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Duke Biochemistry
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Protein Geometry	Poor rotamers	8	3.10%	Goal: <0.3%
	Favored rotamers	234	90.70%	Goal: >98%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	287	96.63%	Goal: >98%
	C β deviations >0.25Å	3	1.09%	Goal: 0
	Bad bonds:	0 / 2372	0.00%	Goal: 0%
	Bad angles:	15 / 3225	0.47%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 13	0.00%	Expected: ≤ 1 per chain, or $\leq 5\%$
Low-resolution Criteria	CaBLAM outliers	2	0.7%	Goal: <1.0%
	CA Geometry outliers	0	0.00%	Goal: <0.5%
Additional validations	Chiral volume outliers	0/364		

In the two column results, the left column gives the raw count, right column gives the percentage.

Key to table colors and cutoffs here: [🔑](#)

#	Alt	Res	High B	Ramachandran	Rotamer	C β deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non-Trans: 0 of 298
A 3		PHE	0.76	-	Allowed (0.7%) <i>t80</i> chi angles: 218.8,54.8	0.10Å	-	-	-	-
A 4		ARG	0.74	Favored (49.34%) General / -110.2,136.5	Favored (5.8%) <i>mmt180</i> chi angles: 275.7,271,183.7,209.5	0.04Å	-	-	-	-
A 5		LYS	0.83	Allowed (0.52%) General / -68.6,93.5	Favored (4.9%) <i>mtpt</i> chi angles: 290.5,219.6,183.9,78.9	0.08Å	Favored (54.759%)	-	-	-
A 6		MET	0.88	Favored (39.25%) General / -94.6,132.5	Favored (3.1%) <i>mtm</i> chi angles: 298,193.7,328.5	0.17Å	Favored (45.772%)	-	-	-
A 7		ALA	0.94	Favored (24.17%) General / -82.3,156.8	-	0.08Å	Favored (36.995%)	-	-	-
A 8		PHE	0.93	Favored (88.7%) Pre-Pro / -59.8,141.9	Favored (70.7%) <i>m-80</i> chi angles: 290.6,287.2	0.06Å	Favored (17.032%)	-	OUTLIER(S) worst is CA-CB-CG: 4.6 σ	-
A 9		PRO	0.94	Favored (39.27%) Trans-Pro / -53.7,130.5	Favored (10.5%) <i>Cg_exo</i> chi angles: 346.6,27.4,328.7	0.09Å	Favored (46.801%)	-	-	-
A 10		SER	0.94	Favored (51.18%) General / -91.5,-7.1	Allowed (0.9%) <i>p</i> chi angles: 38.4	0.09Å	Favored (15.614%)	-	-	-

A 11	GLY	0.93	Favored (63.17%) Glycine / -56.3,-34.5	-	-	Favored (38.885%)	-	-	-	
A 12	LYS	0.91	Favored (73.87%) General / -67.3,-32.7	Favored (31%) <i>mttp</i> chi angles: 287.5,179.1,168.6,82	0.06Å	Favored (77.149%) alpha helix	-	-	-	
A 13	VAL	0.97	Favored (11.62%) Ile or Val / -82.9,-34.6	Favored (38%) <i>t</i> chi angles: 183.8	0.07Å	Favored (45.885%) alpha helix	-	-	-	
A 14	GLU	0.93	Favored (75.83%) General / -57.9,-38.5	Favored (42.3%) <i>mt-10</i> chi angles: 292.9,171.3,51.6	0.07Å	Favored (70.784%) alpha helix	-	-	-	
A 15	GLY	0.96	Favored (61.14%) Glycine / -74.7,-1.1	-	-	Favored (44.735%) alpha helix	-	-	-	
A 16	CYS	0.98	Favored (15.09%) General / -114.0,2.7	Favored (62.7%) <i>m</i> chi angles: 301.6	0.09Å	Favored (51.885%)	-	-	-	
A 17	MET	0.95	Favored (33.67%) General / -86.5,134.6	Favored (74.9%) <i>mmm</i> chi angles: 298.6,314,297.6	0.10Å	Favored (15.603%)	-	-	-	
