Solution NMR Determination of the CDHR3 Rhinovirus-C Binding Domain, EC1

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Supplemental Material

Table S1. Experimental details for 3D spectra collected for backbone, side-chains assignments and structure calculation.[a]

Experiment	# Scans	Spectral Window (ppm) $^{1}H\times^{13}C(^{1}H^{\#})\times^{15}N(^{13}C^{\&})$	Complex Points $^{1}H\times^{13}C(^{1}H^{\#})\times^{15}N(^{13}C^{\&})$	Offset (ppm) $^{1}H\times^{13}C(^{1}H^{\#})\times^{15}N(^{13}C^{\&})$	NUS sampling rate (%)
HNCACB	128	16×66.3×27	1024×64×32	4.82, 45.3, 119.1	32
CBCA(CO)NH	128	16×66.3×27	1024×60×30	4.82, 45.3, 119.1	32
HNCA	48	16×26.5×27	1024×64×39	4.82, 54.0, 119.1	36
HN(CO)CA	48	16×26.5×27	1024×64×39	4.82, 54.0, 119.1	36
HN(CA)CO	128	20×13.9×28	1024×40×32	4.82, 175.6, 119.3	49
HNCO	32	20×13.9×28	1024×40×32	4.82, 175.6, 119.3	49
HBHA(CO)NH	128	20×6.7$^{\#}$×28	1024×40$^{\#}$×32	4.82, 4.82$^{\#}$, 119.3	49
H(C)CH-TOCSY	32	20×8$^{\#}$×69.6$^{\&}$	1024×64$^{\#}$×64$^{\&}$	4.82, 4.82$^{\#}$, 41.6$^{\&}$	36
(H)CCH-TOCSY*	32	16.3×72.1×72.1$^{\&}$	1024×64×64$^{\&}$	4.82, 42.2, 42.2$^{\&}$	36
H(C)CH-COSY*	64	16.3×7.5$^{\#}$×72.1$^{\&}$	1024×48$^{\#}$×48$^{\&}$	4.82, 4.82$^{\#}$, 42.2$^{\&}$	36
NOESY ^{15}N-HSQC	32	20×13.3$^{\#}$×28	1024×72$^{\#}$×38	4.82, 4.82$^{\#}$, 119.3	49
NOESY ^{13}C-HSQC	32	20×12.1$^{\#}$×58.3$^{\&}$	1024×64$^{\#}$×64$^{\&}$	4.82, 4.82$^{\#}$, 41.6$^{\&}$	49

[a]All spectra were collected with a cryogenic probe at 600 or 800* MHz (^{1}H) and at 293 K.

Table S2. NMR structure statistics. Structural quality was evaluated by PSVS 1.5 for the selected residues † by STRIDE.

Parameter	Value
NOE derived distance constraints	
Short range ($\|i-j\| \leq 1$)	1085
Medium range ($1 < \|i-j\| < 5$)	133
Long range ($\|i-j\| \geq 5$)	800
Total	2018
Hydrogen bond constraints	25
Dihedral angle constraints	
Φ	101
Ψ	110
Total	211
Average root mean square deviations against lowest energy model coordinates (Å)†	
Backbone atoms (N, Cα, C, O)	0.68±0.16
All heavy atoms	1.36±0.22
PROCHECK *Z* scores (φ and ψ/all)	-0.90/-1.24
Ramachandran plot summary from MolProbity†	
Most favored	99.2
Allowed	0.8
Disallowed	0
MolProbity Clashscore (raw score / Z-score)	16.05 / -1.23
Root mean square deviations from ideal geometry	
For bond lengths (Å)	0.015
For angles (°)	1.3
XPLOR-NIH pseudopotential *E*(kJ/mol)	4743.01±32.65
Consistent violations (>30%)	
Distance constraints (>0.5 Å)	0
Dihedral angle constraints (>5°)	0
van der Waals constraints (>0.2 Å)	0

† Selected residues by STRIDE: 22, 23, 30, 31, 39-46, 62-65, 72-78, 81-86, 94-96, 100-108, 114-123.

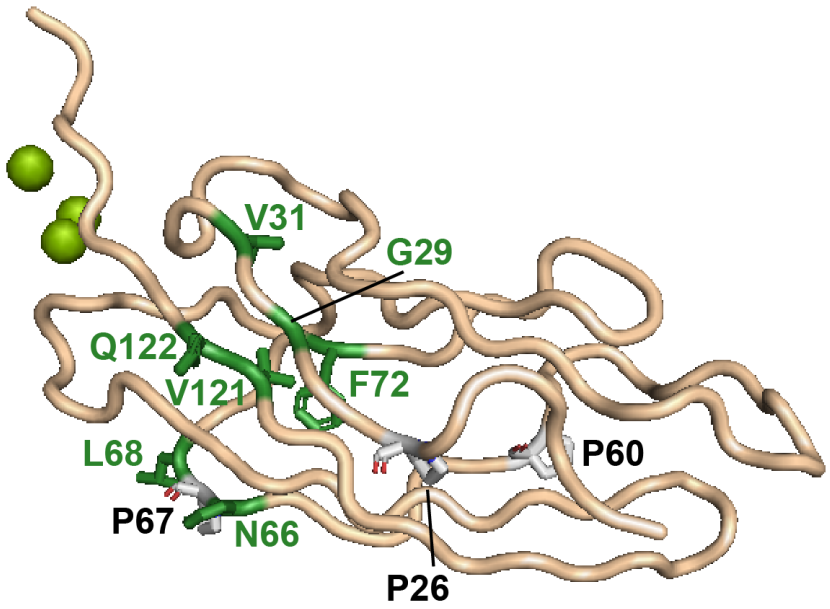

Figure S1: Conformational variability. The 7 residues showing doublets or elongated signals cluster in loop and ⊚-regions near the Ca^{++} end of EC1, and particularly near cisPro67.