Supplementary Table 1. Data collection and refinement statistics for *Ph*DS mutants

	K26R	K26Y	E54H	E54K	E54R	L65A
Data collection						
X-ray wavelength (Å)	1.0	1.0	1.0	1.0	1.0	1.0
Space group	$P4_12_12$	$P4_12_12$	$P4_12_12$	$P4_12_12$	$P4_12_12$	$P4_12_12$
Unit-cell parameters						
a, *b* (Å)	105.1	104.8	105.0	105.0	104.9	105.2
c (Å)	137.2	135.8	137.2	137.0	136.6	137.3
Resolution range (Å)	30.0-2.00 (2.07-2.00)	30.0-2.00 (2.07-2.00)	30.0-1.90 (1.97-1.90)	30.0-1.80 (1.86-1.80)	30.0-1.80 (1.86-1.80)	30.0-2.20 (2.28-2.20)
Unique reflections	52641 (5158)	51715 (5070)	60900 (5951)	71268 (6995)	70711 (6970)	39886 (3905)
Redundancy	11.7 (11.8)	11.8 (12.0)	10.3 (9.6)	9.6 (9.0)	10.8 (10.9)	11.7 (12.0)
Completeness (%)	100 (100)	100 (100)	99.7 (99.5)	99.9 (100)	99.7 (100)	100 (100)
$\langle I/\sigma(I)\rangle$	12.4 (4.99)	11.3 (3.39)	14.6 (5.52)	19.0 (5.31)	21.0 (8.28)	12.0 (5.08)
R_{merge} (%) [a]	6.9 (28.3)	7.6 (40.8)	10.8 (39.1)	9.8 (45.6)	6.2 (27.0)	8.4 (34.5)
Refinement						
Resolution (Å)	30.0-2.00	30.0-2.00	30.0-1.90	30.0-1.80	30.0-1.80	30.0-2.20
No. of atoms	4778	4803	4726	4808	5009	4705
R_{work} / R_{free} (%) [b]	18.8 / 21.1	19.4 / 21.8	20.2 / 21.9	19.5/ 20.3	19.9 / 21.6	19.8 / 22.8
Estimated coordinate error (Å) [c]	0.21	0.23	0.23	0.20	0.21	0.25
rmsd bonds (Å)	0.005	0.005	0.006	0.006	0.006	0.006
rmsd angles (º)	1.3	1.3	1.3	1.3	1.3	1.3
Ramachandran plot						
Most favoured region (%)	92.2	92.2	92.0	92.7	92.2	93.3
Additional allowed region (%)	7.8	7.8	8.0	7.3	7.8	6.7

Values for the highest resolution shell are shown in parentheses.

[a] $R_{merge} = \Sigma_{hkl}\Sigma_j |I_j(hkl) - \langle I(hkl)\rangle| / \Sigma_{hkl}\Sigma_j I_j(hkl)$, where $I_j(hkl)$ and $\langle I(hkl)\rangle$ are the observed intensity of measurement *j* and the mean intensity of the reflection with indices *hkl*, respectively.

[b] $R_{work} = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$, where F_o and F_c are observed and calculated native structure factors, respectively. $R_{free} = R$ calculated using 5% of total reflections, which were chosen randomly and omitted from the refinement.

[c] Coordinate error was estimated by the Luzzati plot (Luzzati, 1952).

	L65Q	E140K	E140N	E140R	E171R	R173A
Data collection						
X-ray wavelength (Å)	1.0	1.0	1.0	1.0	1.0	1.0
Space group	$P4_12_12$	$P4_12_12$	$P4_12_12$	$P4_12_12$	$P4_12_12$	$P4_12_12$
Unit-cell parameters						
a, b (Å)	105.0	105.0	105.0	105.0	105.2	105.0
c (Å)	137.0	137.2	137.0	137.1	137.7	136.8
Resolution range (Å)	30.0-2.20 (2.28-2.20)	30.0-2.00 (2.07-2.00)	30.0-1.90 (1.97-1.90)	30.0-2.00 (2.07-2.00)	30.0-2.20 (2.28-2.20)	30.0-1.90 (1.97-1.90)
Unique reflections	39601 (3890)	52513 (5152)	59809 (5924)	51865 (5127)	39610 (3898)	60416 (5959)
Redundancy	11.7 (12.0)	10.8 (11.0)	9.5 (9.4)	11.3 (10.9)	11.7 (12.0)	10.2 (10.4)
Completeness (%)	100 (100)	99.9 (100)	98.1 (99.4)	99.3 (100)	99.2 (99.6)	99.4 (100)
$\langle I/\sigma(I)\rangle$	11.2 (4.42)	16.6 (7.42)	16.1 (5.31)	18.1 (6.66)	12.3 (4.18)	15.4 (6.94)
R_{merge} (%) [a]	7.0 (36.1)	11.2 (31.7)	6.7 (39.3)	9.3 (34.7)	8.2 (36.8)	10.4 (34.2)
Refinement						
Resolution (Å)	30.0-2.20	30.0-2.00	30.0-1.90	30.0-2.00	30.0-2.20	30.0-1.90
No. of atoms	4648	4699	4865	4642	4724	4773
R_{work} / R_{free} (%) [b]	19.7 / 22.5	20.3 / 23.1	20.1 / 22.3	20.3 / 22.8	20.6 / 23.8	19.2 / 20.9
Estimated coordinate error (Å) [c]	0.25	0.24	0.23	0.24	0.27	0.21
rmsd bonds (Å)	0.006	0.006	0.005	0.007	0.006	0.006
rmsd angles (º)	1.3	1.3	1.3	1.3	1.3	1.3
Ramachandran plot						
Most favoured region (%)	92.5	92.5	91.8	91.8	92.0	92.2
Additional allowed region (%)	7.5	7.5	8.2	8.2	8.0	7.8