A 18	VAL	0.97	Favored (19.98%) Ile or Val / -139.4,167.4	Favored (32.5%) <i>m</i> chi angles: 297.5	0.06Å	Favored (39.605%)	-	-	-	
A 19	GLN	0.93	Favored (50.96%) General / -109.0,134.9	Favored (58%) <i>tt0</i> chi angles: 179.3,183.7,33.7	0.10Å	Favored (49.078%) beta sheet	-	-	-	
A 20	VAL	0.97	Favored (72.88%) Ile or Val / -123.0,125.9	Favored (99.9%) <i>t</i> chi angles: 175.5	0.03Å	Favored (70.672%) beta sheet	-	-	-	
A 21	THR	0.95	Favored (53.69%) General / -121.8,130.8	Favored (23.5%) <i>m</i> chi angles: 307.9	0.09Å	Favored (55.438%)	-	-	-	
A 22	CYS	0.96	Favored (20.11%) General / -135.8,121.9	Favored (58.5%) <i>t</i> chi angles: 182.6	0.03Å	Favored (10.055%)	-	-	-	
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non-Trans: 0 of 298
A 23	GLY	0.92	Favored (35.11%) Glycine / 64.0,-126.9	-	-	Favored (49.543%)	-	-	-	
A 24	THR	0.92	Favored (37.15%) General / -102.8,3.9	Favored (75.1%) <i>p</i> chi angles: 60	0.02Å	Favored (9.262%)	-	-	-	
A 25	THR	0.92	Favored (45.01%) General / -102.8,122.7	Favored (5.6%) <i>m</i> chi angles: 287	0.07Å	Favored (26.497%)	-	-	-	
A	THR	0.93	Favored	Favored (10.1%) <i>m</i>	0.11Å	Favored	-	-	-	

26				(52.18%) General / -128.7,139.6	chi angles: 312.4		(21.229%)			
A 27	LEU	0.95		Favored (7.72%) General / -156.6,-178.9	Allowed (0.5%) <i>pp</i> chi angles: 43,63.6	0.12Å	Favored (16.039%) beta sheet	-	-	-
A 28	ASN	0.96		Favored (24.5%) General / -83.8,152.7	Favored (26%) <i>m-40</i> chi angles: 308,284.8	0.04Å	Favored (16.21%) beta sheet	-	-	-
A 29	GLY	0.99		Favored (24.29%) Glycine / -133.8,165.3	-	-	Favored (50.129%) beta sheet	-	-	-
A 30	LEU	0.98		Favored (33.9%) General / -110.3,117.5	Favored (27.9%) <i>tp</i> chi angles: 183.2,70.2	0.08Å	Favored (50.672%) beta sheet	-	-	-
A 31	TRP	0.94		Favored (20.31%) General / -101.7,108.7	Favored (22.1%) <i>t60</i> chi angles: 182.4,25.4	0.06Å	Favored (53.96%)	-	-	-
A 32	LEU	0.96		Favored (52.23%) General / -125.3,135.2	Favored (45.2%) <i>mt</i> chi angles: 299.7,167.1	0.14Å	CaBLAM Disfavored (1.975%)	-	-	-
A 33	ASP	0.94		Allowed (1.81%) General / 49.4,-122.9	Favored (13.1%) <i>m-30</i> chi angles: 311.7,304.9	0.20Å	CaBLAM Disfavored (3.231%)	-	OUTLIER(S) worst is CA- CB-CG: 4.2 σ	-
A 34	ASP	0.93		Favored (29.85%) General / -100.5,14.9	Favored (36.8%) <i>p0</i> chi angles: 71,170.6	0.08Å	Favored (9.996%)	-	-	-
A 35	VAL	0.96		Favored (57.95%) Ile or Val / -122.9,137.0	Allowed (0.9%) <i>p</i> chi angles: 50.2	0.12Å	Favored (37.047%)	-	-	-
A 36	VAL	0.98		Favored (67.43%) Ile or Val / -110.2,126.0	Favored (87.1%) <i>t</i> chi angles: 177.5	0.05Å	Favored (72.361%)	-	-	-
A 37	TYR	0.98		Favored (51.1%) General / -104.3,132.0	Favored (77.1%) <i>m-80</i> chi angles: 299.1,263.5	0.13Å	Favored (42.129%)	-	-	-
