

Supporting information for:

A Rotamer Library to Enable Modeling and Design of Peptoid Foldamers

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Rotamer Library Coverage Plots for Individual Positions

Rotamer library coverage plots for KMC and QMS rotamers of each individual position of all ROSETTA compatible structures are shown in figures S16–S108.

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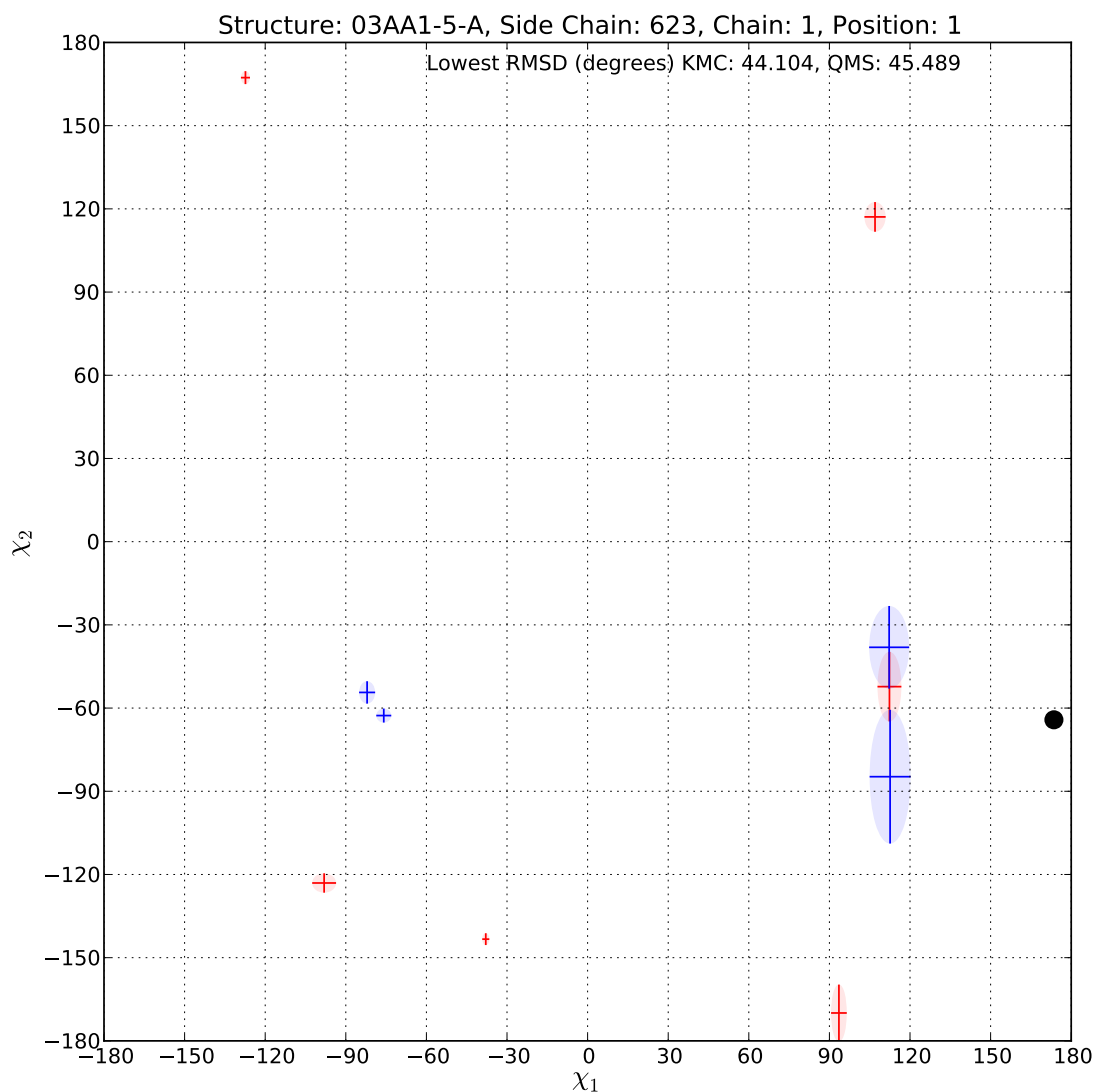


Figure S16: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 03AA1-5-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

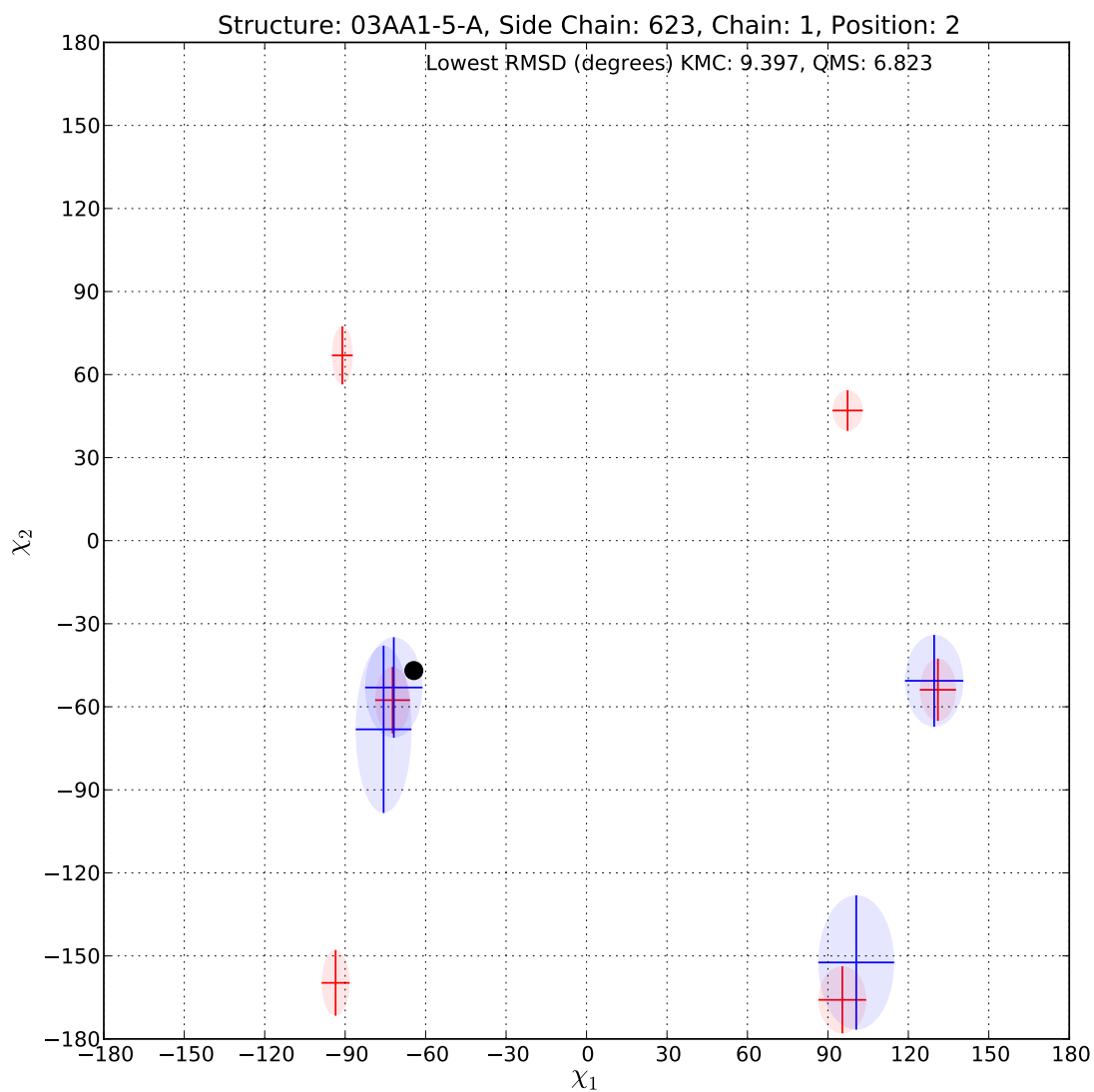


Figure S17: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 03AA1-5-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

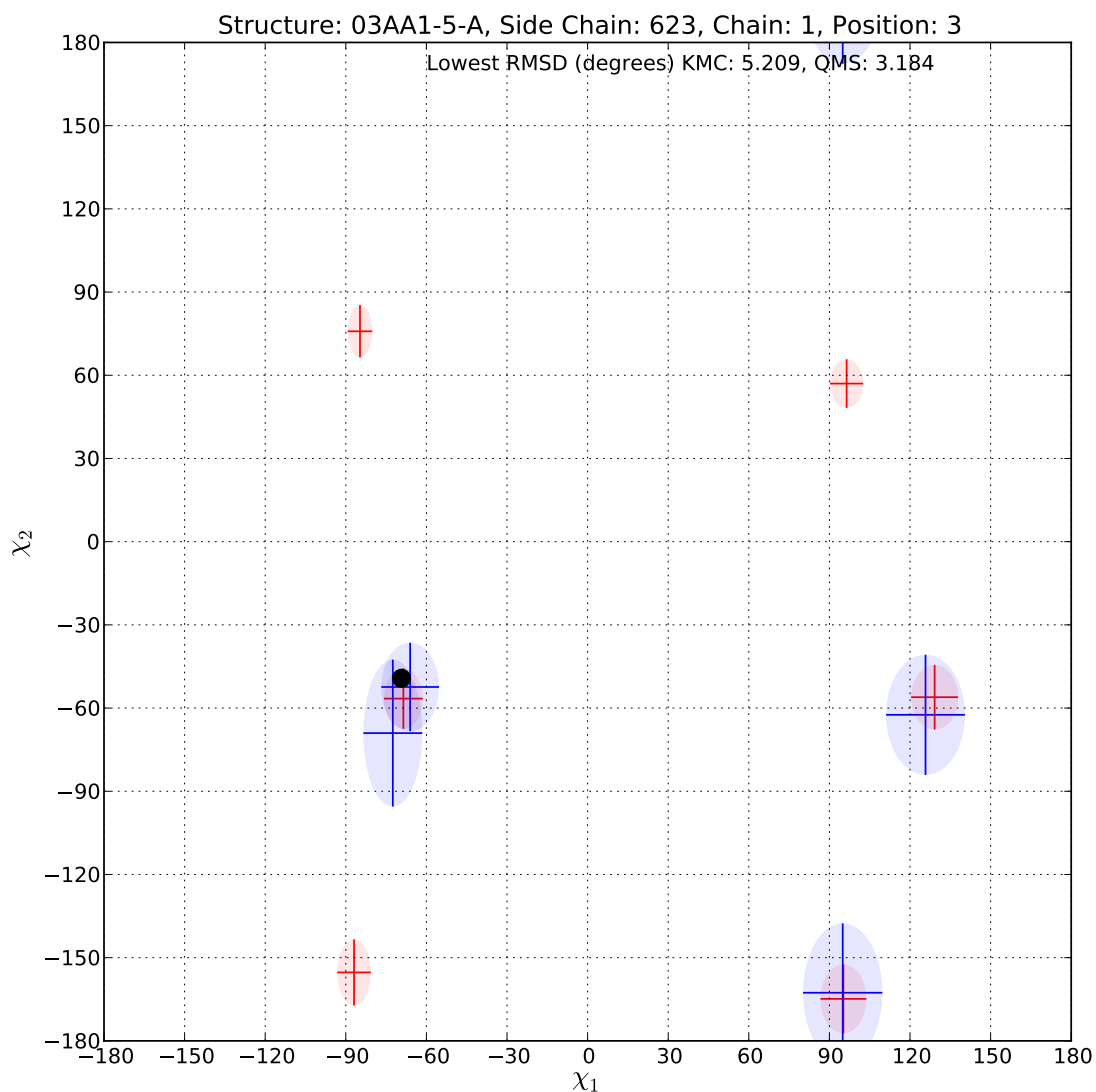


Figure S18: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 03AA1-5-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

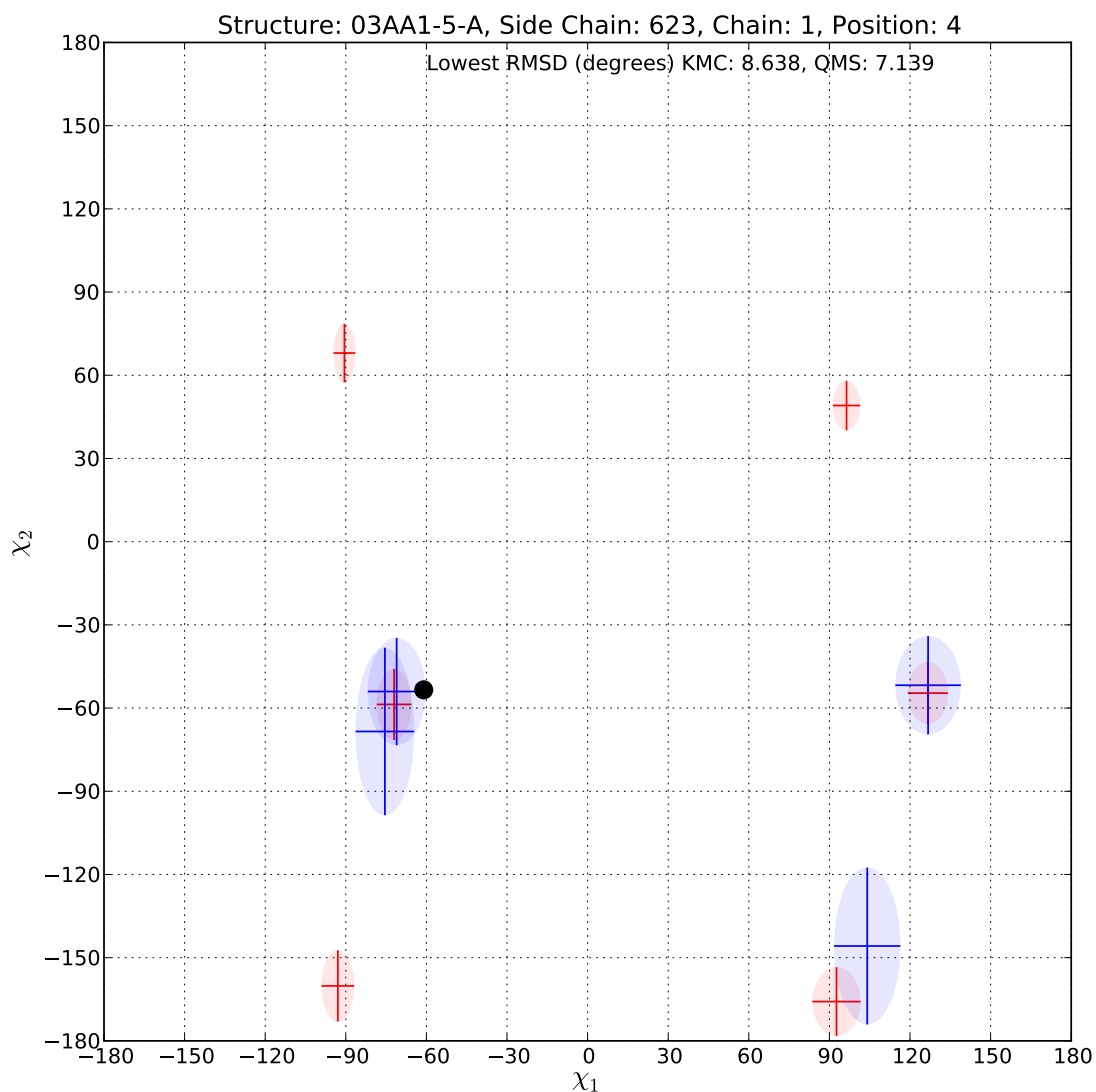


Figure S19: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 03AA1-5-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

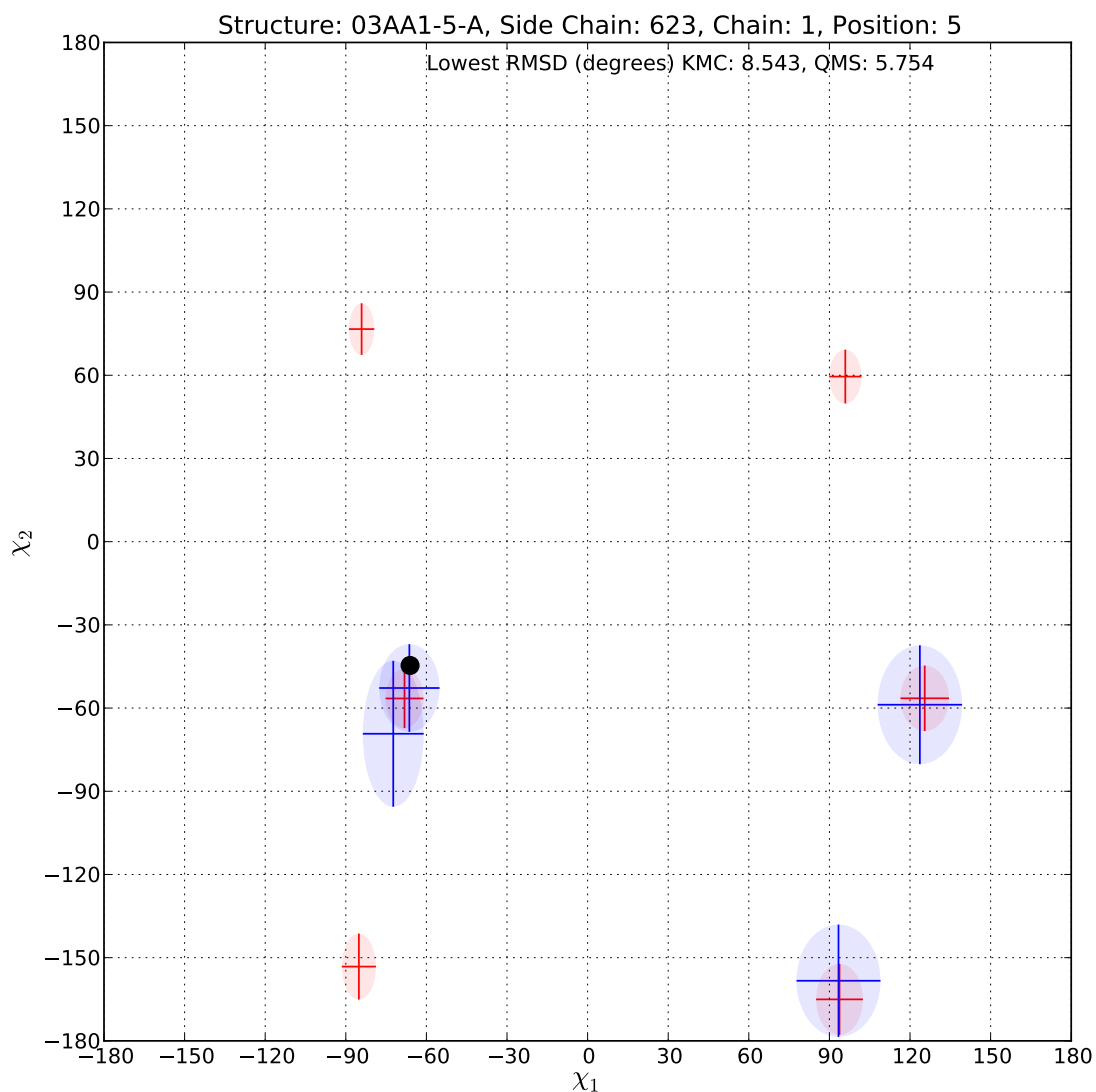


Figure S20: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 03AA1-5-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

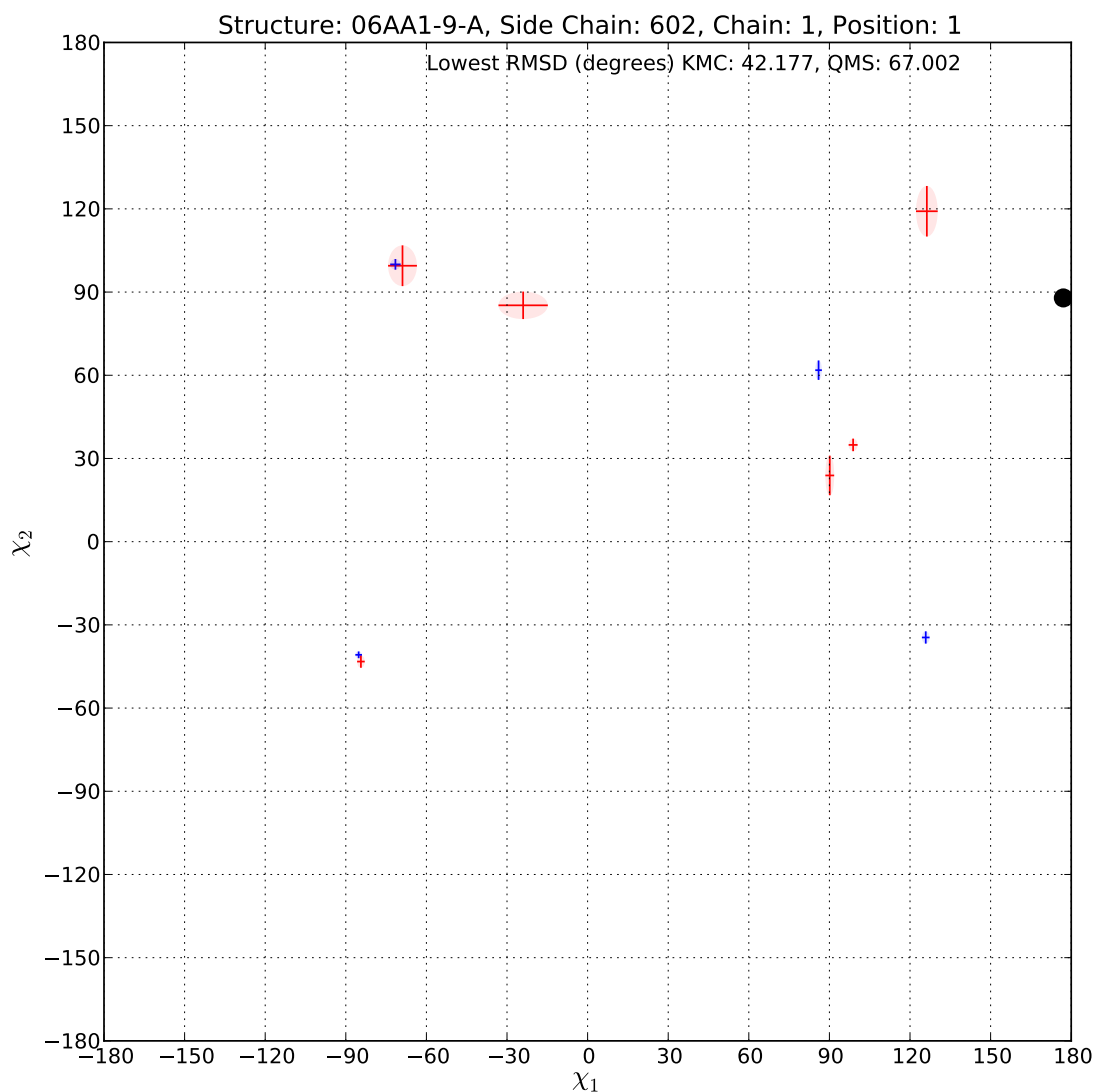


Figure S21: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 06AA1-9-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

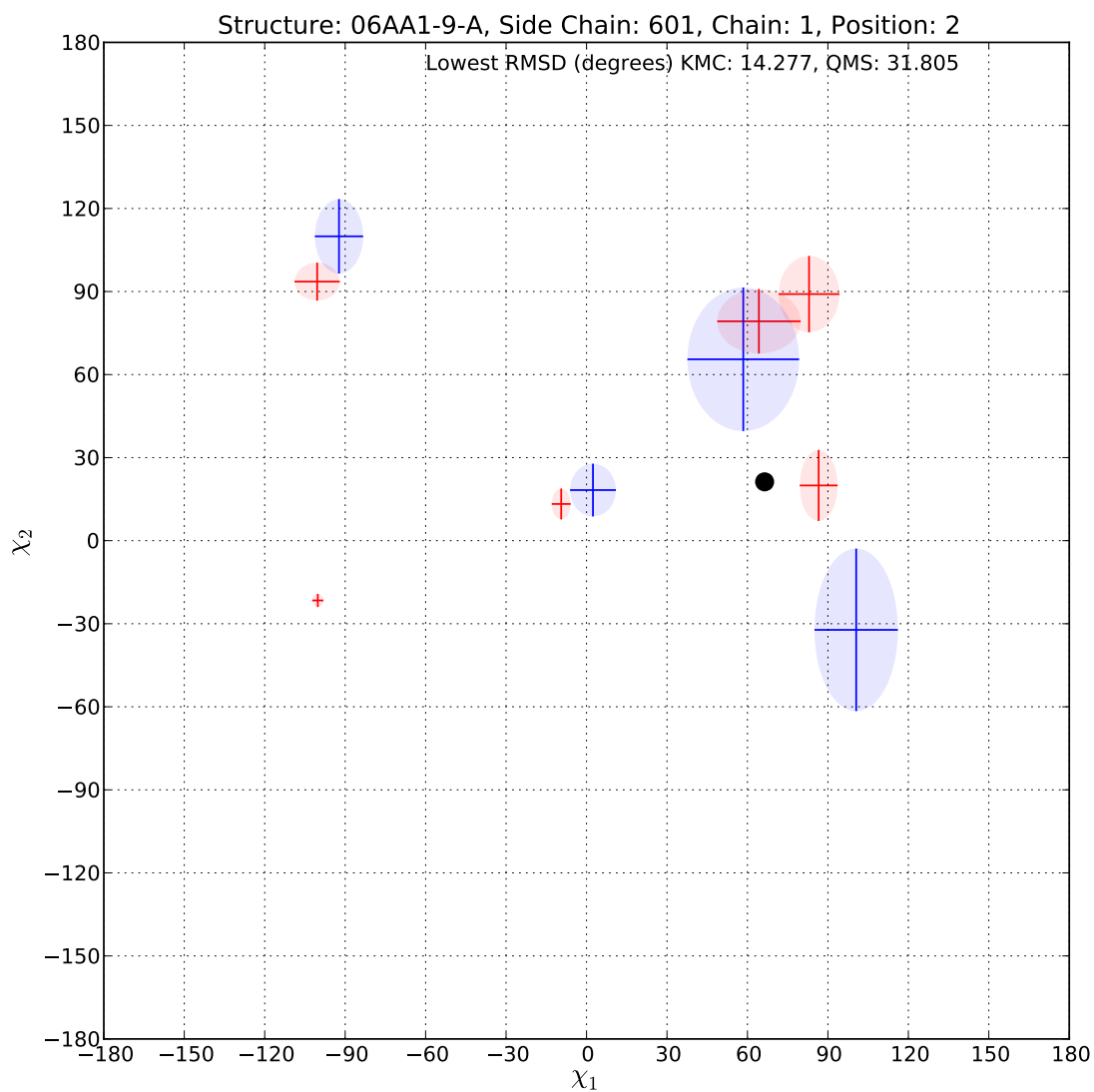


Figure S22: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 06AA1-9-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

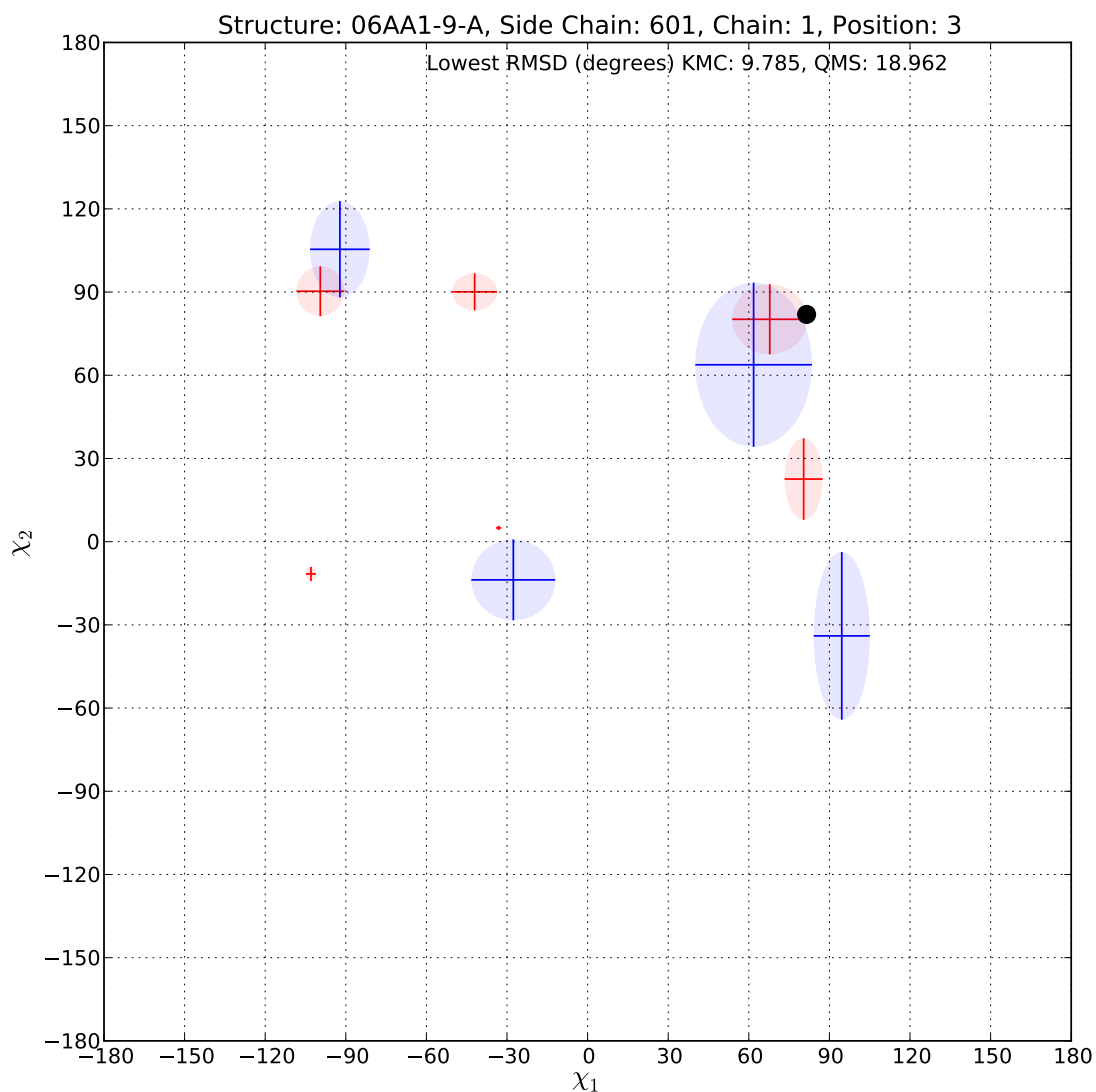


Figure S23: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 06AA1-9-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

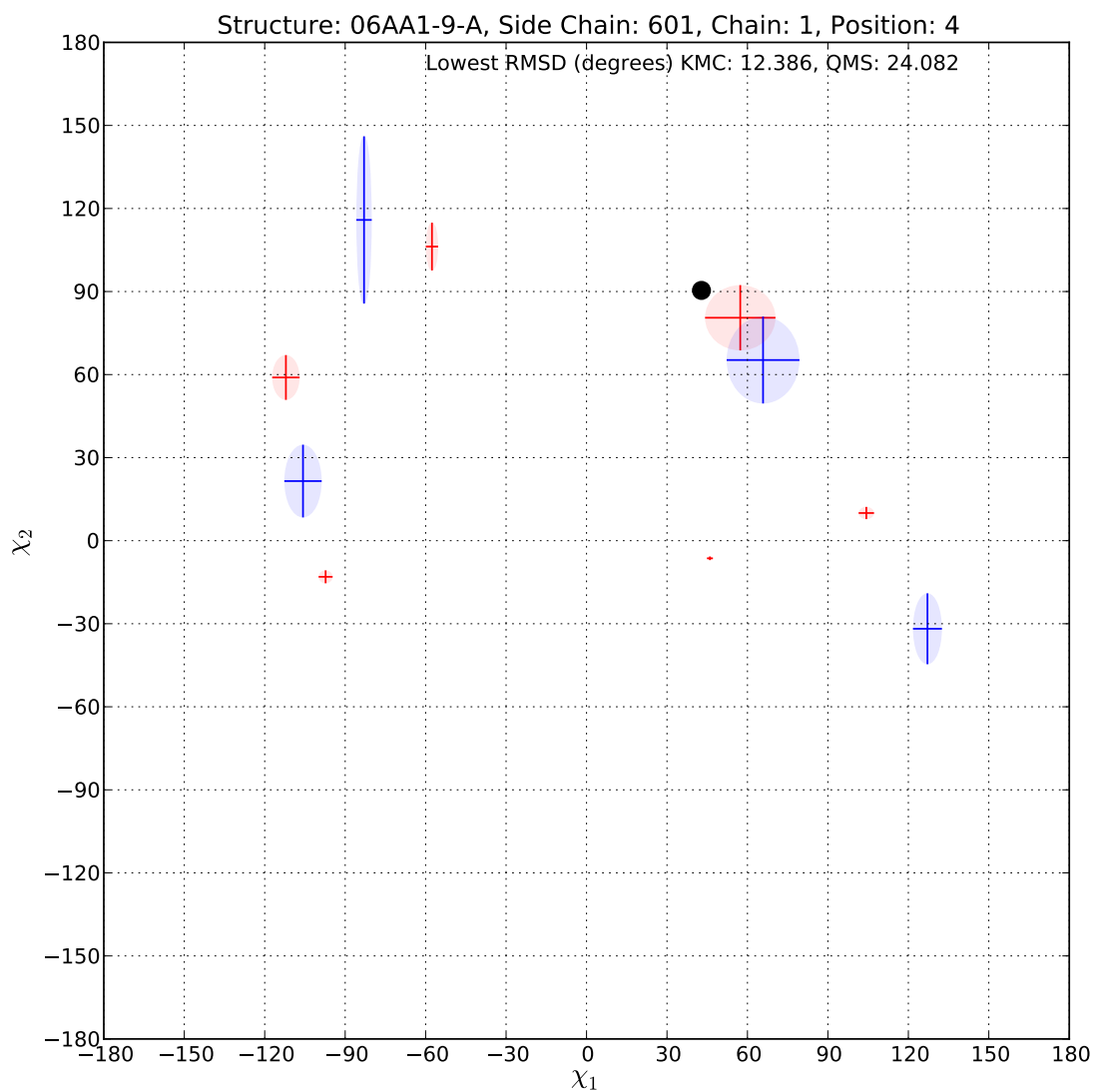


Figure S24: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 06AA1-9-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

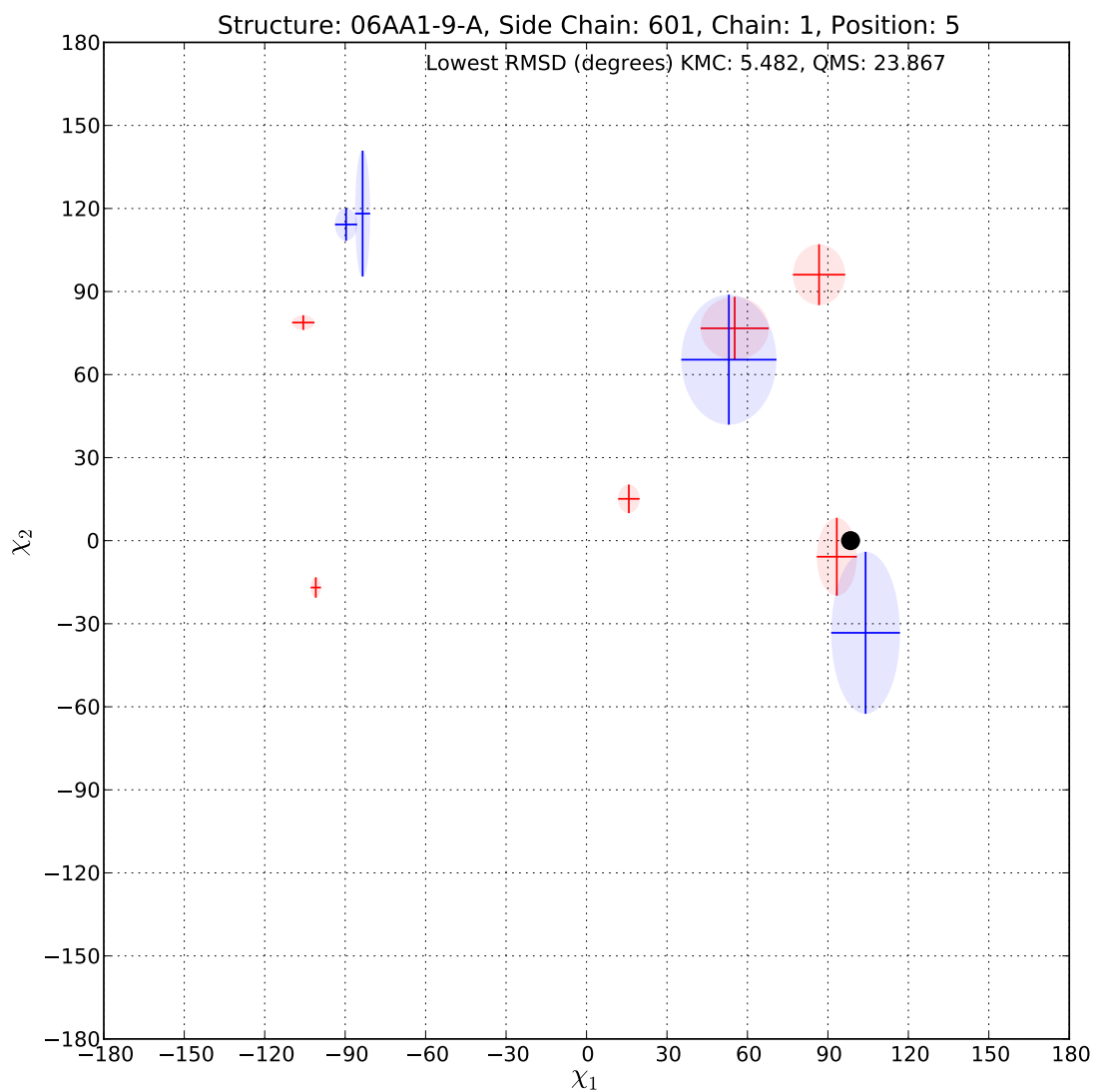


Figure S25: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 06AA1-9-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

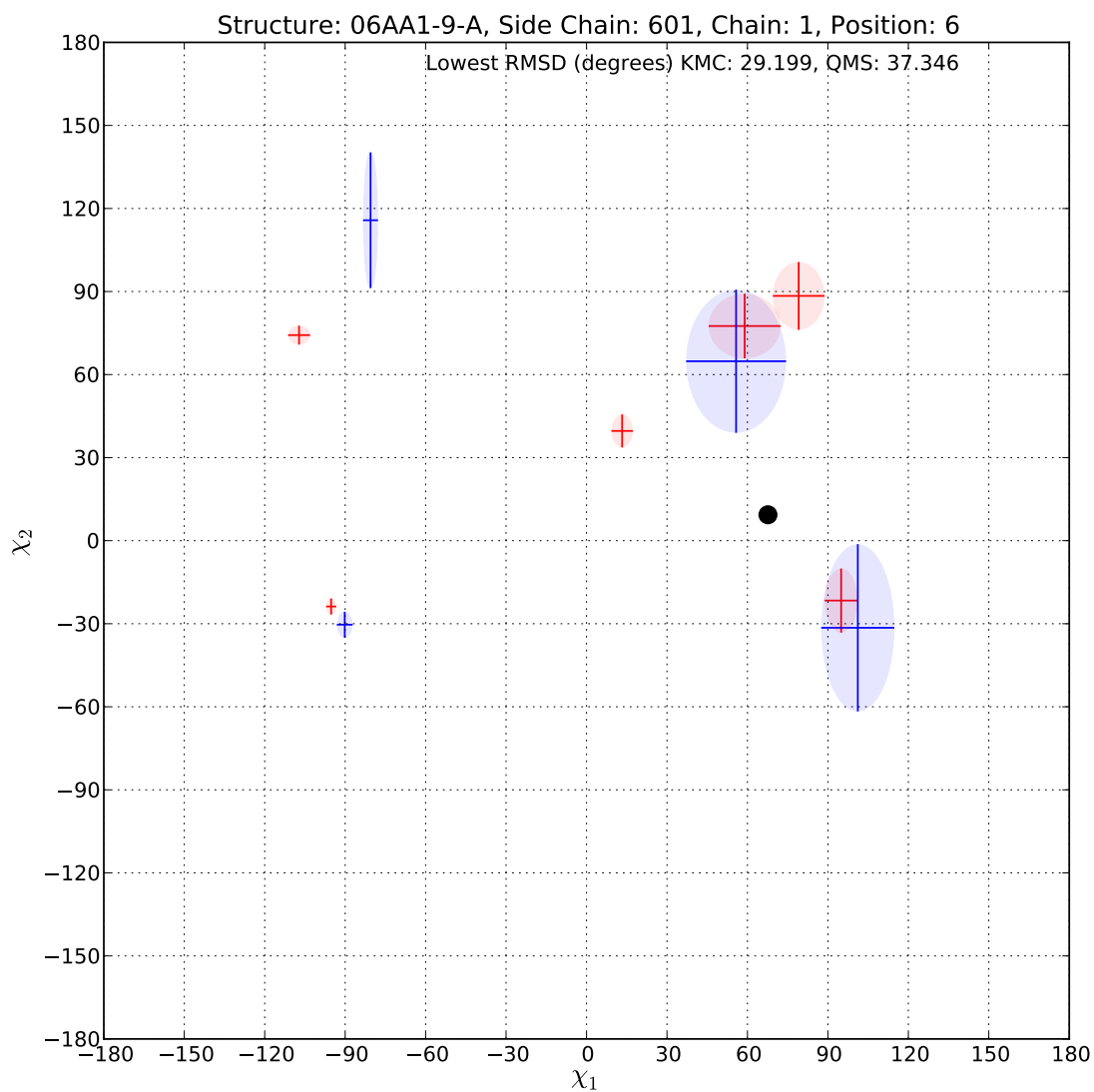


Figure S26: The rotamer library coverage plot for residue number 6 in chain 1 of peptoid databank structure 06AA1-9-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

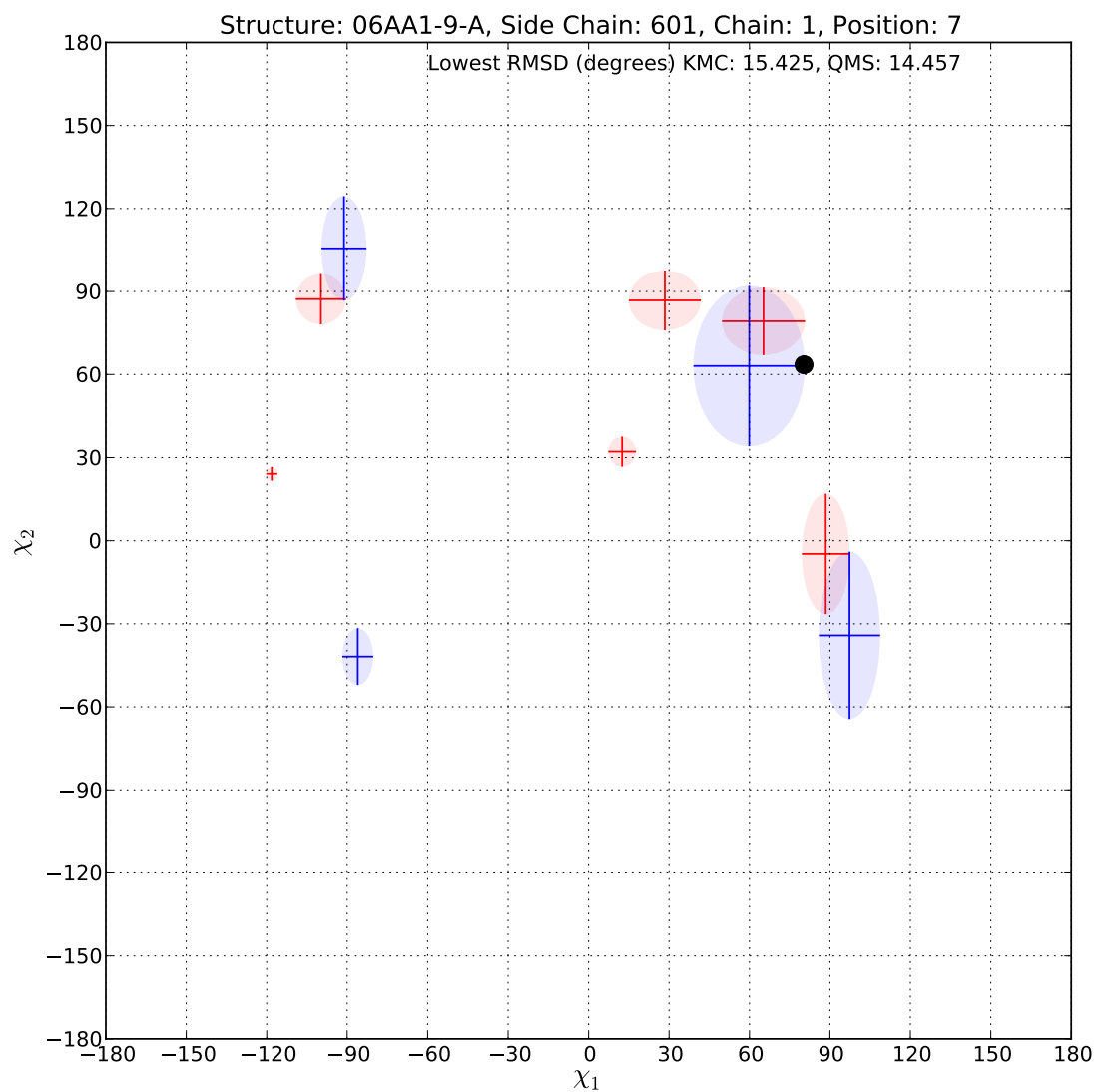


Figure S27: The rotamer library coverage plot for residue number 7 in chain 1 of peptoid databank structure 06AA1-9-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