Values for the highest resolution shell are shown in parentheses.

[a] $R_{merge} = \Sigma_{hkl}\Sigma_j |I_j(hkl) - \langle I(hkl)\rangle| / \Sigma_{hkl}\Sigma_j I_j(hkl)$, where $I_j(hkl)$ and $\langle I(hkl)\rangle$ are the observed intensity of measurement j and the mean intensity of the reflection with indices hkl, respectively.

[b] $R_{work} = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$, where F_o and F_c are observed and calculated native structure factors, respectively. $R_{free} = R$ calculated using 5% of total reflections, which were chosen randomly and omitted from the refinement.

[c] Coordinate error was estimated by the Luzzati plot (Luzzati, 1952).

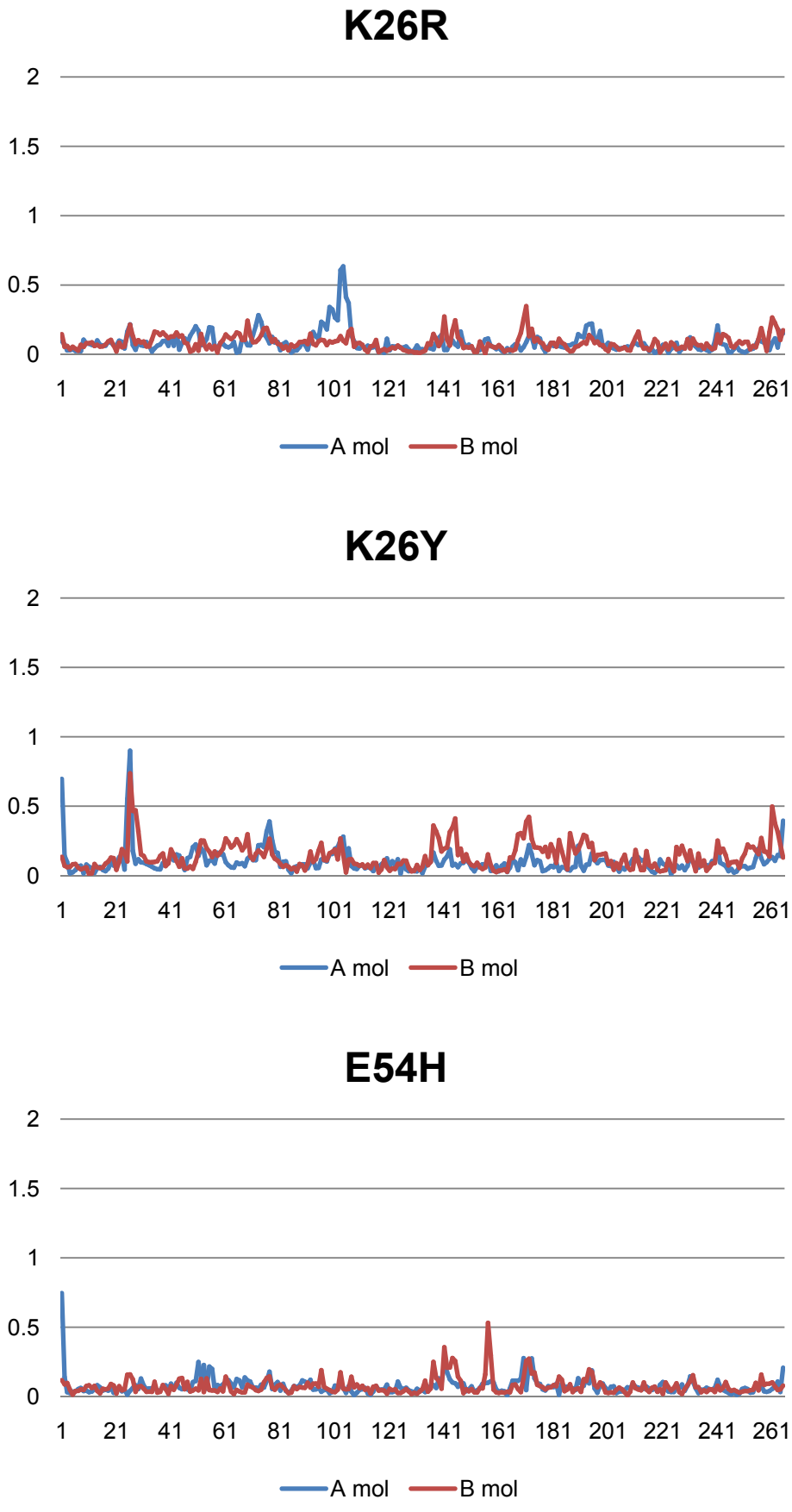
	R173N	K187R	L261M
Data collection			
X-ray wavelength (Å)	1.0	1.0	1.0
Space group	$P4_12_12$	$P4_12_12$	$P4_12_12$
Unit-cell parameters			
a, *b* (Å)	105.1	105.8	104.9
c (Å)	136.9	138.2	137.1
Resolution range (Å)	30.0-1.80 (1.86-1.80)	30.0-2.30 (2.38-2.30)	30.0-1.90 (1.97-1.90)
Unique reflections	71531 (7026)	35614 (3484)	60517 (5946)
Redundancy	10.8 (11.0)	11.6 (12.0)	10.2 (9.6)
Completeness (%)	99.9 (99.9)	100 (100)	99.2 (99.5)
$\langle I/\sigma(I)\rangle$	15.3 (6.04)	11.8 (4.23)	17.1 (4.71)
R_{merge} (%) [a]	14.3 (42.0)	10.4 (36.2)	6.4 (50.0)
Refinement			
Resolution (Å)	30.0-1.80	30.0-2.30	30.0-1.90
No. of atoms	4834	4594	4850
R_{work} / R_{free} (%) [b]	19.7 / 21.1	21.5 / 24.1	22.1 / 24.2
Estimated coordinate error (Å) [c]	0.21	0.31	0.26
rmsd bonds (Å)	0.006	0.007	0.009
rmsd angles (°)	1.3	1.3	1.5
Ramachandran plot			
Most favoured region (%)	92.0	91.2	91.6
Additional allowed region (%)	8.0	8.8	8.4