A 38	CYS	1		Favored (37.17%) Pre-Pro / -150.4,156.9	Favored (29.9%) <i>p</i> chi angles: 66.2	0.07Å	Favored (18.943%)	-	OUTLIER(S) worst is CA-C- N: 4.3 σ	-
A 39	PRO	1		Favored (30.37%) Trans-Pro / -49.1,135.3	Favored (54.1%) <i>Cg_exo</i> chi angles: 337.2,36.6,322.9	0.08Å	Favored (50.355%)	-	-	-
A 40	ARG	0.91		Favored (63.77%) General / -69.4,-20.6	Favored (27.7%) <i>ptt180</i> chi angles: 74.8,180.8,171.9,167.2	0.10Å	Favored (31.783%)	-	-	-
A 41	HIS	0.92		Allowed (1.37%) General / -67.2,2.8	Favored (4.5%) <i>p-80</i> chi angles: 74.7,248.3	0.11Å	Favored (7.247%)	-	OUTLIER(S) worst is ND1- CG-CD2: 4.5 σ	-
A	VAL	0.95		Favored	Favored (3.3%) <i>p</i> chi angles: 73.9	0.11Å	Favored	-	-	-

42				(45.11%) Ile or Val / -60.0,-30.2			(44.759%) three-ten			
#	Alt	Res	High B	Ramachandran	Rotamer	C β deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non- Trans: 0 of 298
A 43		ILE	0.94	Favored (14%) Ile or Val / -77.8,-13.2	Favored (9.9%) <i>pt</i> chi angles: 70.9,182.3	0.13Å	Favored (56.629%)	-	-	-
A 44		CYS	0.94	Favored (23.62%) General / -94.6,147.1	Favored (68.9%) <i>m</i> chi angles: 298.9	0.09Å	Favored (21.583%)	-	-	-
A 45		THR	0.79	Favored (9.46%) General / -106.5,168.0	Favored (44.9%) <i>p</i> chi angles: 55.3	0.14Å	Favored (29.74%)	-	-	-
A 46		SER	0.75	Favored (65.47%) General / -57.9,-29.9	Favored (64.8%) <i>p</i> chi angles: 58.3	0.11Å	Favored (44.27%)	-	-	-
A 47		GLU	0.66	Favored (71.57%) General / -65.2,-48.9	Favored (92.2%) <i>tt0</i> chi angles: 183.6,178.8,179.1	0.05Å	Favored (73.878%) alpha helix	-	-	-
A 48		ASP	0.59	Favored (36.17%) General / -92.6,9.1	Favored (54.8%) <i>p0</i> chi angles: 63.1,355.9	0.11Å	Favored (44.308%)	-	OUTLIER(S) worst is CA- CB-CG: 4.7 σ	-
A 49		MET	0.82	Favored (59.57%) General / -70.9,-10.4	Favored (96.9%) <i>mtp</i> chi angles: 293,180.8,70.2	0.06Å	CaBLAM Disfavored (3.832%)	-	-	-
A 50		LEU	0.8	Favored (95.94%) General / -64.0,-43.3	Favored (20.2%) <i>tp</i> chi angles: 190.4,57.7	0.06Å	Favored (15.726%)	-	-	-
A 51		ASN	0.81	Favored (6.79%) Pre-Pro / -137.3,53.5	OUTLIER (0%) chi angles: 236.8,112.2	0.10Å	Favored (13.615%)	-	-	-
A 52		PRO	0.91	Favored (45.02%) Trans-Pro / -66.8,137.3	Favored (78.7%) <i>Cg_endo</i> chi angles: 30.7,323.1,29.7	0.03Å	Favored (9.415%)	-	-	-
A 53		ASN	0.86	Favored (15.43%) General / -109.9,106.0	Favored (25%) <i>t0</i> chi angles: 182.2,291.5	0.03Å	Favored (58.213%) beta sheet	-	-	-
A 54		TYR	0.89	Favored (91.64%) General / -65.4,-39.0	Favored (55.5%) <i>m-80</i> chi angles: 284.5,100.1	0.09Å	Favored (52.317%)	-	-	-
A 55		GLU	0.85	Favored (90.08%) General / -60.5,-46.5	Favored (40.8%) <i>mp0</i> chi angles: 299.2,83.2,340	0.05Å	Favored (87.777%) alpha helix	-	-	-
A 56		ASP	0.86	Favored (97.74%) General / -63.8,-42.4	Favored (6.1%) <i>t70</i> chi angles: 199.5,76.9	0.10Å	Favored (84.213%) alpha helix	-	-	-
