

Label #	C(Me) SAS In Donut (Å) ³	C(Me) SAS in protomer (Å) ³	Buried / Exposed	Mid-protomer / Interface	Methyl direction	Structure group	Sources of $\Delta\delta_s$ and $\Delta\omega_s$	Sources of $\Delta\delta_s$ and $\Delta\omega_s$	Limits		Limits		Limits			Info source	Apo MRD	Apo MRD	Apo MRD	Apo dynamics in μ s-ms time window (hypothesis)
									0 ppm	0.37	0 ppm	1.3	0 ppm	1.47	1000 Hz					
Info source	TRAP+Trp+RNA crystal 1CS5 ^{***}																			
	TRAP+Trp+RNA structure and $\Delta\delta$ for removal of Trp																			
	Average apo structure in ms time window (hypothesis)																			
	TRAP+Trp+RNA structure and $\Delta\delta$ for removal of Trp																			
	Info source																			
Val 10 _y	0.0	11.8	Buried	Interface	To interface	Interface (I)	Phe9(Nbr) 5.6Å Phe48(Self) 4.4Å	Ile45 _y (Nbr), Thr65 _y (Self)	3%	10%	• Small $\Delta\delta_s$ (+ small $\Delta\omega_s$) → Phe9 and Phe48 too far and/or same orientation as in holo • Small $\Delta\omega_s$ → this apo interface is like holo			Val 10 _y	?	?	> 0	• Non-zero k_{ex} → some structural freedom at this interface		
Val 10 _y	0.0	1.6	(Same as above)	Mid-protomer	To core	Core (C)	Phe48(Self) 6.1Å	Ile120 _y , Ile550 _y	7%	41%	• Small $\Delta\delta_s$ → Phe 48 too far and/or same orientation as in holo TRAP • Modest $\Delta\omega_s$ → this apo core is uniquely packed			Val 10 _y	?	?	40%	• Moderate k_{ex} → moderate rate of motion at this interface		
Val 11 _y	0.0	15.6	Buried	Interface	To interface	Interface (I)	Phe9(Self) 6.2Å Tyr62(Self) 6.4Å	Val43 _y , Ile45 _y , Ile70 _y , δ_s	6%	5%	• Small $\Delta\delta_s$ and $\Delta\omega_s$ → this apo interface is like holo			Val 11 _y	No Disp.	No Disp.	No Disp.	• No dispersion → rigidity at this interface		
Val 11 _y	0.0	15.8	(Same as above)	(Same as above)	(Same as above)	Interface (I)	Phe9(Self) 3.8Å His67(Nbr) 3.8Å	Phe9, Ile45 _y , His67(Nbr)	20%	9%	• Modest $\Delta\delta_s$ (+ small $\Delta\omega_s$) → Phe9 and/or Tyr62 unique apo orientation • Small $\Delta\omega_s$ → this apo interface is like holo			Val 11 _y	?	?	> 0	• Non-zero k_{ex} → some structural freedom at this interface		
Ile 120 _y	0.0	0.0	Buried	Mid-protomer (Center)	To core	Core (C)	Trp ring 7Å	Val10, Val21, Val57, Ile63	2%	56%	• Small $\Delta\delta_s$ → Trp too far to alter δ_s • Modest $\Delta\omega_s$ → center of apo core uniquely packed			Ile 120 _y	?	?	54%	• Moderate k_{ex} → moderate rate of motion in the core		
Leu 150 _y	10.3	10.3	Exposed	Mid-protomer (at base)	To surface (from base)	Surface (S)	Solvent renders local field uniform (no $\Delta\delta_s$ nor $\Delta\omega_s$)	Lys13, Lys40, Lys60, Tyr62, Glu17 all on self	4%	5%	• Small $\Delta\delta_s$ → consistent with solvent exposure • Small $\Delta\omega_s$ → surface of apo base is like holo			Leu 150 _y	No Disp.	No Disp.	No Disp.	• No dispersion → rigid or flexible with constant solvent exposure		
Leu 150 _y	24.1	24.6	(Same as above)	(Same as above)	(Same as above)	Surface (S)	(Same as above)	(Same as above)	1%	3%	(Same as above)			Leu 150 _y	No Disp.	No Disp.	No Disp.	(Same as above)		