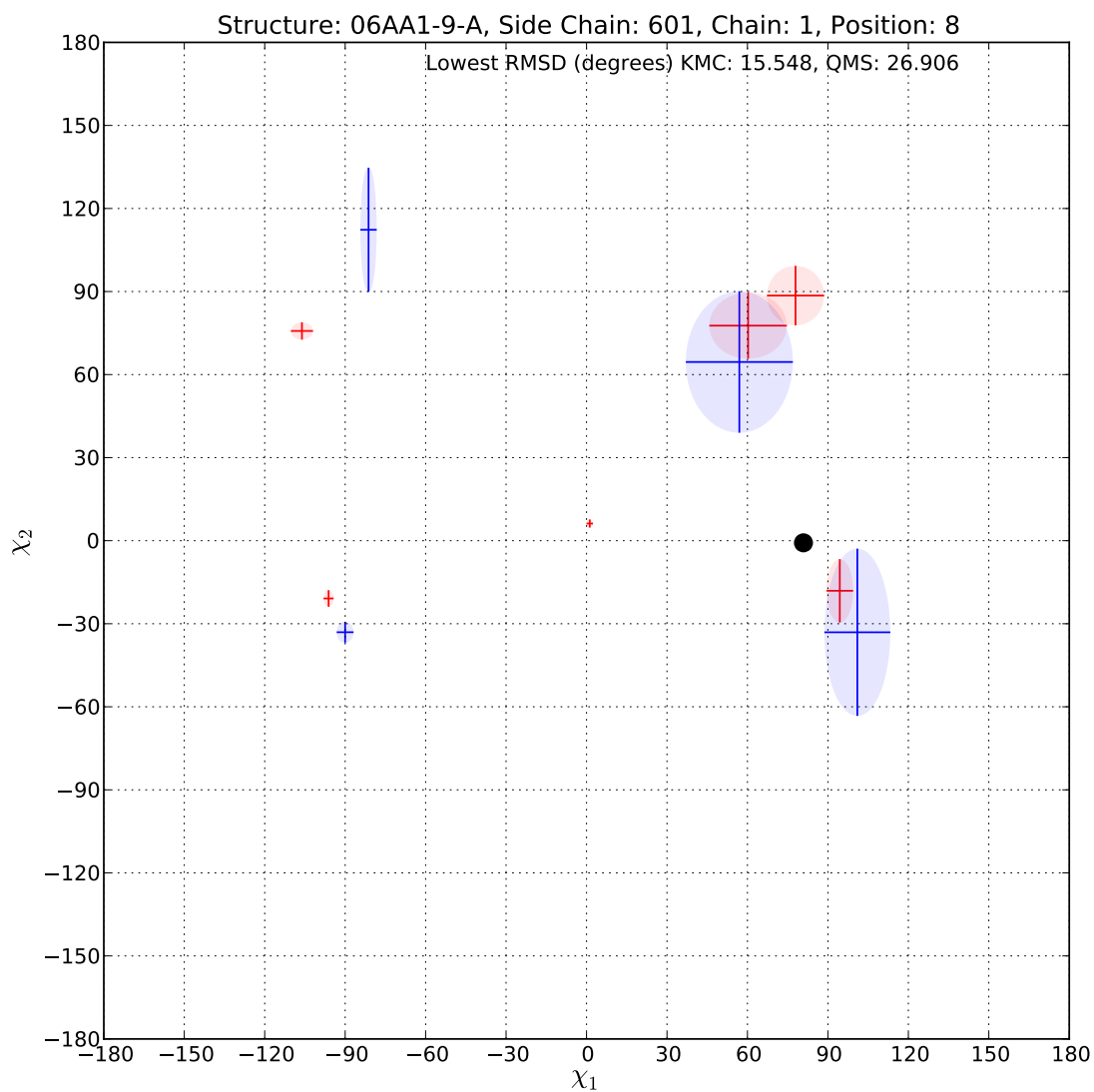


Figure S28: The rotamer library coverage plot for residue number 8 in chain 1 of peptoid databank structure 06AA1-9-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

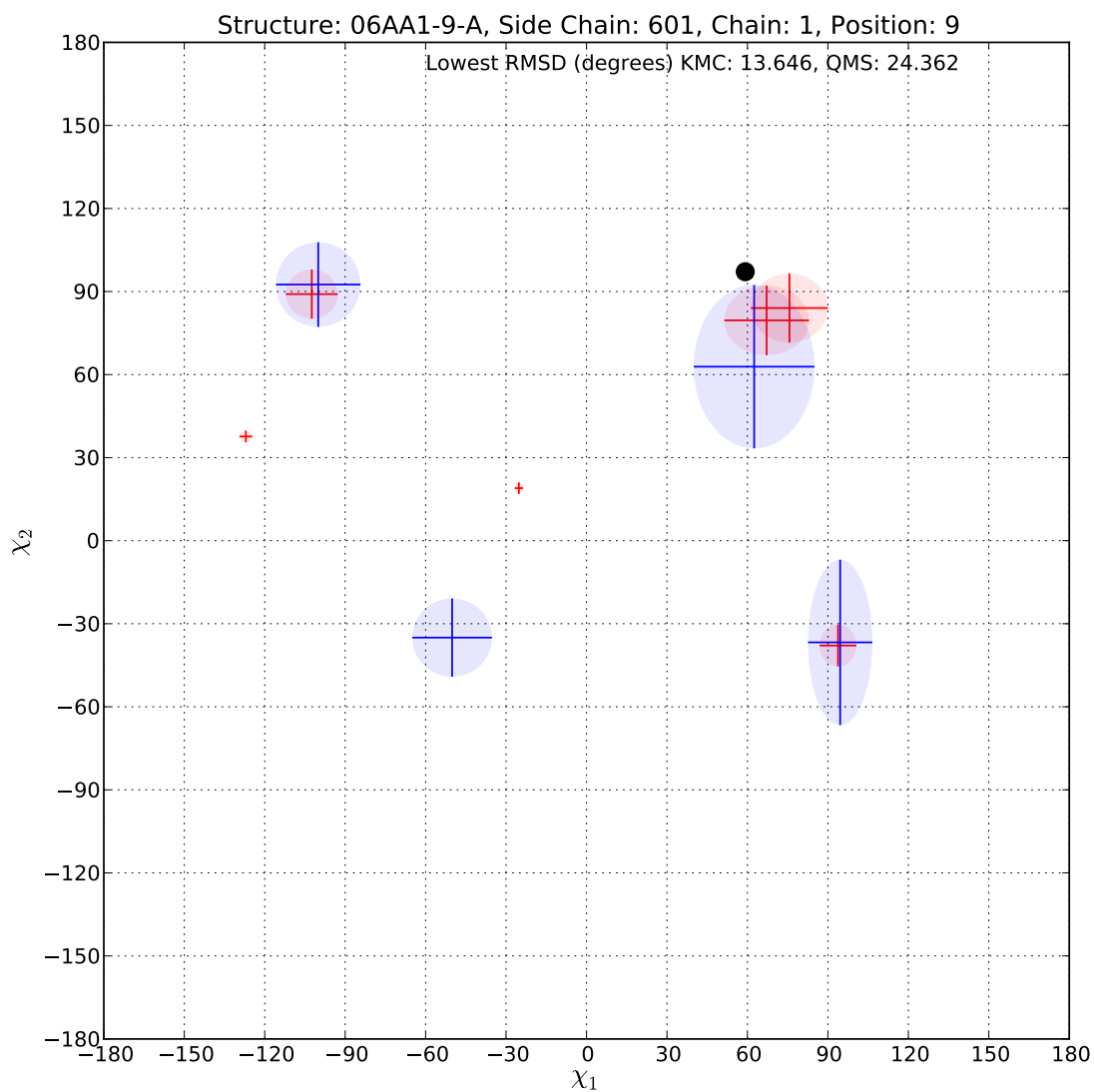


Figure S29: The rotamer library coverage plot for residue number 9 in chain 1 of peptoid databank structure 06AA1-9-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

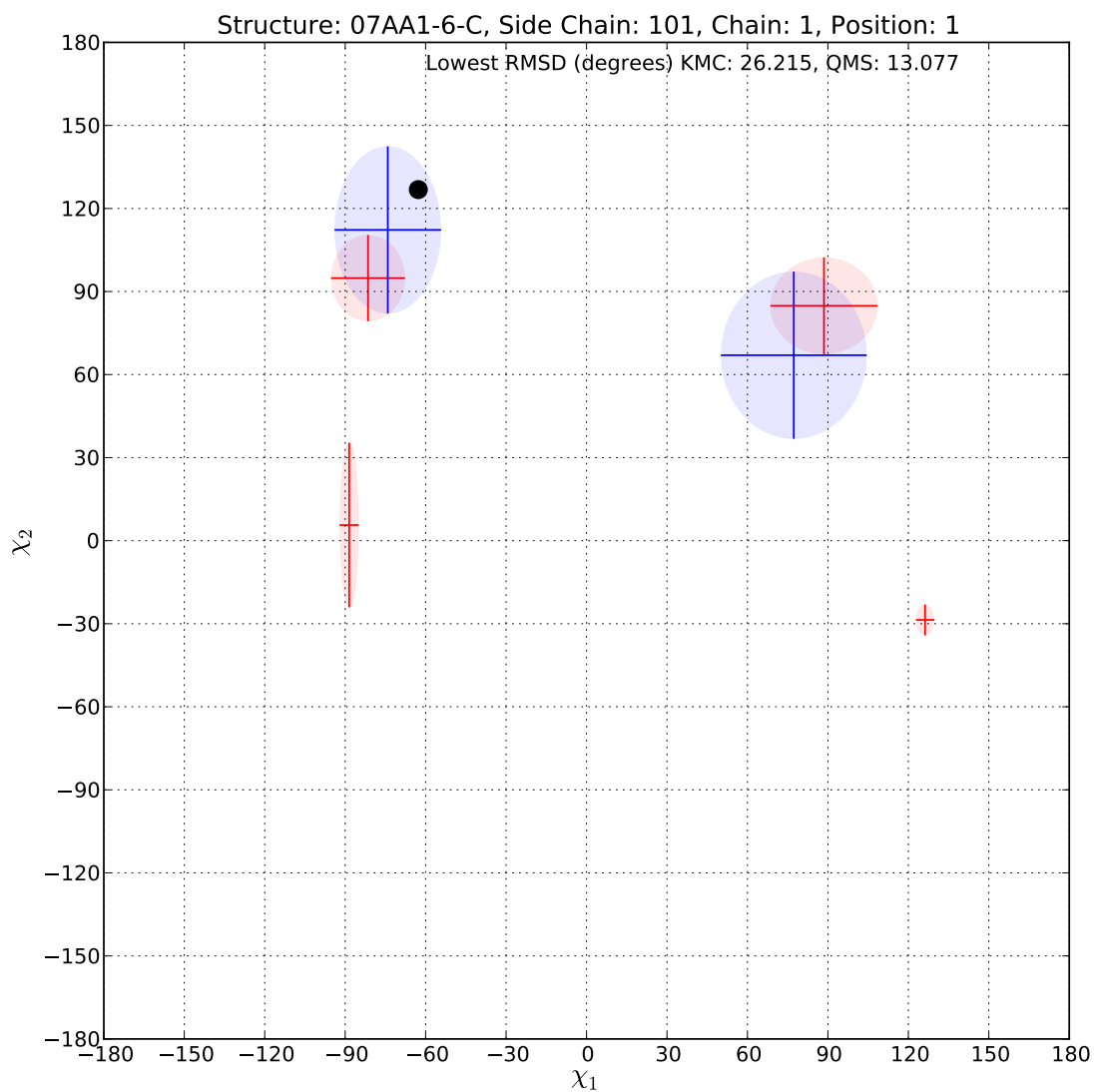


Figure S30: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 07AA1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

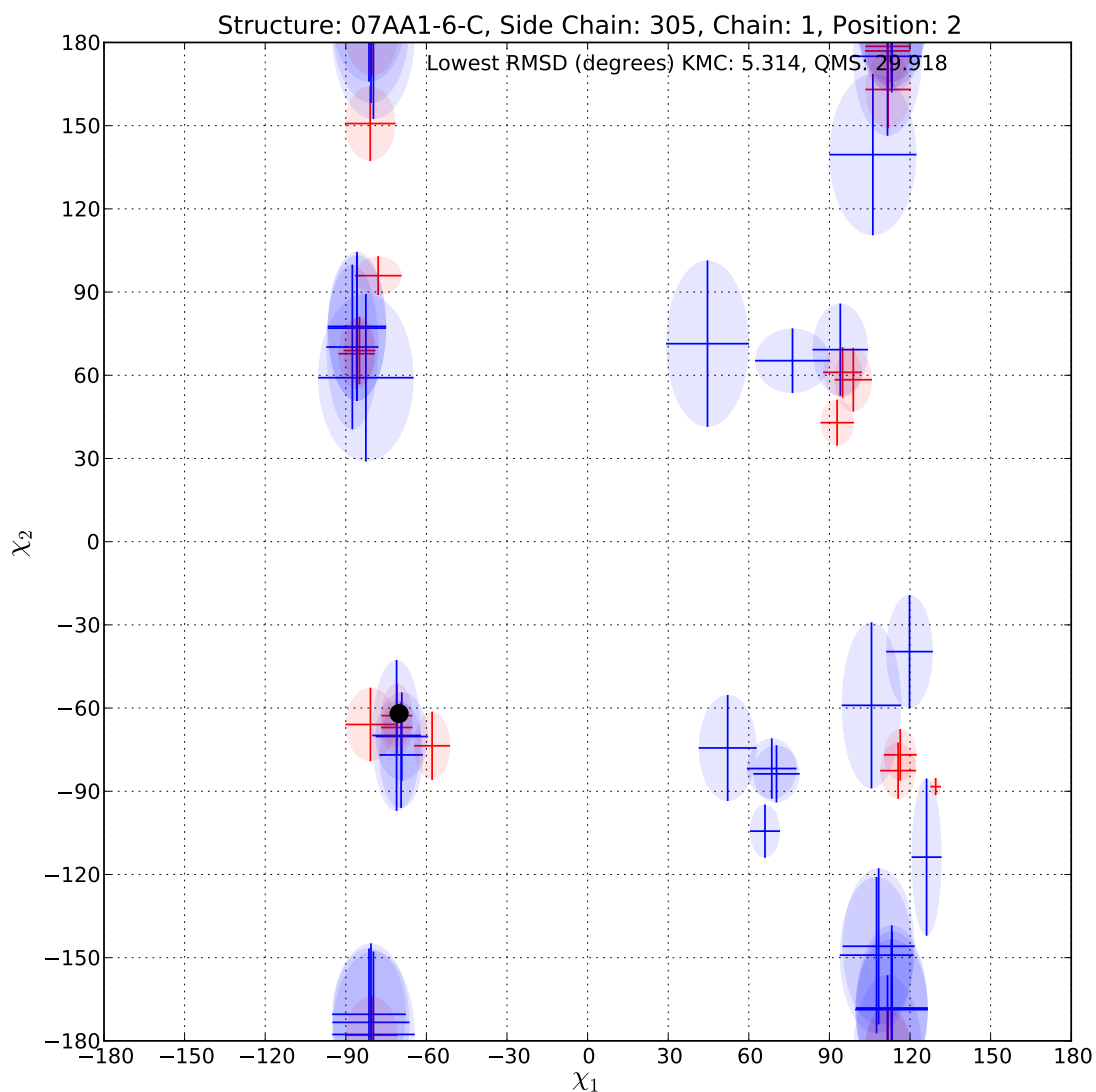


Figure S31: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 07AA1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

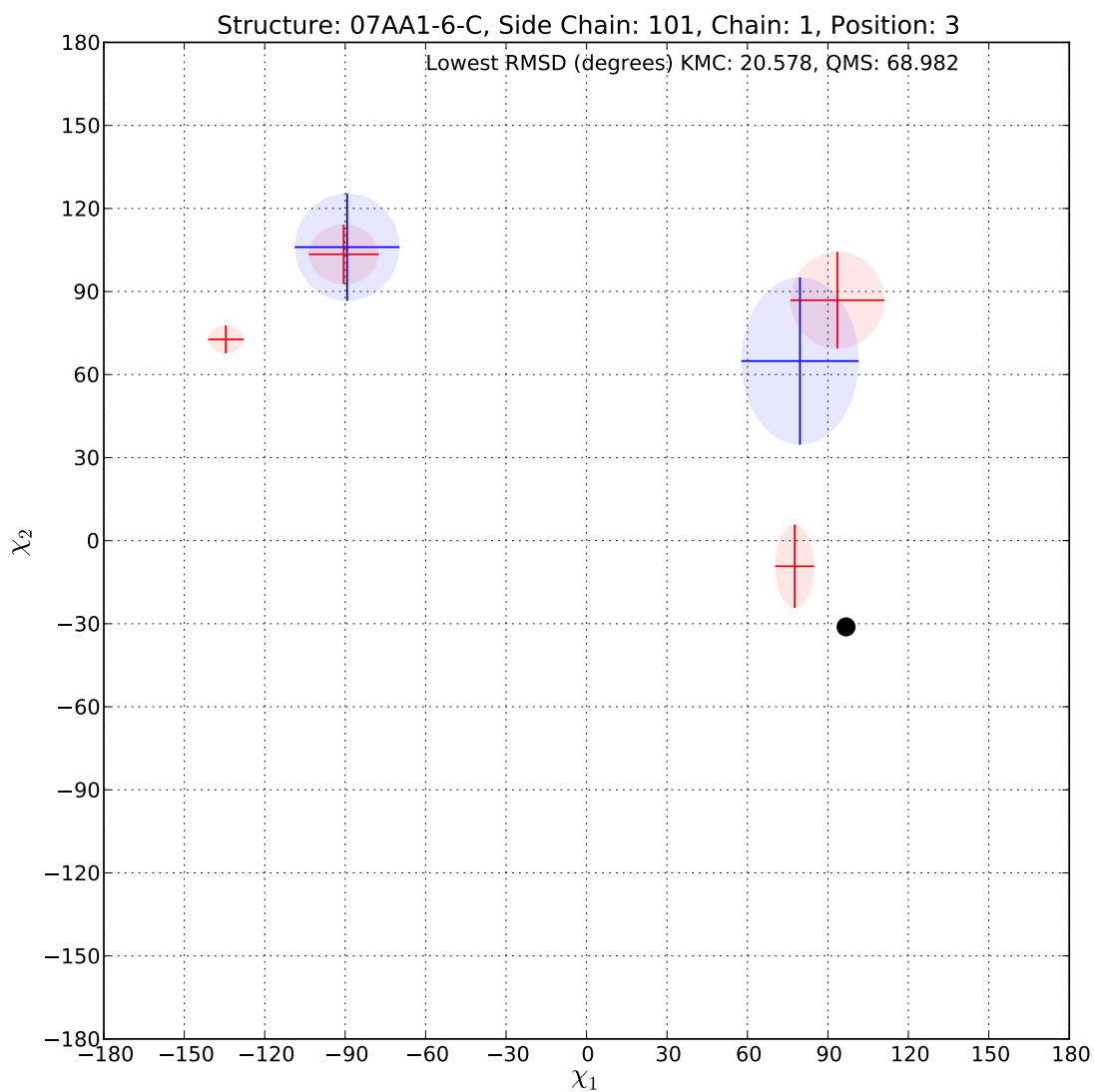


Figure S32: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 07AA1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

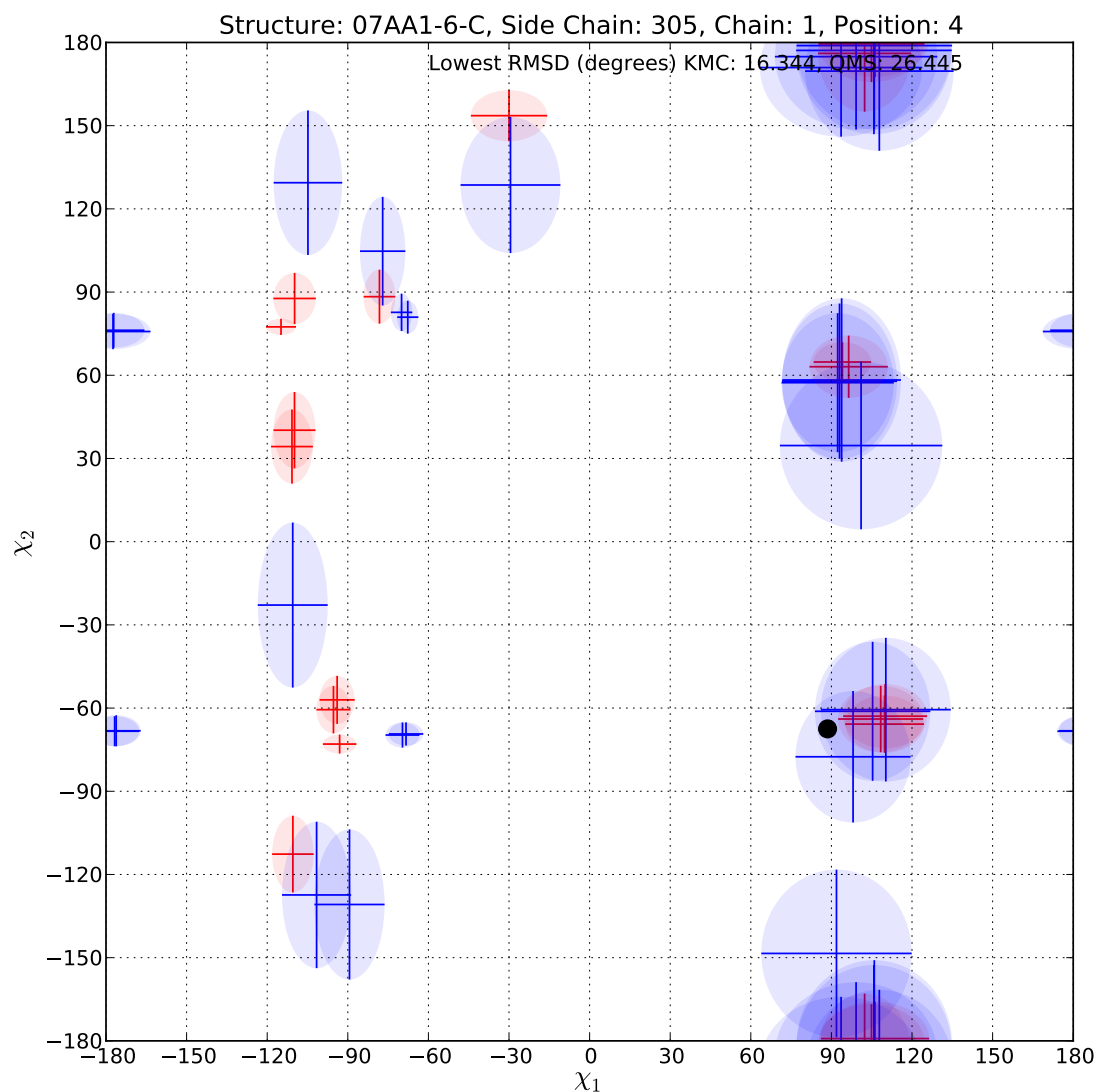


Figure S33: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 07AA1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

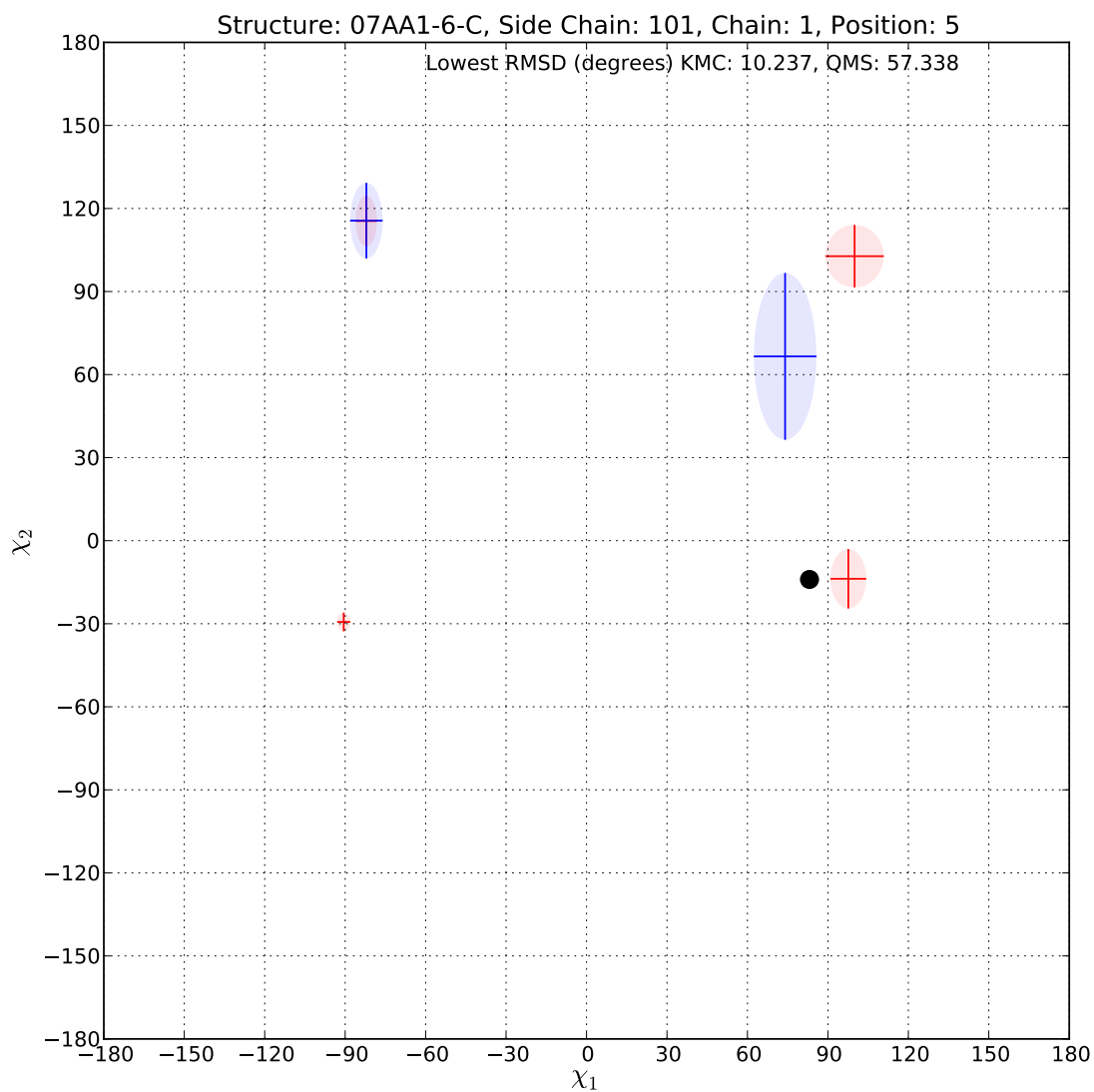


Figure S34: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 07AA1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

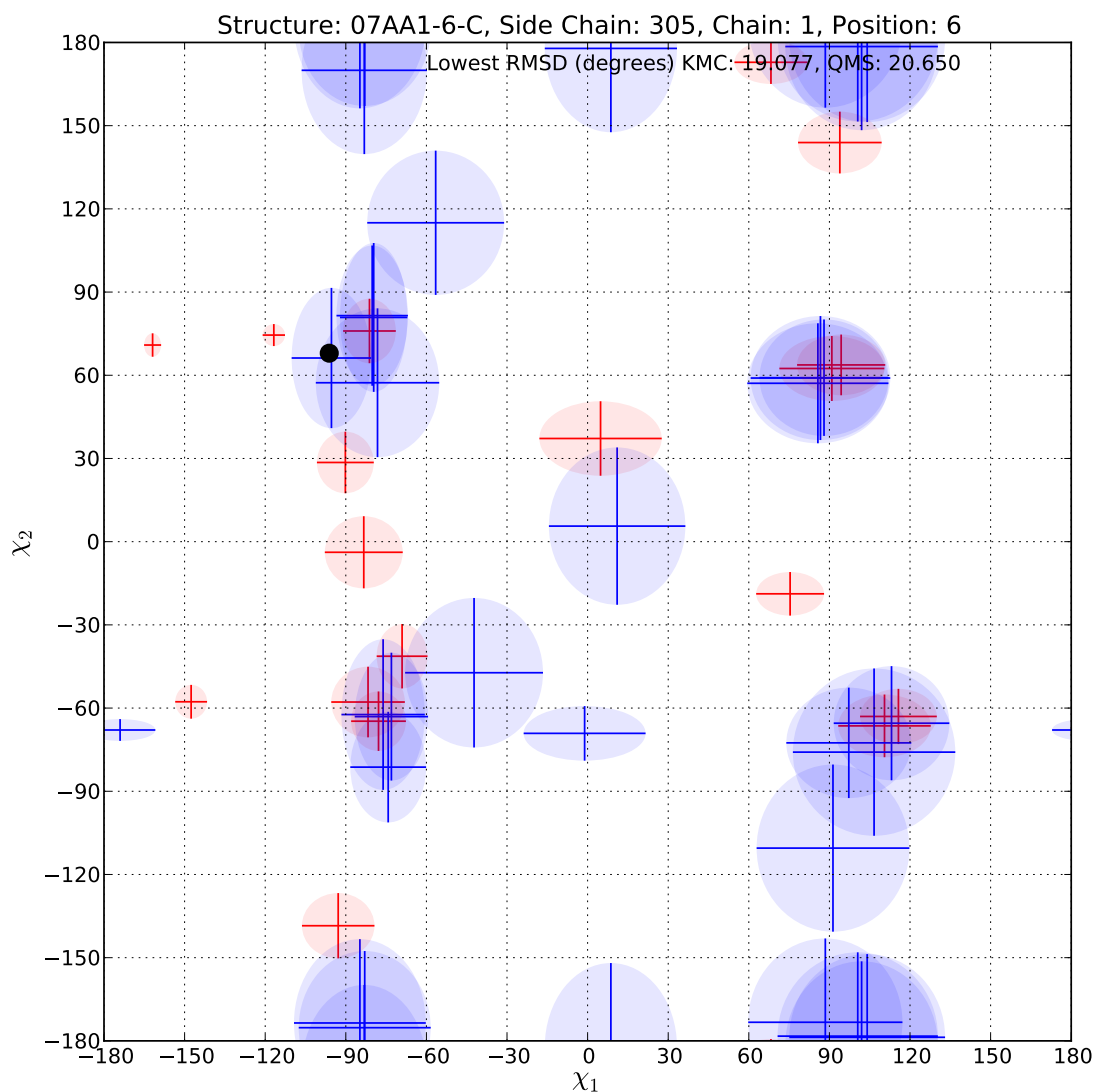


Figure S35: The rotamer library coverage plot for residue number 6 in chain 1 of peptoid databank structure 07AA1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