Values for the highest resolution shell are shown in parentheses.

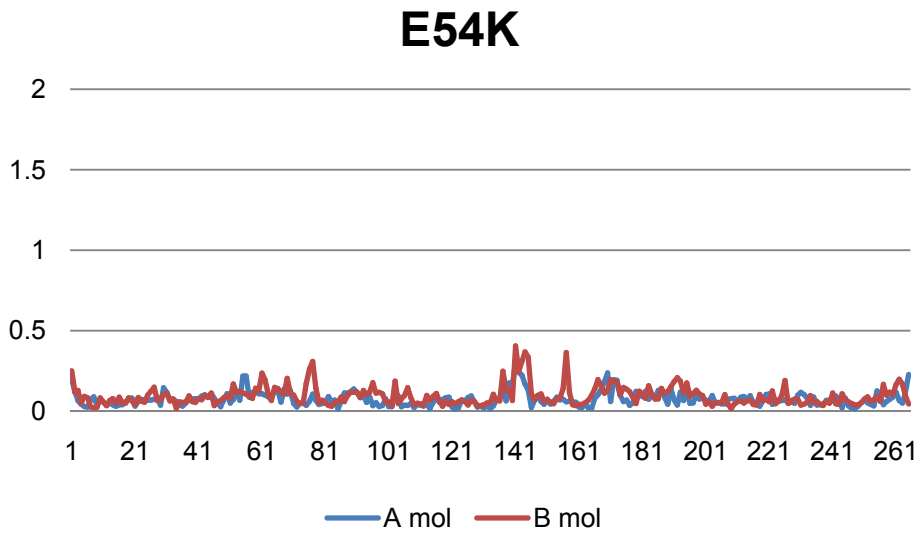
[a] $R_{merge} = \Sigma_{hkl}\Sigma_j |I_j(hkl) - \langle I(hkl)\rangle| / \Sigma_{hkl}\Sigma_j I_j(hkl)$, where $I_j(hkl)$ and $\langle I(hkl)\rangle$ are the observed intensity of measurement *j* and the mean intensity of the reflection with indices *hkl*, respectively.