Val 19 _y	0.0	0.0	Buried	Mid-protomer	To center	Core (C)	No apparent sources of $\Delta\delta_s$ nor $\Delta\omega_s$	Ile12, Val21, Leu38, Ala61	2%	10%	• Small $\Delta\delta_s$ → consistent with lack of $\Delta\delta_s$ sources • Small $\Delta\omega_s$ → this apo core is like holo			Val 19 _y	No Disp.	No Disp.	No Disp.	• No dispersion → core is likely rigid here since little/no adjustment required upon Trp-binding (small $\Delta\delta$)		
Val 19 _y	0.0	0.0	(Same as above)	(Same as above)	To surface	Core (C)	No apparent sources of $\Delta\delta_s$ nor $\Delta\omega_s$	Ala14, Glu16, Gly59	0%	8%	(Same as above)			Val 19 _y	No Disp.	No Disp.	No Disp.	(Same as above)		
Val 21 _y	6.1	6.1	Buried	Center (near interface)	To core (Trp site)	Accessible Core (AC)	His33(Self) 9.3Å His34(Self) 7.3Å Trp ring 4.4Å	Val21, Ile12, Ile55, Val57 _y	6%	10%	• Small $\Delta\delta_s$ and $\Delta\omega_s$ → this apo accessible core is like holo (near Trp!) • Unexpected: small $\Delta\delta_s$ despite proximity to Trp ligand • Small $\Delta\omega_s$ perhaps His 33/34 occupies Trp site in similar orientation as Trp to yield comparable ring shift			Val 21 _y	?	?	42%	• Moderate k_{ex} → Moderate rate of motion at Trp site • Structural location links Trp-site → RNA-site		
Val 21 _y	0.0	0.0	(Same as above)	(Same as above)	To core edge	Core (C)	Glu36(Self) 7.3Å (too far?) His34(Self) 8.4Å Trp ring 7.3Å	Ile120 _y , Leu380 _y , Leu440 _y	1%	28%	• Modest $\Delta\delta_s$ → this apo core is unique (note: γ_s reports holo-like core near Trp)			Val 21 _y	?	?	> 0	• Same as γ_s except rate is unknown • Structural location links Trp-site → RNA-site		
Ile 220 _y	5.5	5.5	Buried (protomer edge)	Mid-protomer (near interface)	To interface	Accessible Core (AC)	Phe32(Self) 3.9Å (covers)	Arg58(Self)	70%	7%	• Large $\Delta\delta_s$ → Phe32 alternate orientation in apo • Small $\Delta\omega_s$ → edge of apo core is like holo			Ile 220 _y	0%	100%	20%	• Small $\Delta\omega_s$ → Phe32 ring is not affecting methyl (perhaps solvated?) • Large $\Delta\omega_s$ → edge of protomer samples wide range of rotameric states • Small k_{ex} → rate of sampling is slow • Ile220 _y solvated and Phe32 flipped outward (?) • Structural location links Trp-site → RNA-site • Large $\Delta\omega_s$ → methyl samples unique orientation to Phe32 • Large $\Delta\omega_s$ → significant structural freedom at this core • Small k_{ex} → rate of exchange is slow • Interface is very mobile here, at a slow rate (δ_s corroborates)		
Leu 240 _y	0.0	0.0	Buried	Mid-protomer	To core	Core (C)	Phe32(Self) 4.1Å	Ile22 _y , Phe32, Lys56	46%	69%	• Large $\Delta\delta_s$ → this apo core has unique orientation to Phe32 • Large $\Delta\omega_s$ → this apo core is unique • Difference less pronounced toward interface (smaller $\Delta\delta_s$ for δ_s)			Leu 240 _y	100%	68%	9%	• Zero $\Delta\omega_s$ → unexpected despite proximity to Phe32 / His34 • $\Delta\omega_s$ k_{ex} → corroborate hypotheses of δ_s methyl		