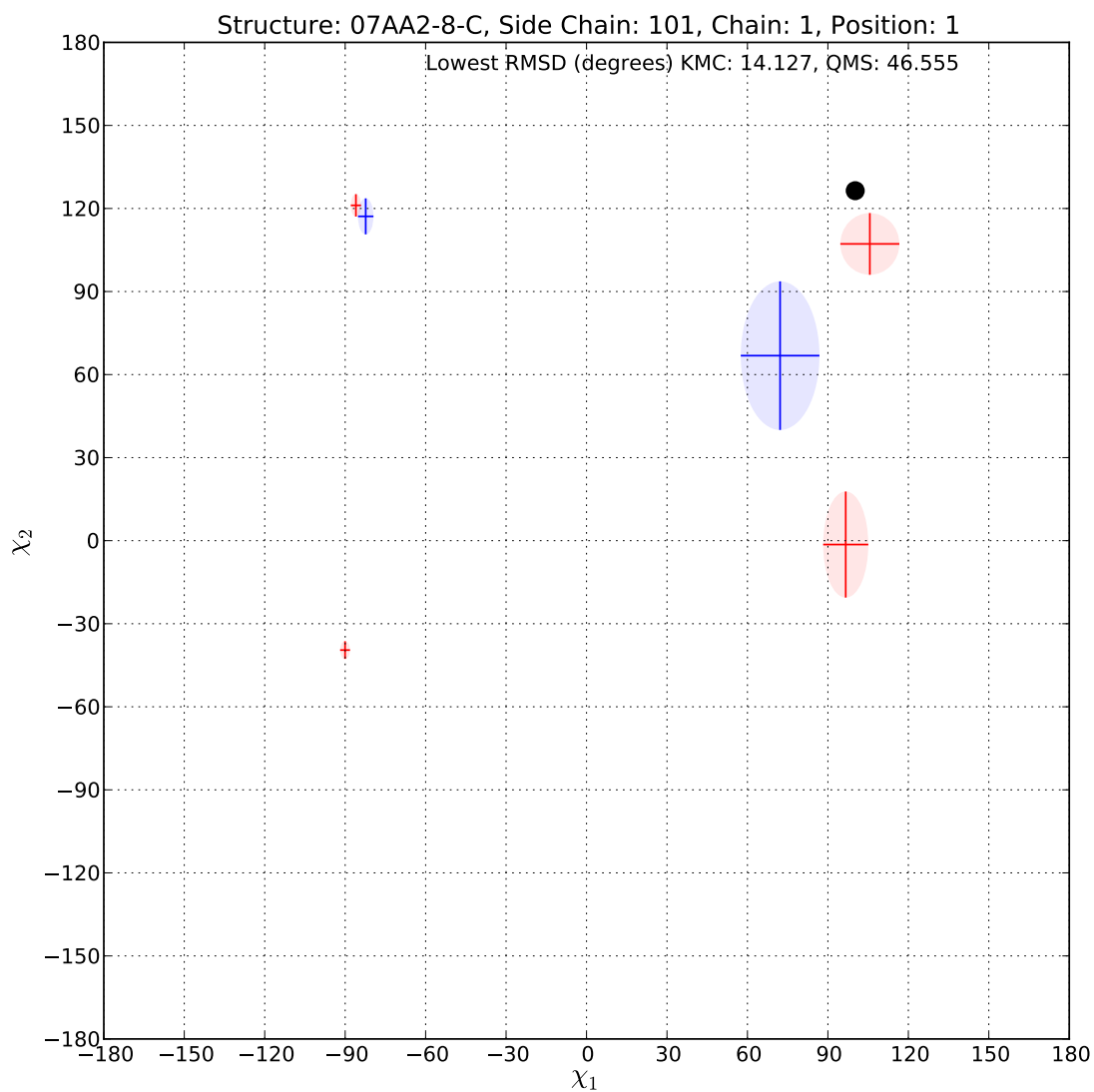


Figure S36: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

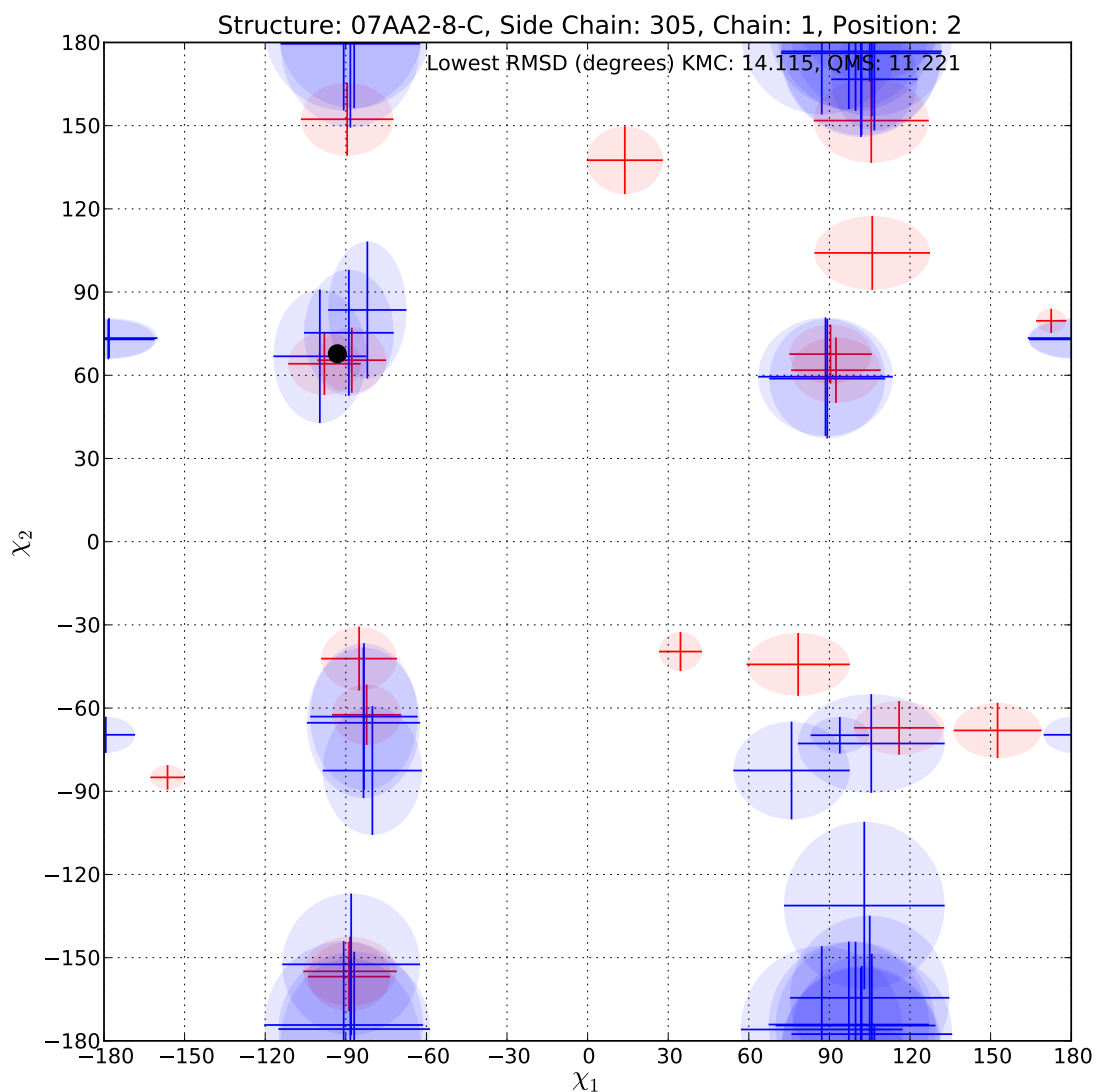


Figure S37: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

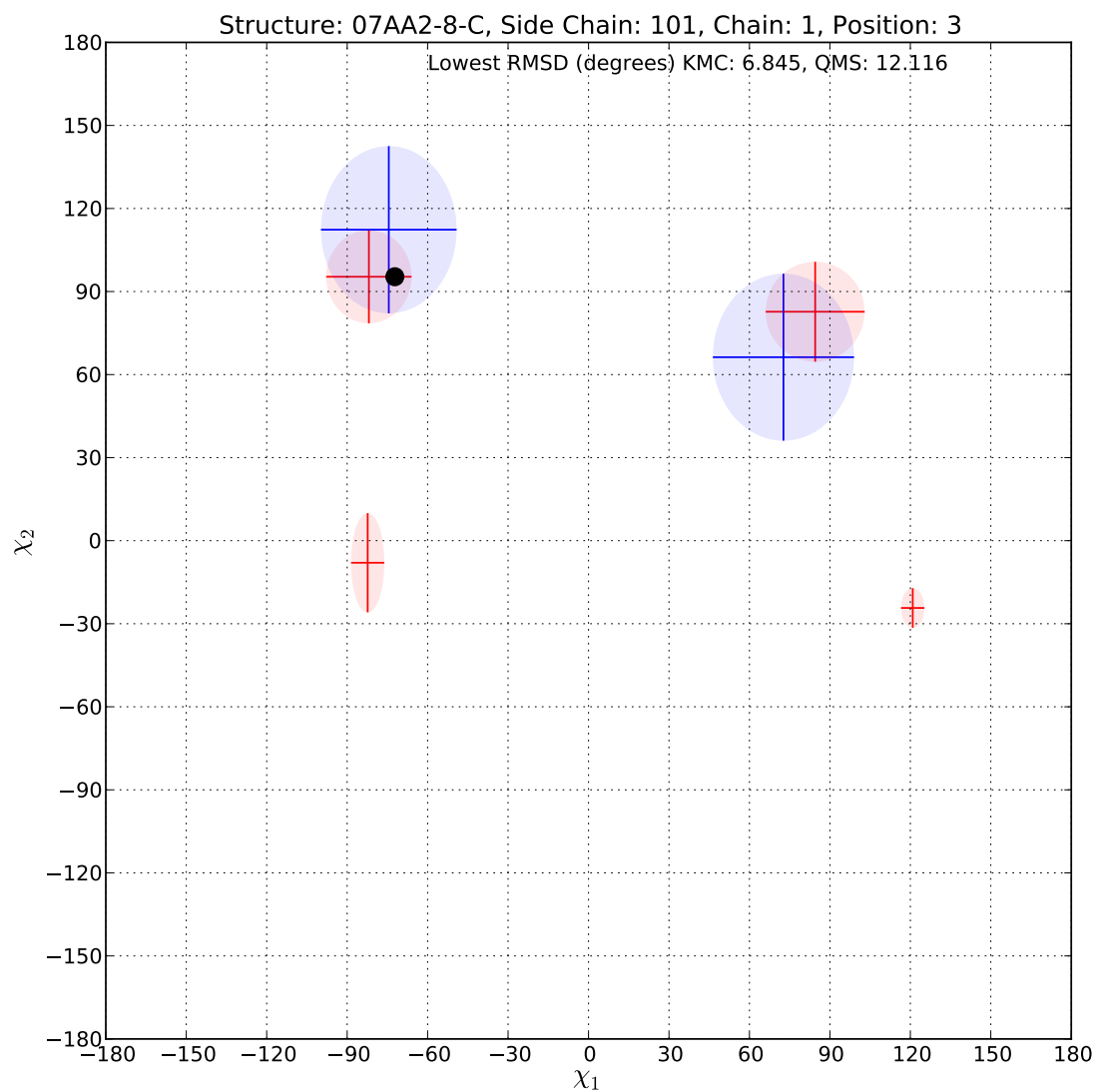


Figure S38: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

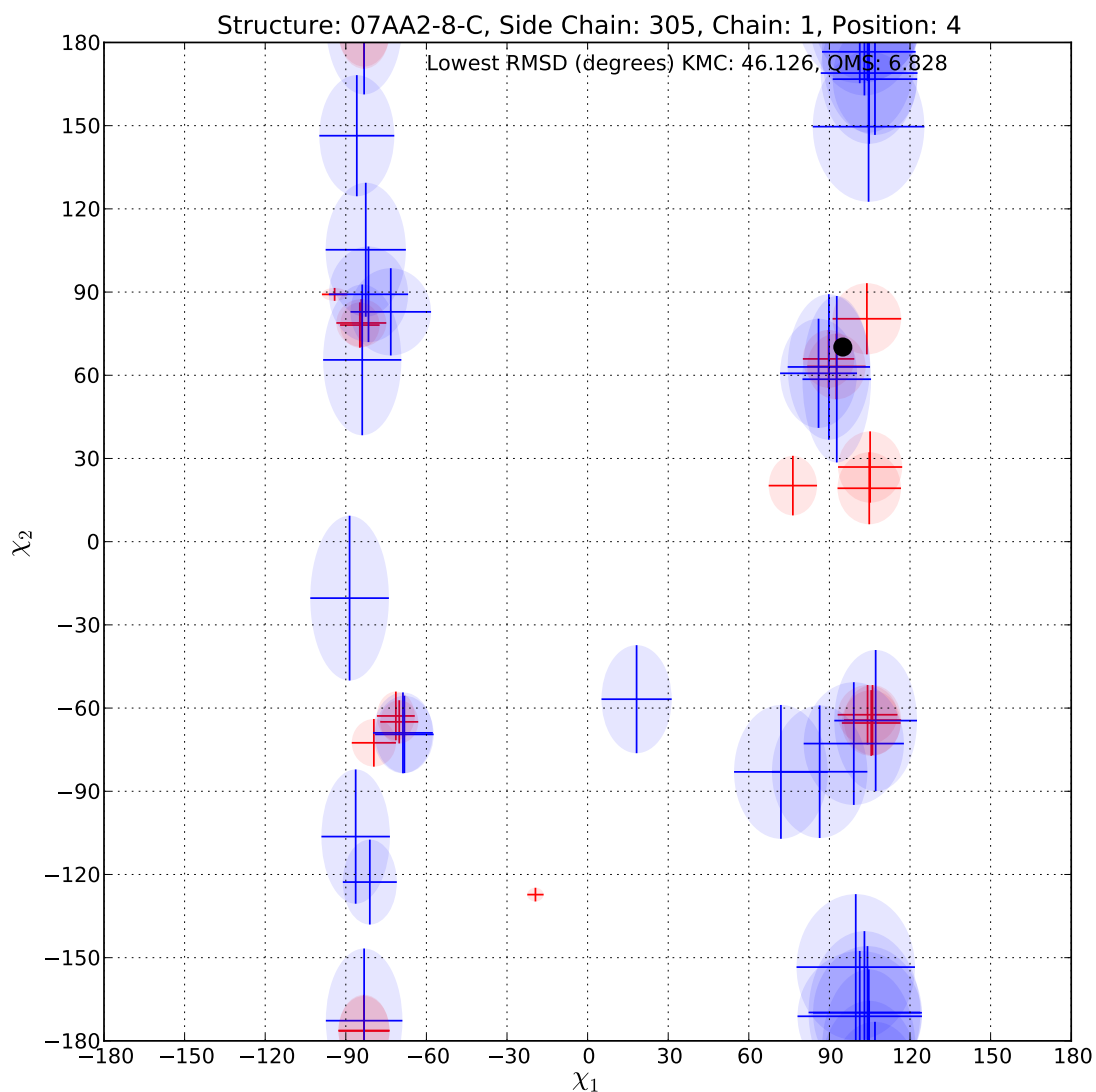


Figure S39: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

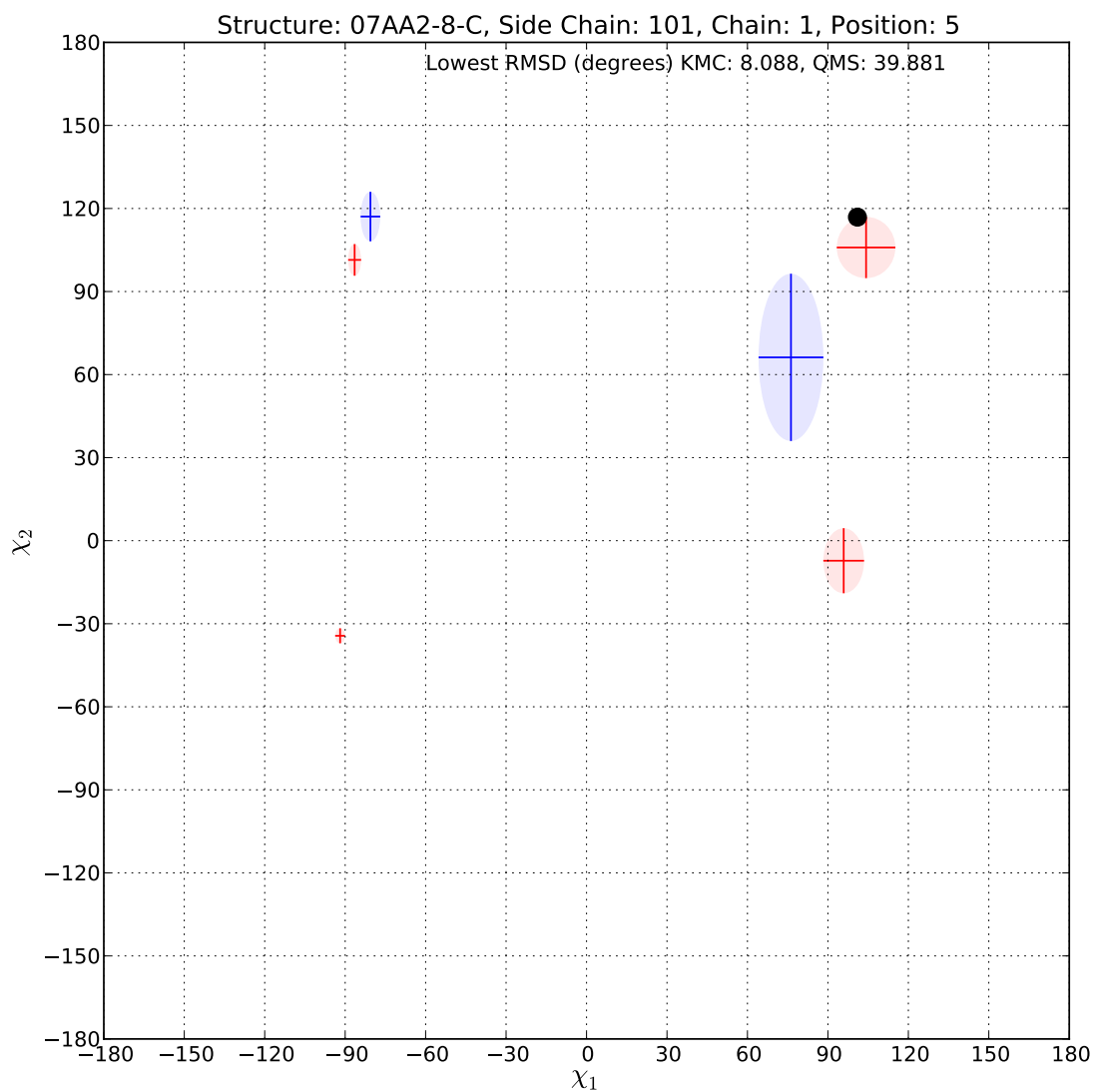


Figure S40: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

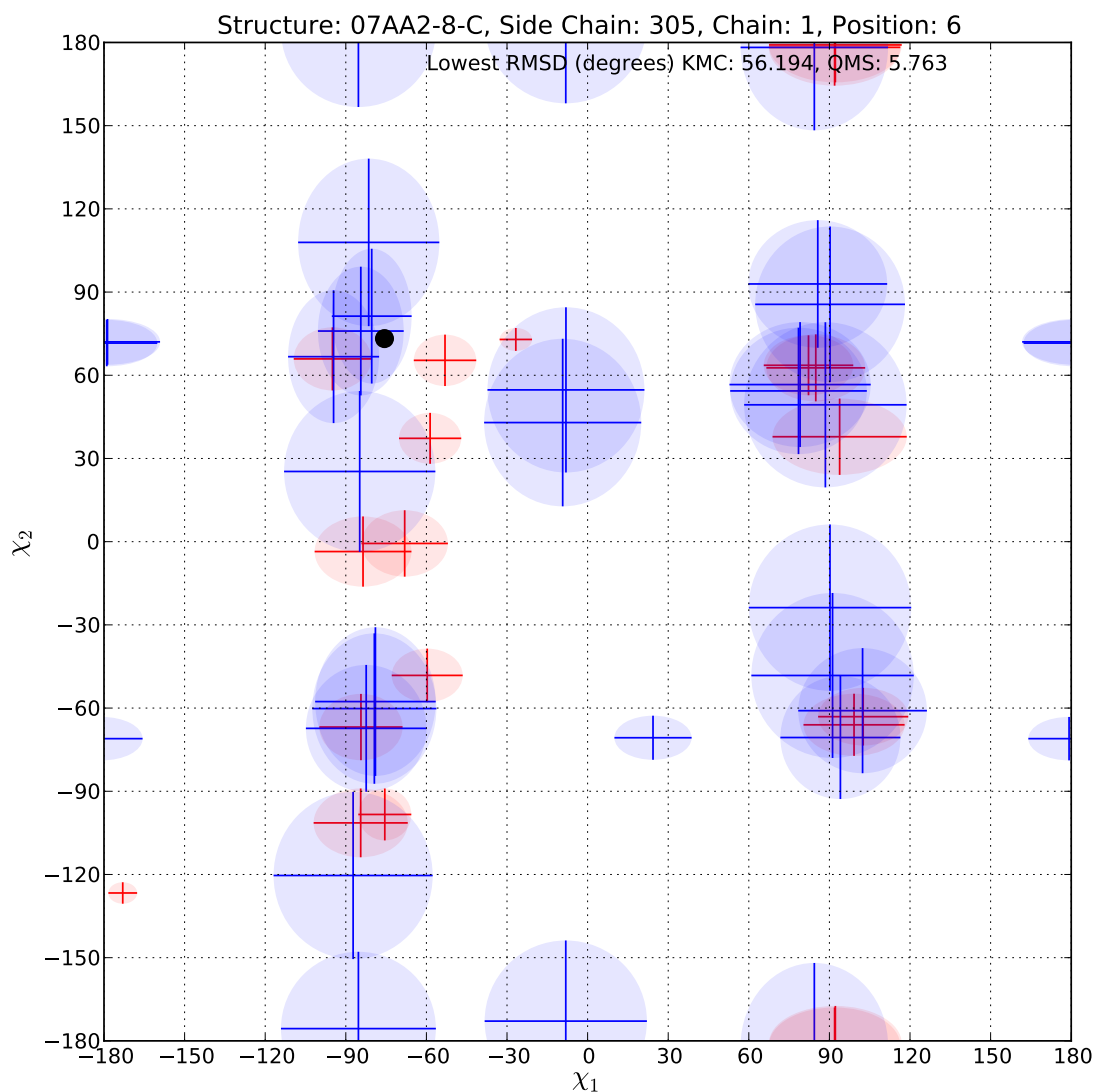


Figure S41: The rotamer library coverage plot for residue number 6 in chain 1 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

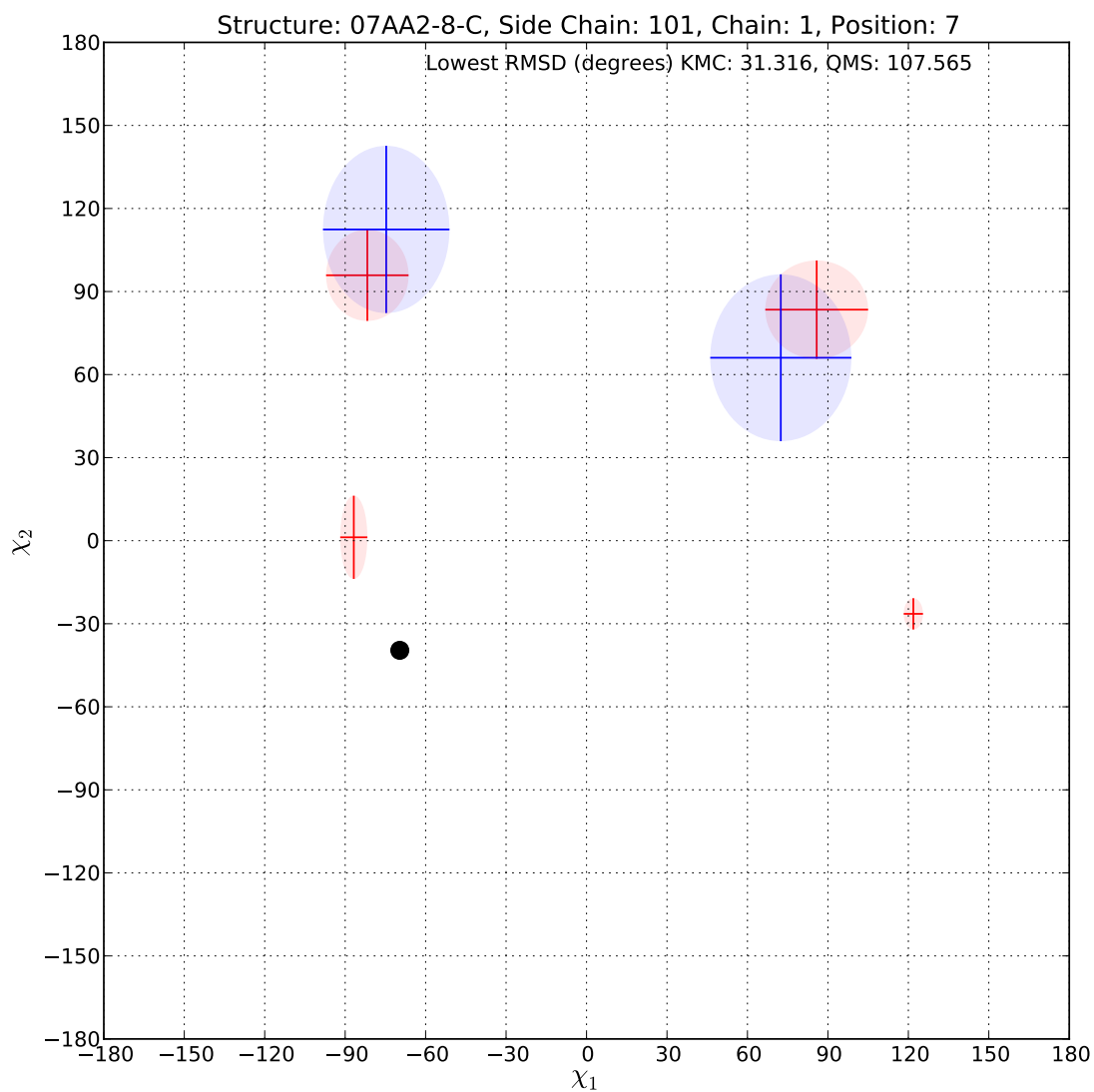


Figure S42: The rotamer library coverage plot for residue number 7 in chain 1 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

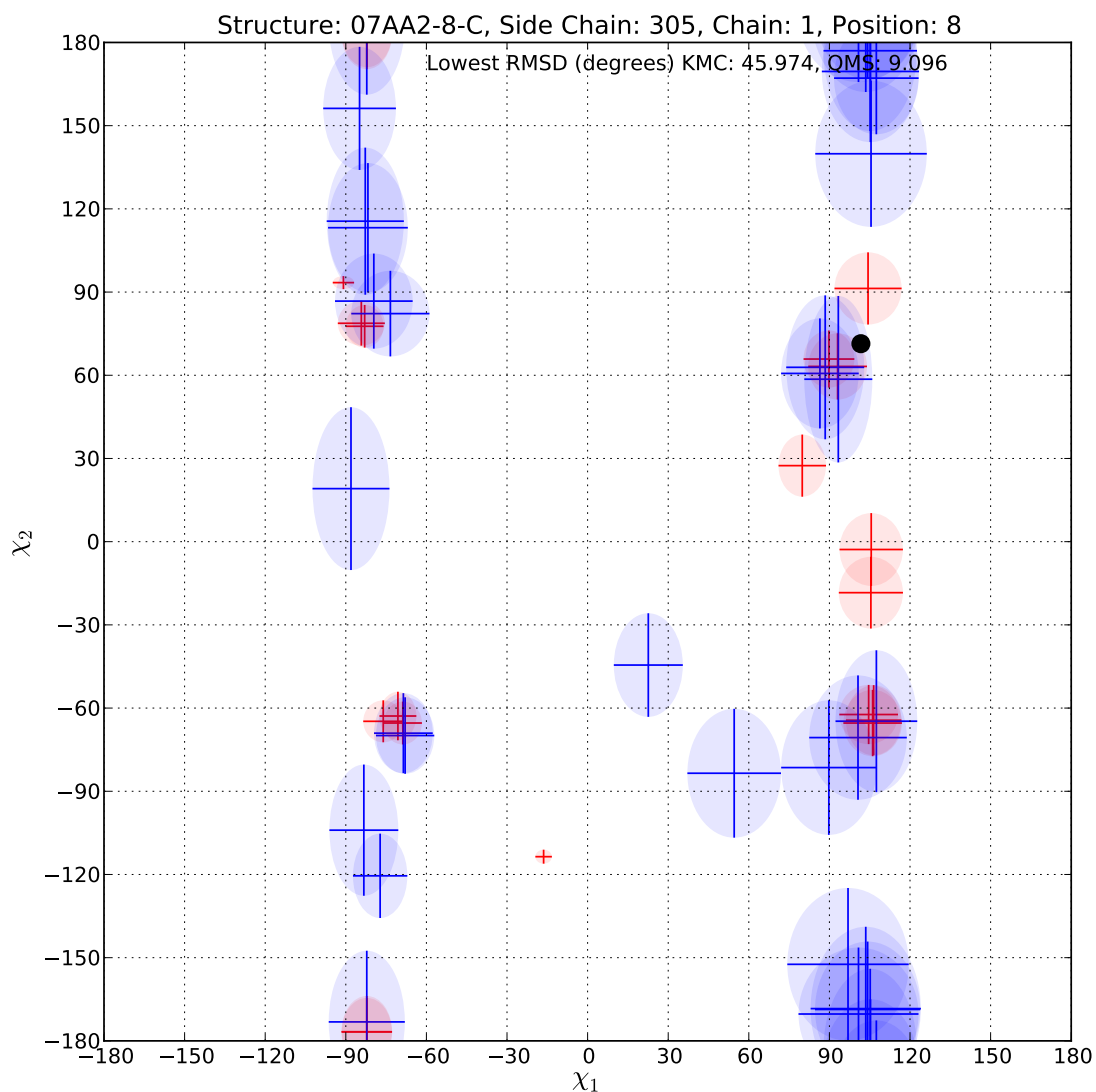


Figure S43: The rotamer library coverage plot for residue number 8 in chain 1 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

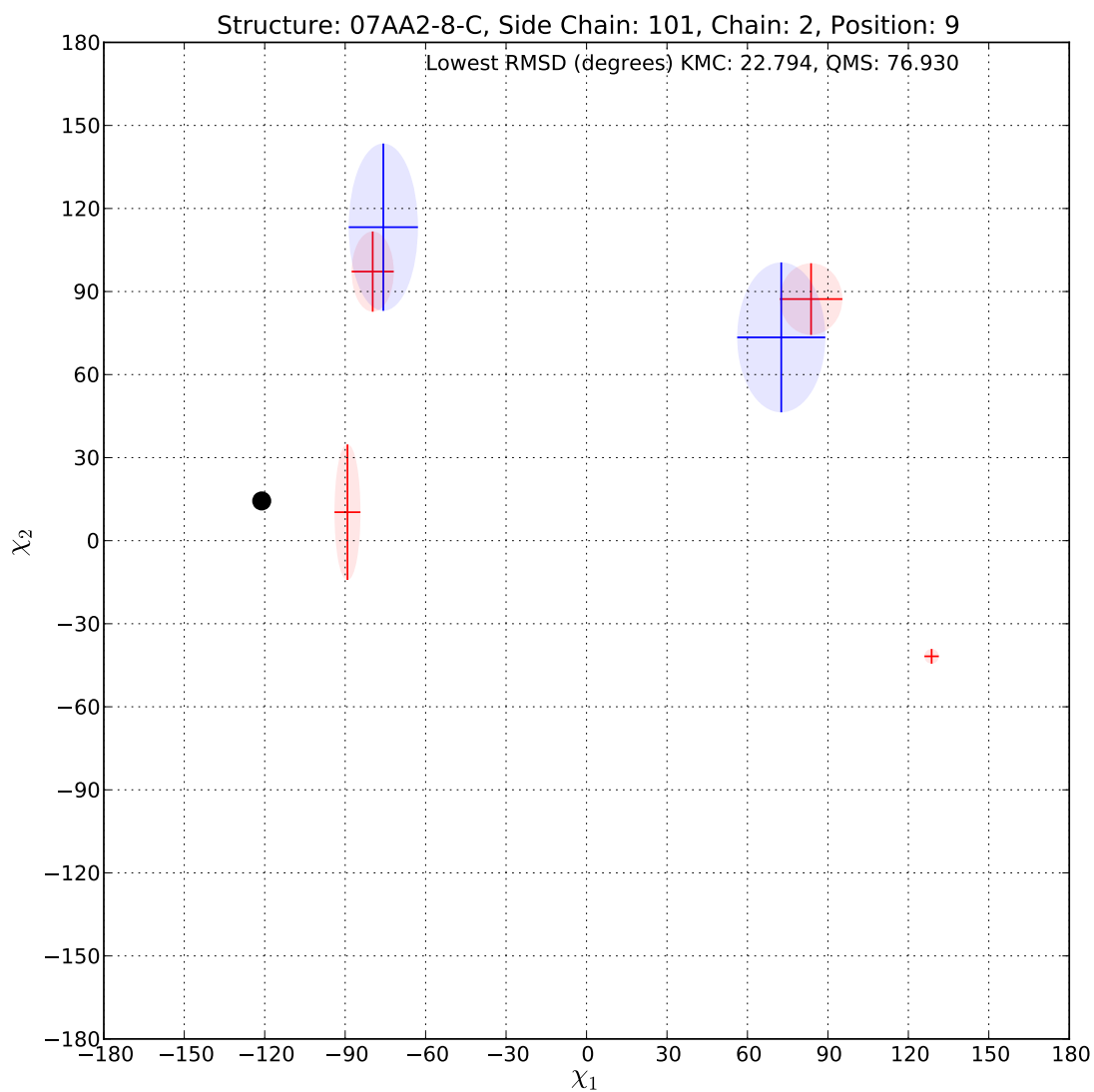


Figure S44: The rotamer library coverage plot for residue number 9 in chain 2 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

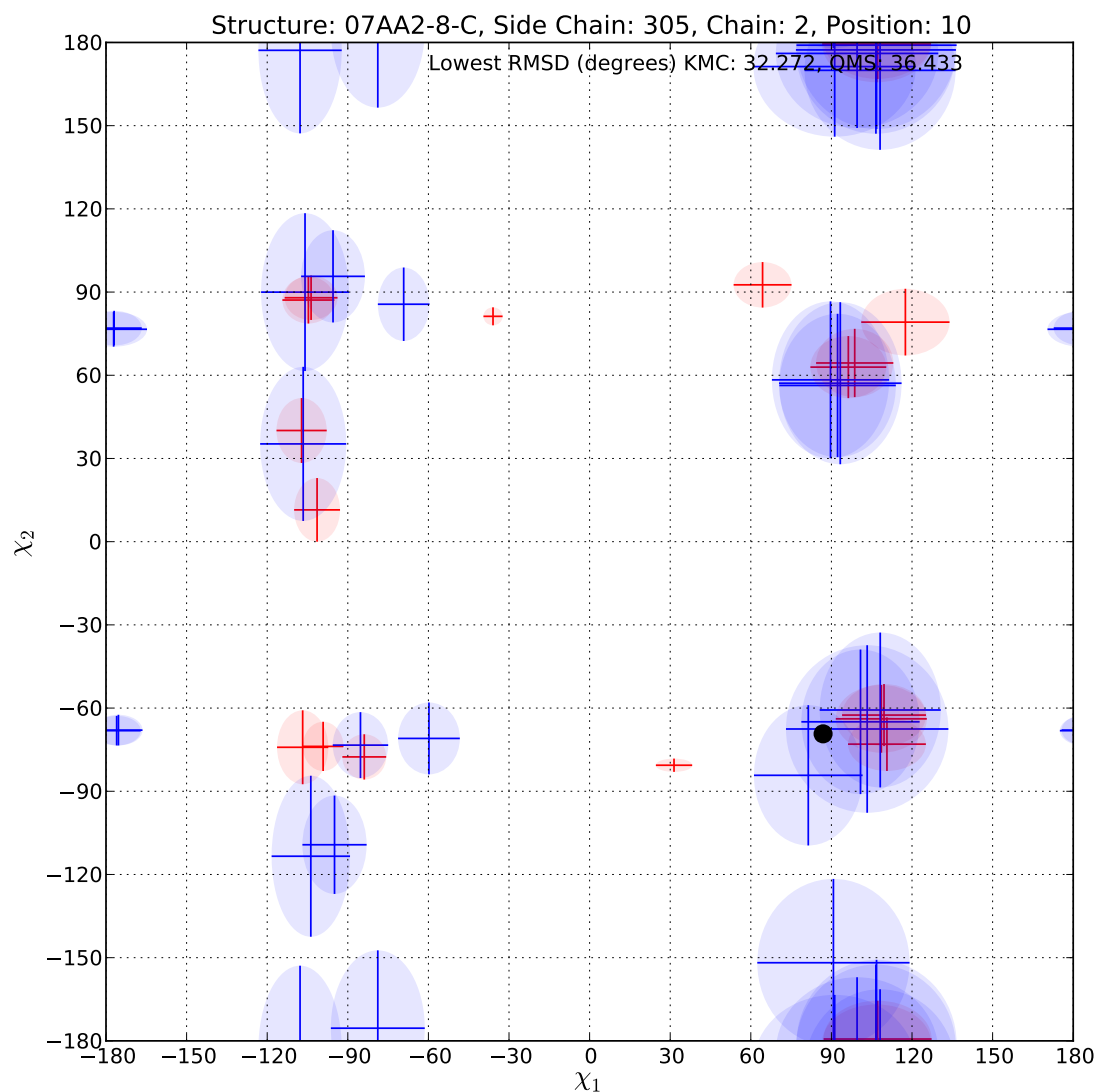


Figure S45: The rotamer library coverage plot for residue number 10 in chain 2 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

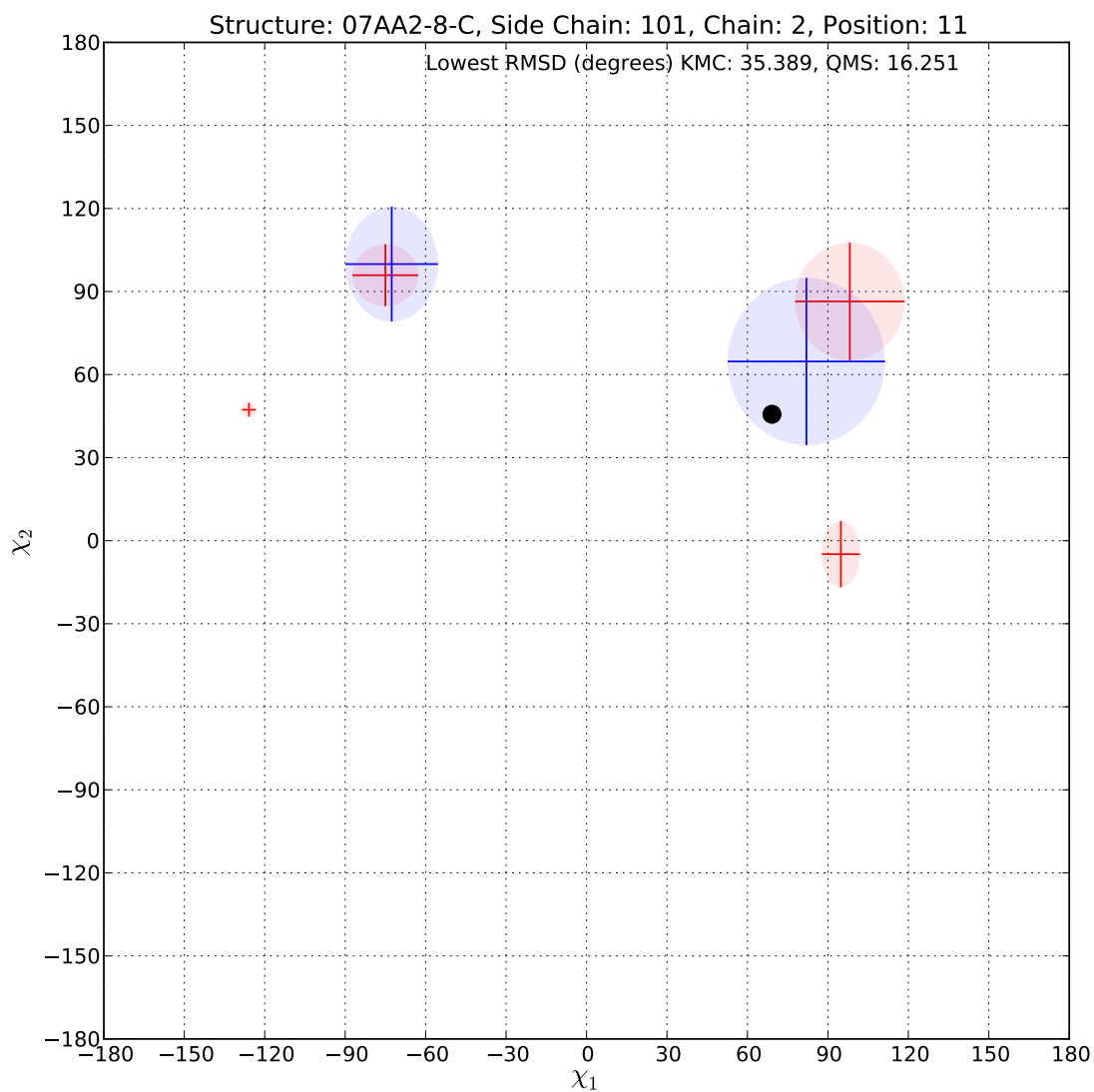


Figure S46: The rotamer library coverage plot for residue number 11 in chain 2 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

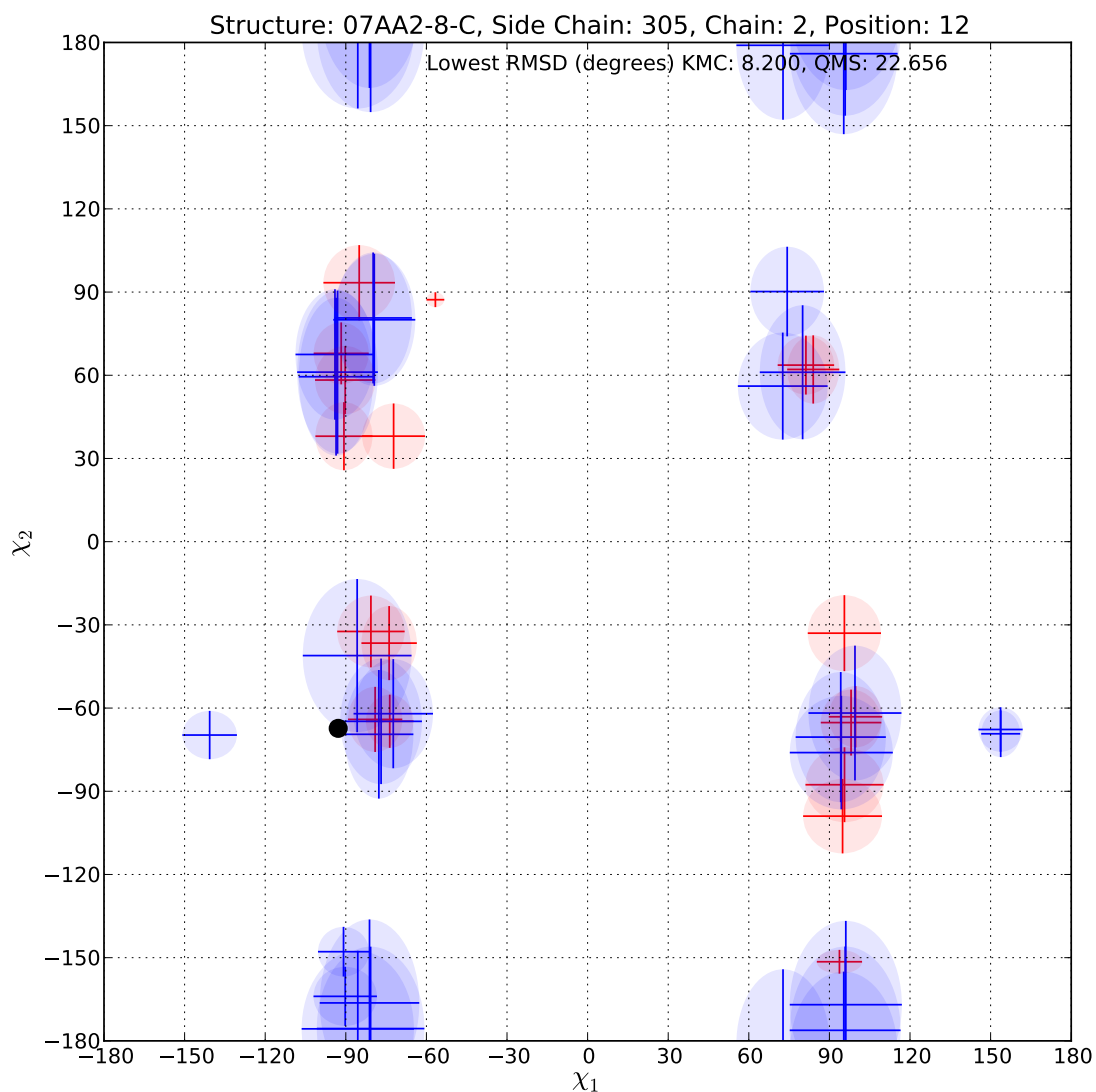


Figure S47: The rotamer library coverage plot for residue number 12 in chain 2 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

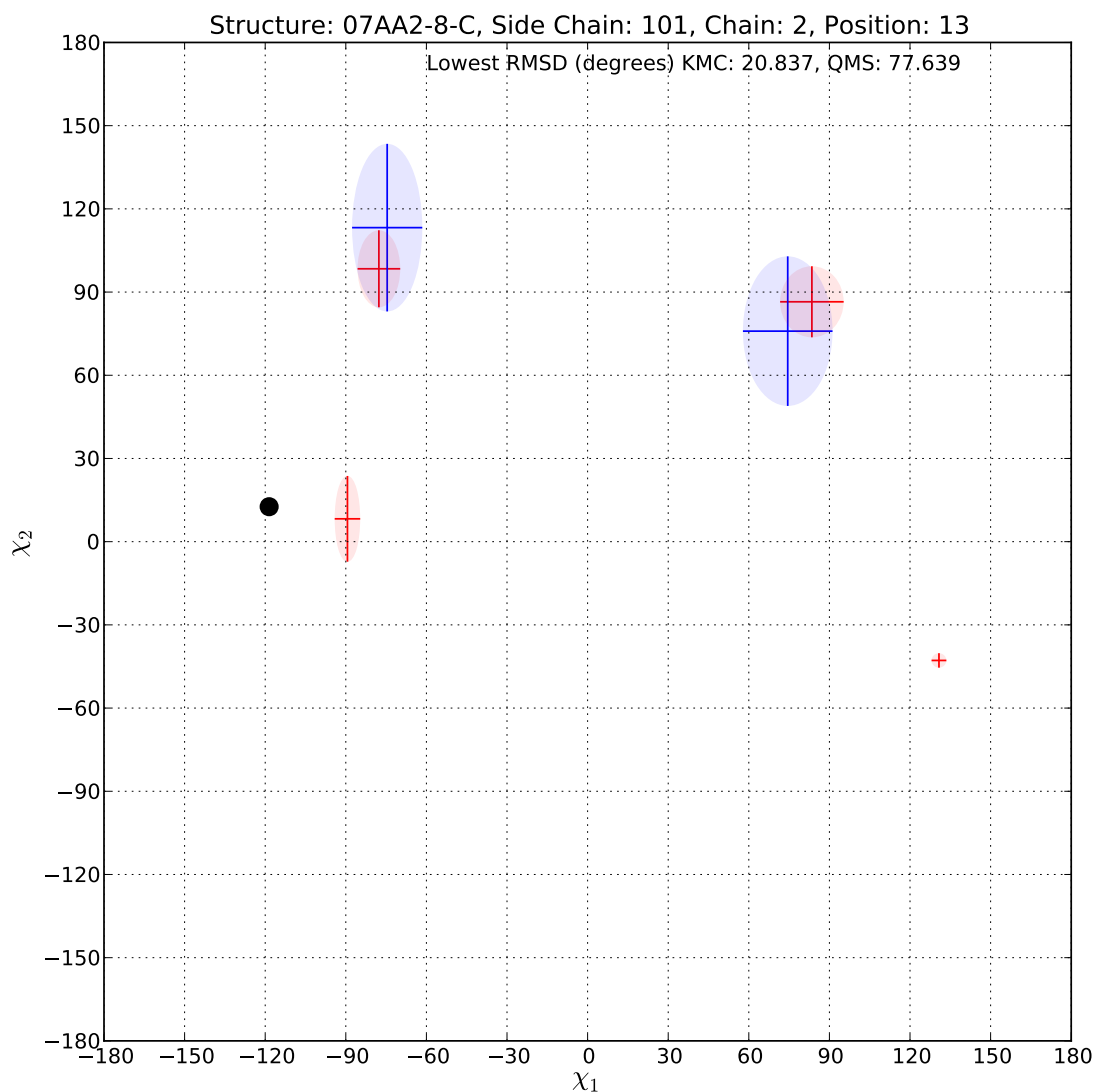


Figure S48: The rotamer library coverage plot for residue number 13 in chain 2 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

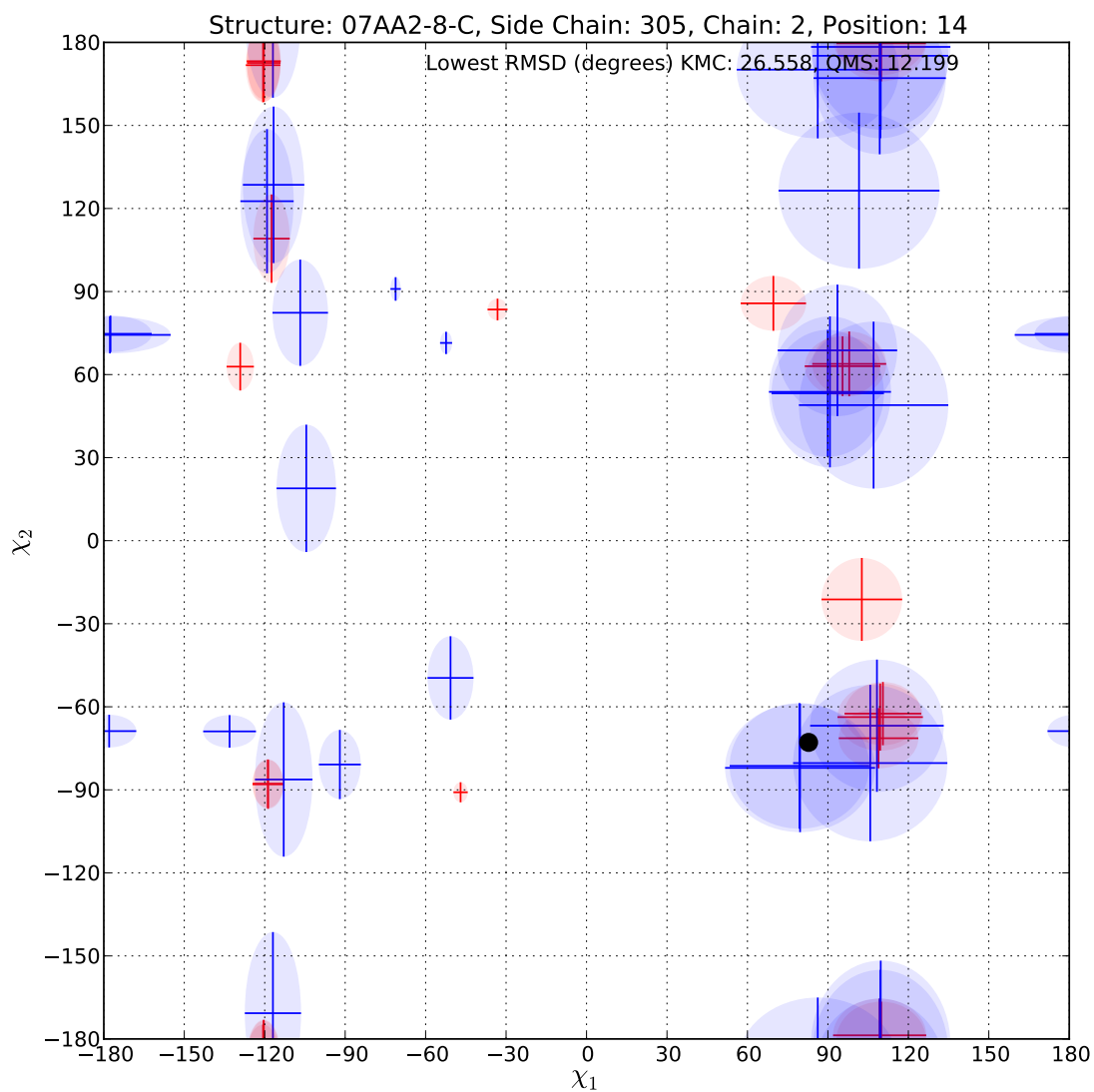


Figure S49: The rotamer library coverage plot for residue number 14 in chain 2 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

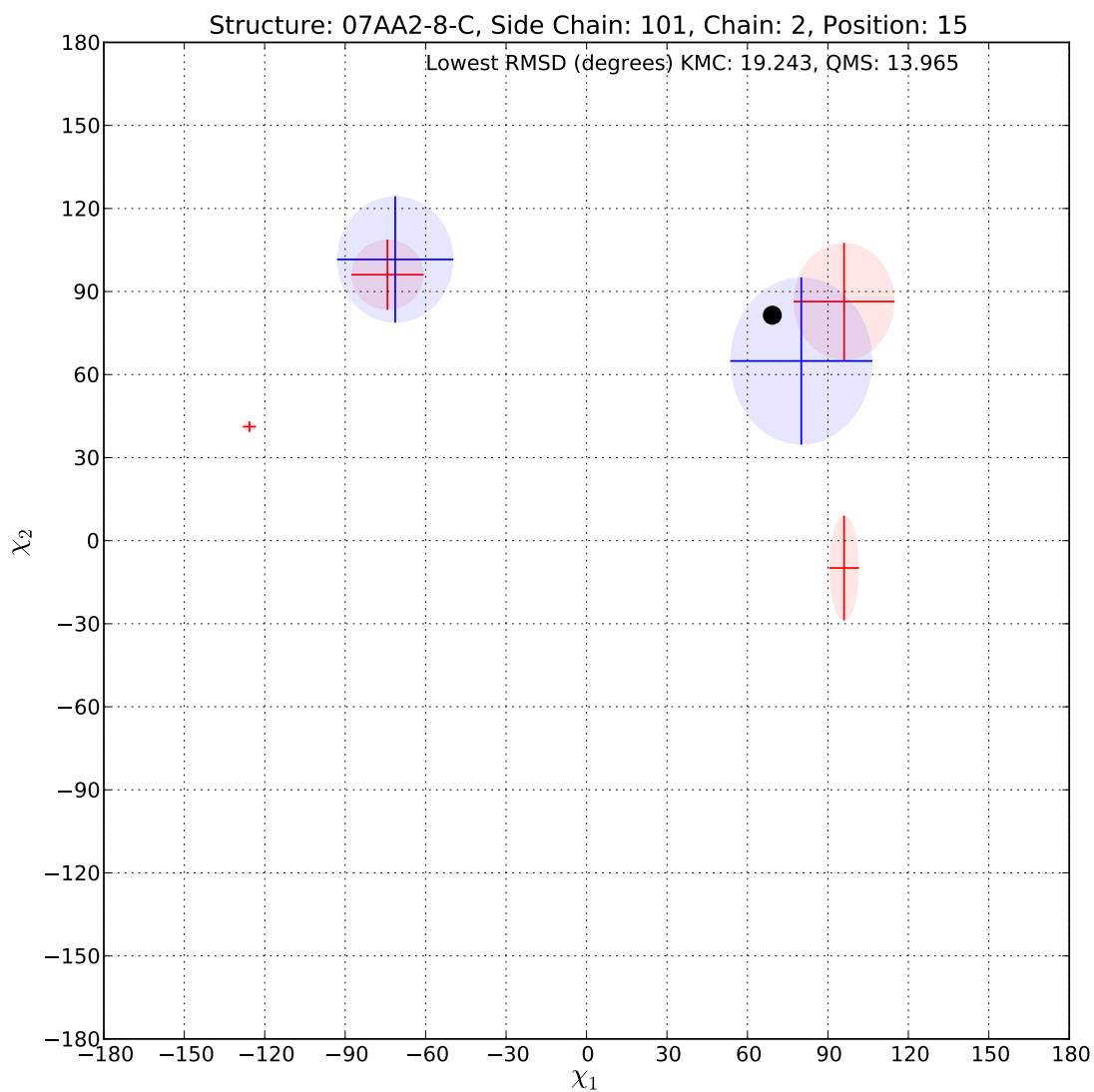


Figure S50: The rotamer library coverage plot for residue number 15 in chain 2 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