A		LEU	0.87	Favored	Favored (91.3%) <i>mt</i>	0.06Å	Favored	-	-	-

57				(90.64%) General / -65.6,-43.1	chi angles: 294.9,171.3		(90.231%) alpha helix			
A 58		LEU	0.89	Favored (77.77%) General / -69.5,-38.8	Favored (28.3%) <i>tp</i> chi angles: 188,60.3	0.09Å	Favored (75.611%) alpha helix	-	-	-
A 59		ILE	0.86	Favored (25.6%) Ile or Val / -65.3,-19.4	Favored (4.8%) <i>tt</i> chi angles: 197.3,154.2	0.10Å	Favored (68.89%) three-ten	-	-	-
A 60		ARG	0.81	Favored (42.22%) General / -87.3,4.6	Favored (71.3%) <i>mtt</i> -85 chi angles: 297.6,172,188.2,259.9	0.17Å	Favored (40.563%)	-	-	-
A 61		LYS	0.86	Favored (36.23%) General / -113.0,147.9	Favored (47.1%) <i>mmtt</i> chi angles: 309.3,281.1,175.6,186.9	0.09Å	Favored (28.961%)	-	-	-
A 62		SER	0.9	Favored (3.25%) General / -108.2,-177.2	Favored (49.2%) <i>p</i> chi angles: 74.7	0.06Å	Favored (22.706%)	-	-	-
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non-Trans: 0 of 298
A 63		ASN	0.9	Favored (79.54%) General / -57.5,-40.8	Favored (95.6%) <i>m</i> -40 chi angles: 289.8,333.3	0.12Å	Favored (39.412%)	-	-	-
A 64		HIS	0.87	Favored (59.76%) General / -74.7,-10.7	Favored (30.5%) <i>p90</i> chi angles: 68.8,76.5	0.18Å	Favored (56.692%) three-ten	-	-	-
A 65		ASN	0.91	Favored (65.58%) General / -67.3,-20.4	Favored (4.6%) <i>m110</i> chi angles: 285.7,65.5	0.12Å	Favored (57.822%)	-	-	-
A 66		PHE	0.94	Favored (47.77%) General / -104.7,123.5	Favored (92.9%) <i>m</i> -80 chi angles: 300,277.5	0.09Å	Favored (30.319%)	-	-	-
A 67		LEU	0.93	Favored (32.5%) General / -105.1,116.8	Allowed (1%) <i>tt</i> chi angles: 201.9,180.2	0.03Å	Favored (71.999%)	-	-	-
A 68		VAL	0.95	Favored (69.19%) Ile or Val / -112.5,128.4	Favored (46.6%) <i>t</i> chi angles: 182.2	0.02Å	Favored (67.668%) beta sheet	-	-	-
A 69		GLN	0.89	Favored (52.9%) General / -124.9,130.7	Favored (60.7%) <i>mt0</i> chi angles: 301.1,177.6,72.9	0.10Å	Favored (70.028%)	-	-	-
A 70		ALA	0.92	Favored (17.83%) General / -106.2,107.0	-	0.03Å	Favored (9.014%)	-	-	-
A 71		GLY	0.88	Favored (23.03%)	-	-	Favored (64.15%)	-	-	-

				Glycine / 59.4,-120.5						
A 72	ASN	0.82		Favored (53.32%) General / -95.6,4.2	OUTLIER (0.1%) chi angles: 78.9,129.5	0.09Å	Favored (12.73%)	-	OUTLIER(S) worst is CA- CB-CG: 5.0 σ	-
A 73	VAL	0.83		Favored (58.6%) Ile or Val / -106.2,121.4	Favored (59%) <i>t</i> chi angles: 170.6	0.03Å	Favored (30.849%)	-	-	-
A 74	GLN	0.86		Favored (55.66%) General / -68.5,139.4	Favored (33.6%) <i>tt0</i> chi angles: 168.8,176.6,338.3	0.12Å	Favored (35.658%) beta sheet	-	-	-
A 75	LEU	0.91		Favored (51.94%) General / -108.3,133.8	OUTLIER (0%) chi angles: 283.2,20.9	0.13Å	Favored (53%) beta sheet	-	-	-
A 76	ARG	0.85		Favored (34.64%) General / -85.8,127.8	Favored (22.5%) <i>ttm-80</i> chi angles: 172.7,189.6,307.6,295.9	0.04Å	Favored (44.161%) beta sheet	-	-	-
