Supplementary material to:

Principles of chemical geometry underlying chiral selectivity in RNA minihelix aminoacylation

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Table S1

Table S1. Number of reactive conformations found in the trajectories of the L-Ala and D-Ala systems using various distances and angles for geometrical criteria with (Nu, R) = ($O_{3'}$, $C_{3'}$)

Conditions	Number of conformations		Ratio (L-Ala/D-Ala)
	L-Ala	D-Ala	
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 25°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 15°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 3.5$ Å	145	48	3.0
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 15°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 15°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 3.5$ Å	121	35	3.5
$\delta^{att} < 3.0$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 25°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 15°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 3.5$ Å	47	9	5.2
$\delta^{att} < 3.5$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 25°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 15°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 3.5$ Å	235	88	2.7
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 25°$, $\lvert\alpha^{FL}\rvert < 25°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 15°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 3.5$ Å	177	84	2.1
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 25°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 25°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 3.5$ Å	245	169	1.4
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 25°$, $\lvert\alpha^{FL}\rvert < 25°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 25°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 3.5$ Å	327	306	1.1
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 25°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 15°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 4.0$ Å	309	135	2.3
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 180°$, $\lvert\alpha^{FL}\rvert < 180°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 180°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 99$ Å	3653	4289	0.9
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 180°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 180°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 99$ Å	2144	2157	1.0
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 25°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 180°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 99$ Å	2023	2009	1.0
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 180°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 15°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 99$ Å	723	564	1.3
$\delta^{att} < 3.2$ Å, $\lvert\alpha^{BD} - 105°\rvert < 15°$, $\lvert\alpha^{FL}\rvert < 180°$, $\lvert\alpha^{Lobe} - 109.5°\rvert < 15°$, $\min(\delta_{OP1}^{SAC}, \delta_{OP2}^{SAC}) < 3.5$ Å	149	49	3.0

Table S2

Table S2. Number of reactive conformations in eight groups classified by dihedral angles of alanyl phosphate

Dihedral angles (°)			Number of conformations*		Group ID
$\tau(C_{5'}\text{-}O_{5'}\text{-}P_{5'}\text{-}O_b)$	$\tau(O_{5'}\text{-}P_{5'}\text{-}O_b\text{-}C_{carb})$	$\tau(P_{5'}\text{-}O_b\text{-}C_{carb}\text{-}C_\alpha)$	L-Ala	D-Ala	
≥ 120	≥ 120	≥ 120	118 (0.81)	8 (0.17)	I
		≤ 60	3 (0.02)	18 (0.38)	II
	< 120	≥ 120	12 (0.08)	4 (0.08)	III
		≤ 60	0 (0)	0 (0)	
< 120	≥ 120	≥ 120	12 (0.08)	10 (0.21)	IV
		≤ 60	0 (0)	7 (0.15)	V
	< 120	≥ 120	0 (0)	1 (0.02)	VI
		≤ 60	0 (0)	0 (0)	

*Fractions of groups are shown in parenthesis.

Figure S1

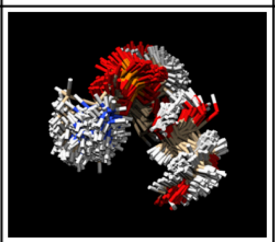
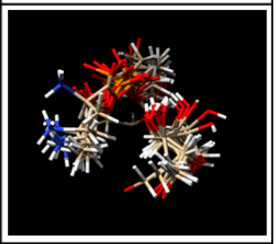
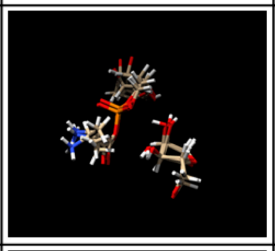
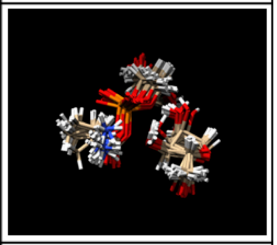
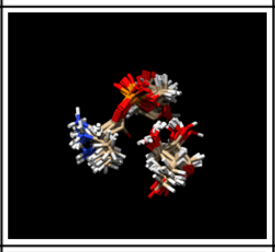
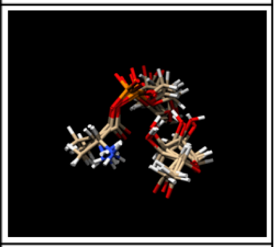
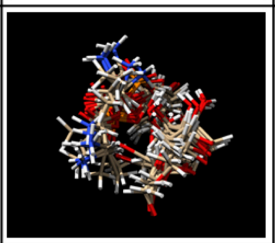
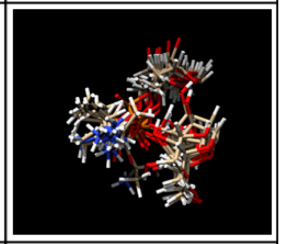
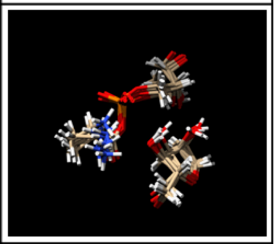
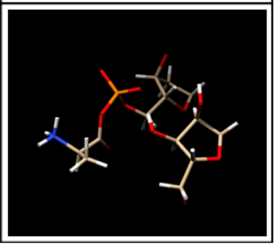
Group ID	L-Ala	D-Ala
I		
II		
III		
IV		
V	-	
VI	-	