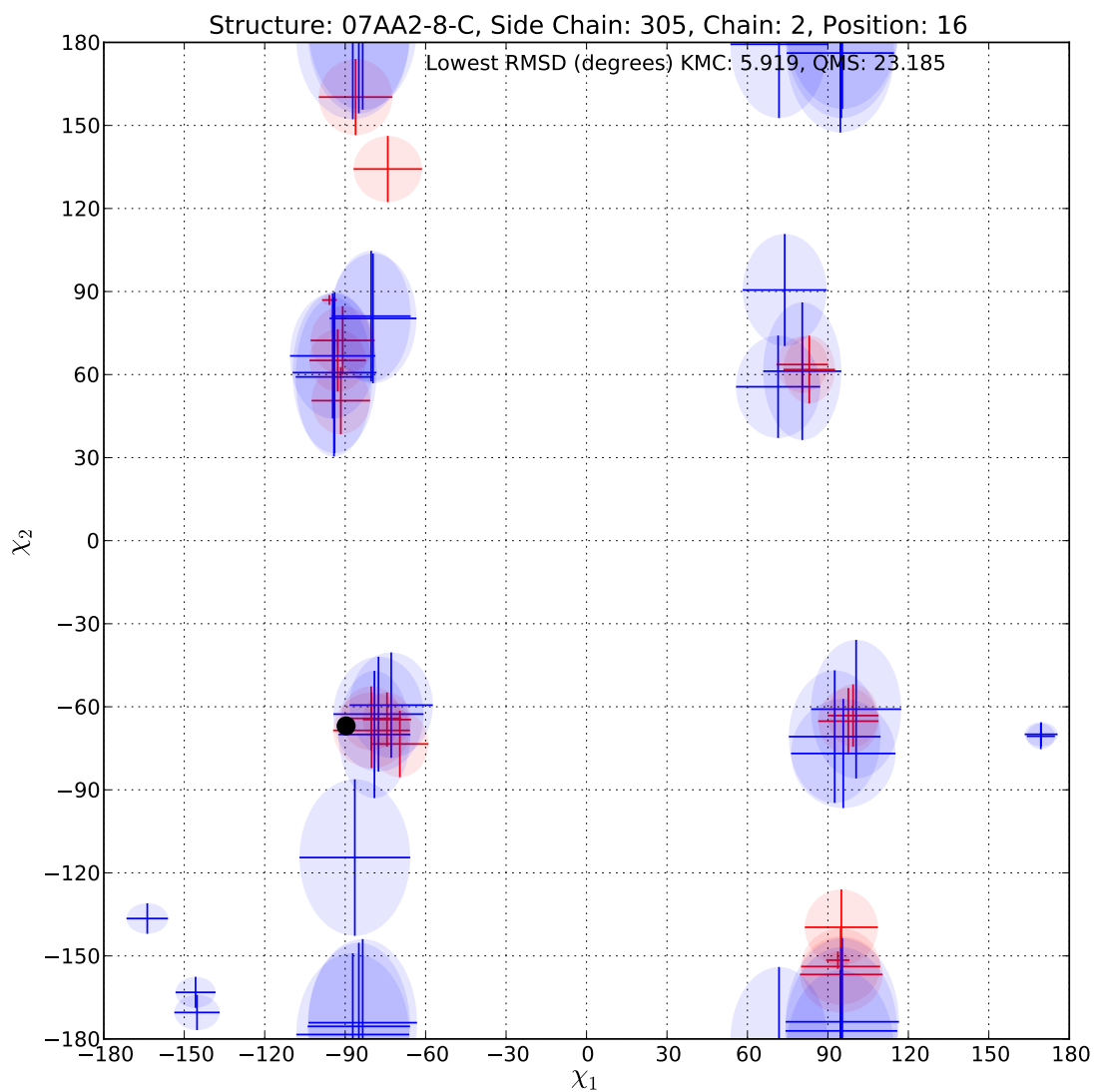


Figure S51: The rotamer library coverage plot for residue number 16 in chain 2 of peptoid databank structure 07AA2-8-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

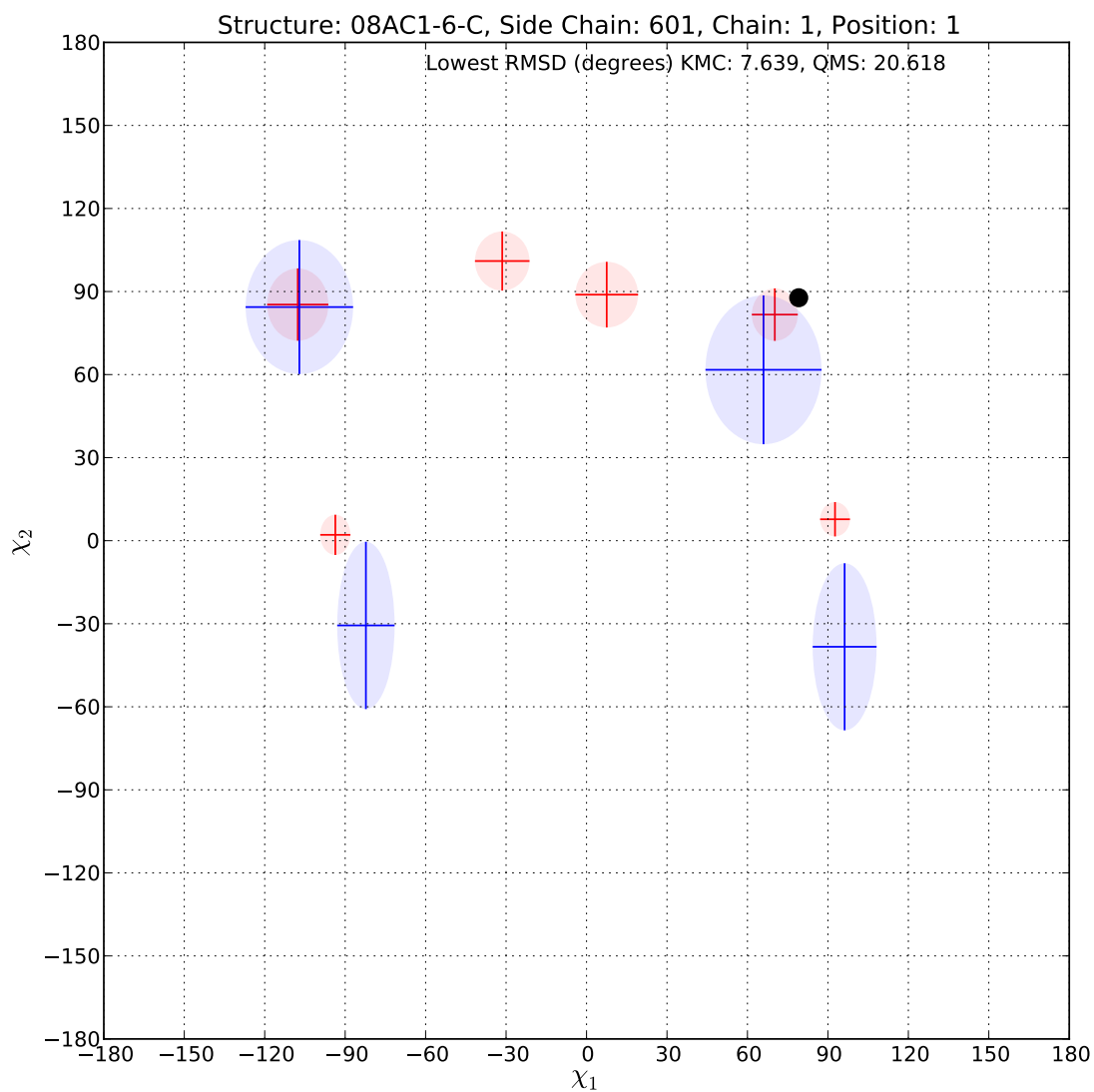


Figure S52: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 08AC1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

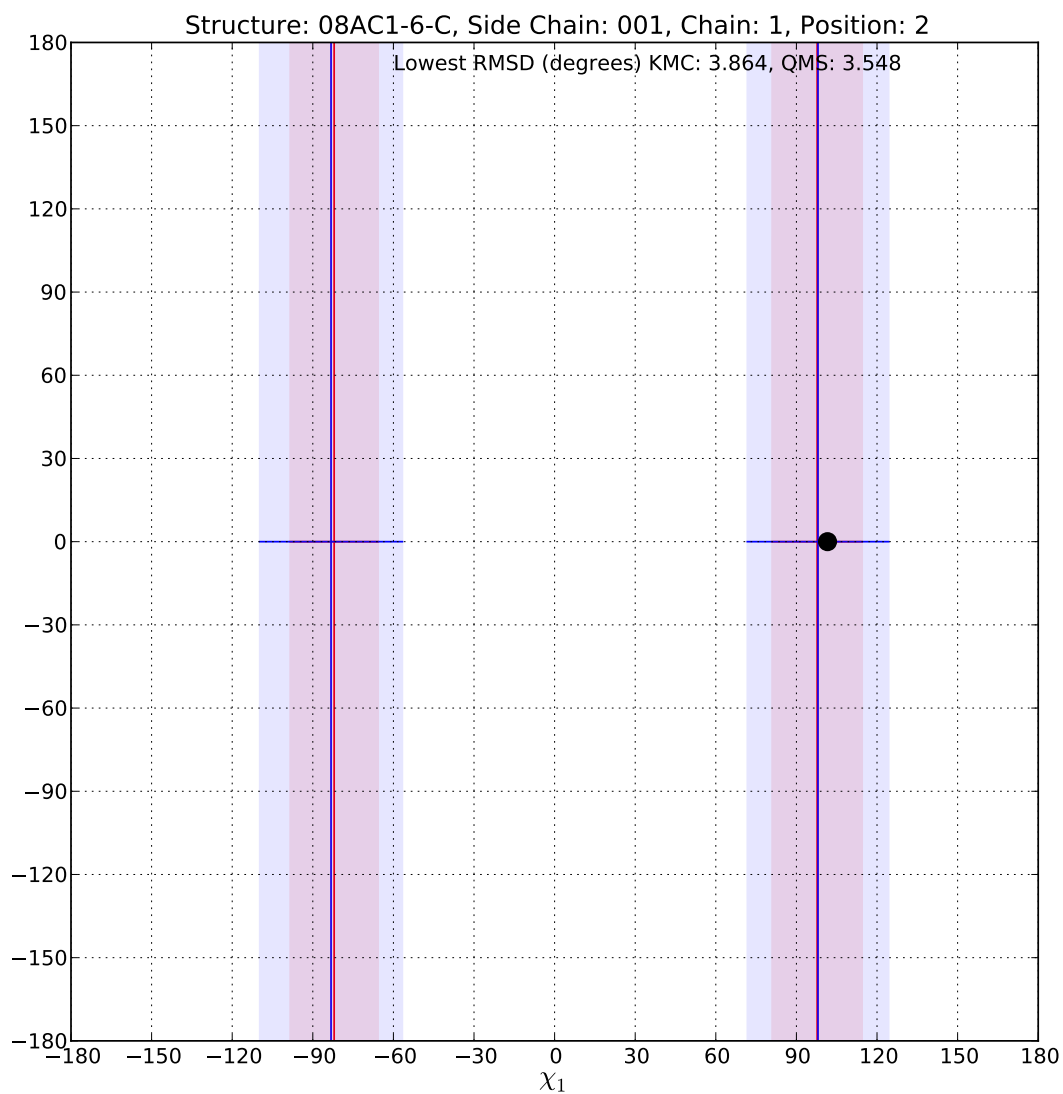


Figure S53: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 08AC1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

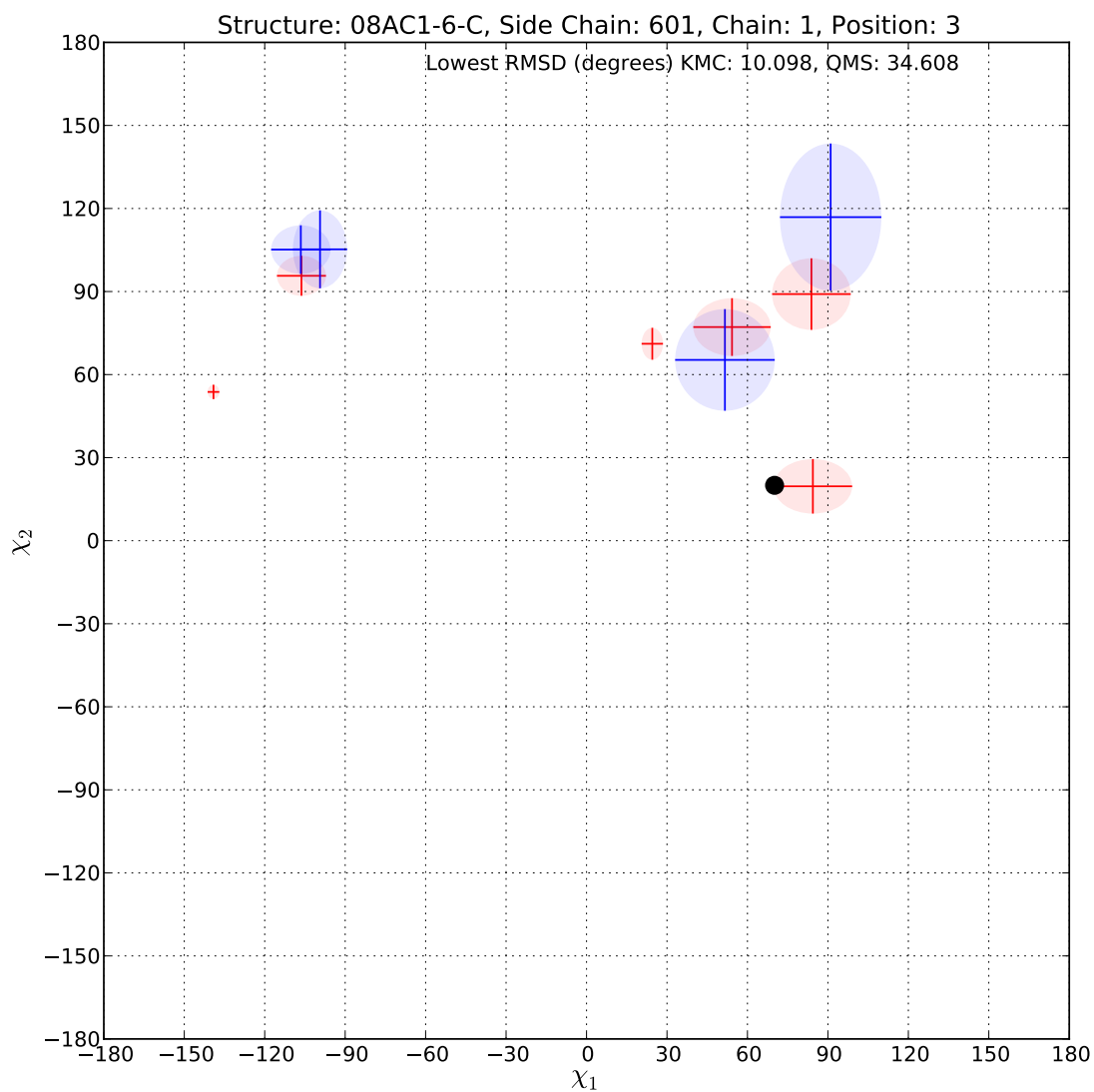


Figure S54: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 08AC1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

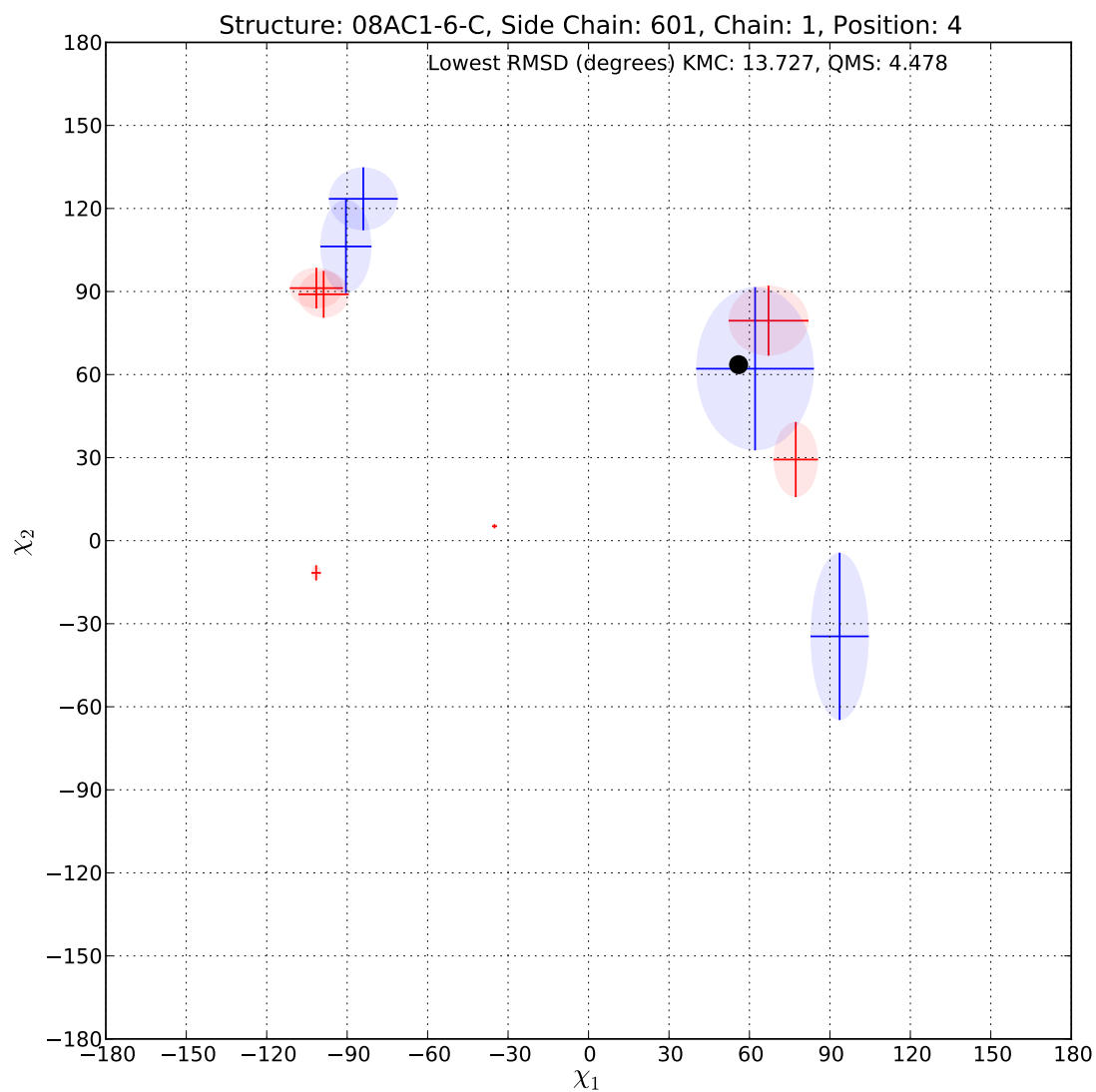


Figure S55: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 08AC1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

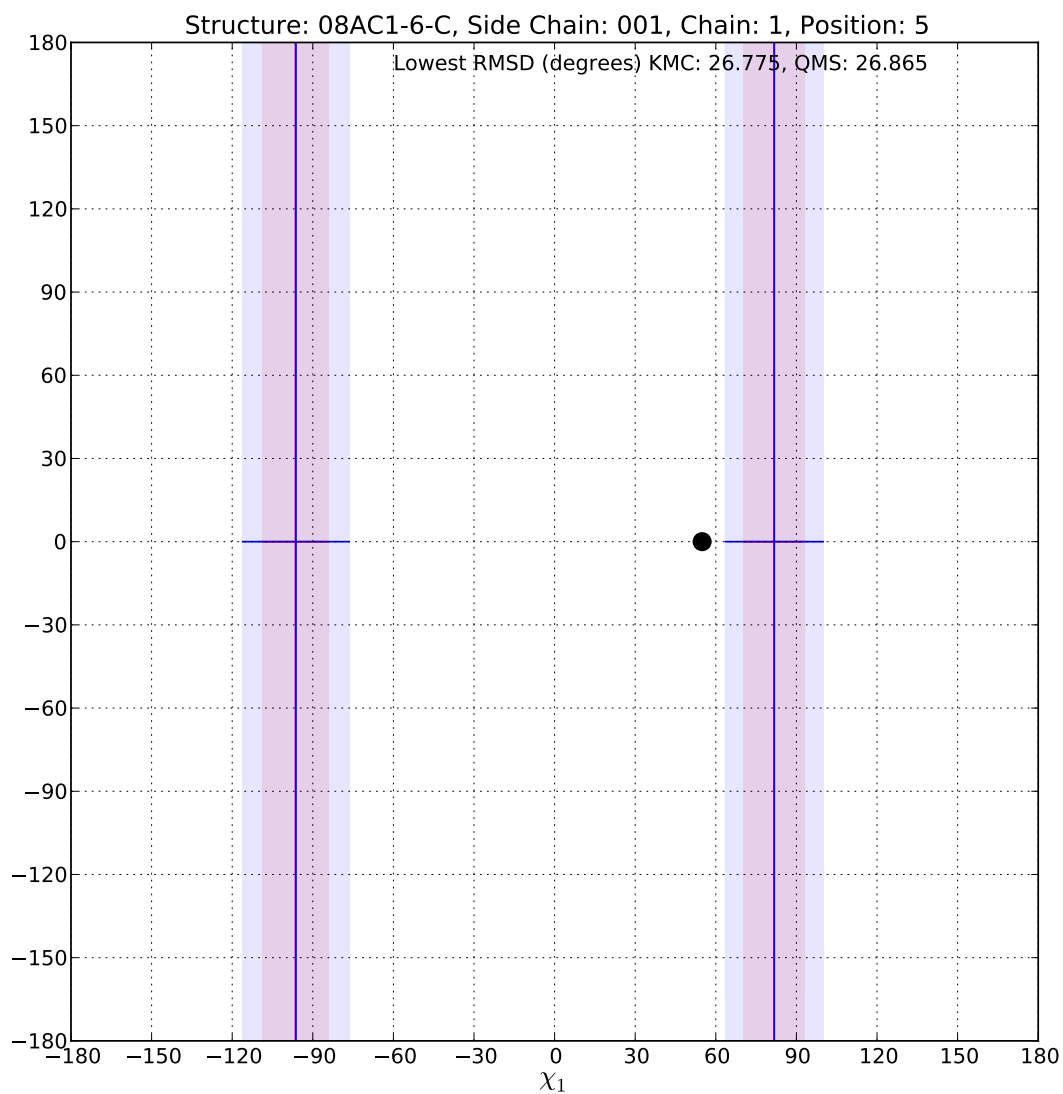


Figure S56: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 08AC1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

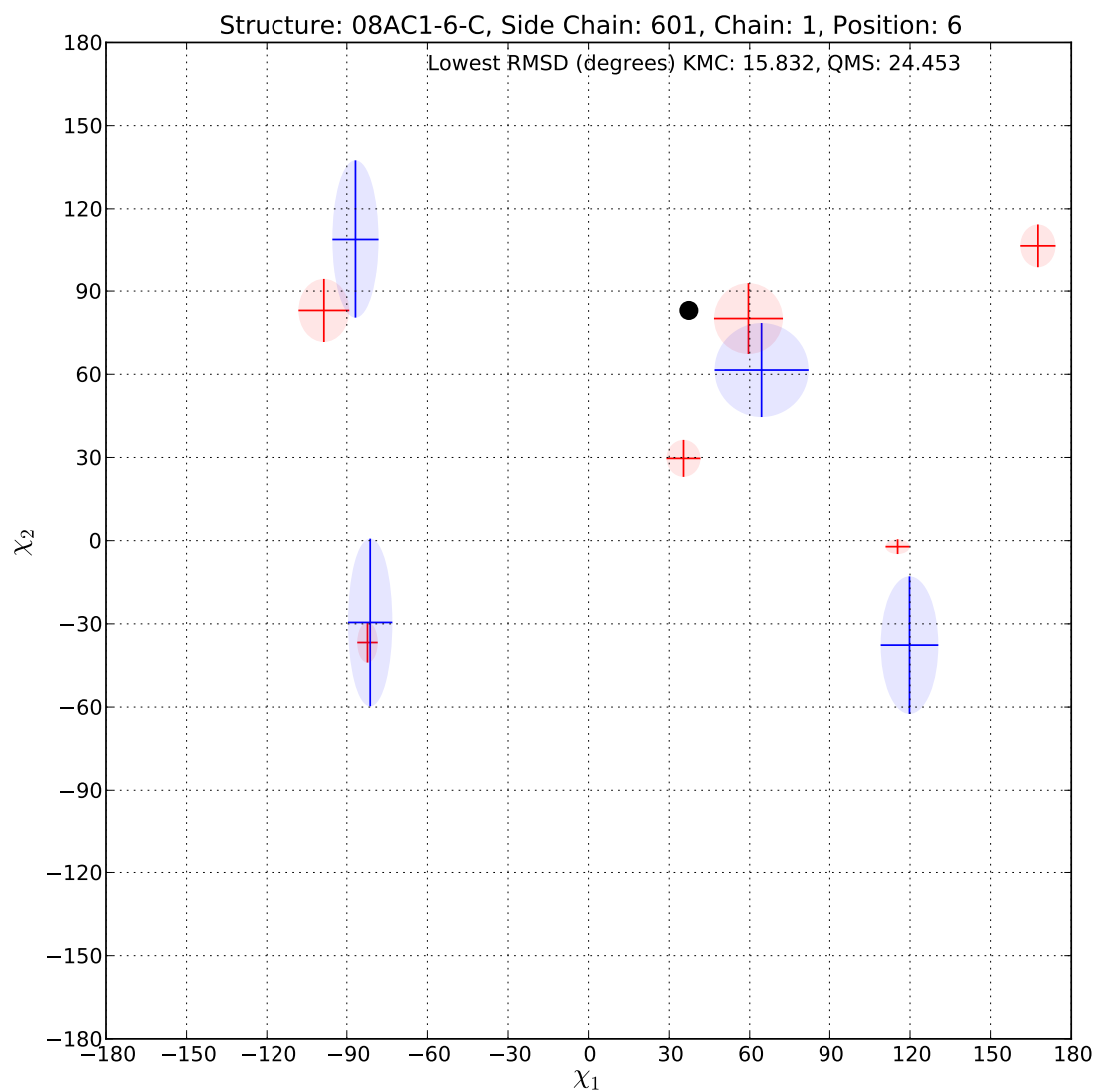


Figure S57: The rotamer library coverage plot for residue number 6 in chain 1 of peptoid databank structure 08AC1-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

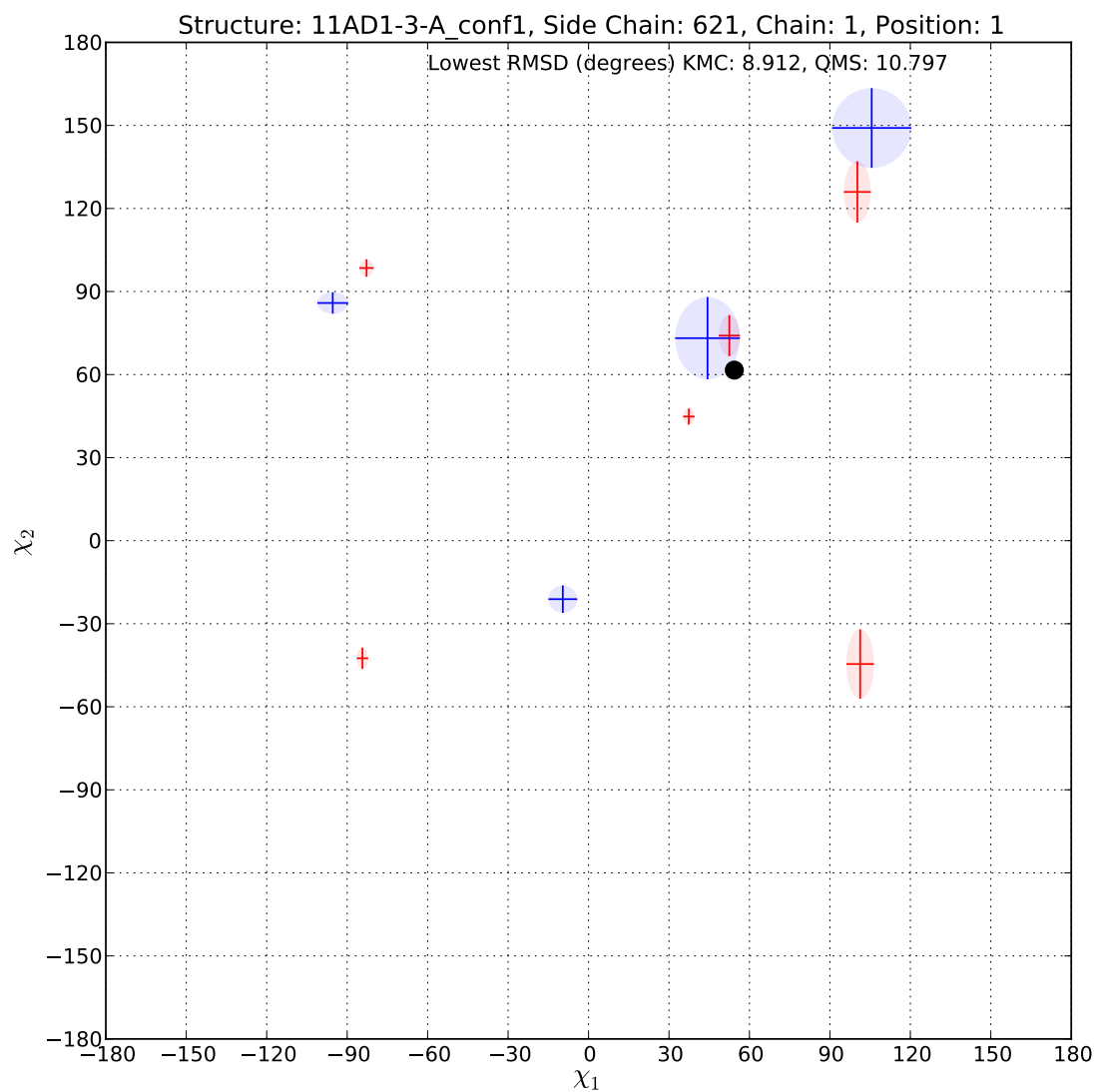


Figure S58: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 11AD1-3-A_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

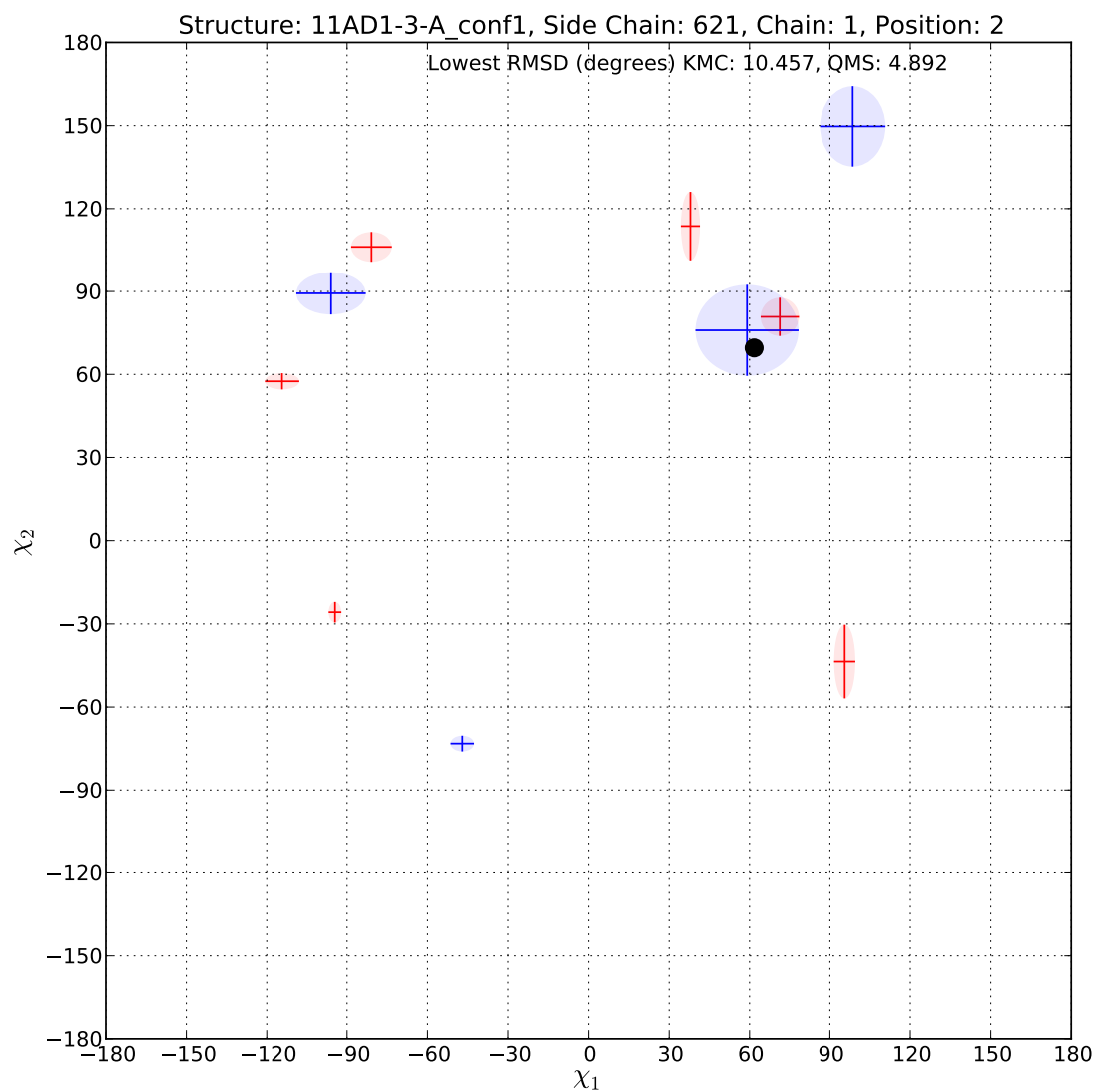


Figure S59: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 11AD1-3-A_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

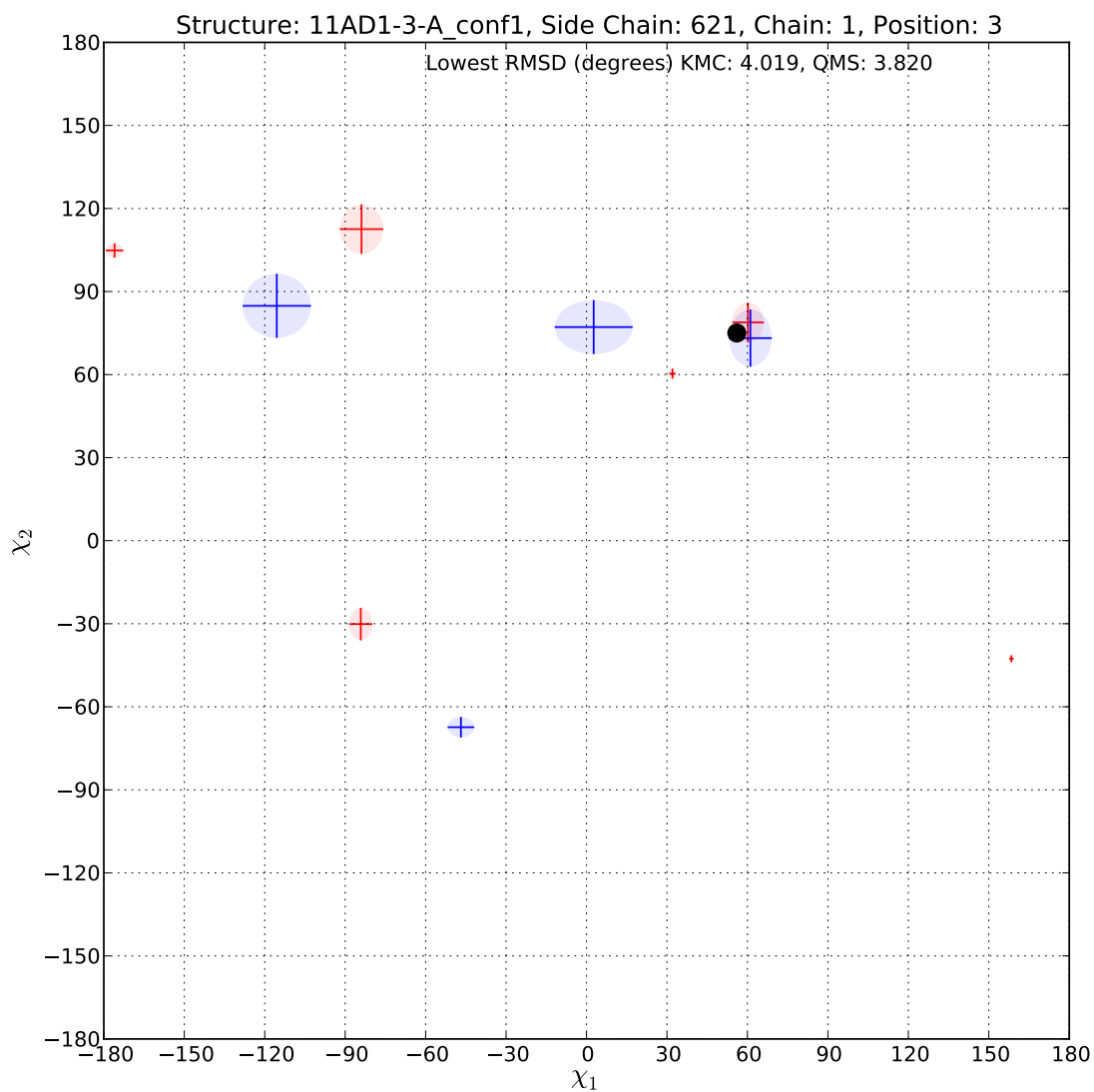


Figure S60: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 11AD1-3-A_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

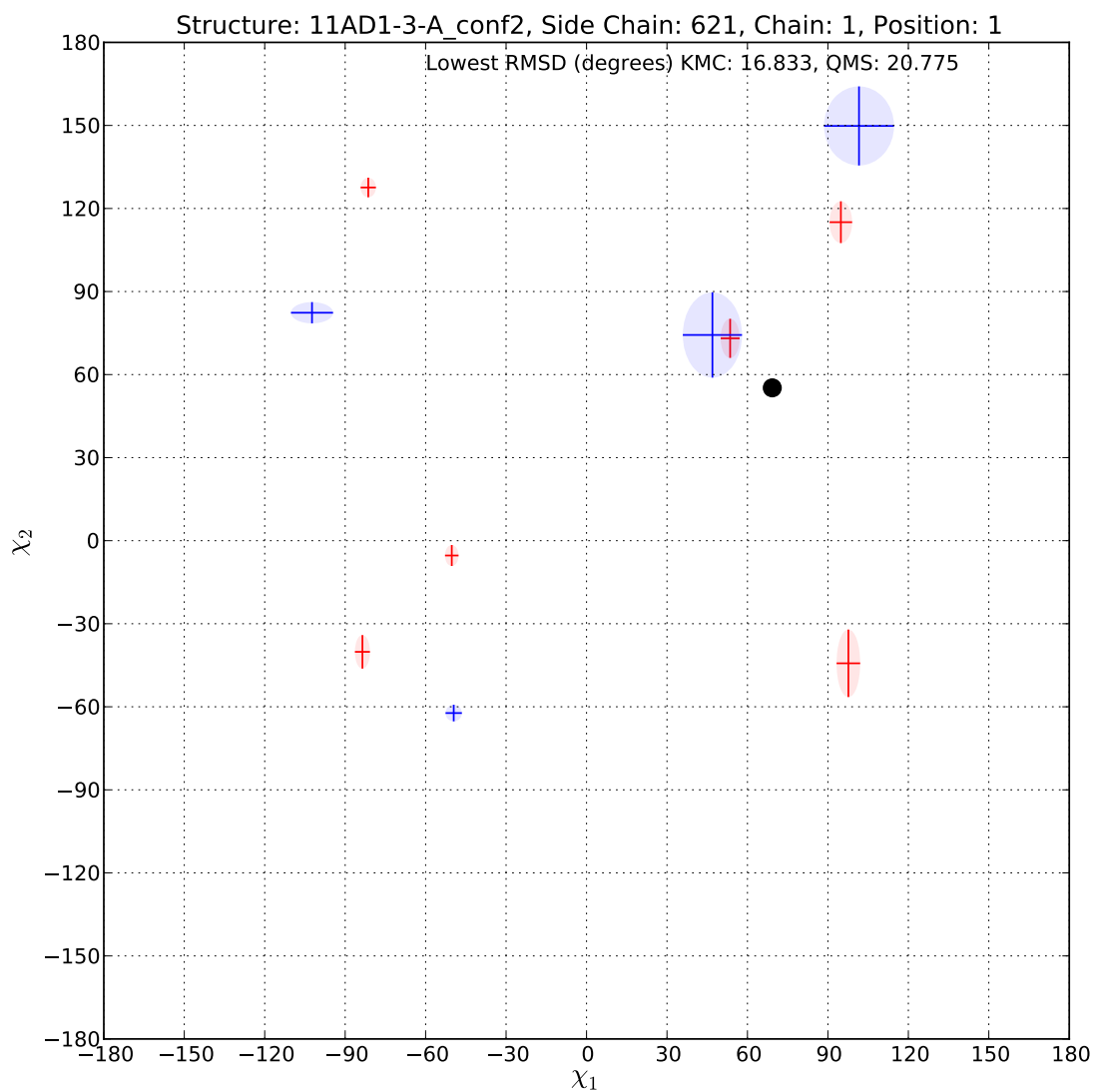


Figure S61: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 11AD1-3-A_conf2. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