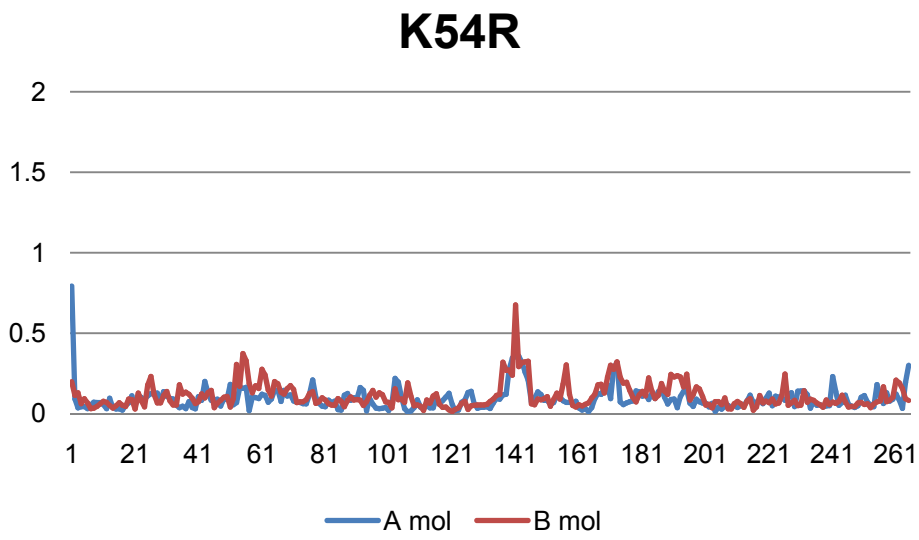
[b] $R_{work} = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$, where F_o and F_c are observed and calculated native structure factors, respectively. $R_{free} = R$ calculated using 5% of total reflections, which were chosen randomly and omitted from the refinement.

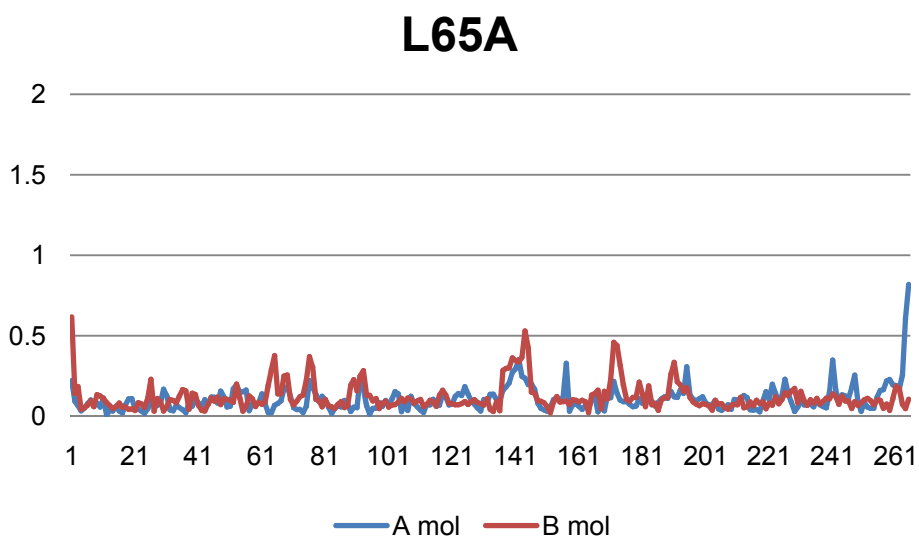
[c] Coordinate error was estimated by the Luzzati plot (Luzzati, 1952).