A 77	VAL	0.93		Favored (34.77%) Ile or Val / -72.5,127.8	Favored (40.4%) <i>t</i> chi angles: 183.3	0.08Å	Favored (46.374%)	-	-	-
A 78	ILE	0.93		Favored (5.35%) Ile or Val / -123.0,8.4	Allowed (1%) <i>pt</i> chi angles: 67,196.2	0.08Å	Favored (12.819%)	-	-	-
A 79	GLY	0.93		Favored (10.4%) Glycine / 179.2,152.2	-	-	Favored (15.811%)	-	-	-
A 80	HIS	0.91		Favored (35.01%) General / -147.9,150.9	Favored (43.4%) <i>p-80</i> chi angles: 59.9,271.6	0.08Å	Favored (59.888%)	-	-	-
A 81	SER	0.93		Favored (42.2%) General / -151.2,157.1	Favored (6.2%) <i>p</i> chi angles: 47.9	0.15Å	Favored (47.301%) beta sheet	-	-	-
A 82	MET	0.92		Favored (52.38%) General / -108.8,133.8	Favored (26.1%) <i>ttp</i> chi angles: 169.1,163.2,75.7	0.03Å	Favored (56.927%)	-	-	-
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			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non- Trans: 0 of 298
A 83	GLN	0.91		Favored (10.89%) General / -129.9,109.4	Favored (53.2%) <i>tt0</i> chi angles: 183.3,186.9,1.7	0.05Å	Favored (12.211%)	-	-	-
A 84	ASN	0.95		Allowed (1.49%) General / 54.0,-119.5	Favored (60.1%) <i>m-40</i> chi angles: 307.1,300.1	0.17Å	CaBLAM Disfavored (4.656%)	-	-	-
A 85	CYS	1		Favored (28.96%) General / -99.8,14.8	Favored (17.1%) <i>m</i> chi angles: 309.1	0.14Å	Favored (8.651%)	-	-	-
A 86	VAL	0.99		Favored (7.18%)	OUTLIER (0.2%) chi angles: 88.1	0.08Å	Favored (27.522%)	-	-	-

				Ile or Val / -107.1,157.9						
A 87	LEU	0.96		Favored (42.85%) General / -110.5,142.0	Favored (33.2%) <i>mt</i> chi angles: 305.4,170.3	0.18Å	Favored (61.819%)	-	-	-
A 88	LYS	0.92		Favored (26.15%) General / -112.1,113.7	Favored (54.8%) <i>mtmt</i> chi angles: 294.2,181.7,289.4,186.8	0.09Å	Favored (67.016%) beta sheet	-	-	-
A 89	LEU	0.94		Favored (40.24%) General / -105.6,119.9	Favored (43.9%) <i>mt</i> chi angles: 305,172.2	0.07Å	Favored (65.701%) beta sheet	-	-	-
A 90	LYS	0.91		Favored (34.41%) General / -83.1,128.3	OUTLIER (0%) chi angles: 316.2,250,98.3,250.3	0.08Å	Favored (58.564%) beta sheet	-	-	-
A 91	VAL	0.93		Favored (15.89%) Ile or Val / -117.7,162.2	Favored (6%) <i>m</i> chi angles: 288.3	0.09Å	Favored (35.404%)	-	-	-
A 92	ASP	0.9		Favored (57.25%) General / -78.7,-16.5	Favored (25.5%) <i>p0</i> chi angles: 63.8,331.9	0.14Å	Favored (55.32%)	-	OUTLIER(S) worst is CA- CB-CG: 6.9 σ	-
A 93	THR	0.89		Favored (50.37%) General / -113.4,123.6	Favored (62.6%) <i>m</i> chi angles: 303.4	0.06Å	Favored (26.534%)	-	-	-
A 94	ALA	0.91		Favored (34.85%) General / -83.0,135.4	-	0.02Å	Favored (38.513%)	-	-	-
A 95	ASN	0.92		Favored (43.32%) Pre-Pro / -67.6,117.0	Favored (48.3%) <i>t0</i> chi angles: 185.2,3.3	0.12Å	Favored (44.813%) beta sheet	-	-	-
A 96	PRO	0.92		Favored (14.98%) Trans-Pro / -78.3,-5.4	Favored (59.8%) <i>Cg_endo</i> chi angles: 26.4,325.5,29.5	0.07Å	Favored (59.94%)	-	-	-