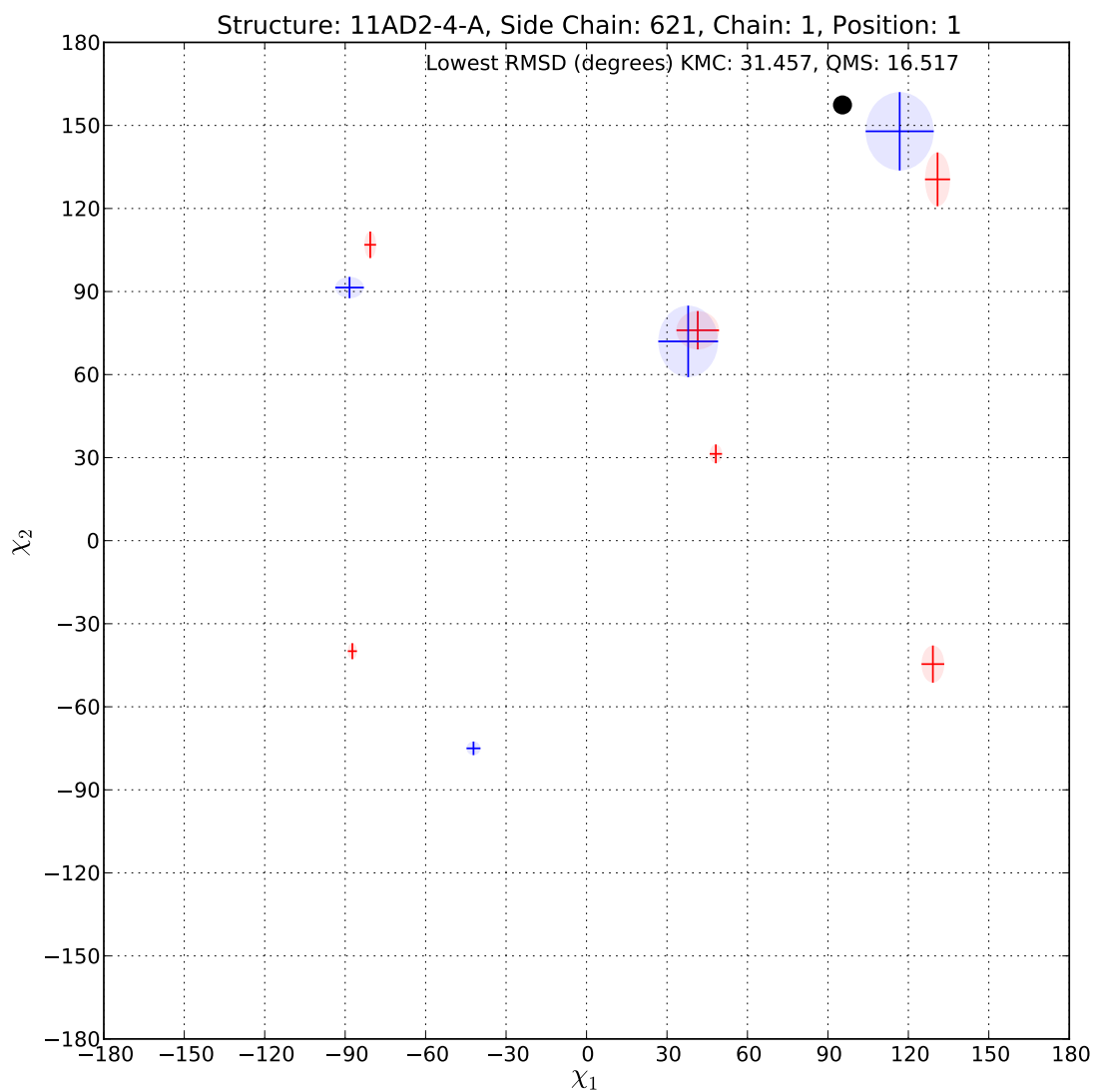


Figure S62: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 11AD2-4-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

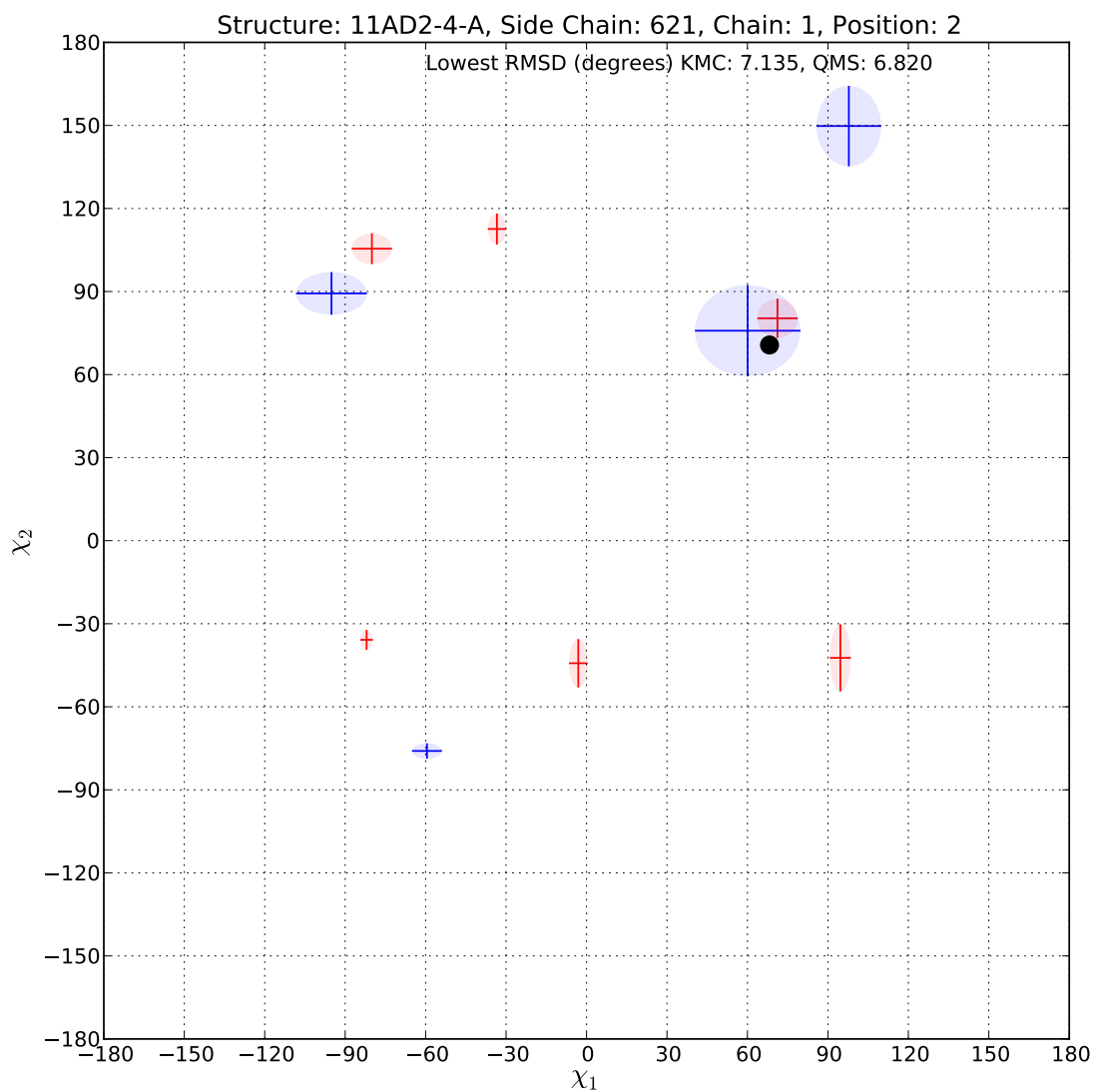


Figure S63: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 11AD2-4-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

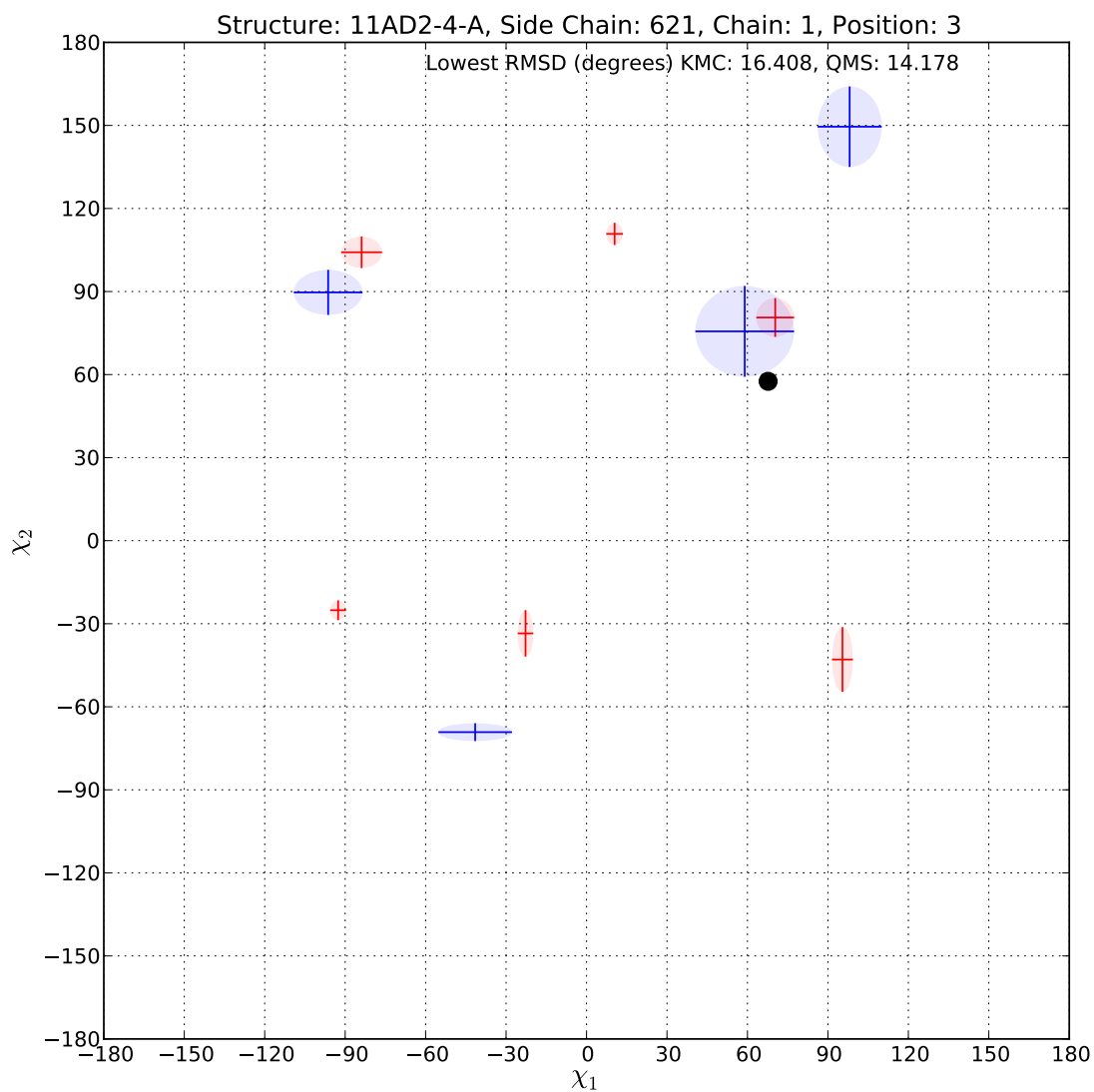


Figure S64: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 11AD2-4-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

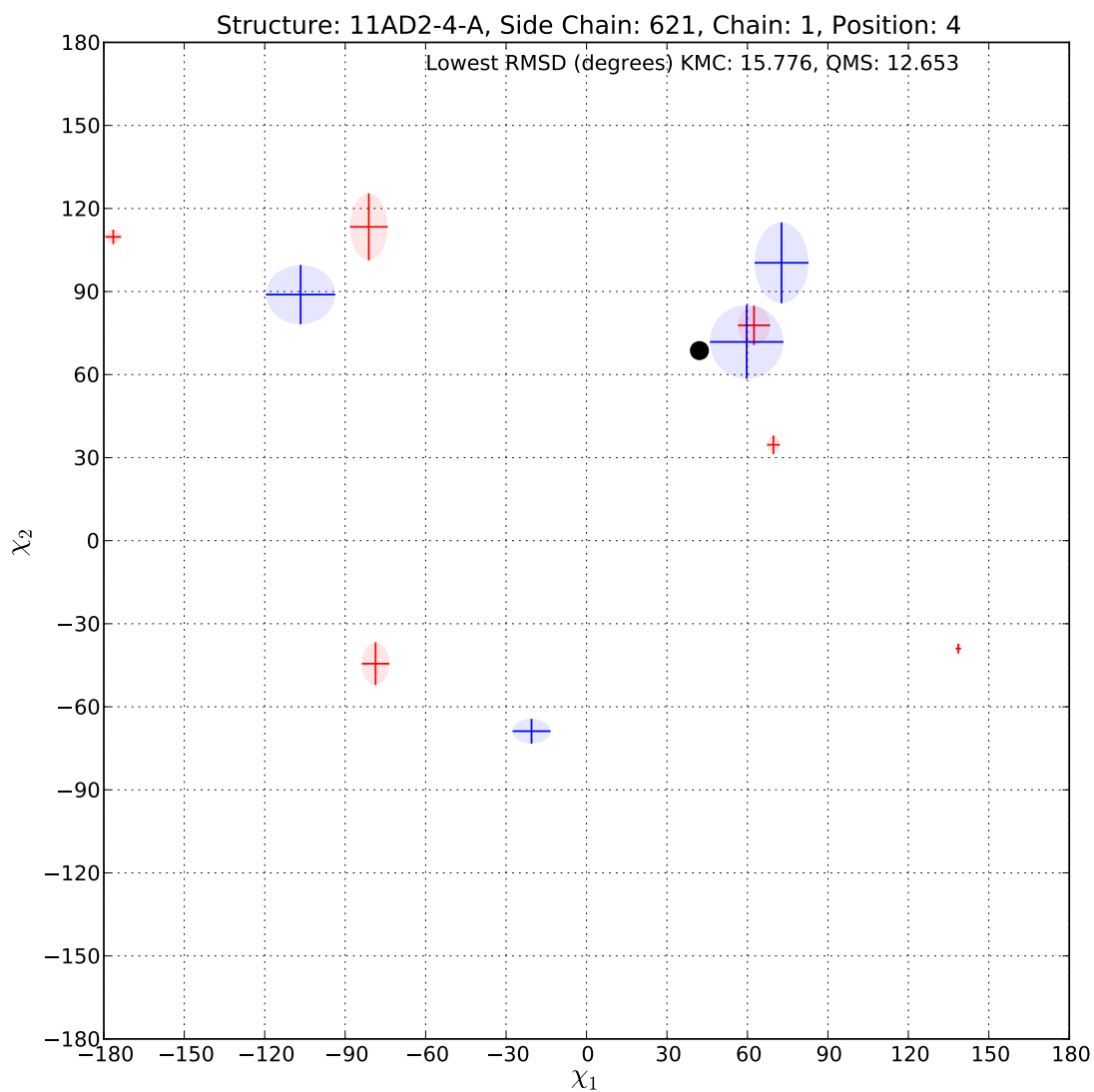
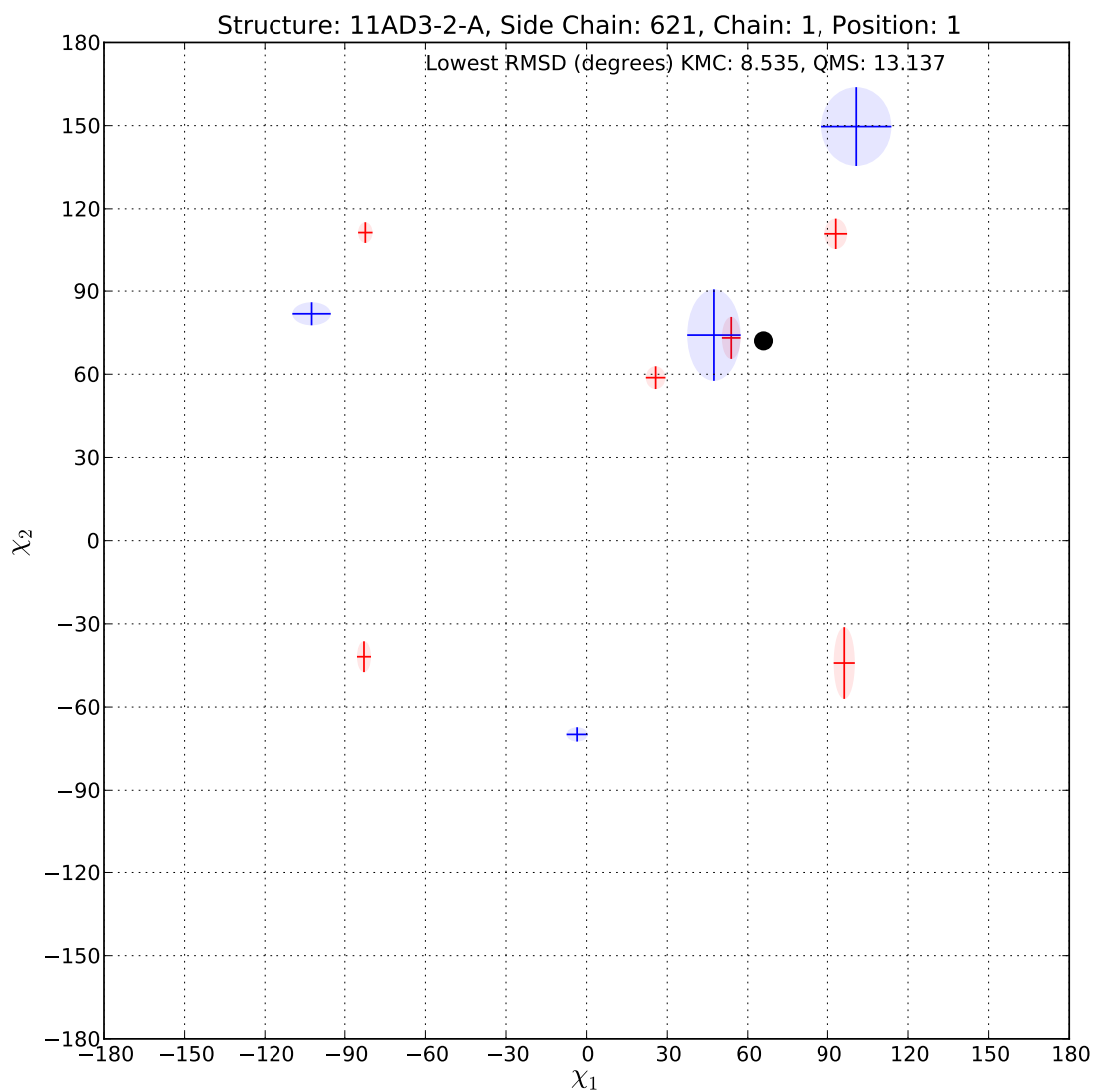


Figure S65: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 11AD2-4-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.



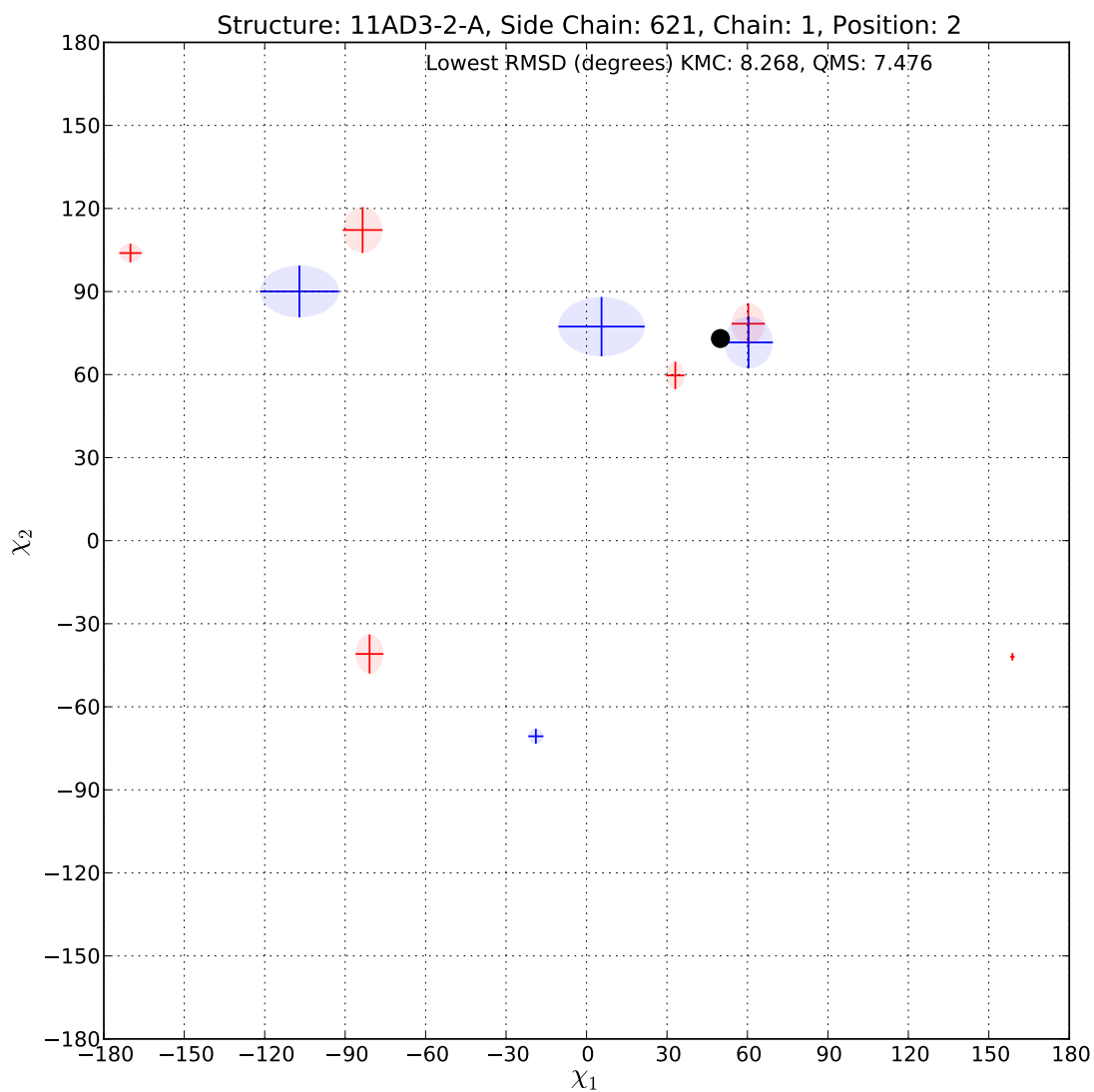


Figure S67: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 11AD3-2-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

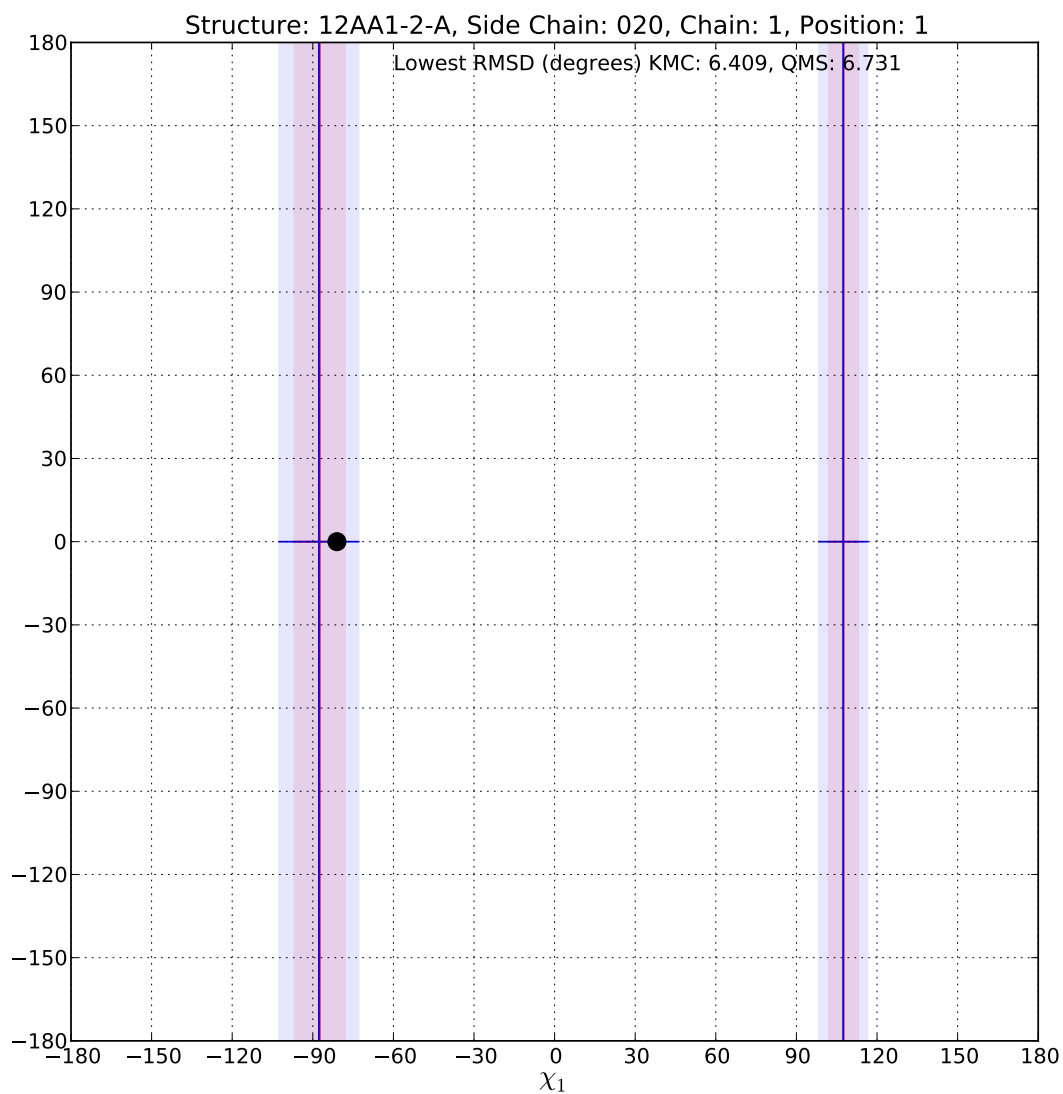


Figure S68: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 12AA1-2-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

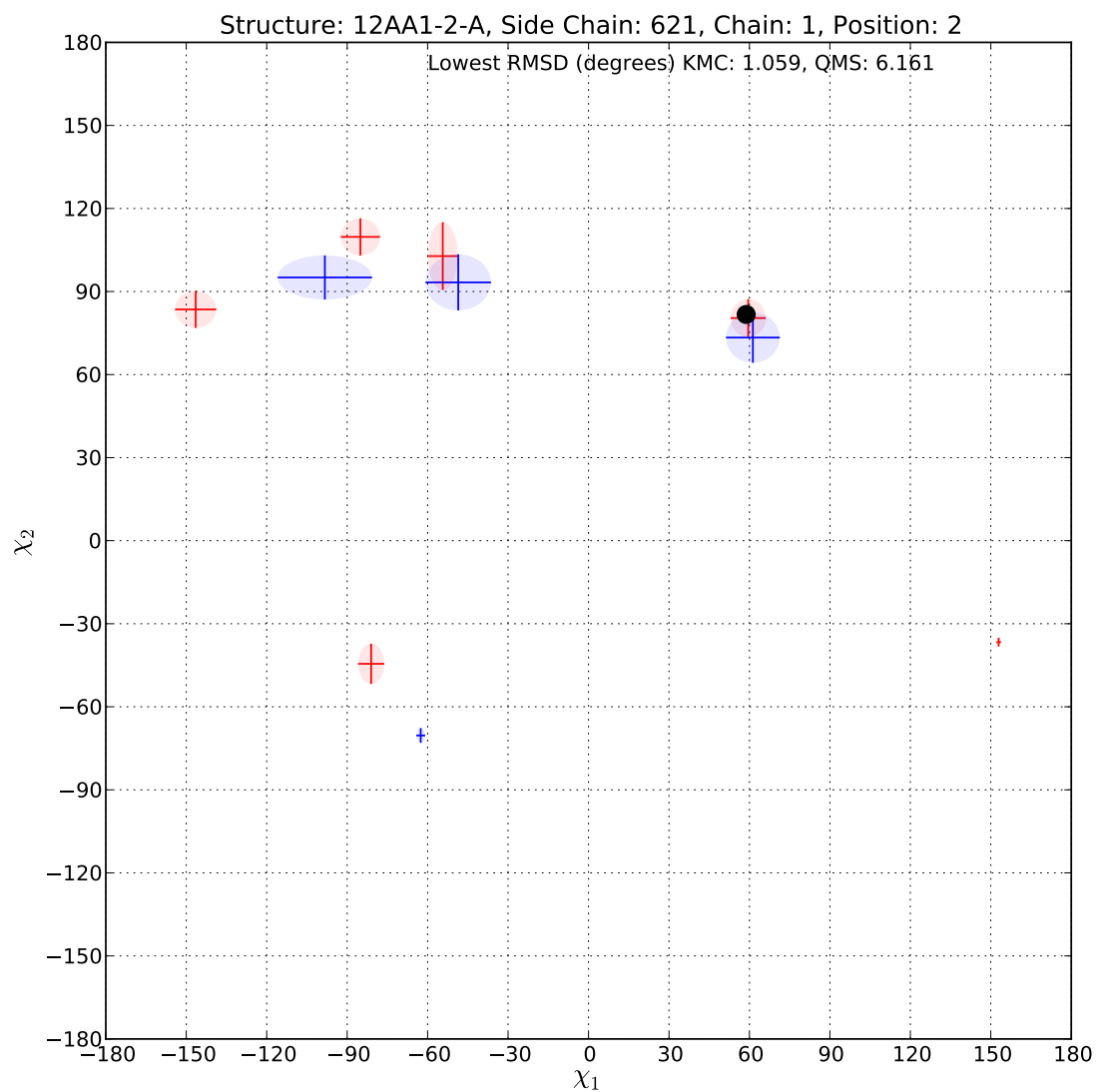


Figure S69: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 12AA1-2-A. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

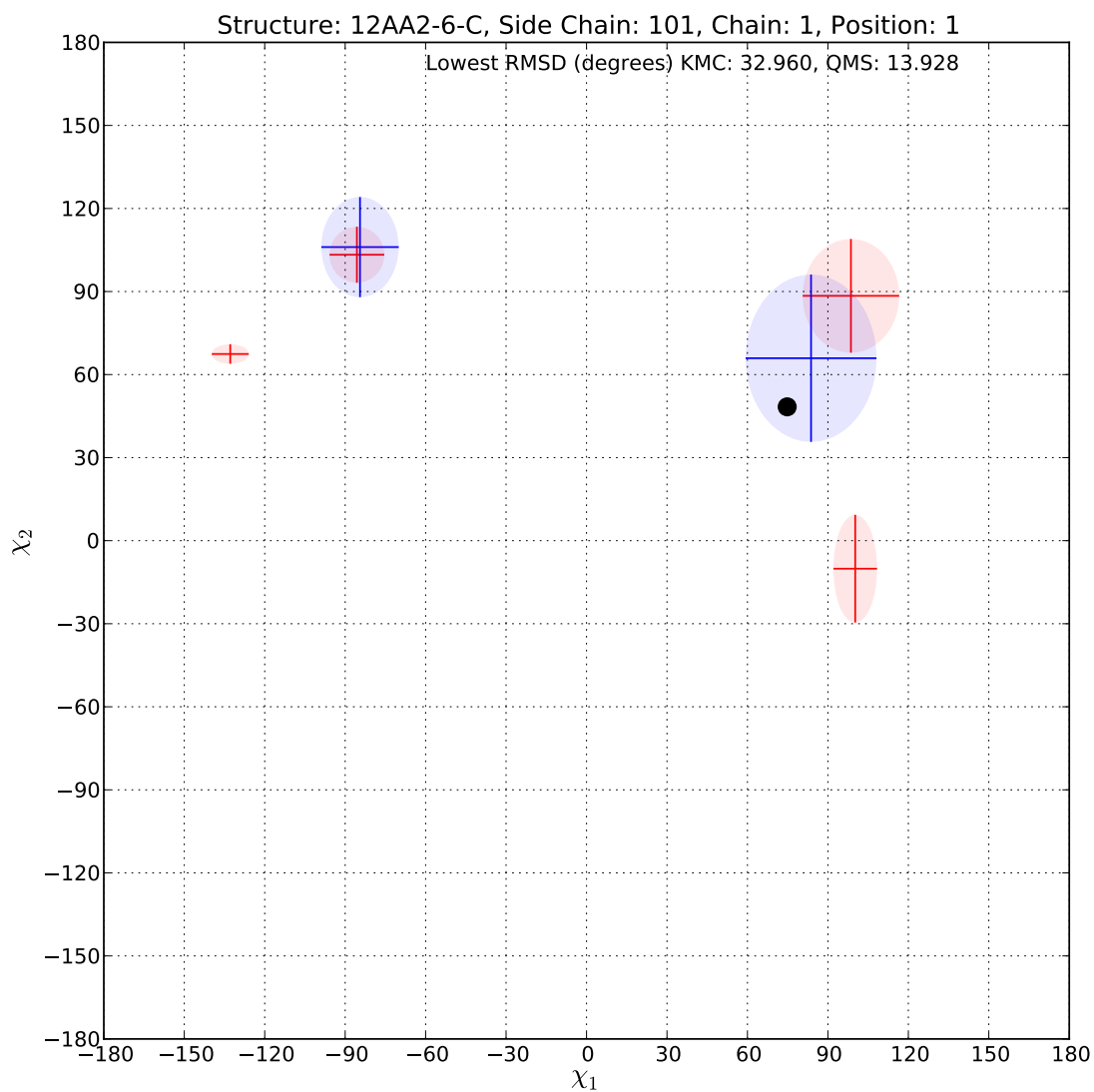


Figure S70: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 12AA2-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

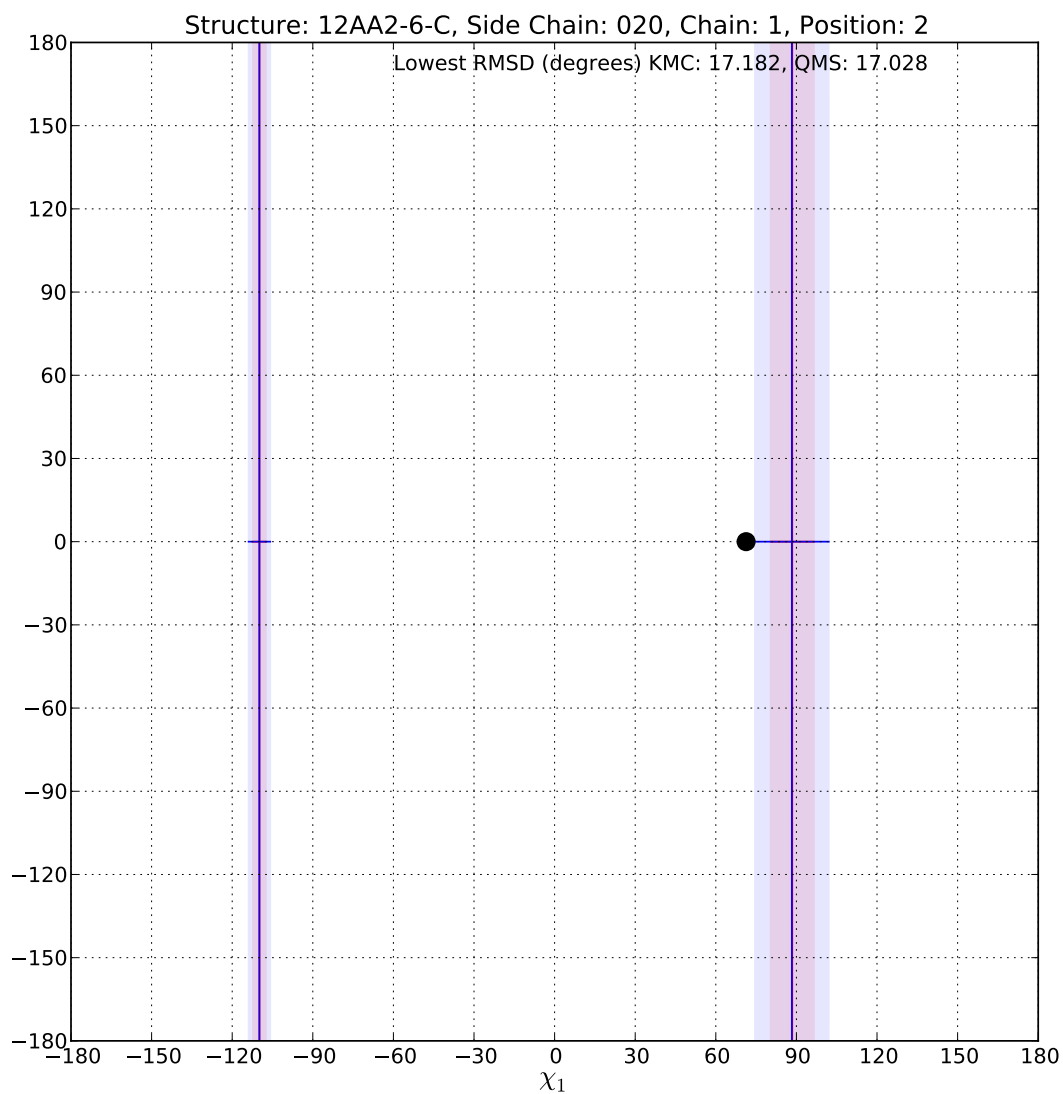


Figure S71: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 12AA2-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

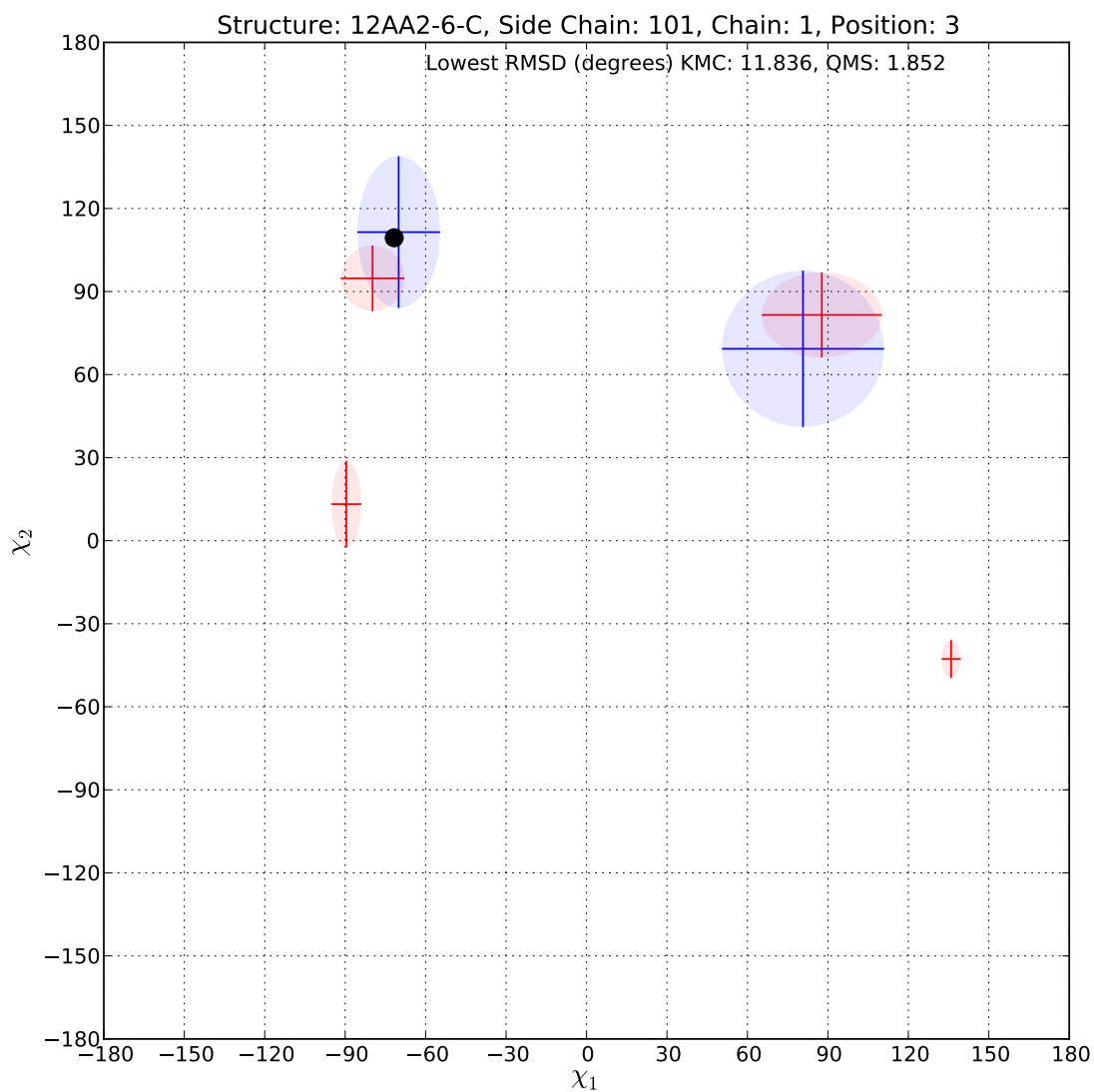


Figure S72: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 12AA2-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

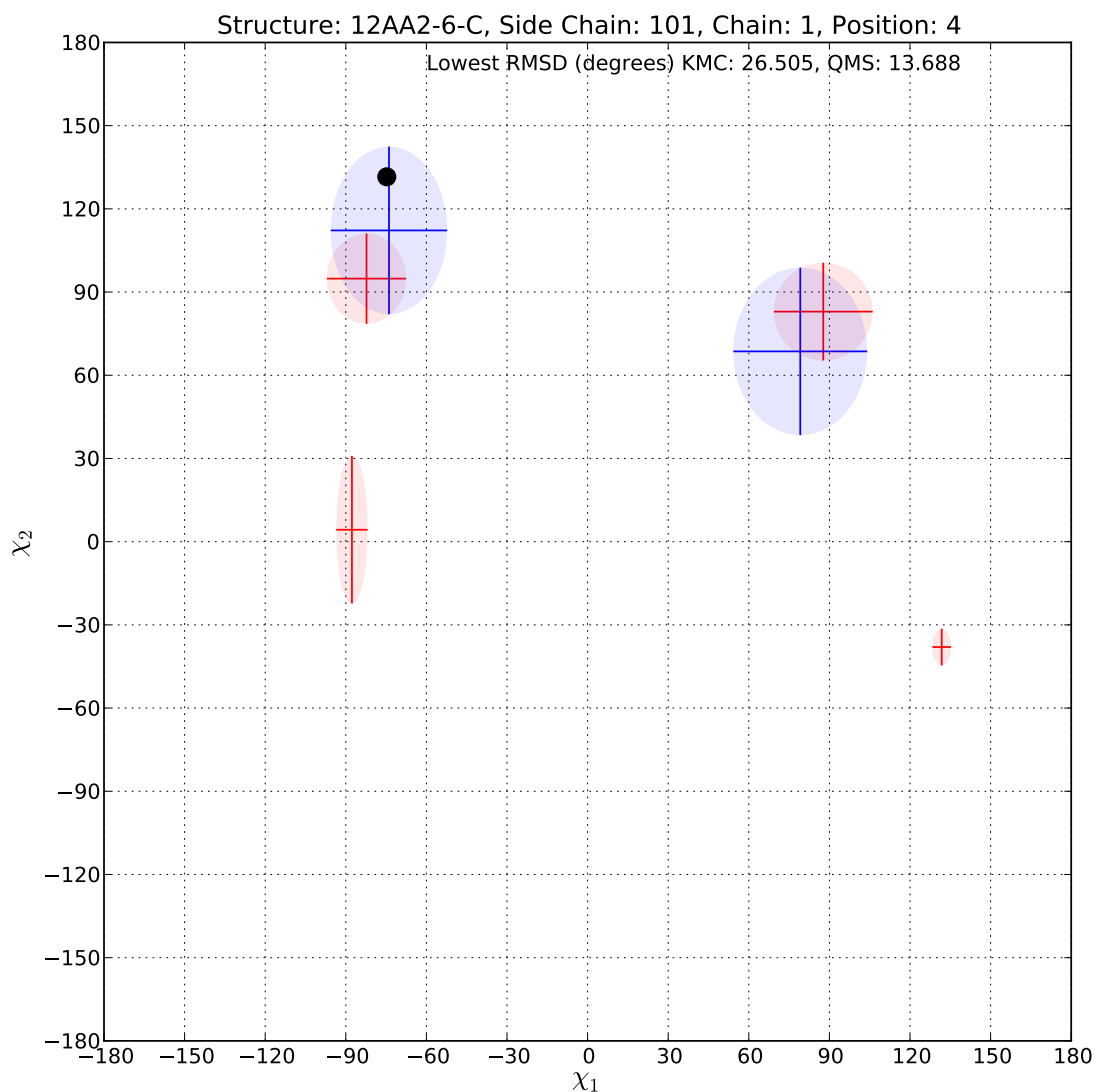


Figure S73: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 12AA2-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