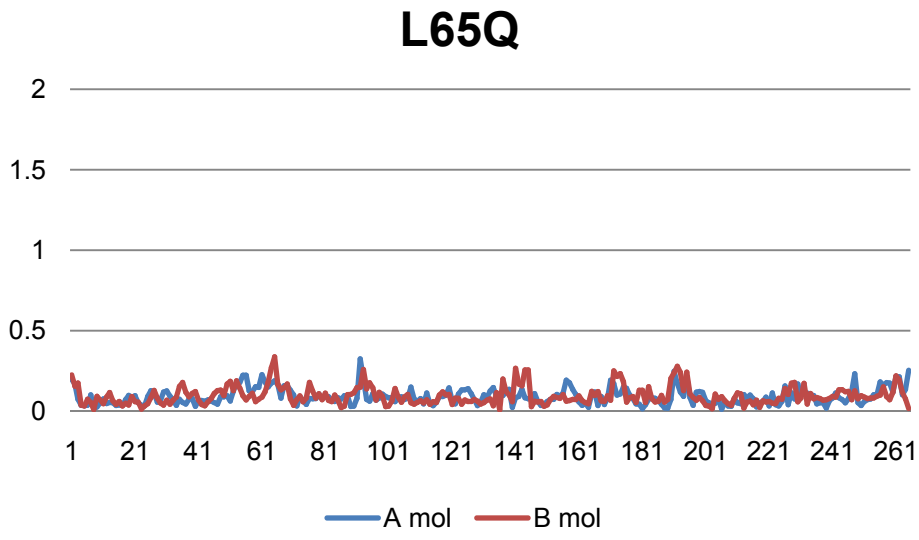
Supplementary Figure 1. Coordinate deviations from the C^{α} superposition (part 1).