Leu 240 _y	2.3	27.0	(Same as above)	(Same as above)	To interface (closer to Trp than δ_s)	Interface (I)	Phe32(Self) 4.8Å His34(Nbr) 4.8Å	Thr30 _y , Phe32	47%	31%	• Large $\Delta\delta_s$ → this interface unique orientation to Phe32 and/or His34 • Modest $\Delta\omega_s$ → this apo interface is unique • Difference more pronounced towards core (larger $\Delta\delta_s$ for δ_s)			Leu 240 _y	0%	68%	0%	• Small k_{ex} → interface is very mobile here, at a slow rate (δ_s corroborates)		
Ile 280 _y	72.7	75.0	Exposed	Interface	To solvent (?)	Trp-Loop (L)	His51(Nbr) 3.9Å Trp 9.7Å (quite far)	Exposed (not packed)	41%	100%	• Modest $\Delta\delta_s$ → this apo loop has unique orientation to His51 • Large $\Delta\omega_s$ → this apo loop has unique packing (closes over empty Trp site?)			Ile 280 _y	0%	93%	100%	• Small $\Delta\omega_s$ → His51 not affecting methyl (perhaps Ile and/or His51 is solvated?) • Large $\Delta\omega_s$, k_{ex} → loop rapidly sampling wide range of rotamers (perhaps Ile is solvated?) • Good example for solvated Ile δ_s dynamics		
Leu 380 _y	0.0	0.0	Buried (protomer edge)	Mid-protomer	To core	Core (C)	Glu36(Self) 7.0Å (too far/indirect)	Val19 _y , Val21 _y , Leu44 _y	16%	6%	• Unexpected: small/modest $\Delta\delta_s$ despite lack of sources of $\Delta\delta_s$ • Small $\Delta\omega_s$ → this apo core is like holo			Leu 380 _y	No Disp.	No Disp.	No Disp.	• No dispersion → core is likely rigid here since little/no adjustment required upon Trp-binding (small $\Delta\delta$)		
Leu 380 _y	0.0	9.4	(Same as above)	Interface	To interface	Interface (I)	Lys56(Nbr) 4.5Å Glu36(Self) 5.6Å	Glu36, Leu440 _y , Lys56	14%	11%	• Small $\Delta\delta_s$ → this apo interface is uniquely orientated to Lys56 and/or Glu36 • Small $\Delta\omega_s$ → this apo interface is like holo			Leu 380 _y	?	?	28%	• Small k_{ex} → this interface has slow rate or motion		
Val 43 _y	0.0	8.1	Very buried	Interface (deeper than γ_s)	To interface	Interface (I)	No apparent sources of $\Delta\delta_s$ nor $\Delta\omega_s$	Val11 _y , Ile45 _y	9%	9%	• Small $\Delta\delta_s$ → consistent with lack of sources of $\Delta\delta_s$ • Small $\Delta\omega_s$ → this apo interface is like holo			Val 43 _y	No Disp.	No Disp.	No Disp.	• No dispersion → interface likely rigid here since little/no adjustment required upon Trp-binding (small $\Delta\delta$)		
Val 43 _y	0.0	29.4	(Same as above)	Interface	To interface	Interface (I)	(Same as above)	Lys15, Ile700 _y (Nbr)	2%	6%	(Same as above)			Val 43 _y	No Disp.	No Disp.	No Disp.	• No dispersion → interface likely rigid here since little/no adjustment required upon Trp-binding (small $\Delta\delta$)		
Leu 440 _y	0.0	42.6	Buried	Interface	To interface	Interface (I)	His 34(Self) 7.2Å Trp ring 7.6Å	Lys56(Nbr), Glu38, Ala54(Nbr), Leu340 _y (Nbr)	55%	53%	• Modest $\Delta\delta_s$ → Trp ligand ring current • Modest $\Delta\omega_s$ → this apo interface is unique • Adjacent Trp-site methyl is less altered (smaller $\Delta\delta_s$ for δ_s)			Leu 440 _y	?	?	35%	• Small k_{ex} → slow exchange rate at this interface		
Leu 440 _y	4.1	5.4	(Same as above)	(Same as above)	To core (Trp site)	Accessible Core (AC)	His 34(Self) 7.0Å Trp ring 5.8Å	Val21 _y , Glu38, Ala46	100%	18%	• Large $\Delta\delta_s$ → Trp ligand ring current • Small/modest $\Delta\omega_s$ → this apo Trp-pocket only slightly different than holo • Adjacent interface methyl is more significantly altered (larger $\Delta\delta_s$ for δ_s)			Leu 440 _y	?	?	> 0	• Same as δ_s except unknown k_{ex}		
