as (a), except chain A of unliganded Kapβ2 is
superimposed with substrate-bound Kapβ2 (pink). (c) same as (a), except chain A of unliganded
Kapβ2 is superimposed with Ran-bound Kapβ2 (red). (d) same as (a), except substrate-bound
Kapβ2 (pink) is superimposed with Ran-bound Kapβ2 (red).



similar to that of Ran-bound Kap β 2, whereas its N-terminal arch is similar to that of native Kap β 2. The selenomethionine model is not refined and thus its coordinates are not deposited in the PDB.