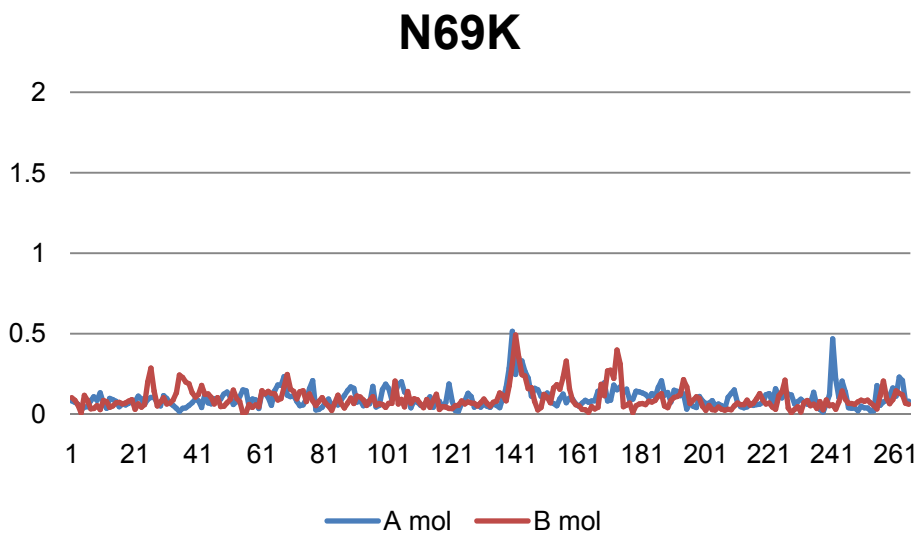


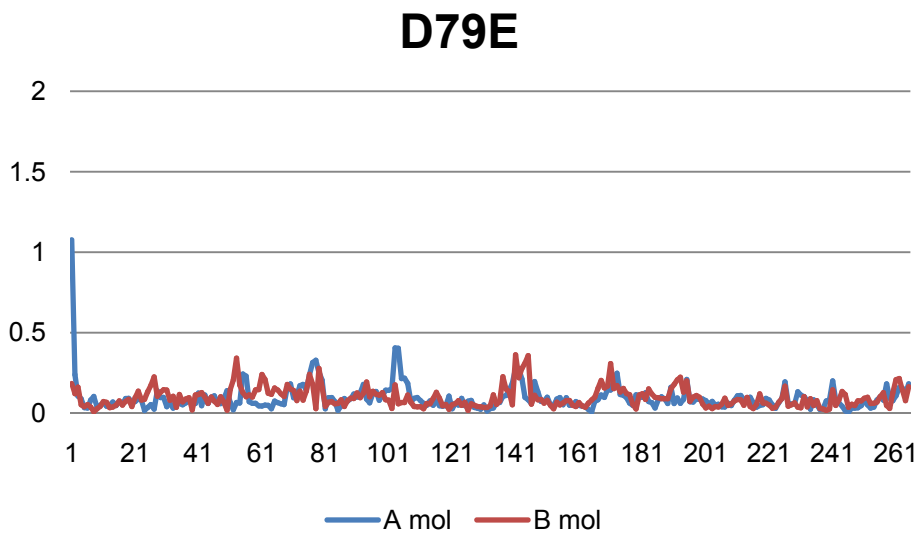




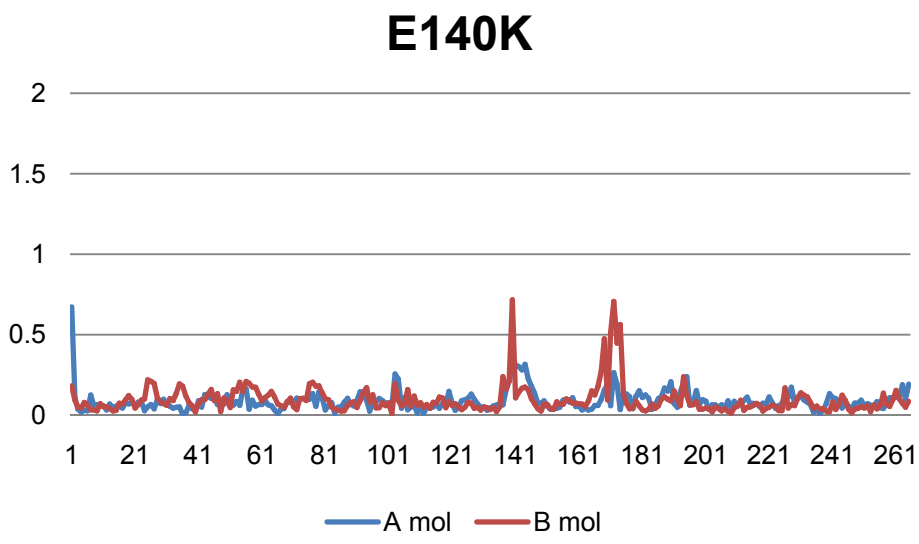
Supplementary Figure 1. Coordinate deviations from the C^{α} superposition (part 2).