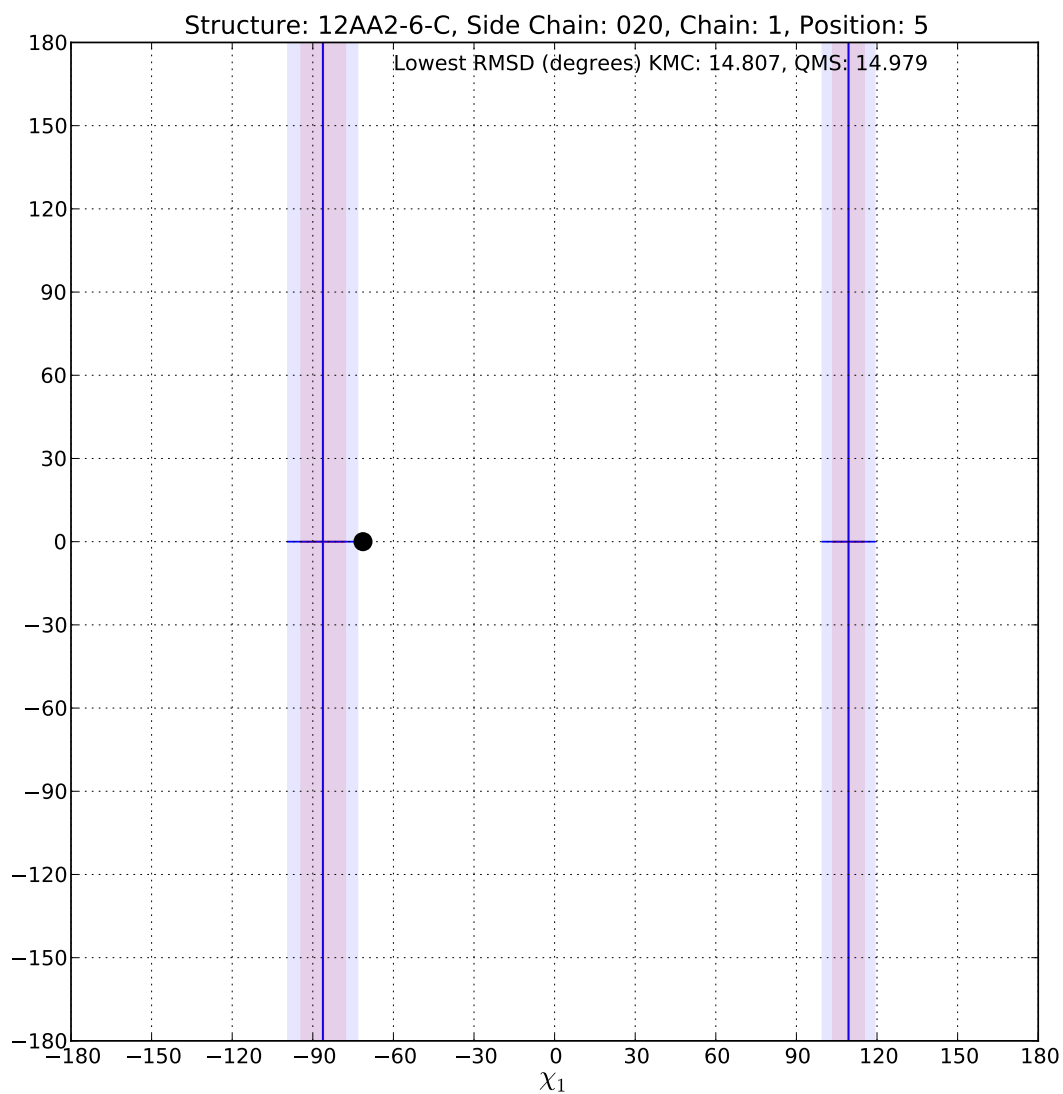


Figure S74: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 12AA2-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

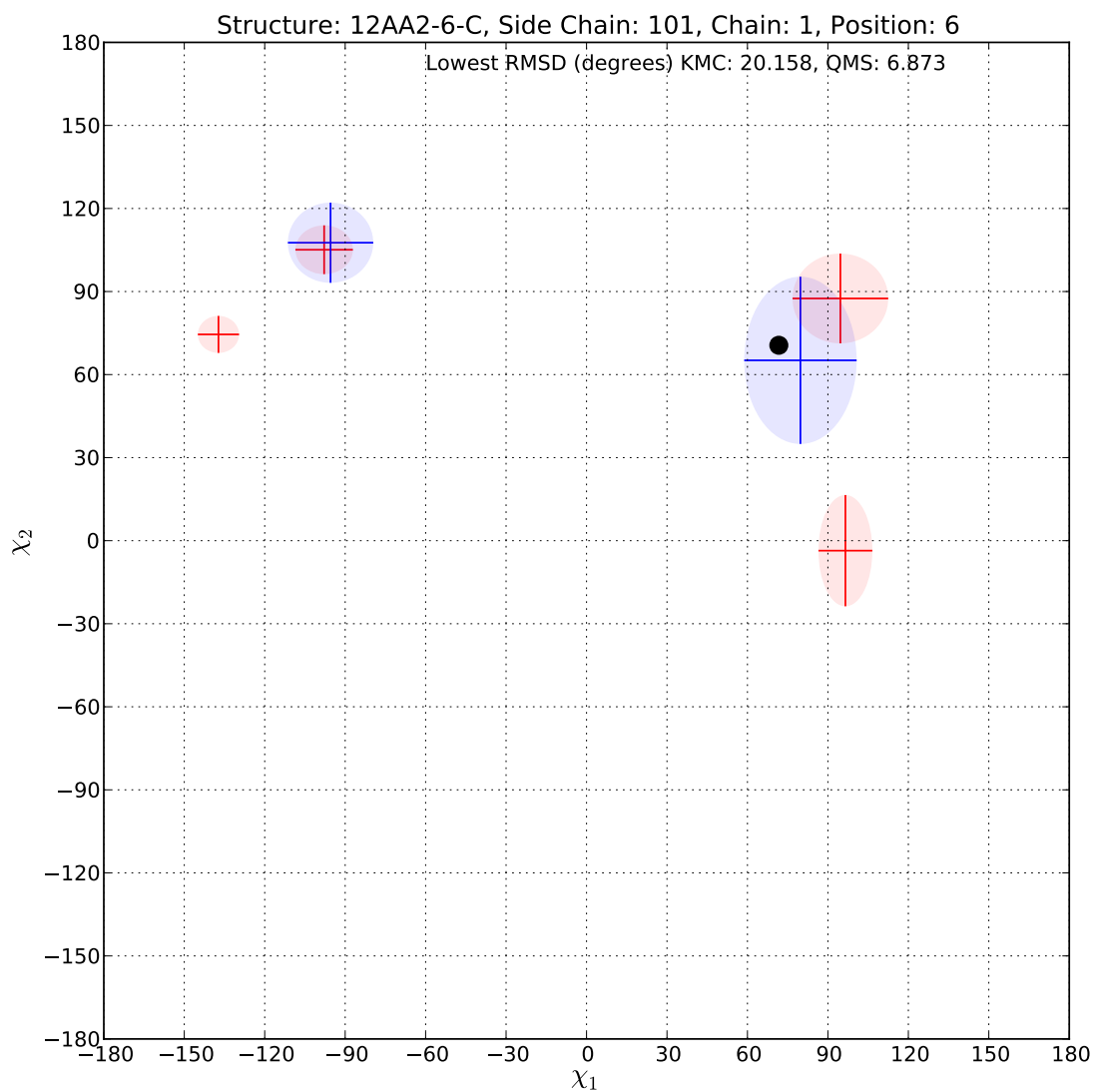


Figure S75: The rotamer library coverage plot for residue number 6 in chain 1 of peptoid databank structure 12AA2-6-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

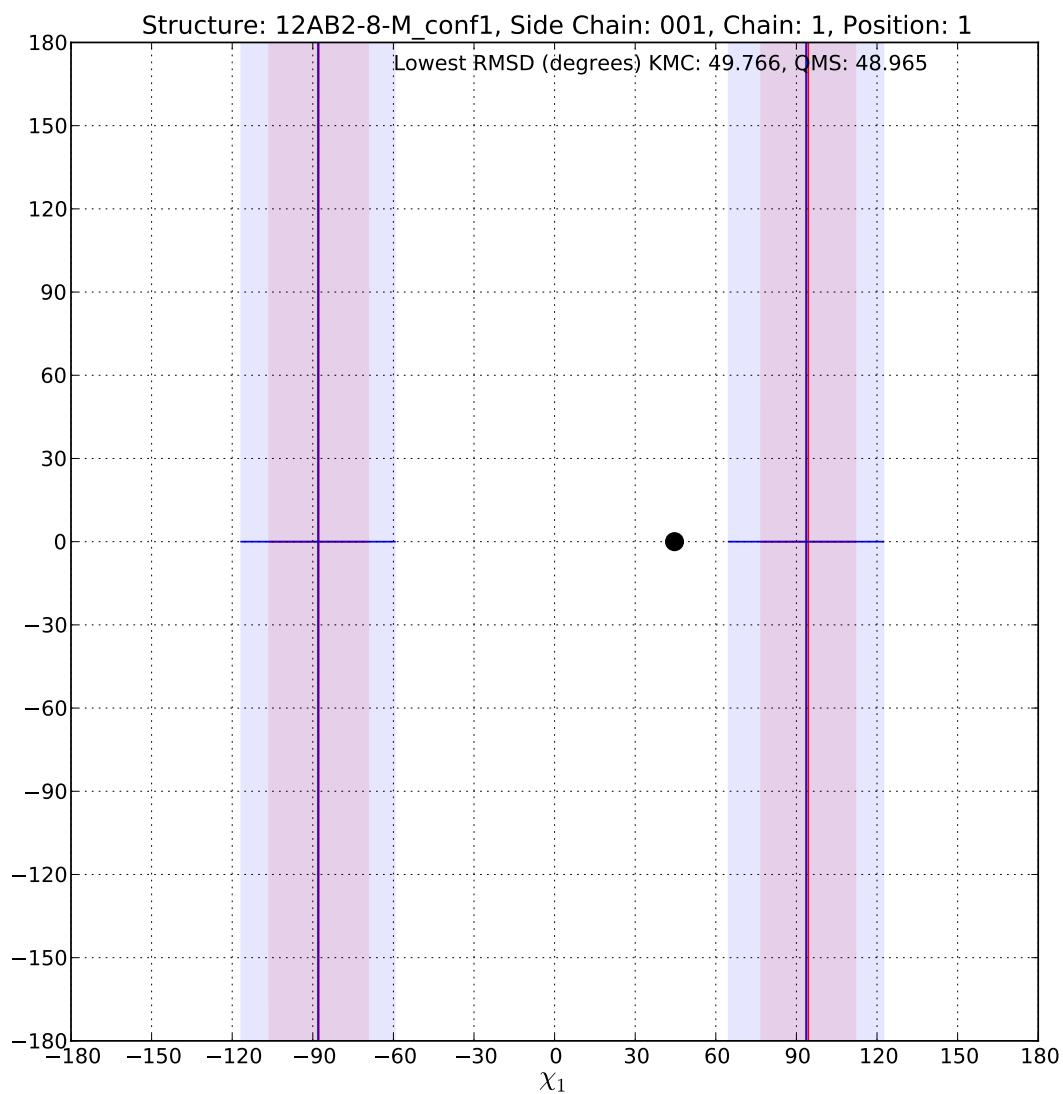


Figure S76: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 12AB2-8-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

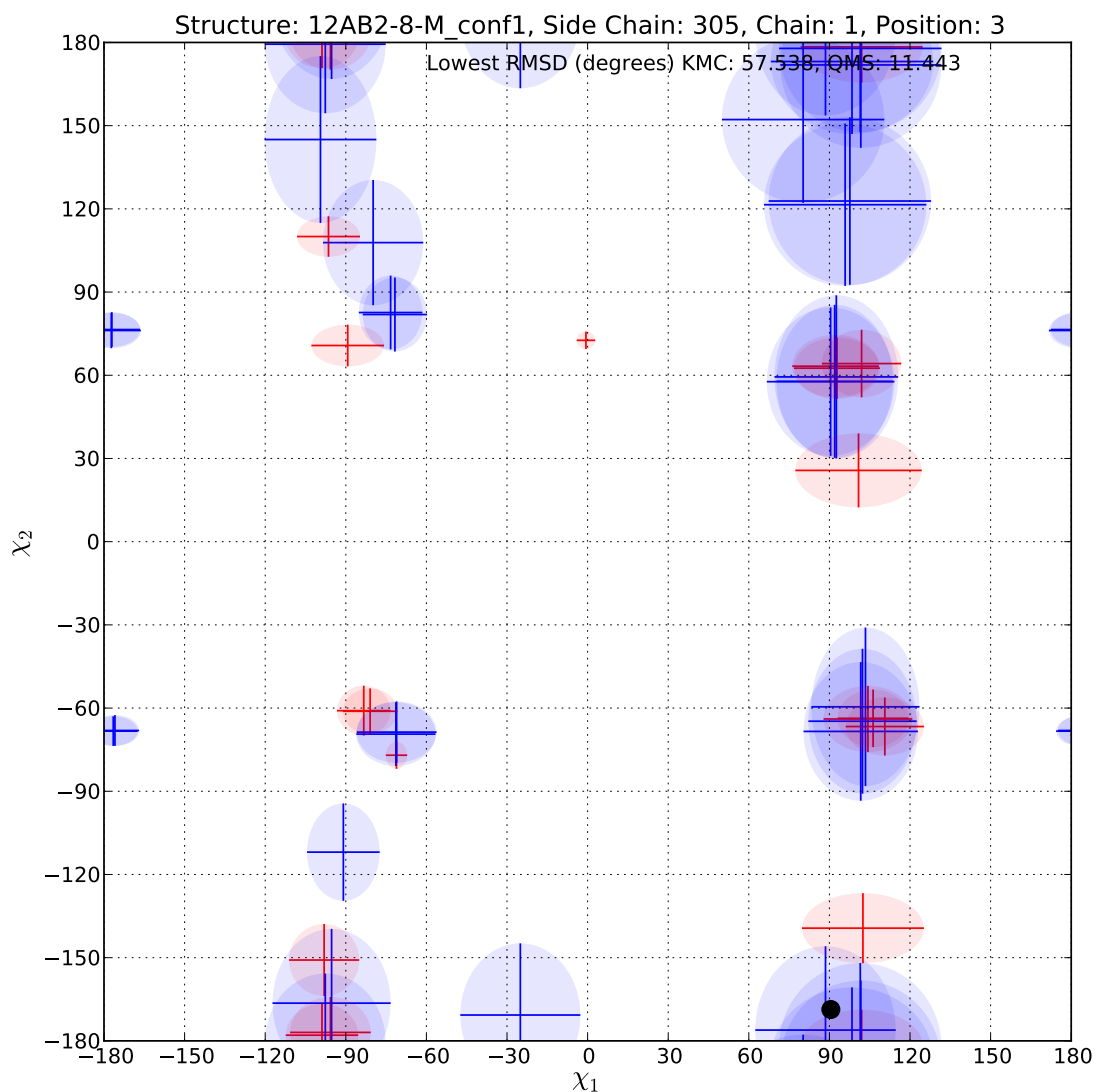


Figure S77: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 12AB2-8-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

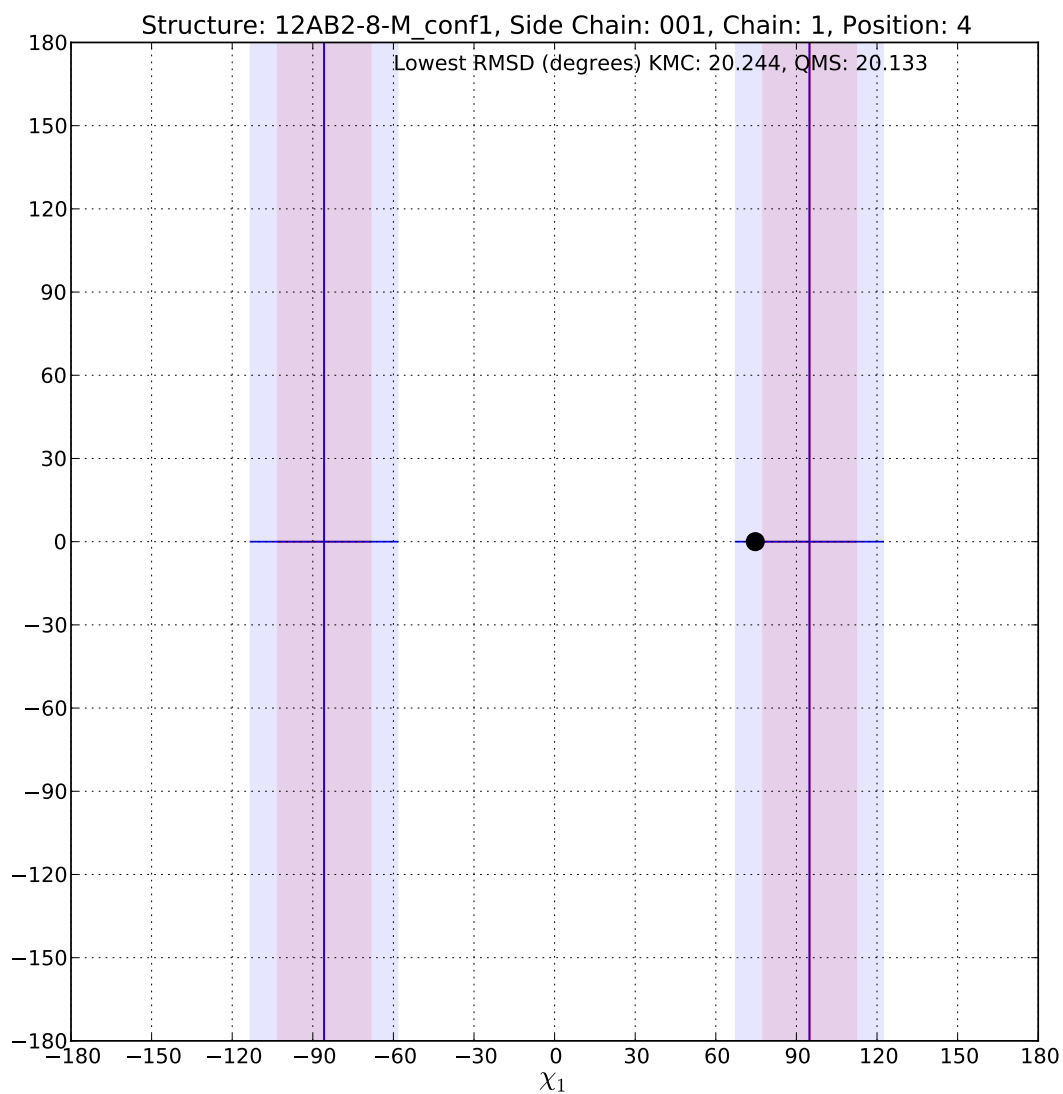


Figure S78: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 12AB2-8-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

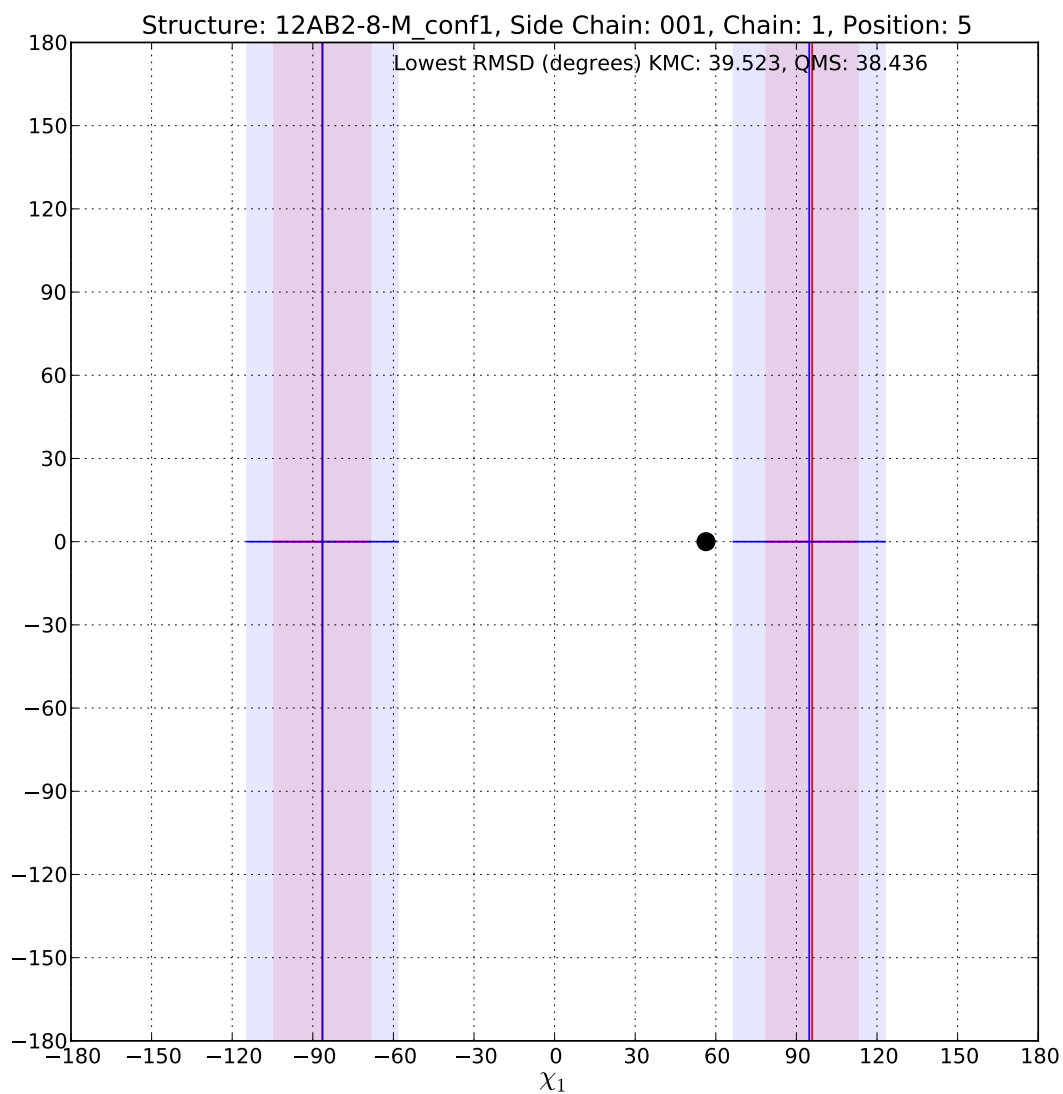


Figure S79: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 12AB2-8-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

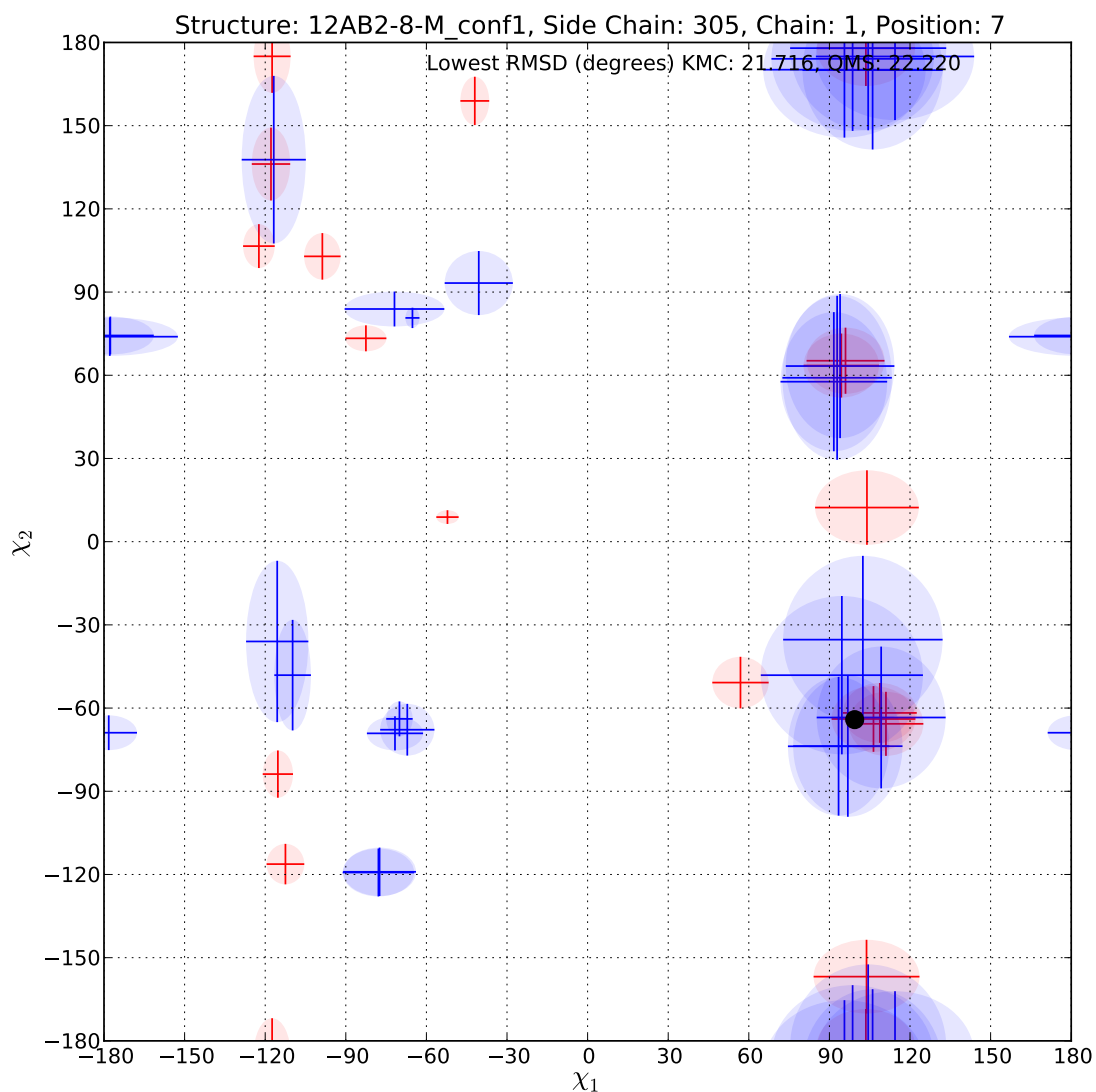


Figure S80: The rotamer library coverage plot for residue number 7 in chain 1 of peptoid databank structure 12AB2-8-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

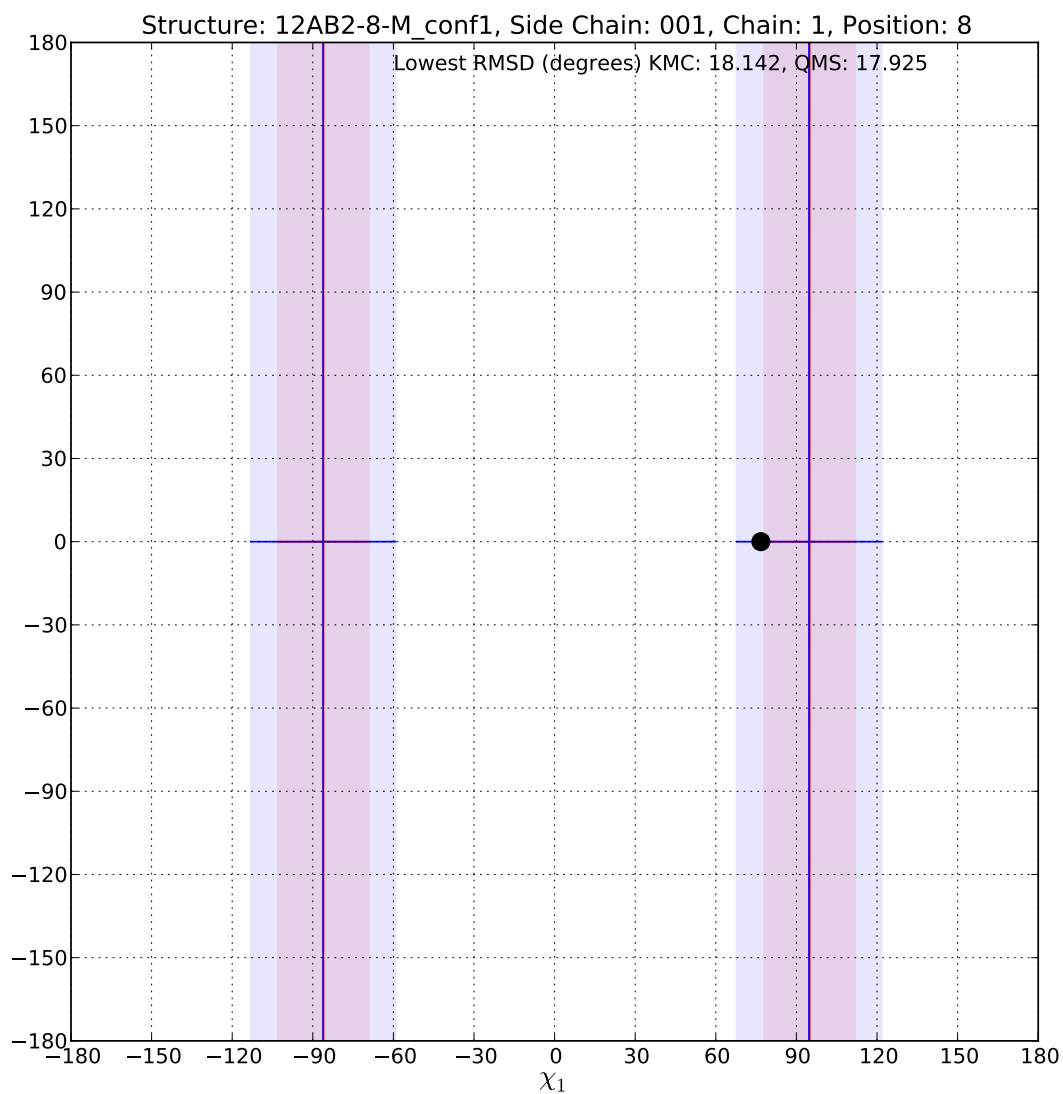


Figure S81: The rotamer library coverage plot for residue number 8 in chain 1 of peptoid databank structure 12AB2-8-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

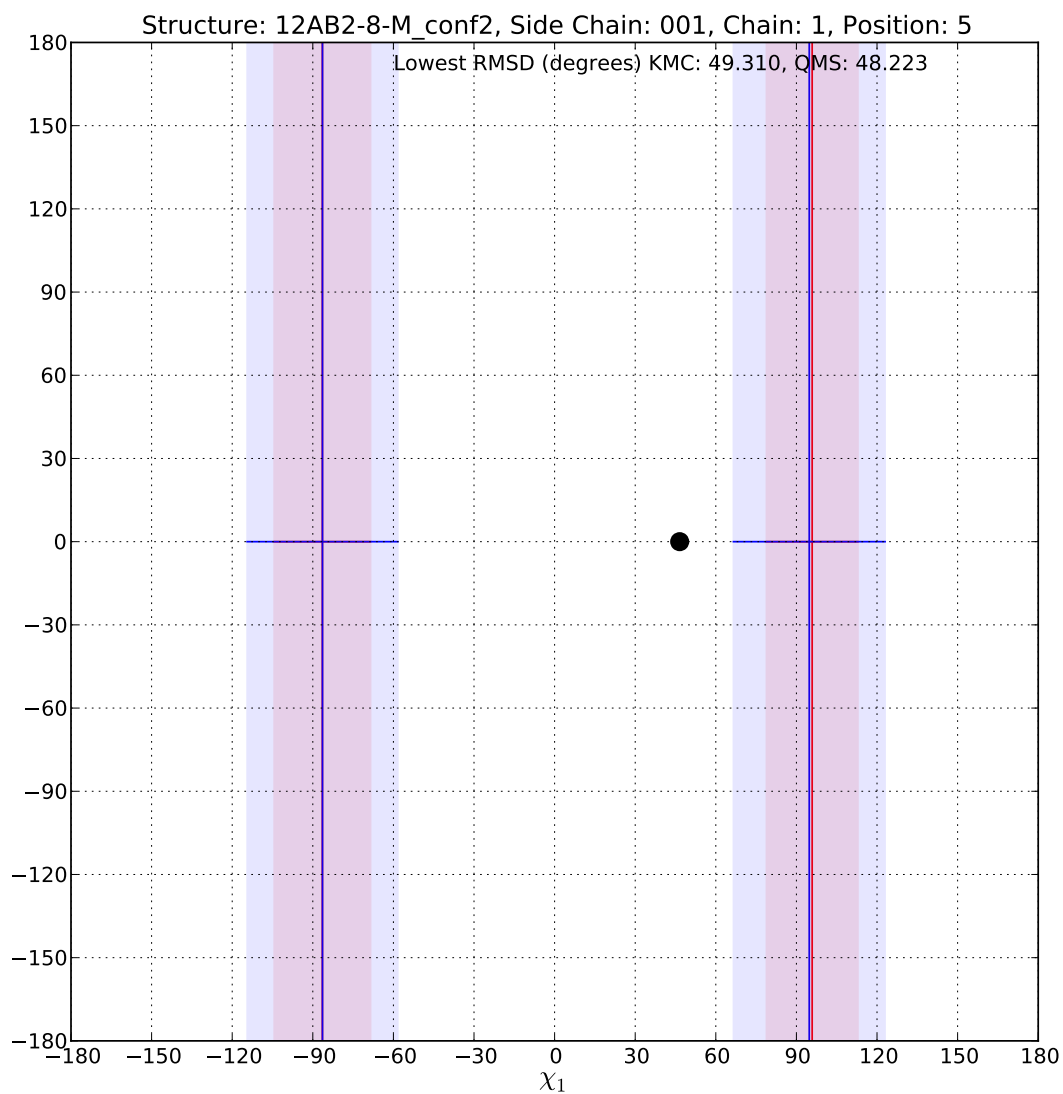


Figure S82: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 12AB2-8-M_conf2. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