Figure S1. Structures of members in eight groups listed in Table S2. Structures in group IV for L-Ala were not well clustered due to heterogeneity in $\tau(C_{4'}\text{-}C_{5'}\text{-}O_{5'}\text{-}P_{5'})$ and $\tau(O_b\text{-}C_{carb}\text{-}C_{\alpha}\text{-}N)$.

Figure S2

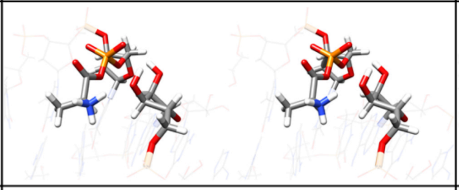
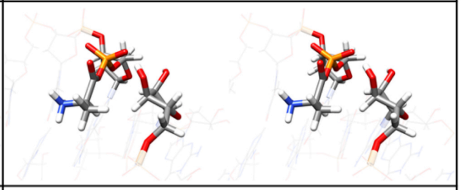
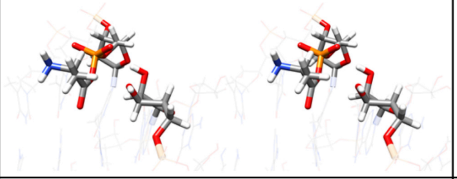
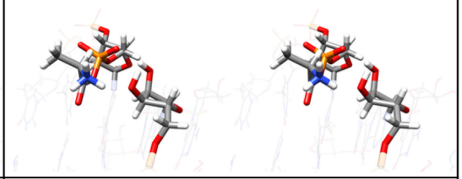
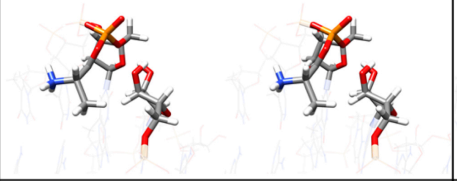
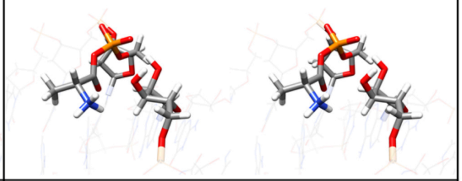
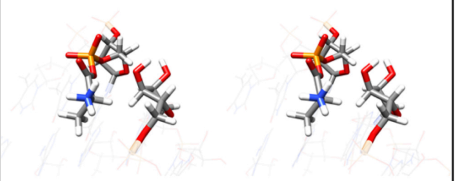
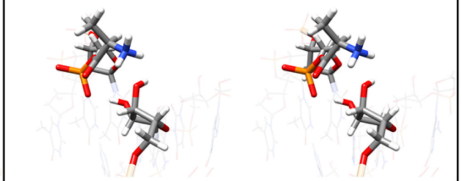
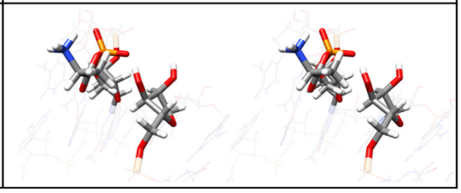
Group ID	L-Ala	D-Ala
I		
II		
III		
IV		
V	-	
VI	-	

Figure S2. Representative structures of eight groups listed in Table S2. The structures are shown as a cross-eyed stereo view.