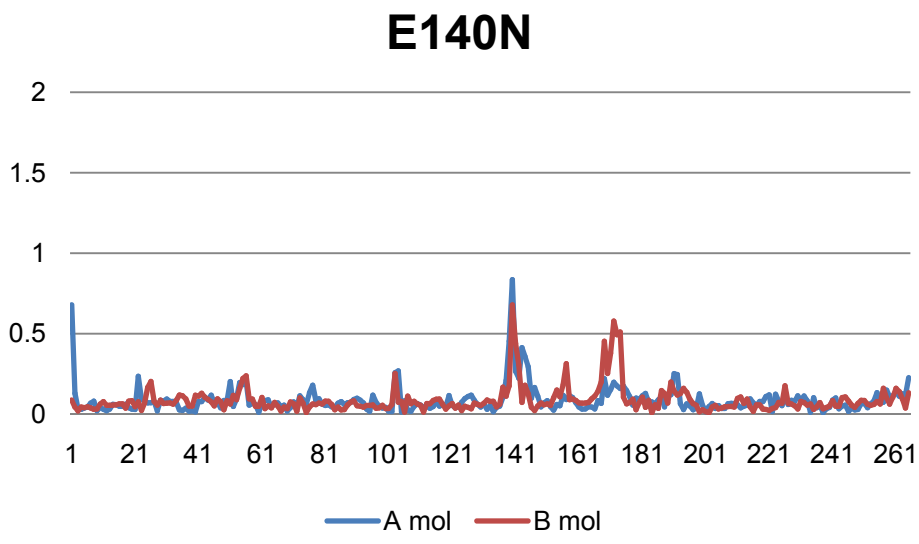


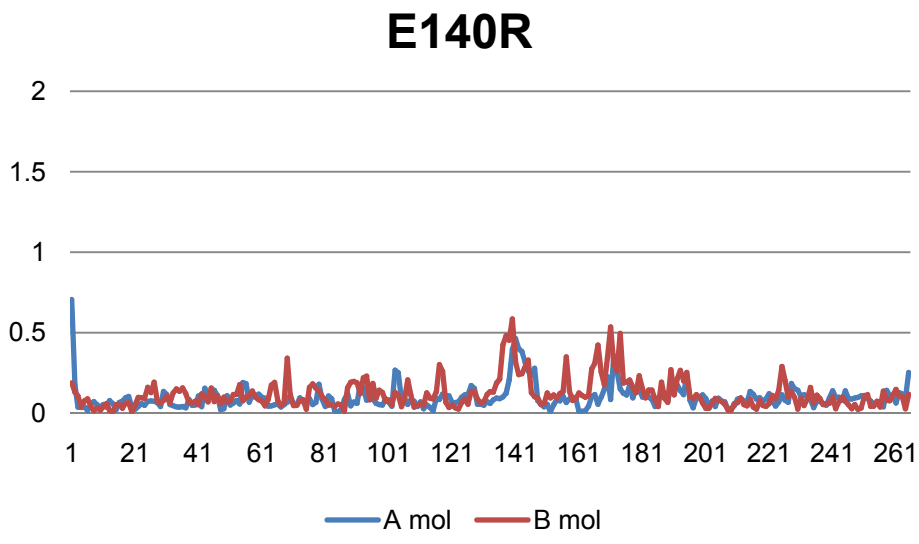




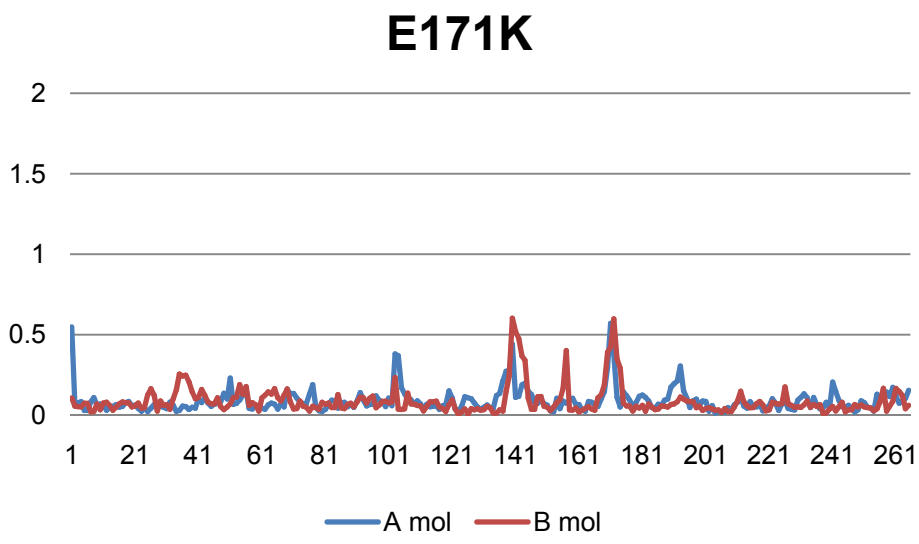
Supplementary Figure 1. Coordinate deviations from the C^{α} superposition (part 3).