A 97	LYS	0.88		Favored (20.95%) General / -111.7,11.0	Favored (2.1%) <i>mmtt</i> chi angles: 311.2,302.9,143.9,206.6	0.04Å	Favored (34.375%)	-	-	-
A 98	THR	0.94		Favored (7.02%) Pre-Pro / -57.7,113.8	Favored (34.1%) <i>m</i> chi angles: 306.1	0.11Å	Favored (29.919%)	-	-	-
A 99	PRO	0.96		Favored (15.87%) Trans-Pro / -72.1,171.9	Favored (58.7%) <i>Cg_endo</i> chi angles: 32,321,31.7	0.08Å	Favored (23.188%)	-	-	-
A 100	LYS	0.91		Favored (49.82%) General / -61.8,131.4	Favored (51%) <i>tttt</i> chi angles: 179.1,172.5,173.9,158.4	0.10Å	Favored (13.464%)	-	-	-
A 101	TYR	0.94		Favored (25.79%) General / -145.5,166.4	Favored (30.4%) <i>p90</i> chi angles: 75.3,94.6	0.15Å	Favored (37.123%) beta sheet	-	-	-
A 102	LYS	0.91		Favored (33.56%)	Allowed (1.8%) <i>mttm</i>	0.11Å	Favored (57.583%)	-	-	-

				General / -141.5,163.2	chi angles: 290.6,171.8,198.1,348.9		beta sheet			
#	Alt	Res	High B	Ramachandran	Rotamer	C β deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non-Trans: 0 of 298
A 103		PHE	0.96	Favored (55.52%) General / -110.7,130.6	Favored (21.2%) <i>m</i> -10 chi angles: 291.6,344.4	0.04Å	Favored (48.71%) beta sheet	-	-	-
A 104		VAL	0.97	Favored (52.24%) Ile or Val / -134.0,137.4	Favored (60%) <i>t</i> chi angles: 170.8	0.02Å	Favored (59.371%) beta sheet	-	-	-
A 105		ARG	0.93	Favored (28.37%) General / -96.0,116.0	Favored (64.3%) <i>ttt90</i> chi angles: 185.8,176.1,177.4,87.8	0.01Å	Favored (60.955%) beta sheet	-	-	-
A 106		ILE	0.96	Favored (3.3%) Ile or Val / -85.6,159.3	Allowed (1.6%) <i>pt</i> chi angles: 54.3,145.9	0.07Å	Favored (27.467%)	-	-	-
A 107		GLN	0.93	Favored (51.38%) Pre-Pro / -87.8,152.5	Favored (25.1%) <i>mm110</i> chi angles: 286.3,288.8,111.1	0.02Å	Favored (23.113%)	-	-	-
A 108		PRO	0.99	Favored (12.75%) Trans-Pro / -45.8,136.9	Favored (84.1%) <i>Cg_exo</i> chi angles: 334.2,37.6,325.1	0.08Å	Favored (25.235%)	-	-	-
A 109		GLY	0.98	Favored (50.04%) Glycine / 95.2,-20.3	-	-	Favored (68.225%)	-	-	-
A 110		GLN	0.95	Favored (37.69%) General / -77.0,146.0	Favored (50%) <i>tp40</i> chi angles: 174.1,57.4,32.3	0.08Å	Favored (39.709%)	-	-	-
A 111		THR	0.97	Favored (15.26%) General / -98.2,158.9	Favored (20.6%) <i>p</i> chi angles: 50.8	0.05Å	Favored (27.263%) beta sheet	-	-	-
A 112		PHE	0.97	Favored (26.2%) General / -163.0,162.8	Favored (25.3%) <i>p90</i> chi angles: 55.7,98.2	0.10Å	Favored (31.813%) beta sheet	-	-	-
A 113		SER	0.96	Favored (31.93%) General / -95.6,139.4	Favored (16.1%) <i>m</i> chi angles: 306	0.25Å	Favored (42.659%) beta sheet	-	OUTLIER(S) worst is C-CA-CB: 4.6 σ	-
A 114		VAL	0.97	Favored (67.41%) Ile or Val / -110.2,126.6	Favored (83.2%) <i>t</i> chi angles: 173.4	0.08Å	Favored (66.83%) beta sheet	-	-	-