Ile 450 _y	0.0	65.3	Very buried	Interface	To interface	Interface (I)	No apparent sources of $\Delta\delta_s$ nor $\Delta\omega_s$	Val59 _y , Ile63 _y , γ_s all on Nbr	1%	14%	• Small $\Delta\delta_s$ → consistent with lack of sources of $\Delta\delta_s$ • Small/modest $\Delta\omega_s$ → this apo interface is slightly different than holo			Ile 450 _y	0%	67%	47%	• Zero $\Delta\omega_s$ → consistent with lack of sources of $\Delta\omega_s$ • Large $\Delta\omega_s$ and modest k_{ex} → significant mobility at this interface		
Ile 550 _y	1.6	1.6	Very buried	Mid-protomer	To core	Core (C)	Phe48 4.3Å Trp ring 3.8Å	Val10 _y , Trp ligand	19%	27%	• Small/modest $\Delta\delta_s$ → Trp ligand ring current • Modest $\Delta\omega_s$ → minor adjustment to pack against Trp ring			Ile 550 _y	?	?	79%	• Large k_{ex} → center of core undergoing rapid exchange • Structural location links Trp-site → RNA-site		
Val 57 _y	0.0	0.0	Buried	Mid-protomer	To core	Core (C)	No apparent sources of $\Delta\delta_s$ nor $\Delta\omega_s$	Ile12 _y , Val19 _y , Ala61 β	0%	16%	• Small $\Delta\delta_s$ → consistent with lack of sources of $\Delta\delta_s$ • Small $\Delta\omega_s$ → this apo core is like holo			Val 57 _y	No Disp.	No Disp.	No Disp.	• No dispersion → core is rigid here		
Val 57 _y	0.0	7.9	(Same as above)	Interface	(Same as above)	Interface (I)	No apparent sources of $\Delta\delta_s$ nor $\Delta\omega_s$	Ile120 _y , Ile450 _y , Ile55 _y	1%	11%	(Same as above)			Val 57 _y	No Disp.	No Disp.	No Disp.	• No dispersion → core is rigid here		
Ile 630 _y	0.0	10.3	Buried	Interface	To interface	Interface (I)	No apparent sources of $\Delta\delta_s$ nor $\Delta\omega_s$	Val45 _y , γ_s , Ile450 _y , Val57 _y , Ser73 β	0%	4%	• Small $\Delta\delta_s$ → consistent with lack of sources of $\Delta\delta_s$ • Small $\Delta\omega_s$ → this apo interface is like holo			Ile 630 _y	?	?	61%	• Modest k_{ex} → modest structural freedom at this interface (near base)		
Val 69 _y	21.4	24.4	Exposed	Mid-protomer (base at back)	Along surface	Surface (S)	Tyr62 4.2Å	Tyr62, Glu64 Relatively exposed	8%	2%	• Small $\Delta\delta_s$ → apo base slightly adjusted relative to Tyr62 • Small $\Delta\omega_s$ → surface of apo base is like holo			Val 69 _y	No Disp.	No Disp.	No Disp.	• No dispersion → flexible with constant solvent exposure (or rigid, which is less likely)		
Val 69 _y	51.6	51.6	(Same as above)	(Same as above)	To surface (unique γ_s)	Surface (S)	Tyr62 4.5Å	Exposed (not packed)	8%	0%	(Same as above)			Val 69 _y	?	?	47%	• Moderate k_{ex} → base mobility about the holo conformation (small $\Delta\delta$)		
Ile 700 _y	0.0	72.4	Buried near surface (at base)	Interface	To interface	Interface (I)	Tyr62(Nbr) 3.4Å	Lys13, Tyr62(Nbr) May be exposed in apo	4%	5%	• Small $\Delta\delta_s$ → apo base slightly adjusted relative to Tyr62 • Small $\Delta\omega_s$ → surface of apo base is like holo			Ile 700 _y	?	?	> 0	• Non-zero k_{ex} → base mobility about the holo conformation (small $\Delta\delta$)		