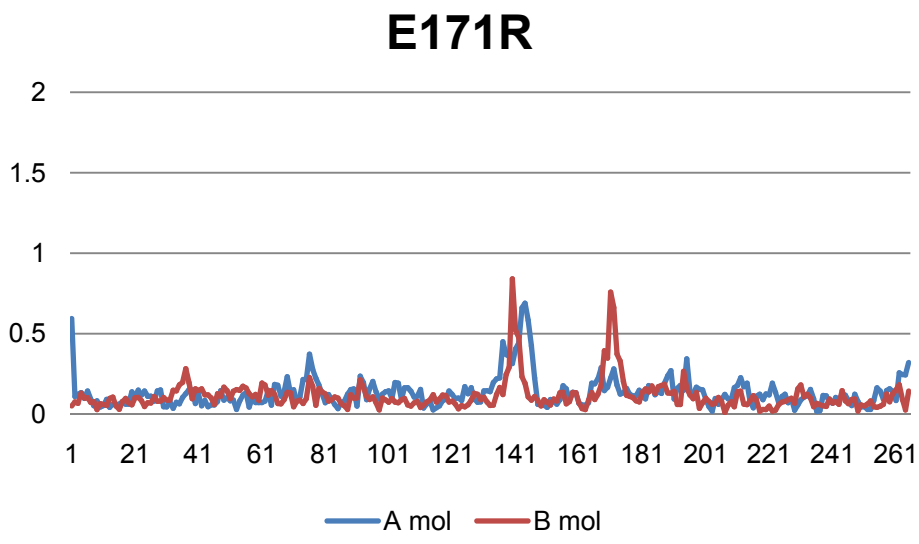


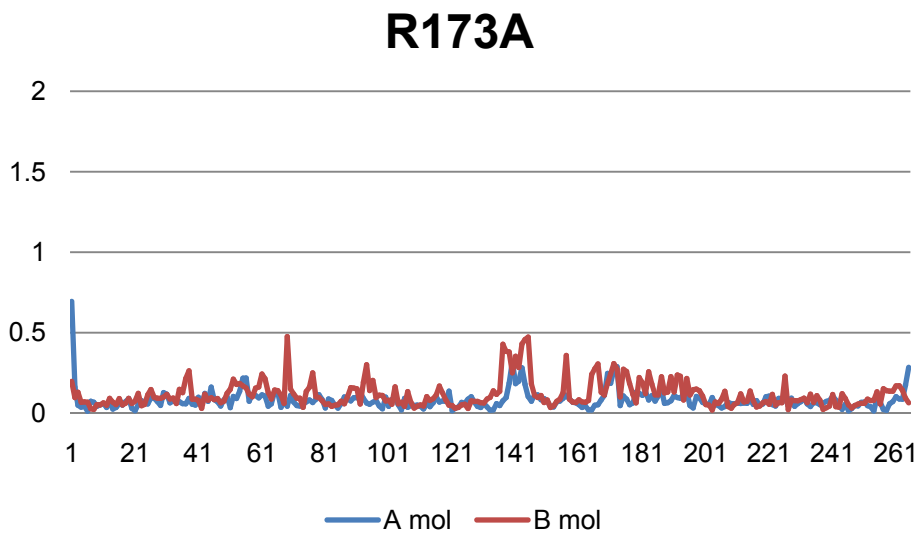




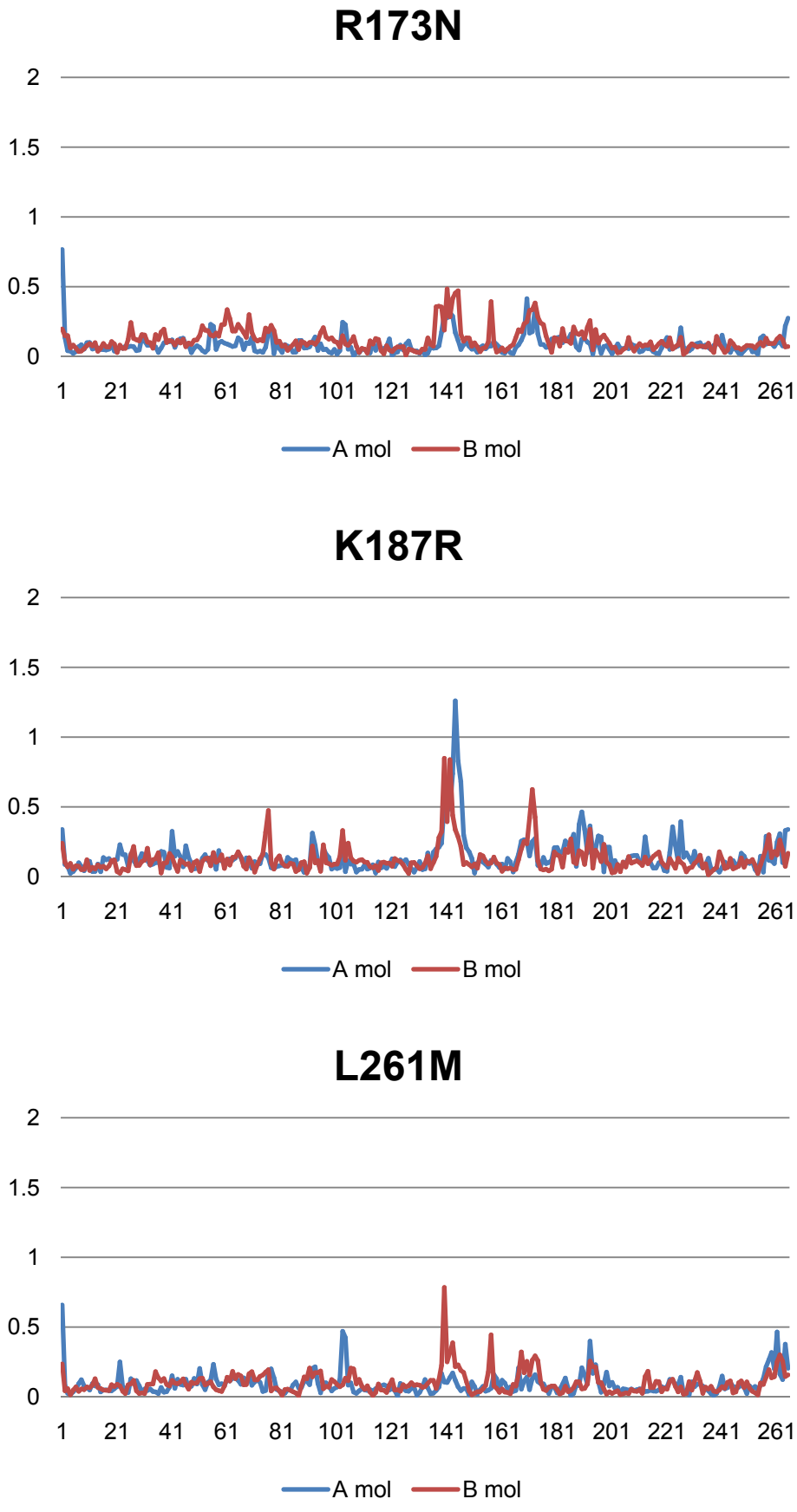
Supplementary Figure 1. Coordinate deviations from the C^{α} superposition (part 4).







Supplementary Figure 1. Coordinate deviations from the C^{α} superposition (part 5).



Supplementary Figure 1. Coordinate deviations from the C^{α} superposition (part 6).