A 115		LEU	0.96	Favored (18.57%) General / -94.9,106.6	Favored (57.5%) <i>tp</i> chi angles: 181.9,59.7	0.03Å	Favored (66.09%) beta sheet	-	-	-
A 116		ALA	0.95	Favored (35.28%) General / -81.7,132.0	-	0.07Å	Favored (45.099%) beta sheet	-	-	-
A 117		CYS	0.97	Favored (41.11%)	Favored (78%) <i>m</i> chi angles: 296.3	0.16Å	Favored (58.071%)	-	-	-

				General / -140.8,148.8						
A 118		TYR	0.92	Favored (23.76%) General / -135.4,124.1	Favored (96.9%) <i>m</i> - 80 chi angles: 293.8,269	0.05Å	Favored (19.715%)	-	-	-
A 119		ASN	0.9	Favored (28.21%) General / 50.9,42.5	Favored (49.3%) <i>m</i> - 40 chi angles: 286.9,4.3	0.17Å	Favored (39.45%)	-	-	-
A 120		GLY	0.95	Favored (85.54%) Glycine / 79.1,1.6	-	-	Favored (83.529%)	-	-	-
A 121		SER	0.91	Favored (38.06%) Pre-Pro / -110.3,122.6	Favored (28.4%) <i>t</i> chi angles: 173.1	0.10Å	Favored (32.812%)	-	-	-
A 122		PRO	0.94	Favored (22.64%) Trans-Pro / -57.1,126.6	Favored (61.5%) <i>Cg_exo</i> chi angles: 335.9,37.7,323	0.07Å	Favored (35.181%)	-	-	-
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non- Trans: 0 of 298
A 123		SER	0.9	Favored (7.88%) General / -112.7,-28.2	Favored (62.9%) <i>p</i> chi angles: 58.1	0.07Å	Favored (20.43%)	-	-	-
A 124		GLY	0.93	Favored (24.68%) Glycine / -174.4,157.2	-	-	Favored (41.6%)	-	-	-
A 125		VAL	0.93	Favored (53.88%) Ile or Val / -125.3,138.6	Favored (10%) <i>p</i> chi angles: 64.2	0.07Å	Favored (48.461%)	-	-	-
A 126		TYR	0.93	Favored (27.81%) General / -146.2,165.9	Favored (43.8%) <i>p90</i> chi angles: 59.2,95.4	0.15Å	Favored (47.719%) beta sheet	-	-	-
A 127		GLN	0.91	Favored (53.46%) General / -112.2,135.0	Favored (24.8%) <i>tp40</i> chi angles: 181.1,72.7,358.3	0.14Å	Favored (35.307%) beta sheet	-	-	-
A 128		CYS	0.96	Favored (22.19%) General / -143.8,167.5	Favored (19.7%) <i>p</i> chi angles: 58.1	0.04Å	Favored (41.27%) beta sheet	-	-	-
A 129		ALA	0.96	Favored (38.11%) General / -110.2,144.9	-	0.08Å	Favored (33.601%) beta sheet	-	-	-
A 130		MET	0.96	Favored (21.32%) General / -71.0,123.1	Favored (37.3%) <i>ttm</i> chi angles: 184,165.2,285.5	0.05Å	Favored (39.61%) beta sheet	-	-	-
A 131		ARG	0.92	Favored (89.13%) Pre-Pro / -66.7,155.5	Favored (26%) <i>mmm160</i> chi angles: 299.8,311.3,306.5,166.5	0.02Å	Favored (47.099%)	-	-	-
A 132		PRO	0.98	Favored (29.58%)	Favored (97%) <i>Cg_exo</i>	0.15Å	Favored (92.89%)	-	-	-

				Trans-Pro / -51.7,-28.4	chi angles: 332.7,36.5,327.8					
A 133	ASN	0.93		Favored (28.58%) General / -87.5,7.6	Favored (39.6%) <i>p0</i> chi angles: 70.4,1.2	0.07Å	Favored (49.874%)	-	-	-
A 134	PHE	0.97		Allowed (1.74%) General / 80.8,2.2	Favored (92.5%) <i>m-80</i> chi angles: 295.5,85.9	0.18Å	CaBLAM Disfavored (3.546%)	-	-	-
A 135	THR	0.98		Favored (15.16%) General / -86.2,167.1	Favored (18.8%) <i>p</i> chi angles: 73.1	0.18Å	Favored (37.703%)	-	-	-