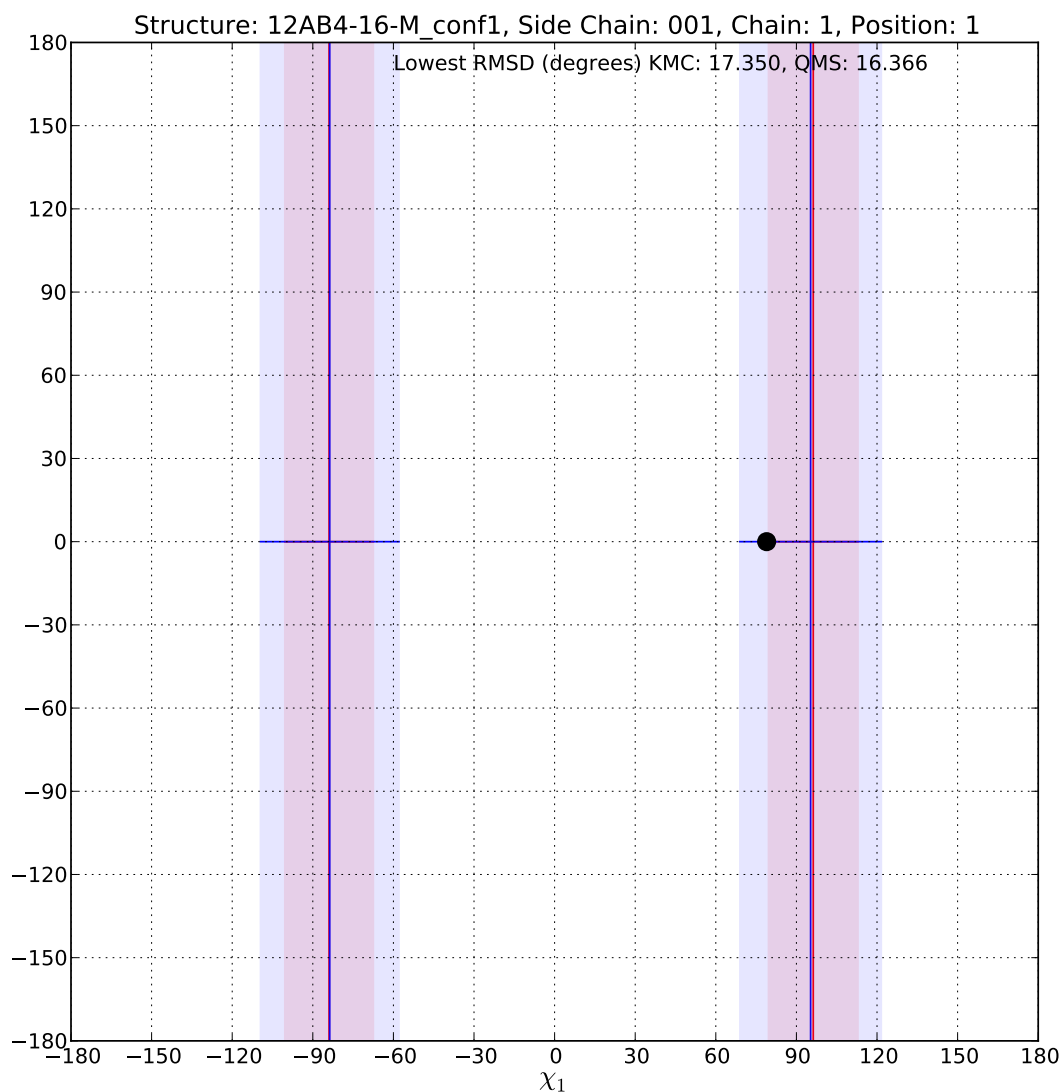


Figure S83: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

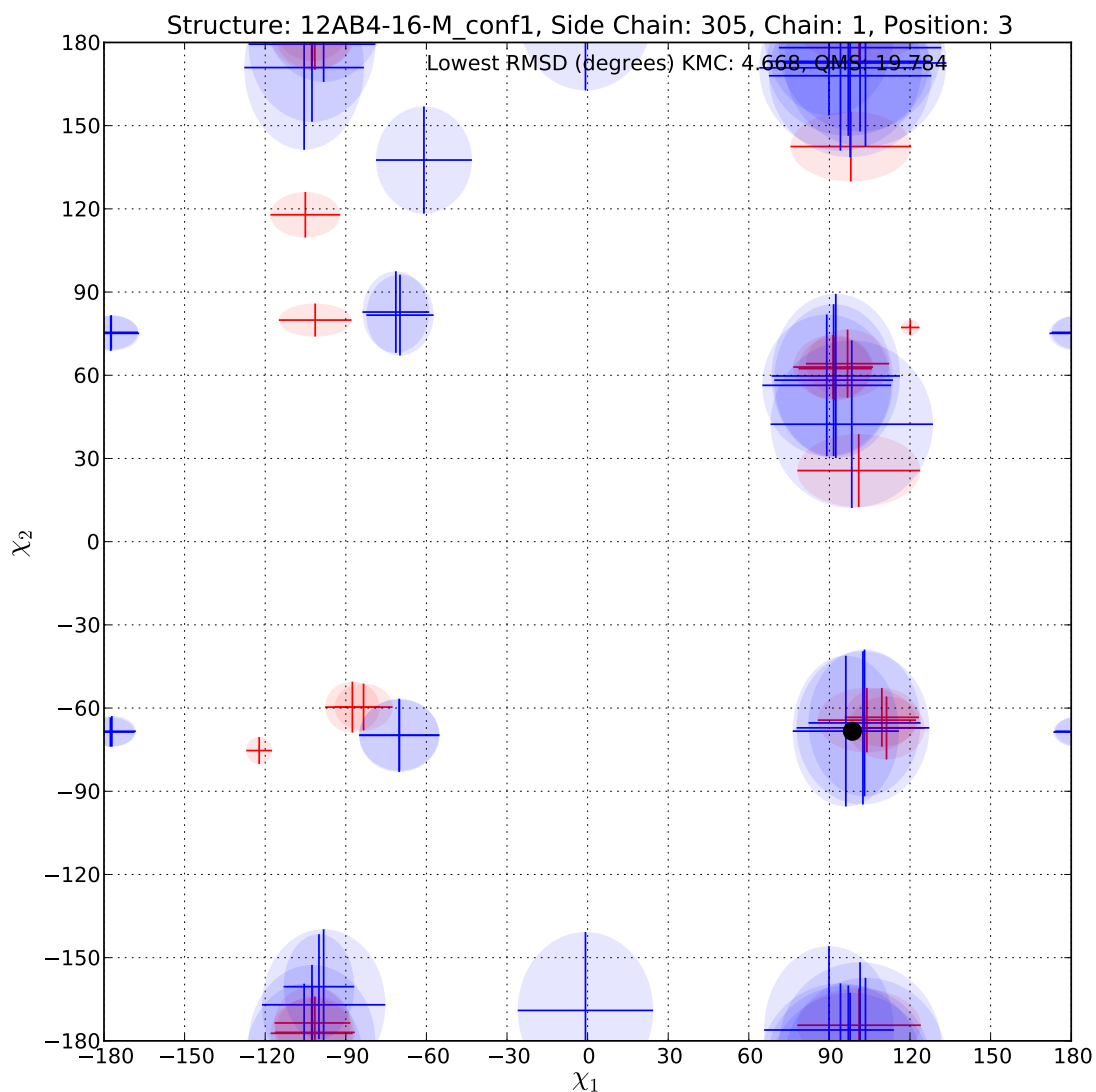


Figure S84: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

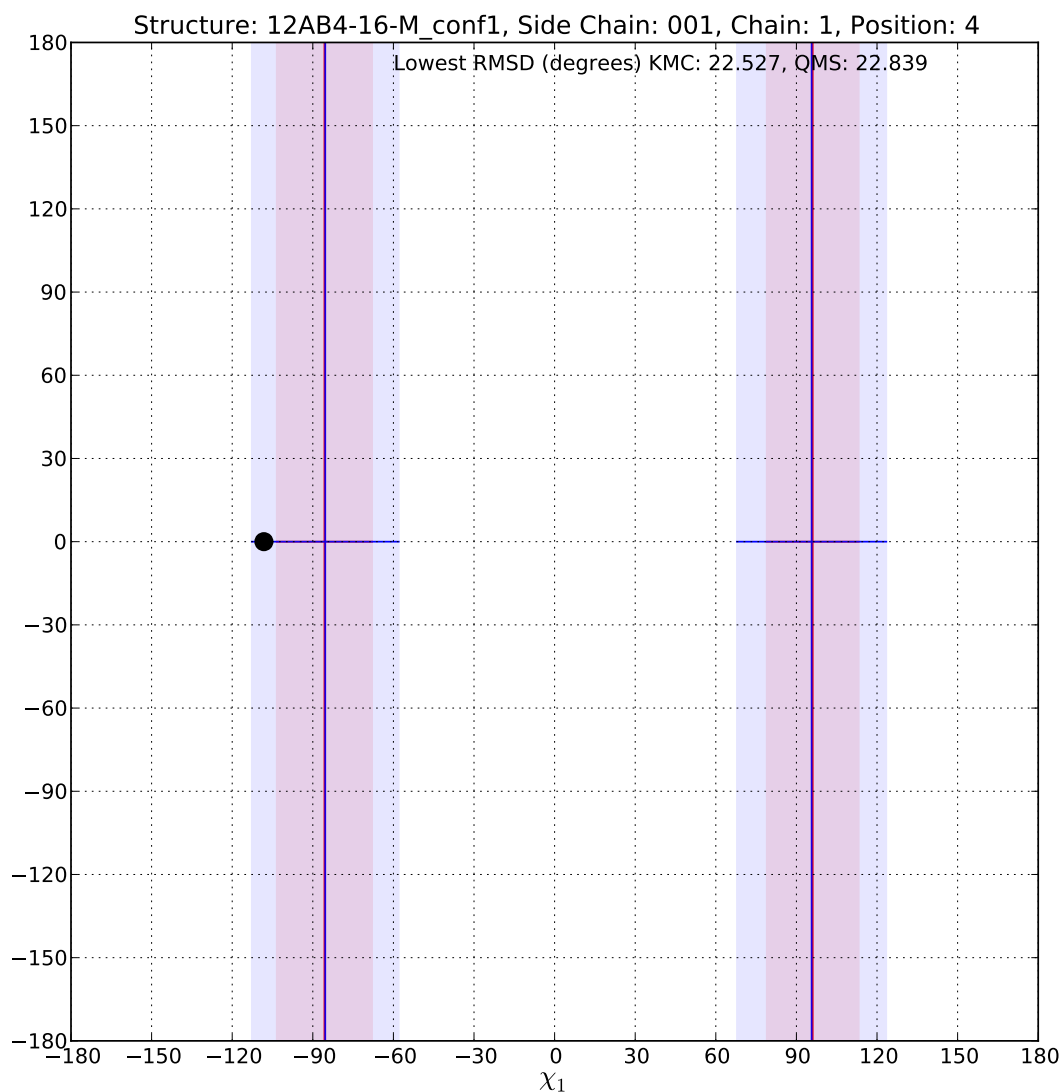


Figure S85: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

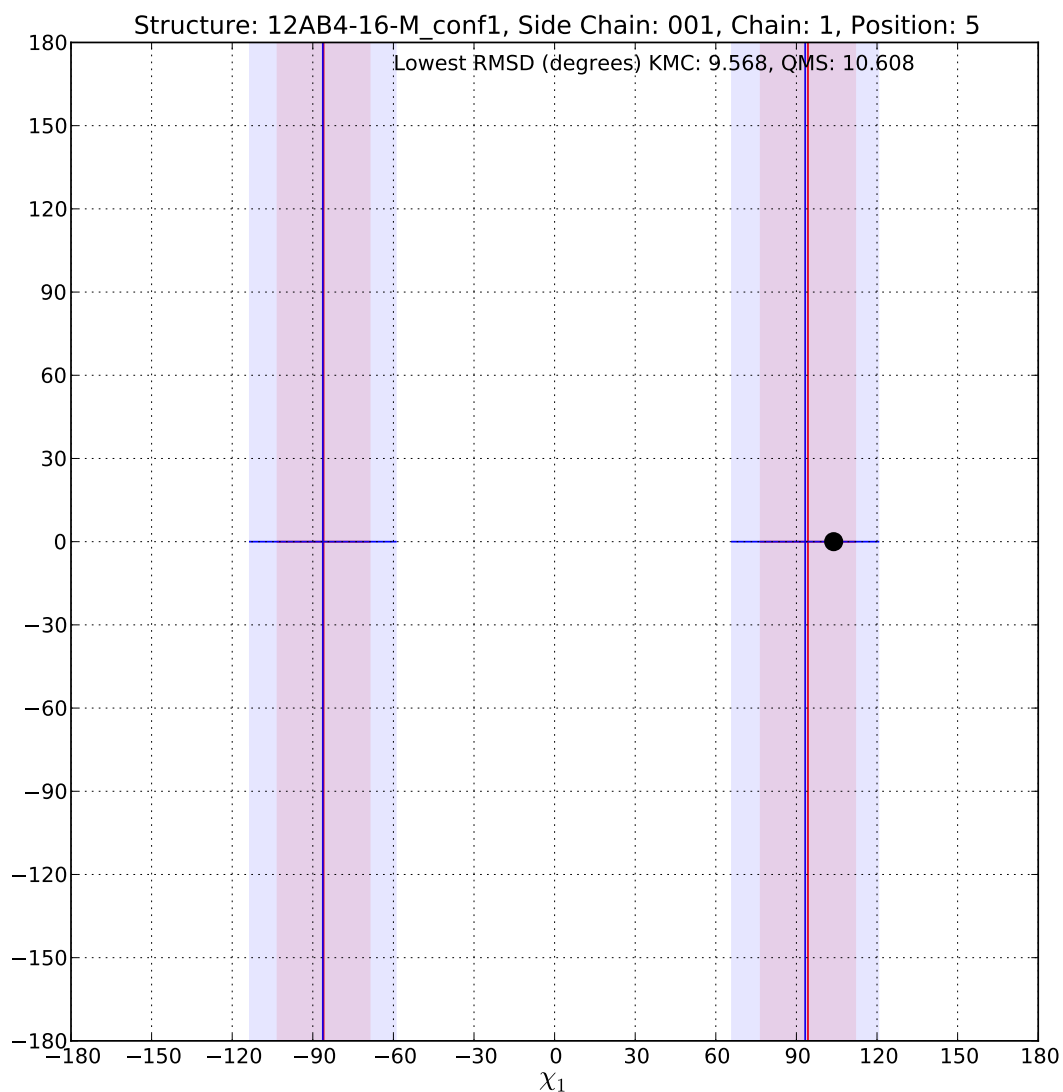


Figure S86: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

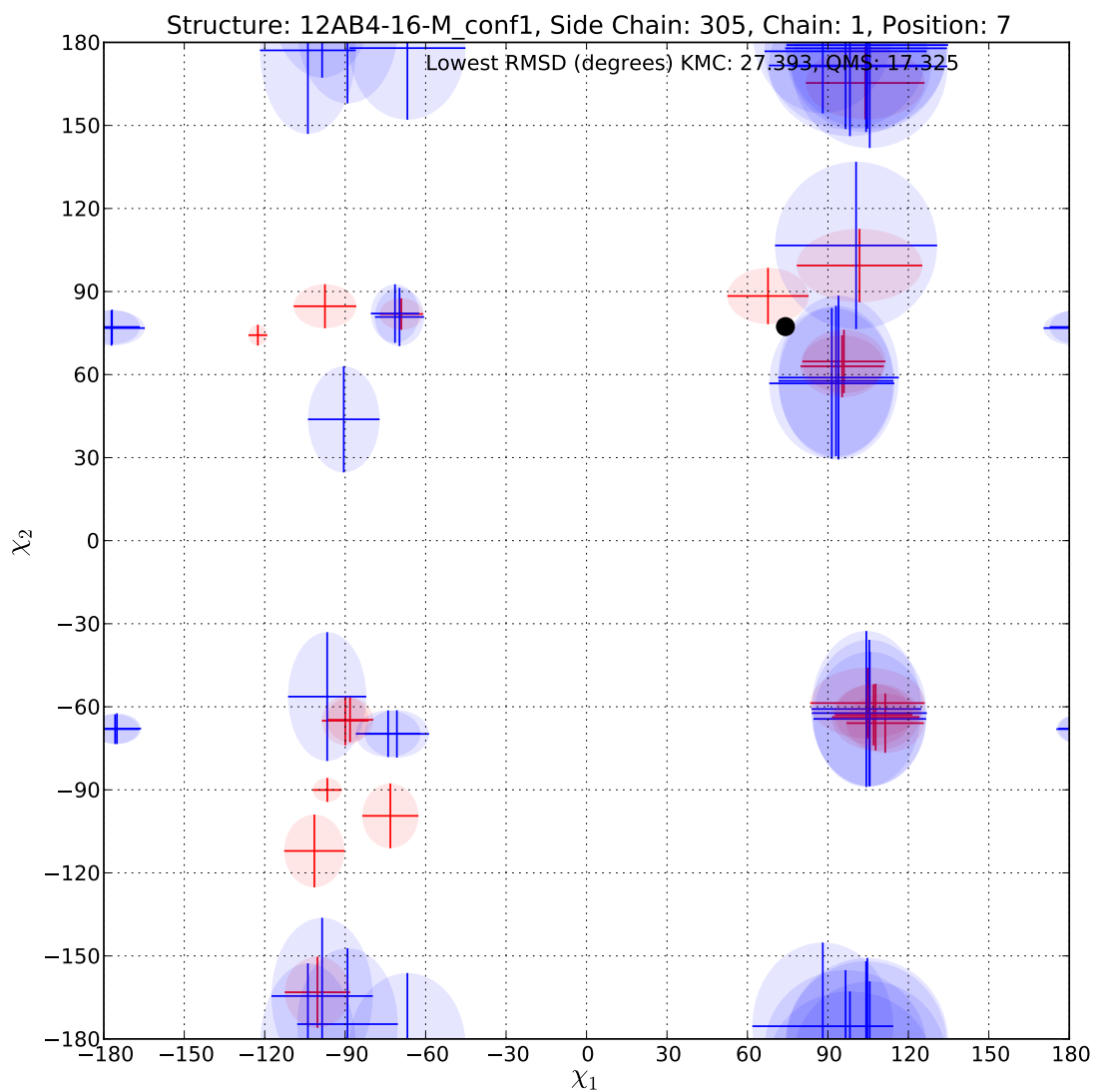


Figure S87: The rotamer library coverage plot for residue number 7 in chain 1 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

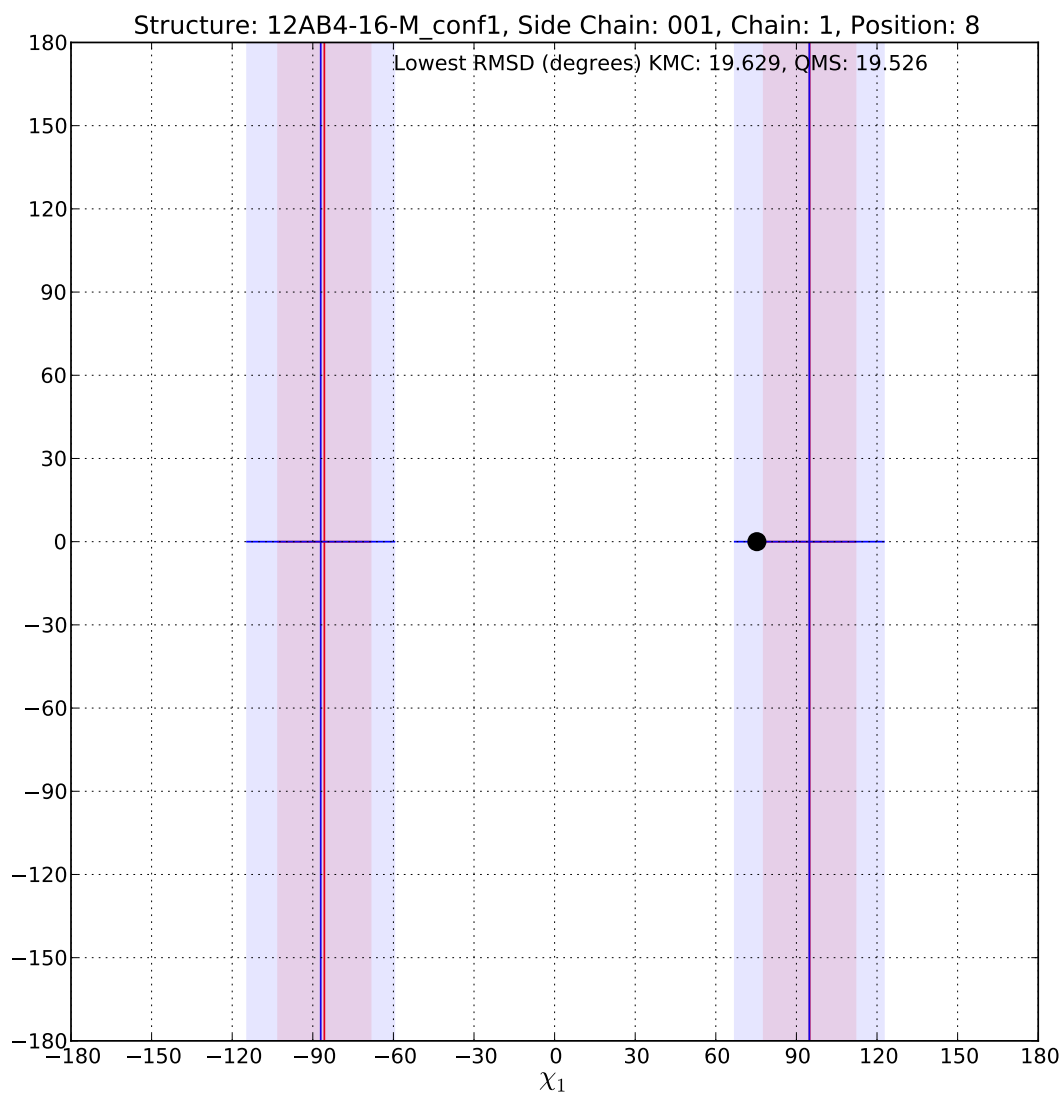


Figure S88: The rotamer library coverage plot for residue number 8 in chain 1 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

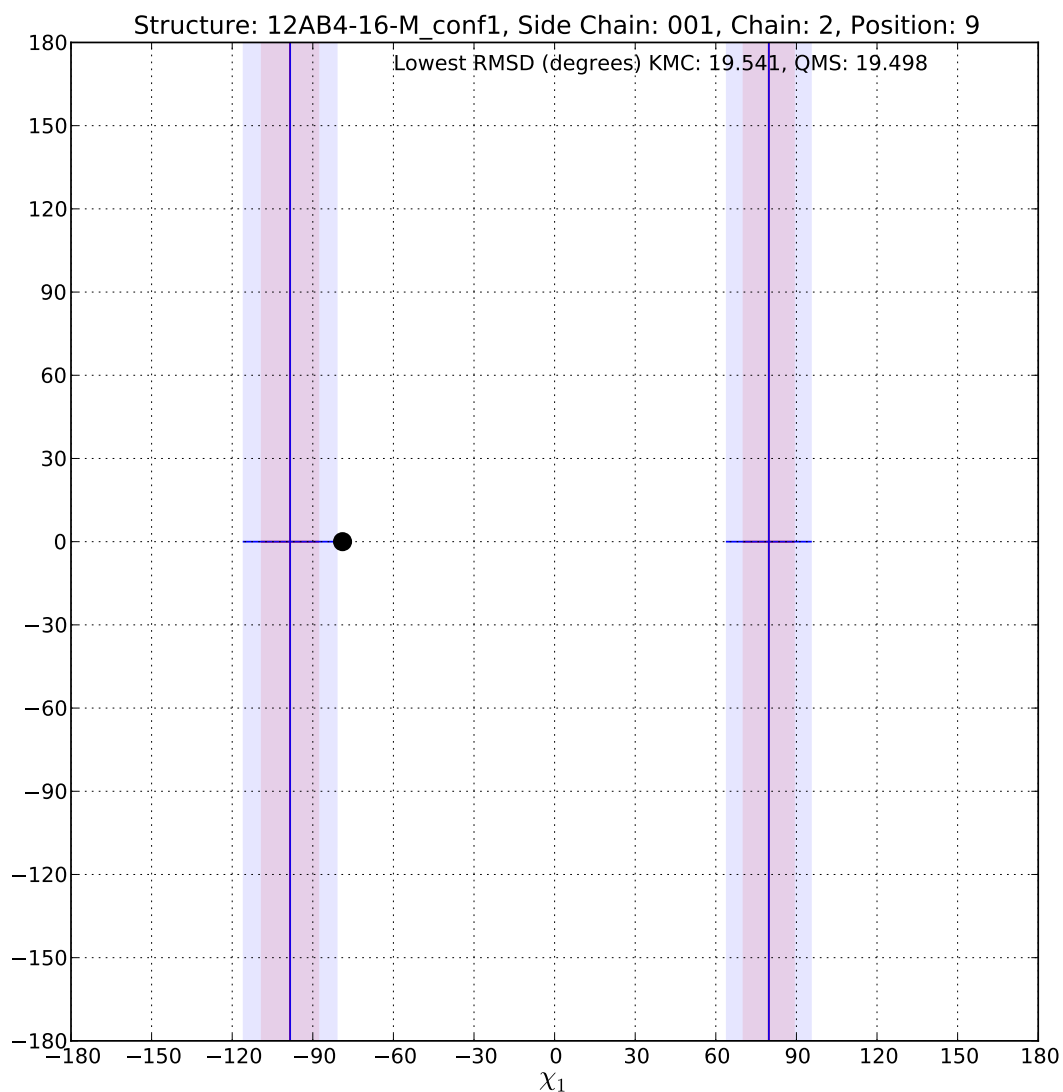


Figure S89: The rotamer library coverage plot for residue number 9 in chain 2 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

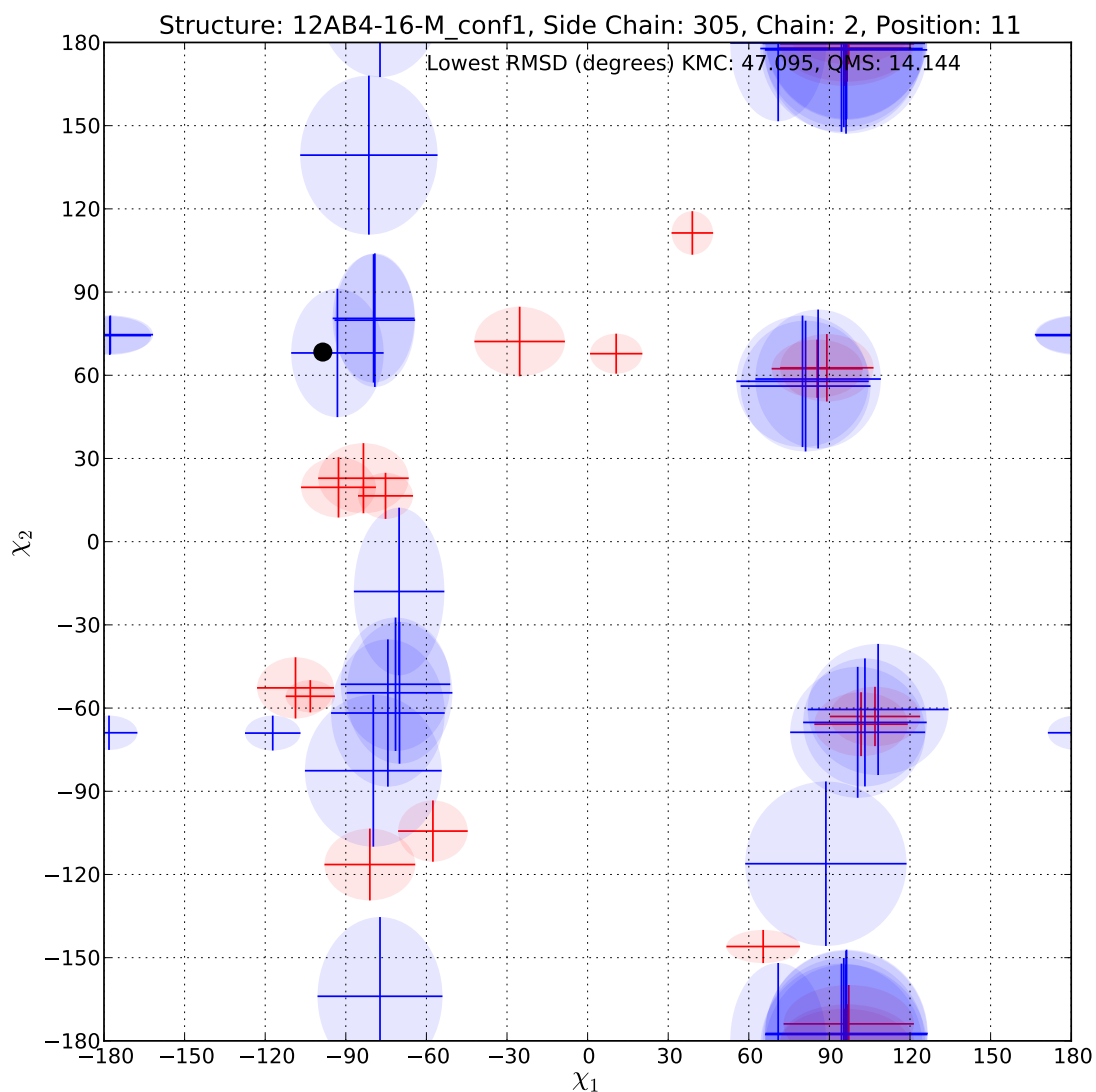


Figure S90: The rotamer library coverage plot for residue number 11 in chain 2 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

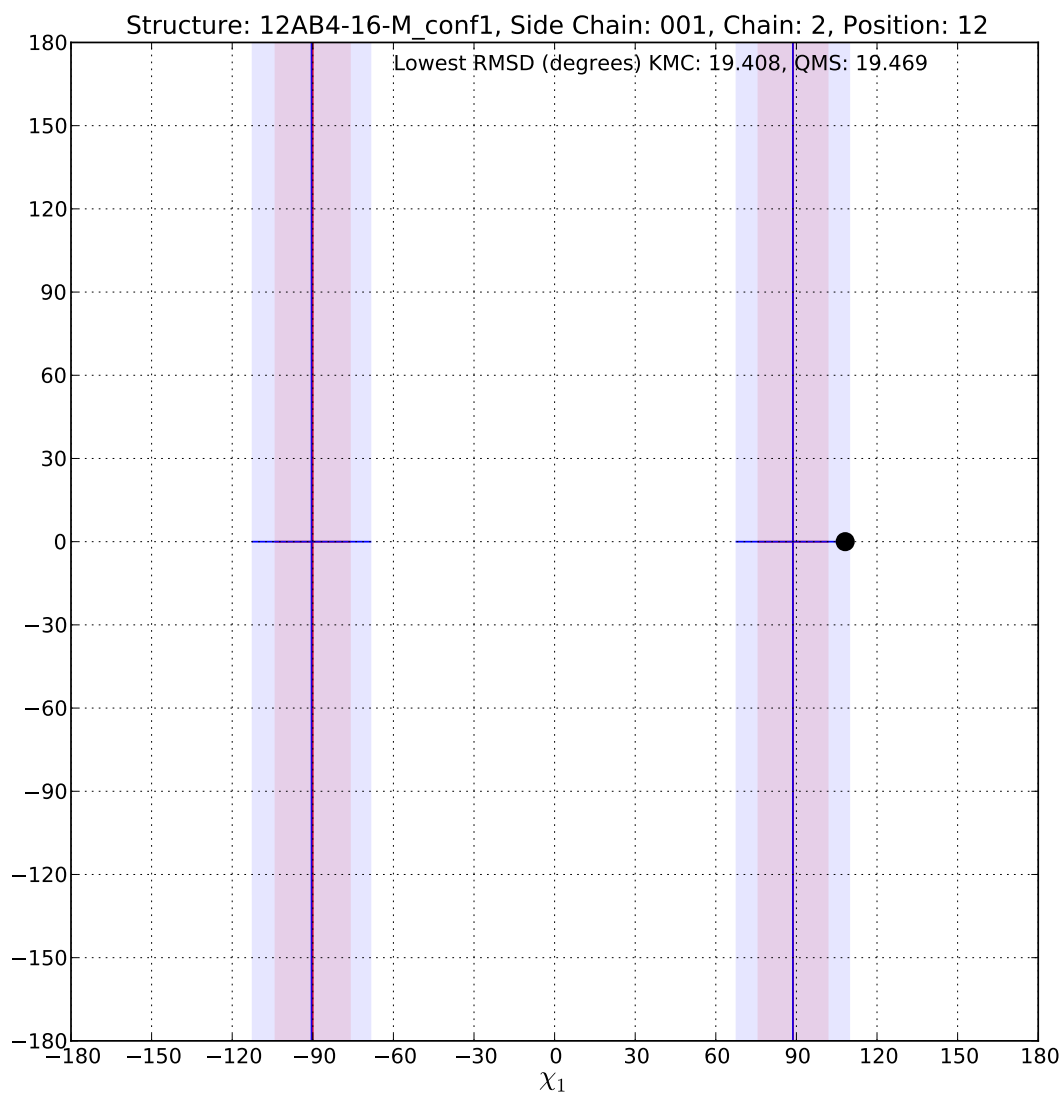


Figure S91: The rotamer library coverage plot for residue number 12 in chain 2 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

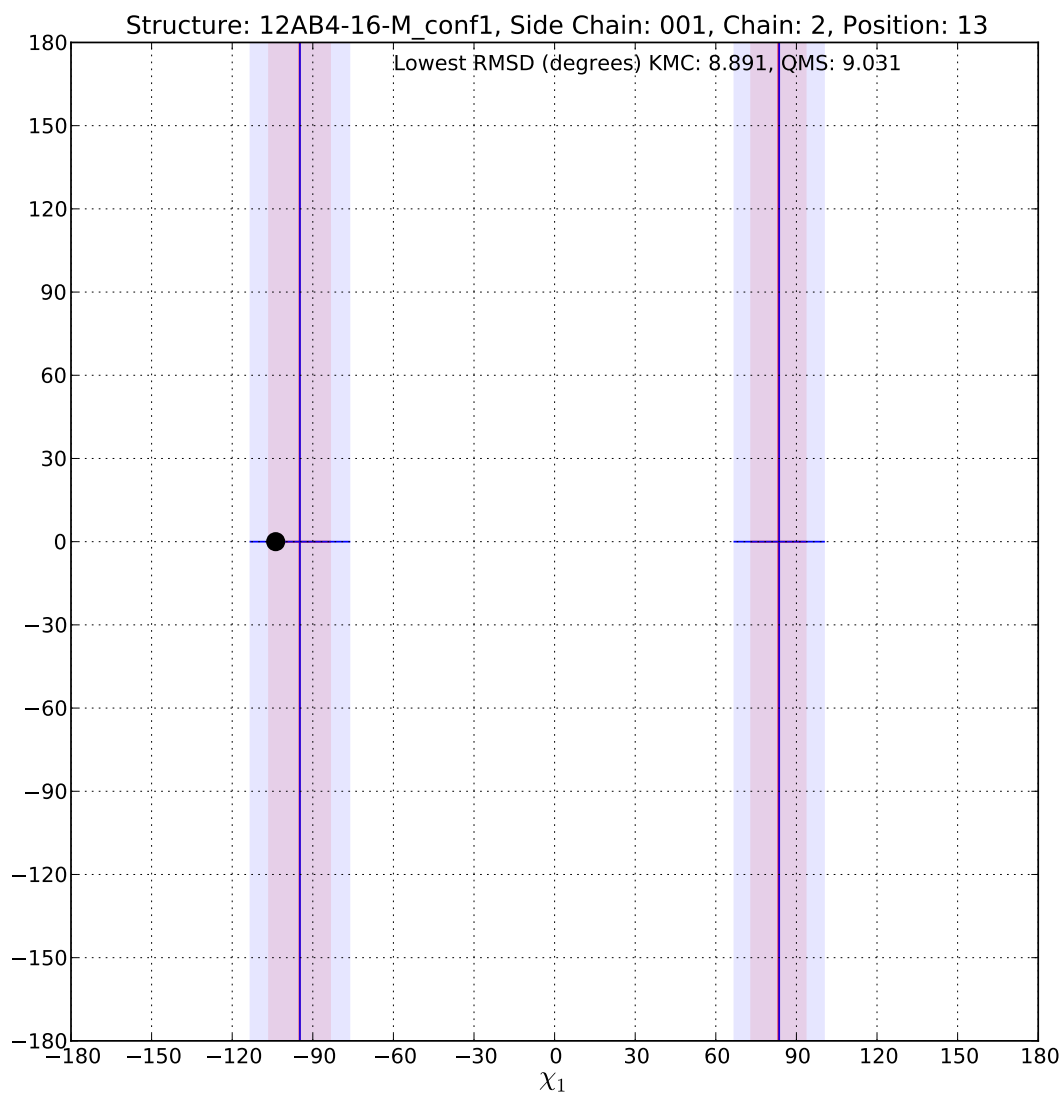


Figure S92: The rotamer library coverage plot for residue number 13 in chain 2 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

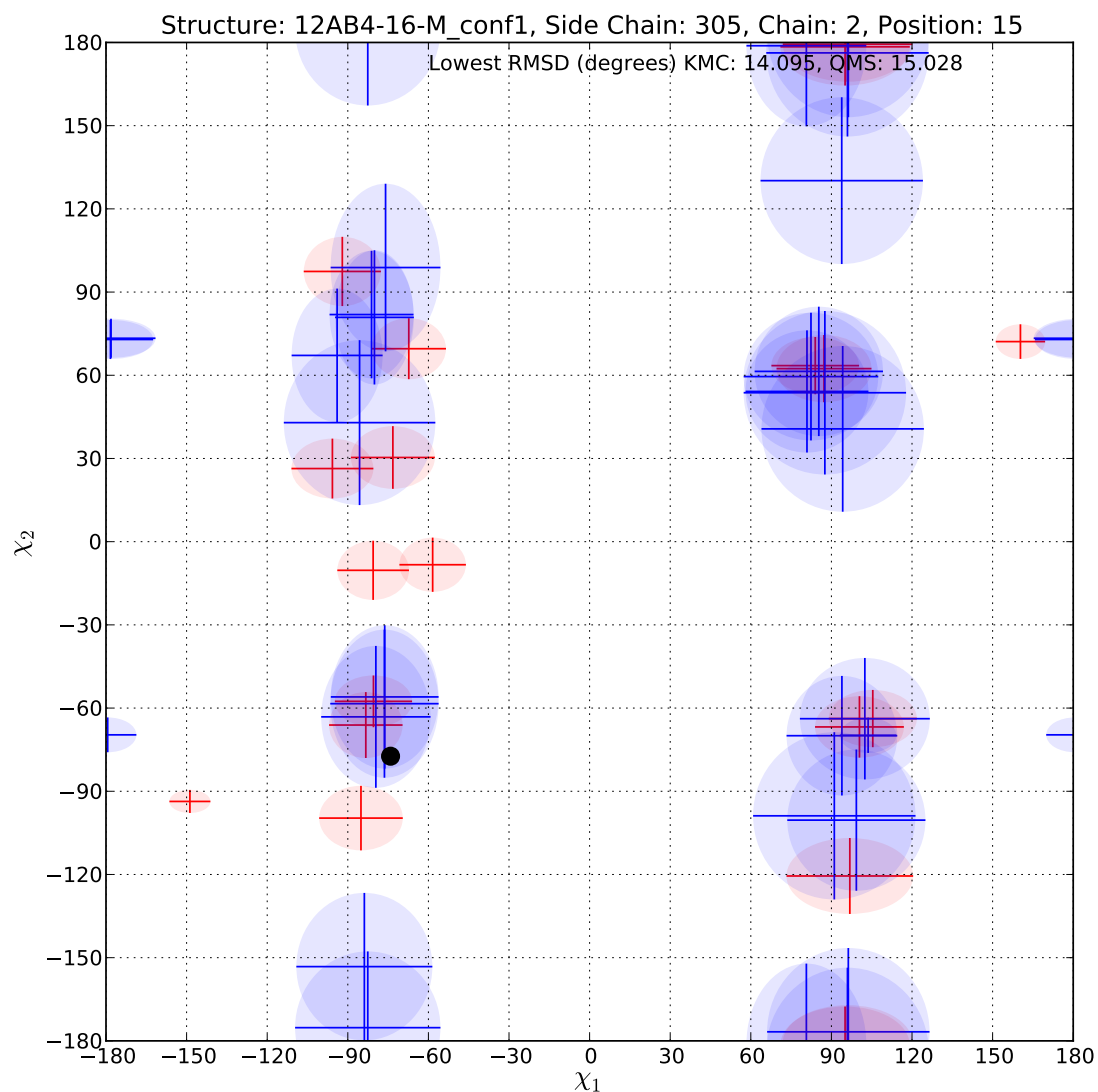


Figure S93: The rotamer library coverage plot for residue number 15 in chain 2 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

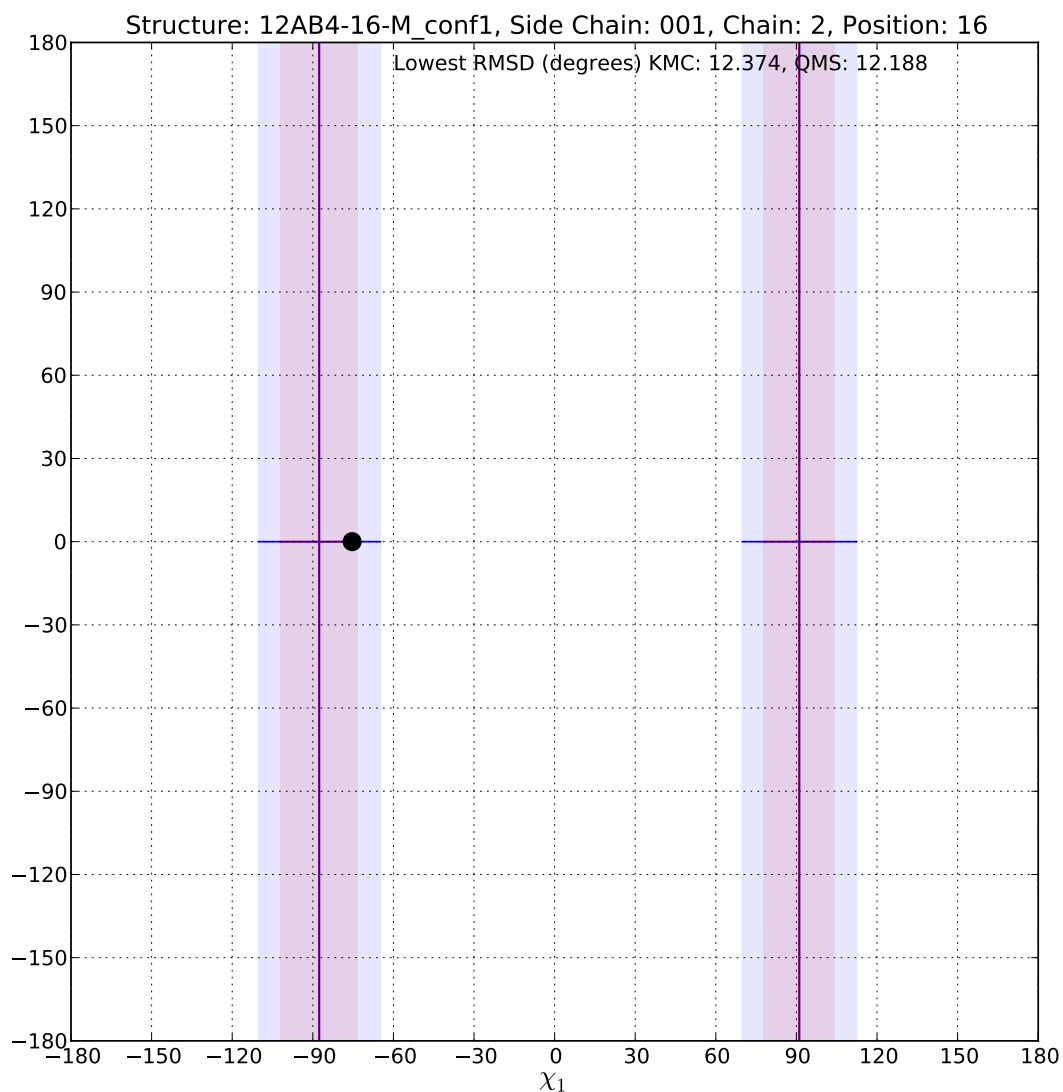


Figure S94: The rotamer library coverage plot for residue number 16 in chain 2 of peptoid databank structure 12AB4-16-M_conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

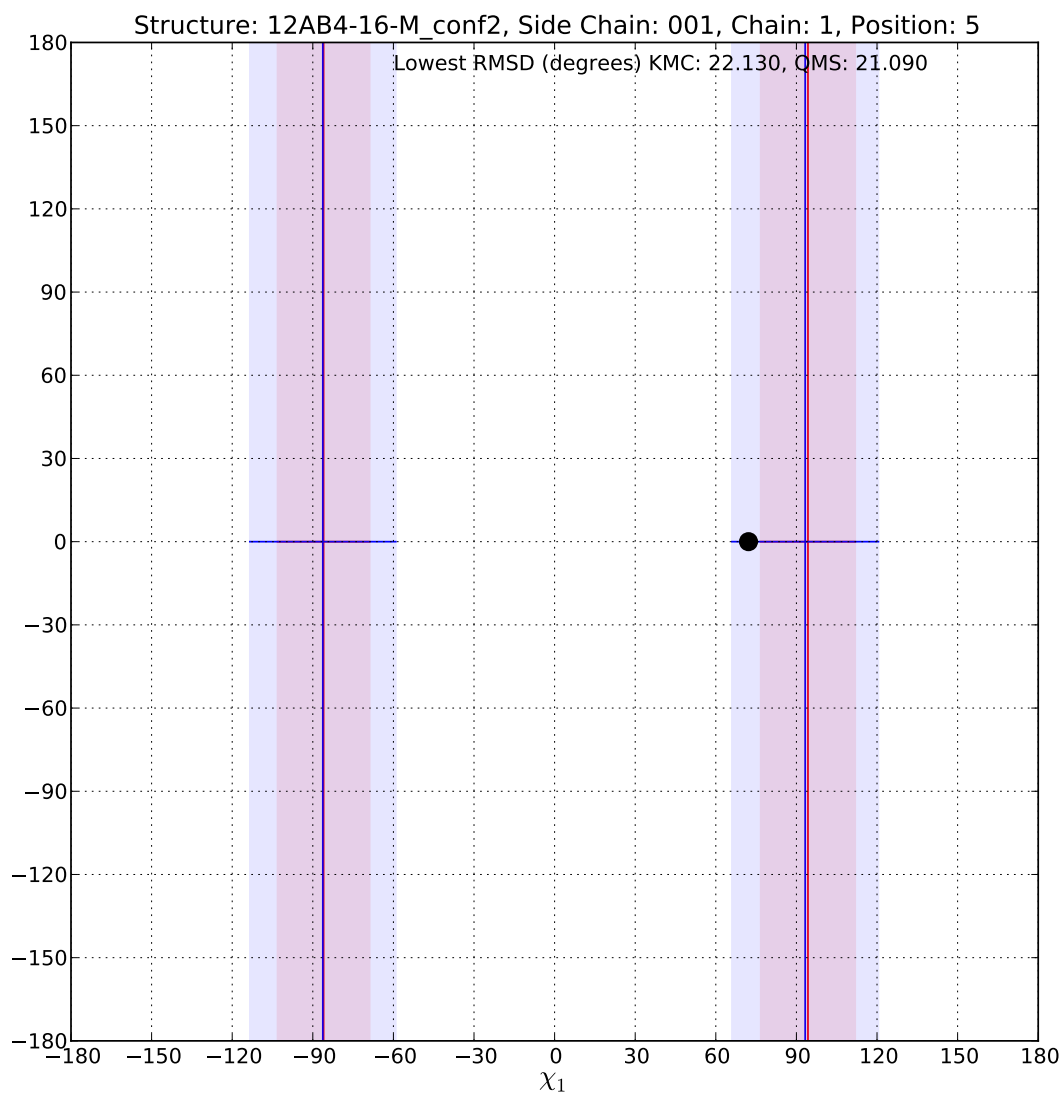


Figure S95: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 12AB4-16-M_conf2. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

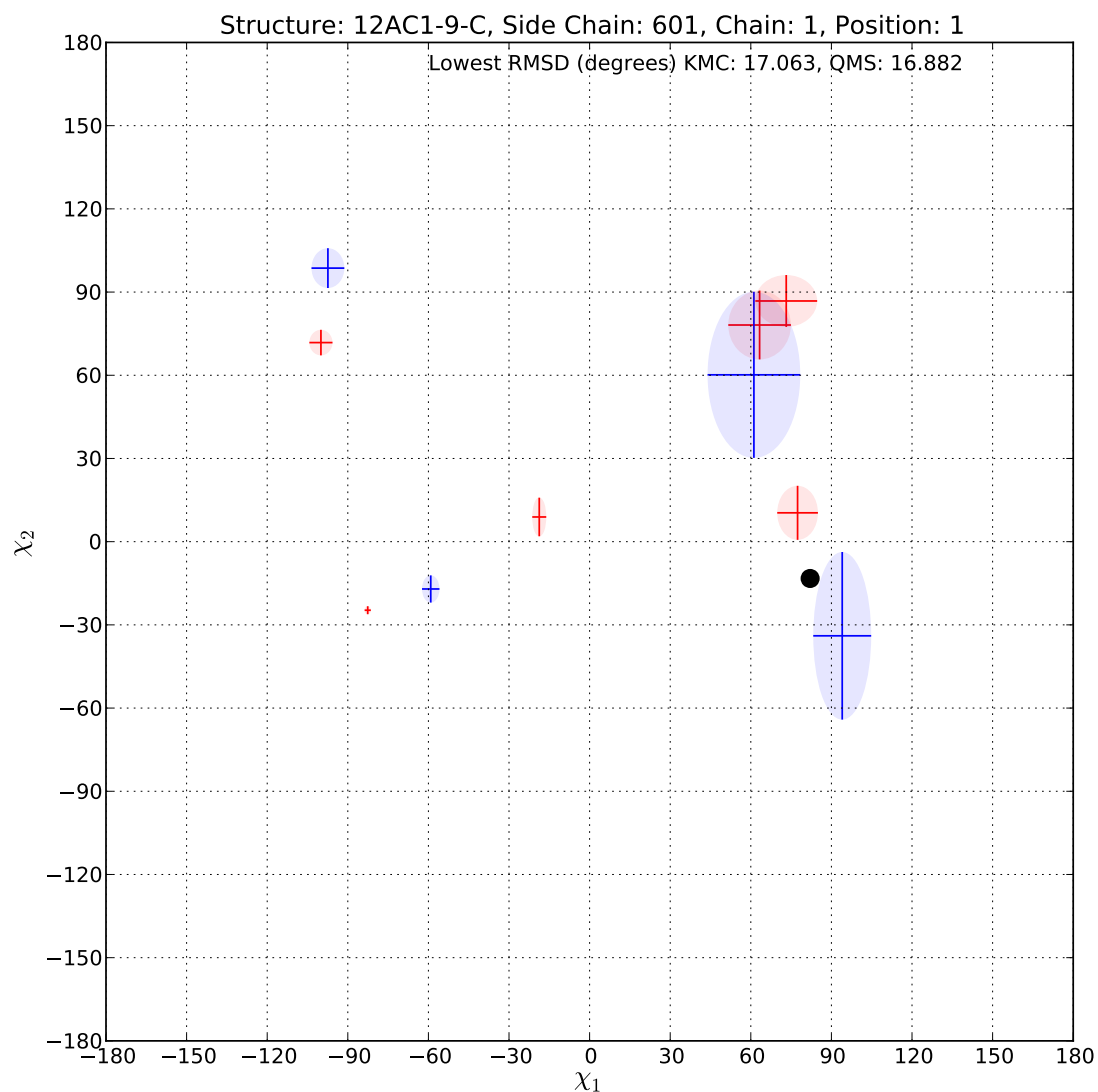


Figure S96: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 12AC1-9-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

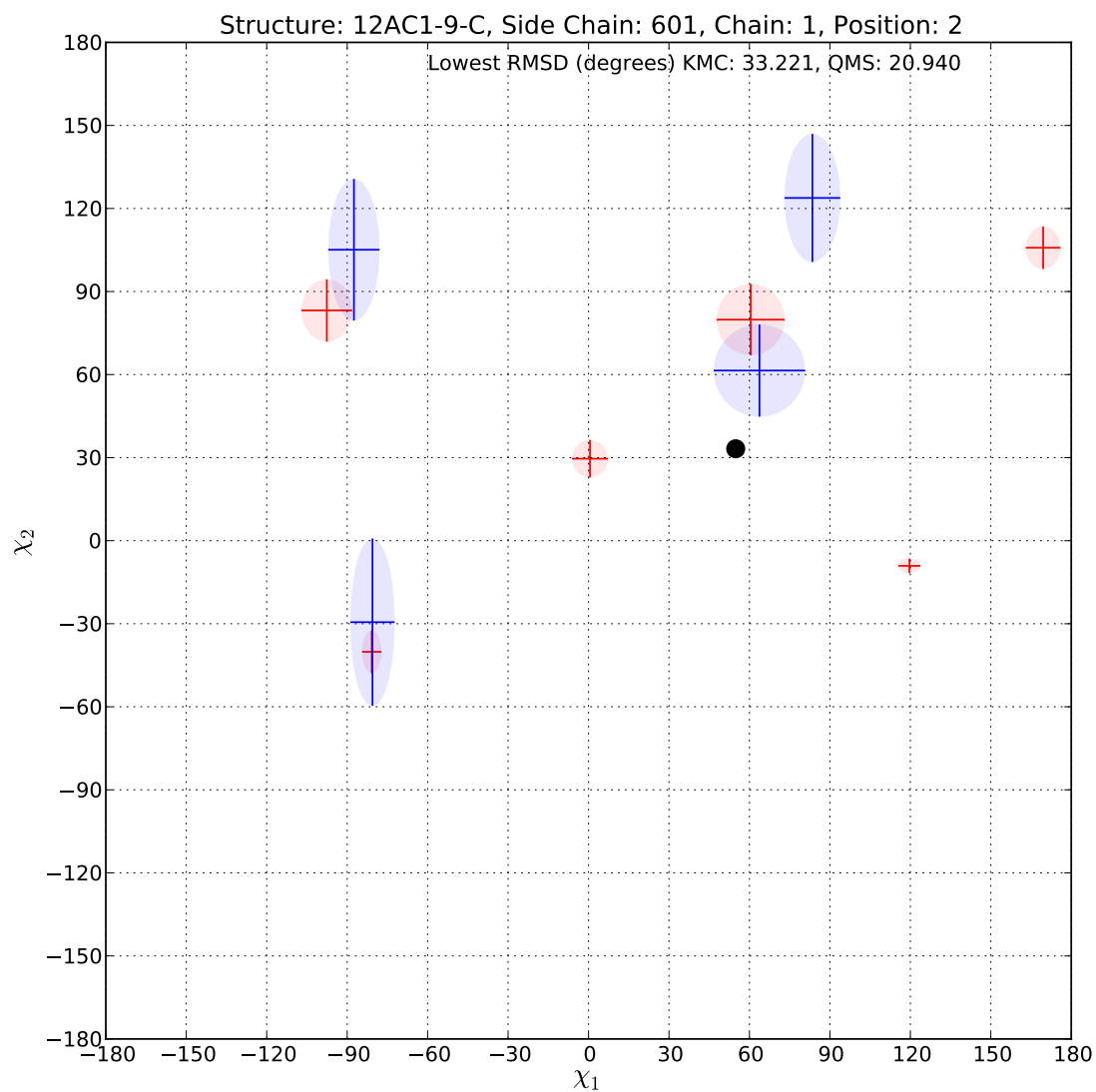


Figure S97: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 12AC1-9-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

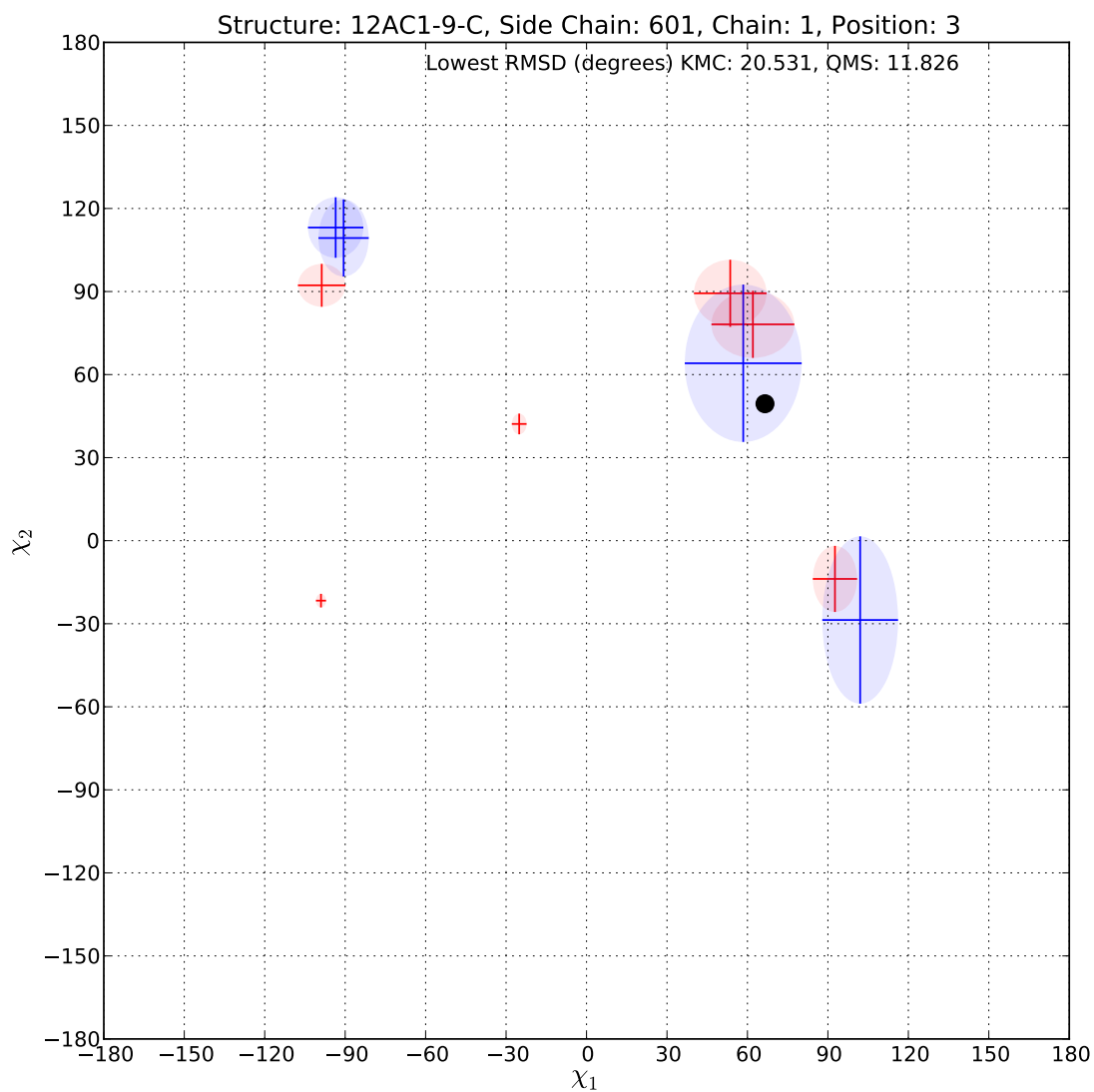


Figure S98: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 12AC1-9-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

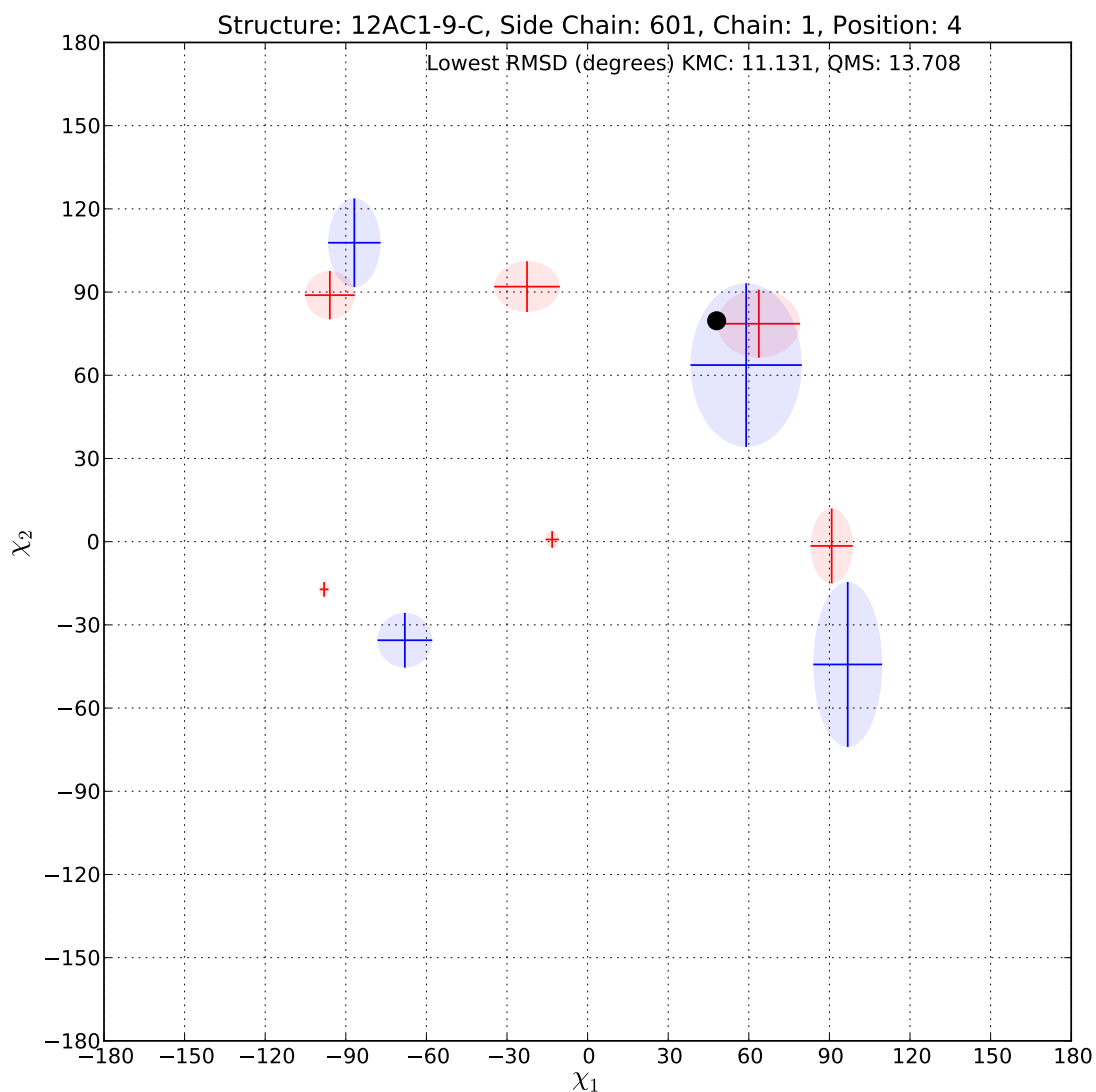


Figure S99: The rotamer library coverage plot for residue number 4 in chain 1 of peptoid databank structure 12AC1-9-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

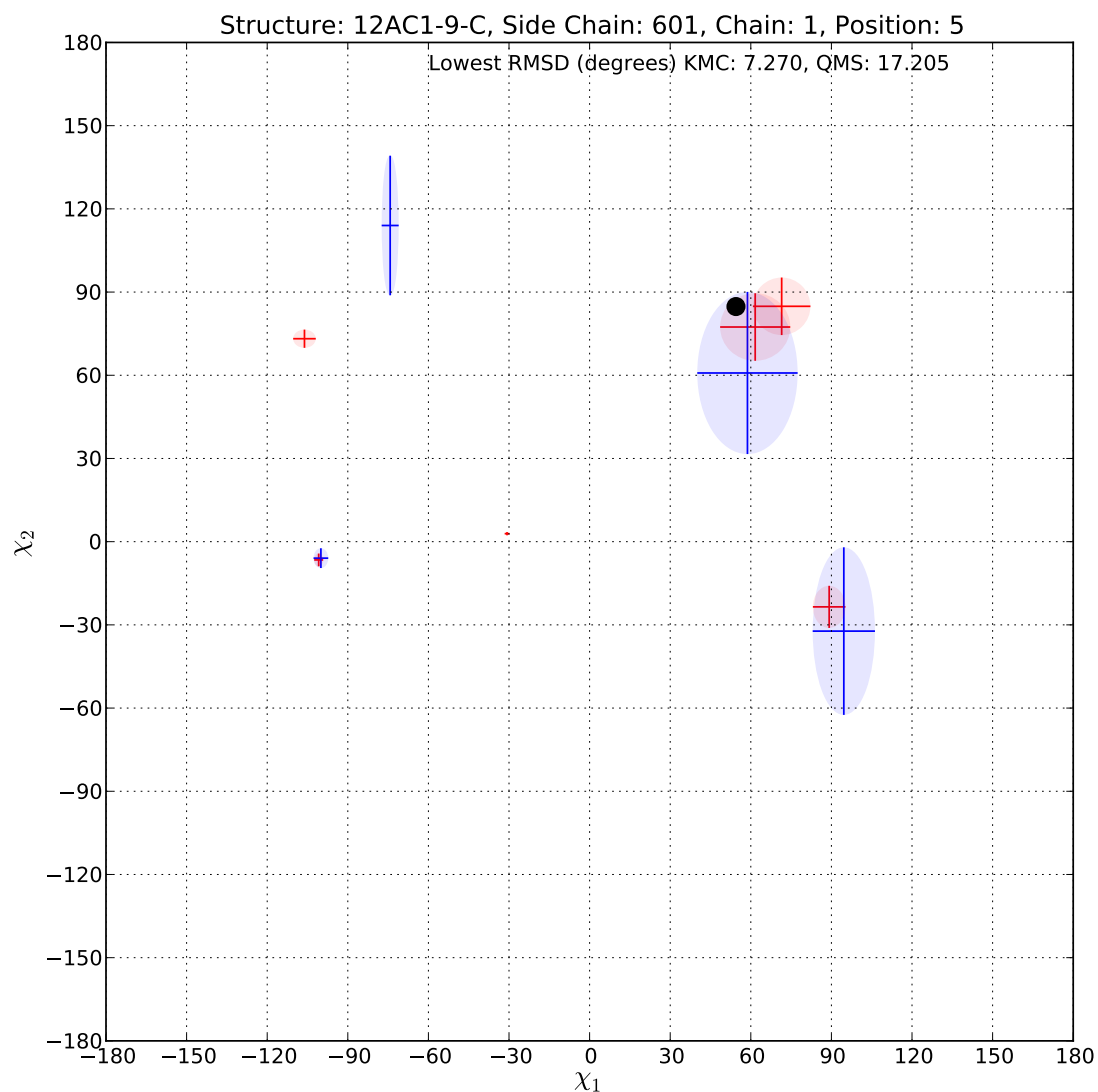


Figure S100: The rotamer library coverage plot for residue number 5 in chain 1 of peptoid databank structure 12AC1-9-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

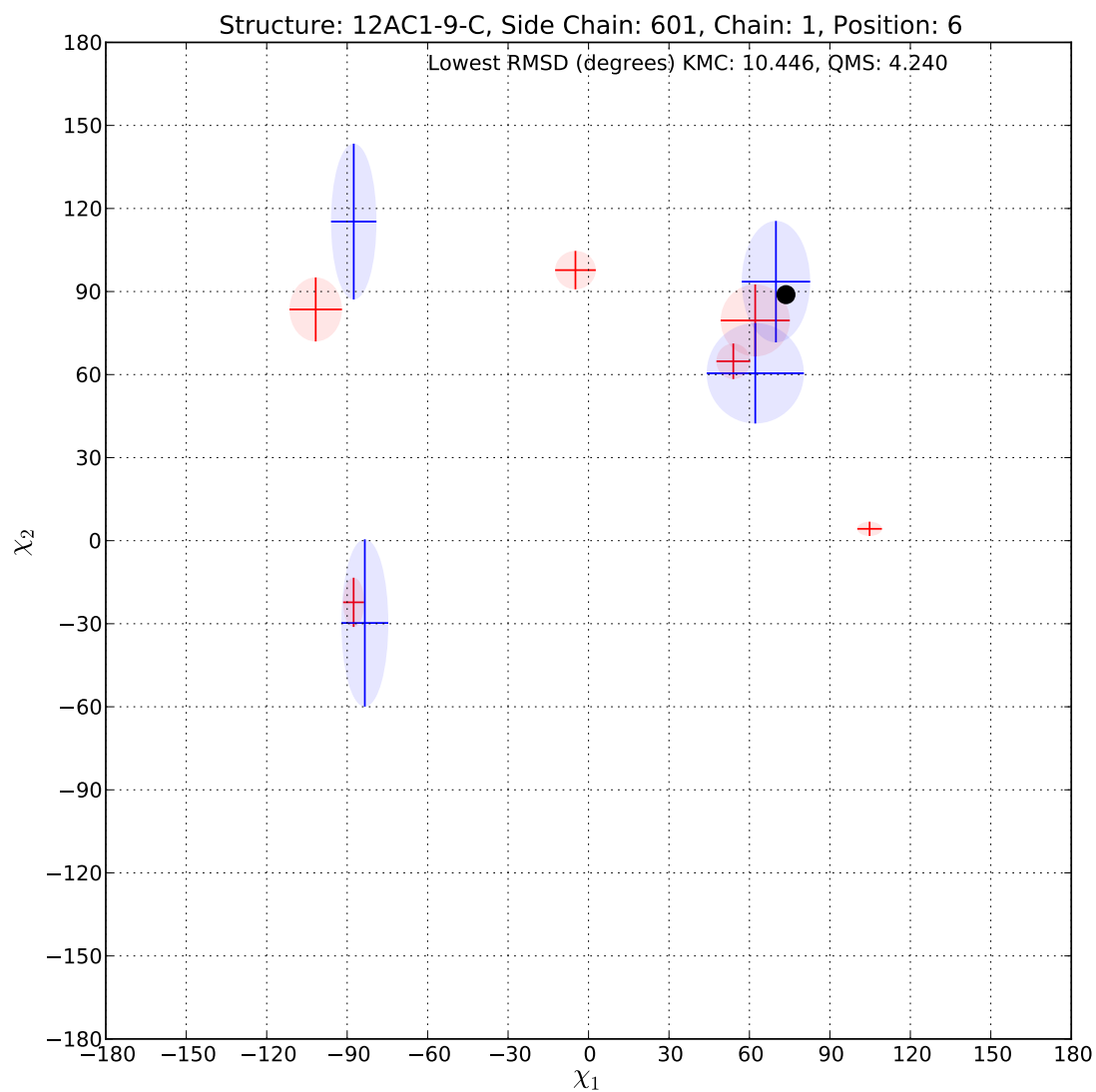


Figure S101: The rotamer library coverage plot for residue number 6 in chain 1 of peptoid databank structure 12AC1-9-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

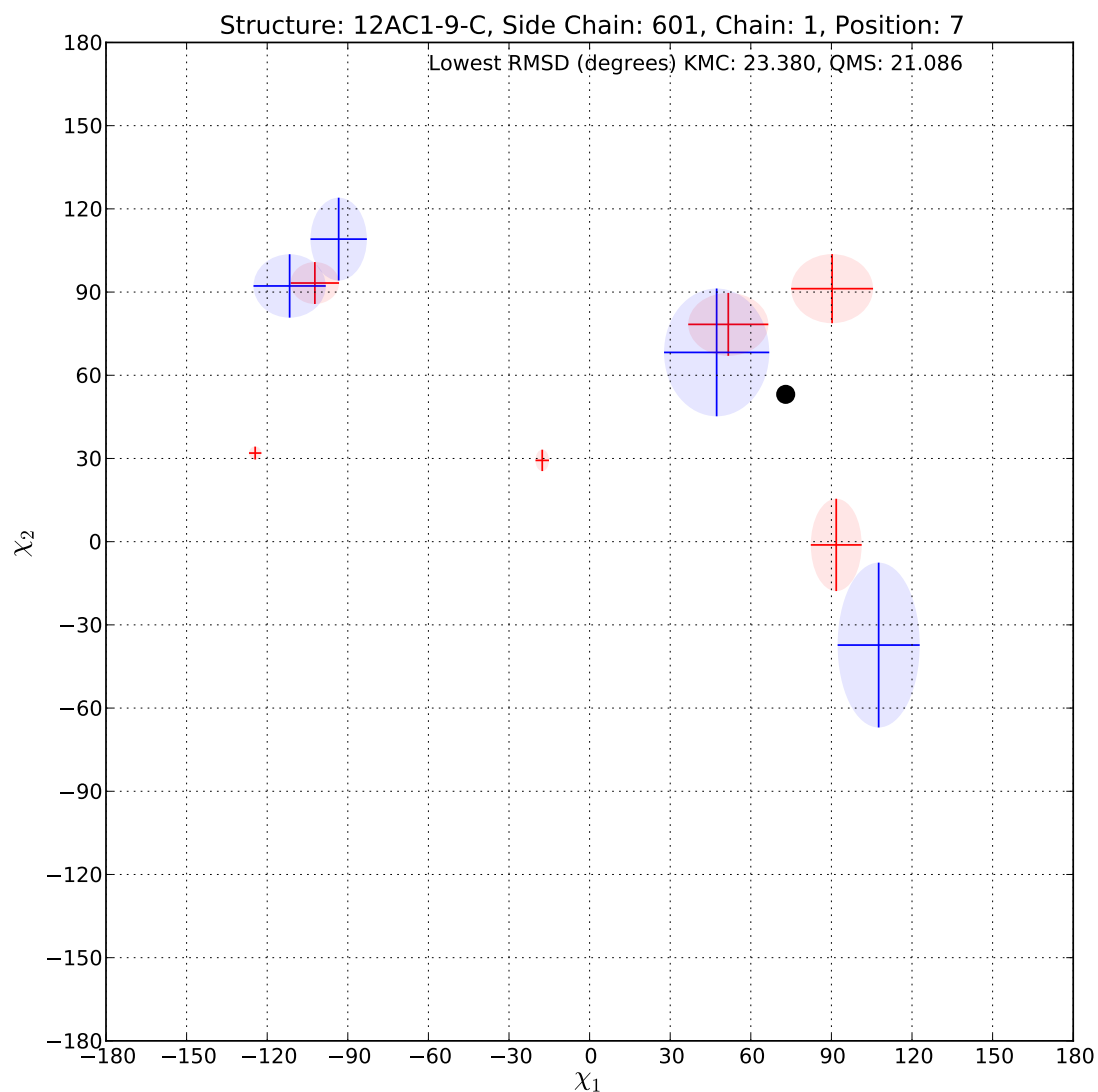


Figure S102: The rotamer library coverage plot for residue number 7 in chain 1 of peptoid databank structure 12AC1-9-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

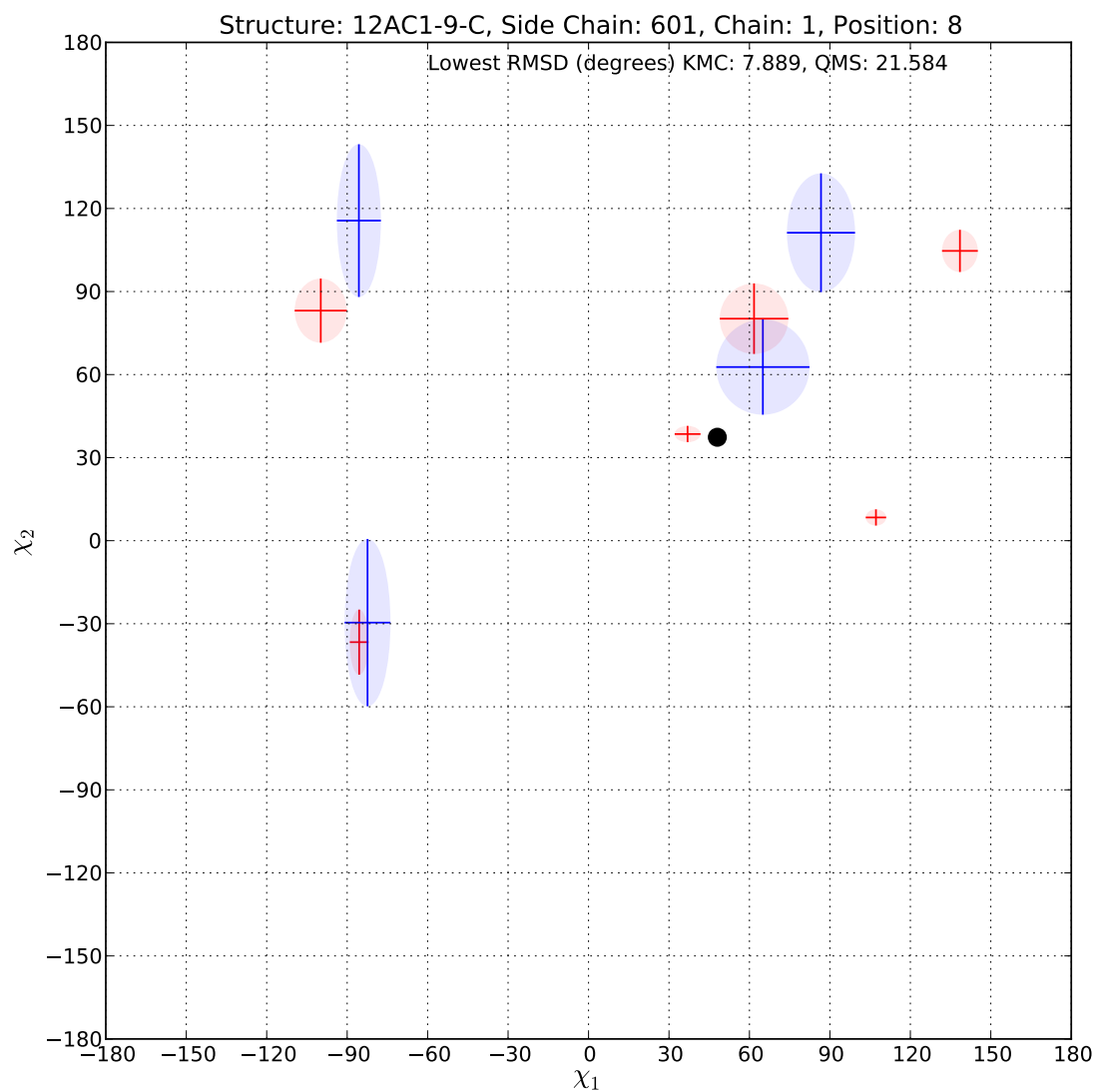


Figure S103: The rotamer library coverage plot for residue number 8 in chain 1 of peptoid databank structure 12AC1-9-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

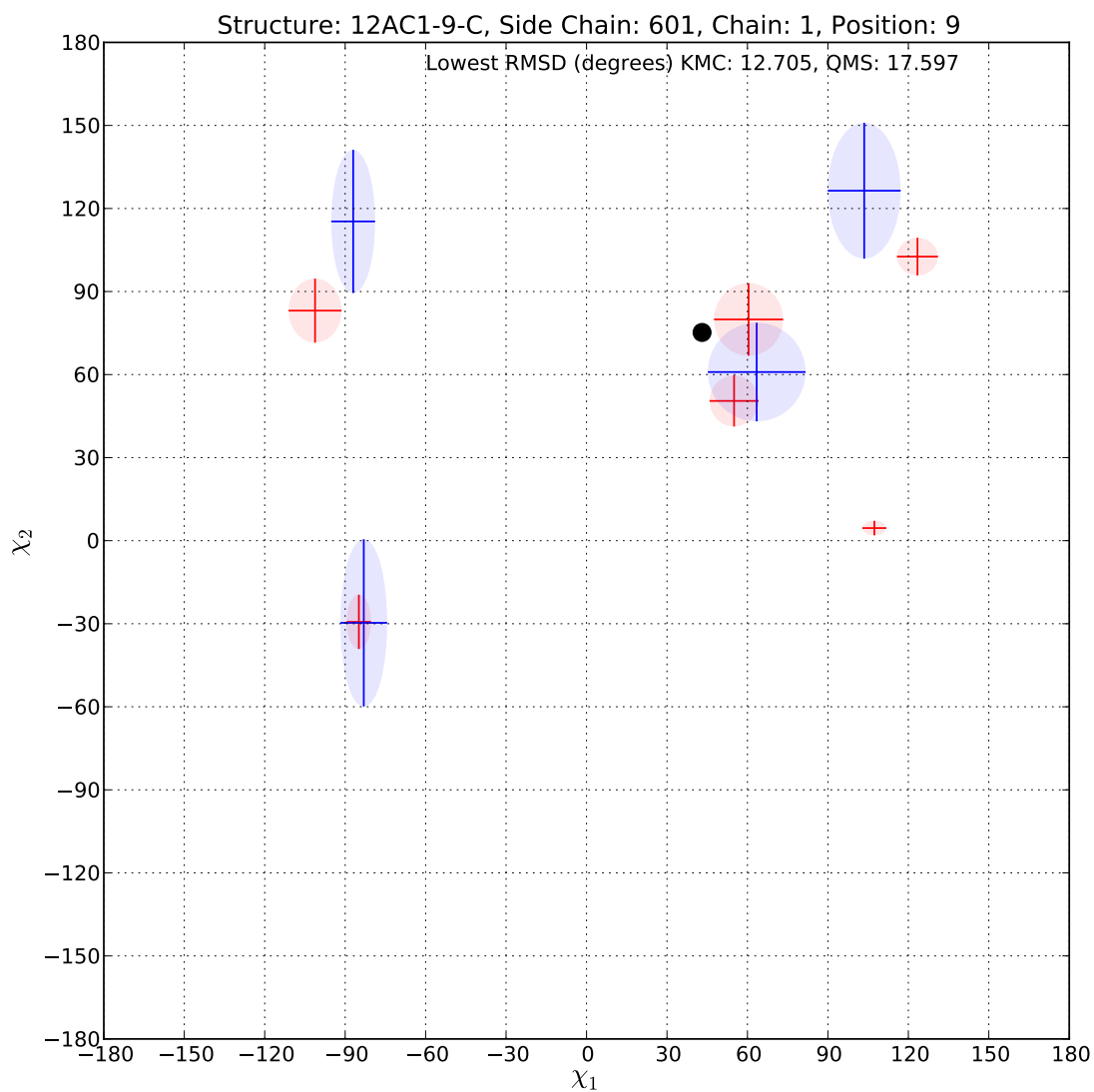


Figure S104: The rotamer library coverage plot for residue number 9 in chain 1 of peptoid databank structure 12AC1-9-C. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

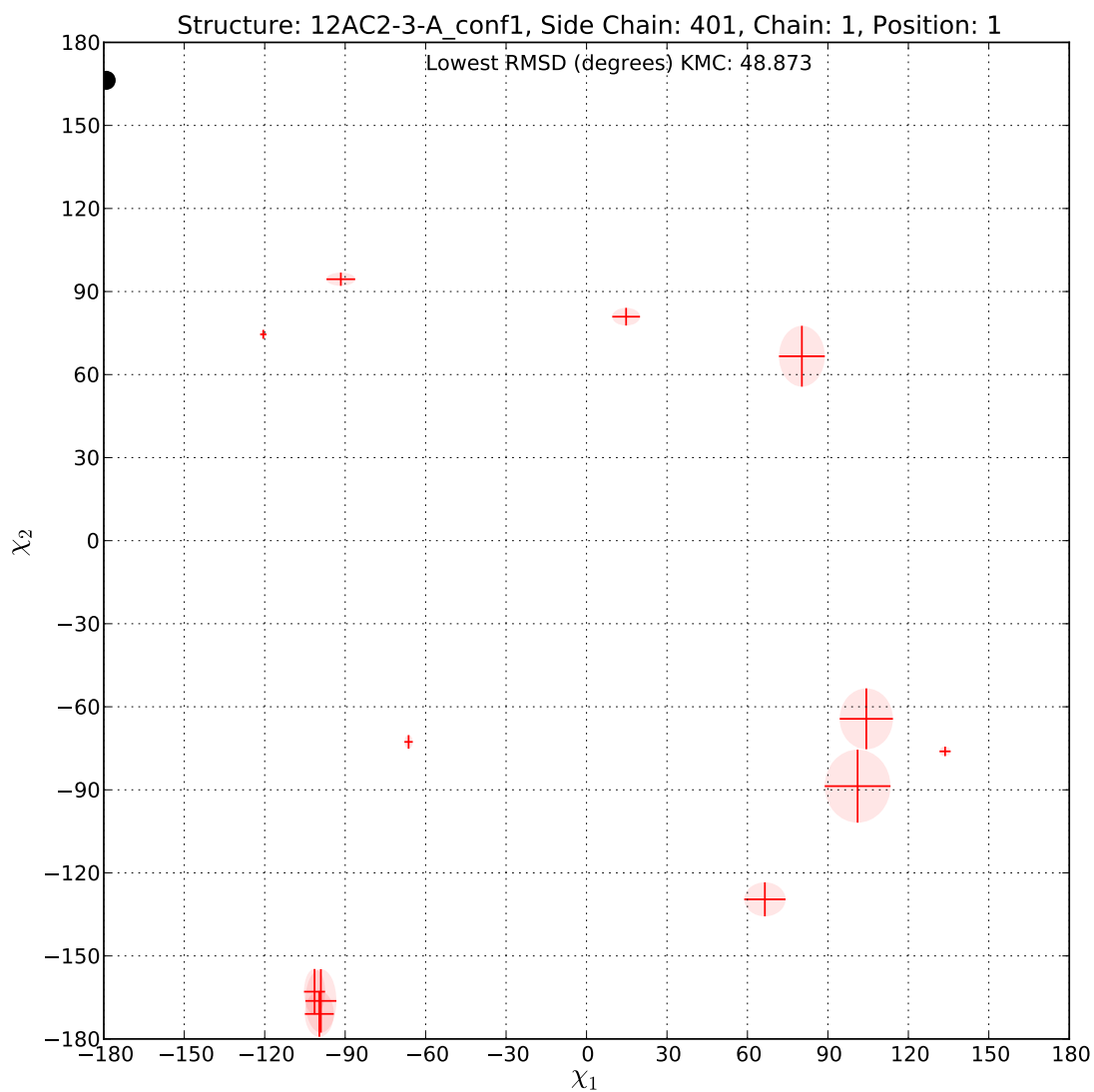


Figure S105: The rotamer library coverage plot for residue number 1 in chain 1 of peptoid databank structure 12AC2-3-A.conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

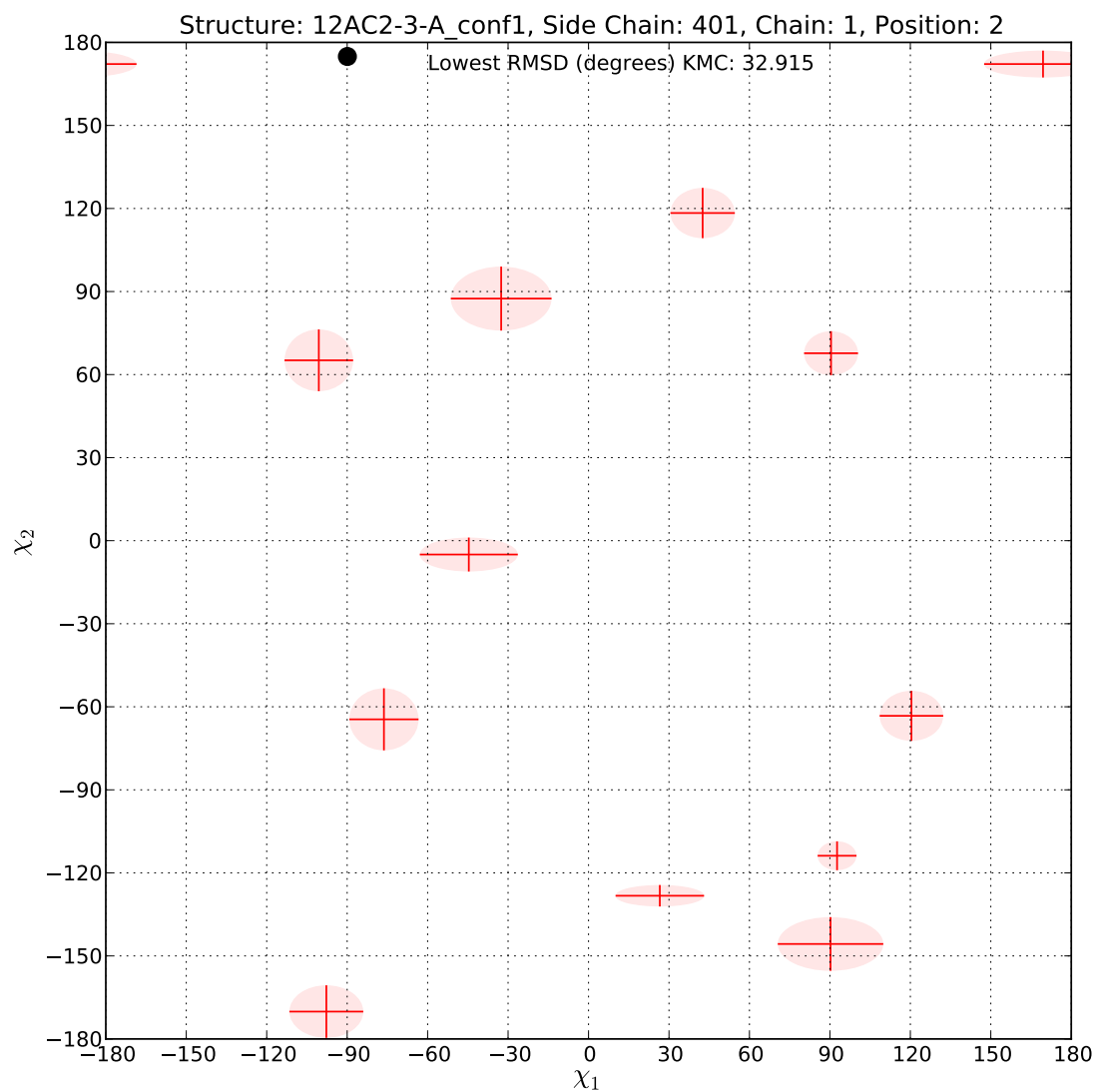


Figure S106: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 12AC2-3-A.conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

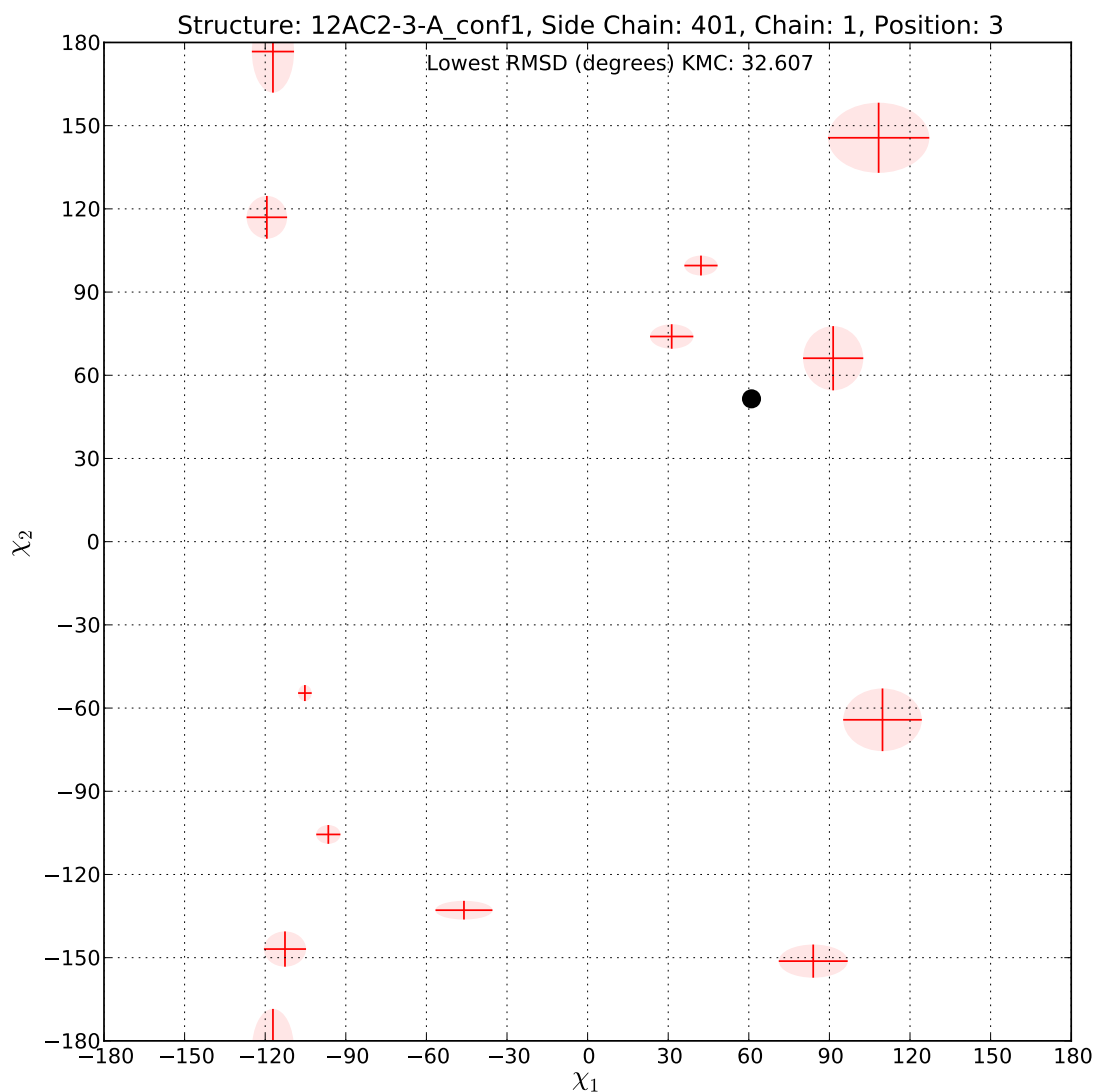


Figure S107: The rotamer library coverage plot for residue number 3 in chain 1 of peptoid databank structure 12AC2-3-A.conf1. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.

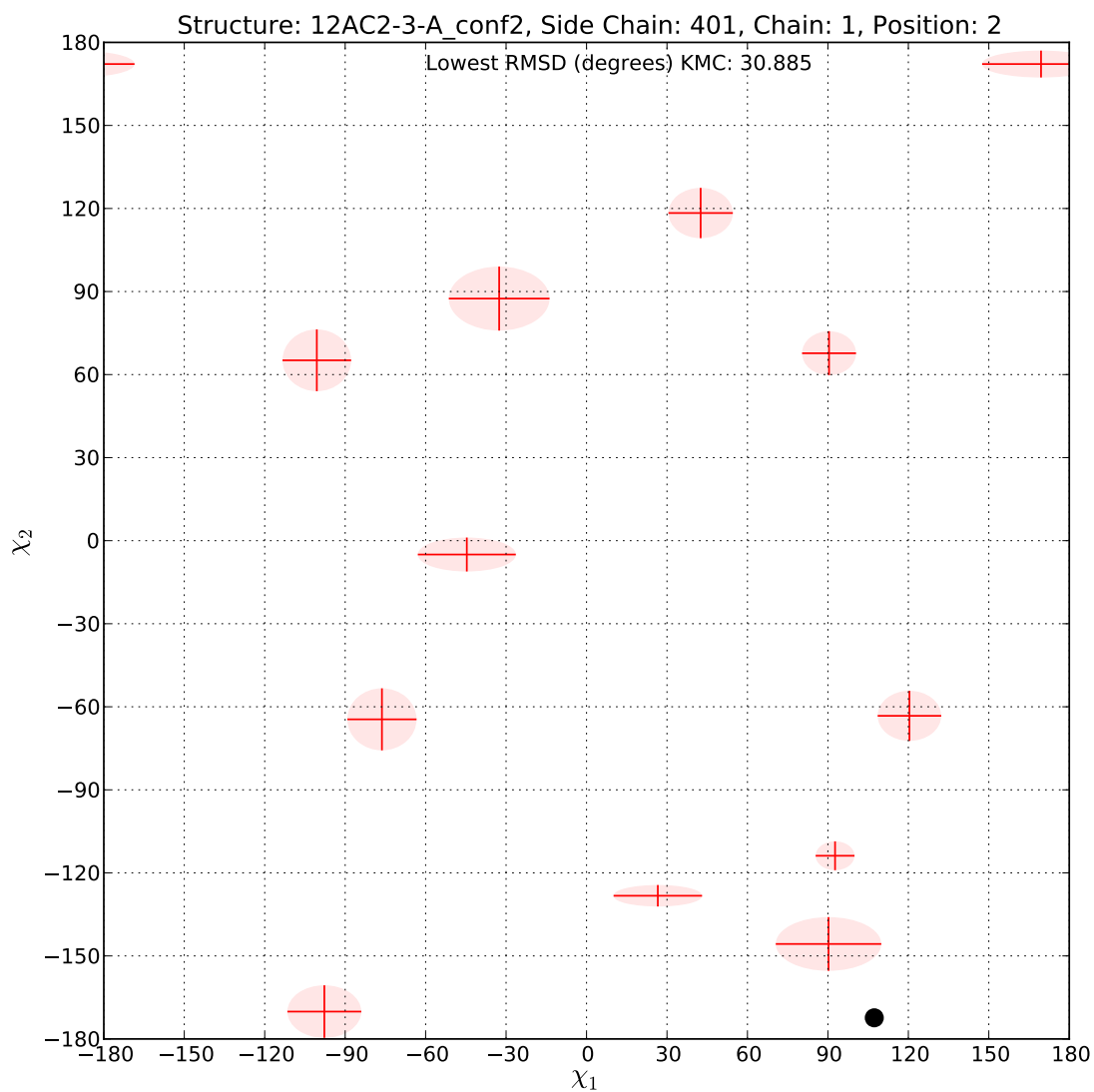


Figure S108: The rotamer library coverage plot for residue number 2 in chain 1 of peptoid databank structure 12AC2-3-A.conf2. Interpolated rotamers from the k-means clustering (KMC) method are shown as red ellipses and rotamers for the quantum mechanically-seeded (QMS) method are shown in blue. Experimental values shown as black circles.