A 136	ILE	0.96		Favored (47.87%) Ile or Val / -124.3,140.3	Allowed (0.7%) <i>mp</i> chi angles: 290.3,106.3	0.07Å	Favored (50.115%) beta sheet	-	-	-
A 137	LYS	0.87		Favored (8.72%) General / -92.1,93.4	Allowed (1.4%) <i>mtp</i> chi angles: 298,185.1,111.2,44.2	0.02Å	Favored (18.405%) beta sheet	-	-	-
A 138	GLY	0.89		Favored (16.13%) Glycine / -113.3,-165.5	-	-	Favored (41.951%) beta sheet	-	-	-
A 139	SER	0.82		Favored (2.85%) General / -136.9,93.5	Allowed (1.6%) <i>t</i> chi angles: 202.3	0.04Å	CaBLAM Disfavored (1.587%) try beta sheet	-	-	-
A 140	PHE	0.82		Favored (49.15%) General / -125.3,129.0	Favored (63.1%) <i>m-80</i> chi angles: 288.3,107.9	0.05Å	Favored (28.048%)	-	-	-
A 141	LEU	0.77		Favored (5.04%) General / -108.9,176.6	Favored (33.4%) <i>mt</i> chi angles: 292,160.4	0.08Å	Favored (6.579%)	-	-	-
A 142	ASN	0.72		Favored (41.9%) General / -58.1,129.4	Favored (5.9%) <i>p0</i> chi angles: 75.5,309.3	0.18Å	CaBLAM Disfavored (4.887%)	-	-	-
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non- Trans: 0 of 298
A 143	GLY	0.84		Favored (48.79%) Glycine / 102.7,-0.8	-	-	Favored (67.136%)	-	-	-
A 144	SER	0.93		Favored (48.68%) General / -96.4,-0.9	Favored (99.9%) <i>p</i> chi angles: 65.5	0.10Å	Favored (7.502%)	-	-	-
A 145	CYS	0.96		Favored (52.79%) General / -59.6,142.5	Favored (48.3%) <i>m</i> chi angles: 303.7	0.10Å	Favored (7.443%)	-	-	-
A 146	GLY	0.98		Favored (84.89%) Glycine / 85.5,-5.0	-	-	Favored (68.699%)	-	-	-
A 147	SER	0.97		Favored (58.83%) General / -62.9,140.9	Favored (42.9%) <i>m</i> chi angles: 290.2	0.16Å	Favored (36.382%)	-	-	-

A 148	VAL	0.99	Favored (16.51%) Ile or Val / -115.1,153.9	Favored (27.7%) <i>m</i> chi angles: 298.8	0.12Å	Favored (41.09%) beta sheet	-	-	-	
A 149	GLY	0.99	Favored (17.85%) Glycine / -111.1,148.4	-	-	Favored (41.037%) beta sheet	-	-	-	
A 150	PHE	0.97	Favored (39.82%) General / -156.7,162.5	Favored (32.8%) <i>p90</i> chi angles: 60.2,99.6	0.05Å	Favored (41.719%) beta sheet	-	-	-	
A 151	ASN	0.95	Favored (40.42%) General / -125.0,154.9	Favored (44.9%) <i>m-40</i> chi angles: 286.9,271.8	0.04Å	Favored (55.498%) beta sheet	-	-	-	
A 152	ILE	0.93	Favored (68.39%) Ile or Val / -124.8,124.7	Favored (9.6%) <i>mt</i> chi angles: 300,189.9	0.04Å	Favored (49.691%)	-	-	-	
A 153	ASP	0.9	Favored (23.05%) General / -127.0,117.7	Favored (3.4%) <i>p0</i> chi angles: 51.4,280.4	0.08Å	Favored (12.969%)	-	-	-	
A 154	TYR	0.77	Favored (2.22%) General / 39.6,57.1	Favored (20.6%) <i>m-80</i> chi angles: 313.4,298.8	0.14Å	Favored (15.845%)	-	-	-	
A 155	ASP	0.86	Allowed (1.4%) General / 69.5,-4.3	Favored (41.6%) <i>m-30</i> chi angles: 275.1,174.7	0.31Å	CaBLAM Disfavored (2.046%)	-	-	-	
A 156	CYS	0.97	Favored (37.44%) General / -92.9,132.0	Favored (31%) <i>t</i> chi angles: 189.4	0.06Å	Favored (29.643%)	-	-	-	
A 157	VAL	0.95	Favored (26.92%) Ile or Val / -96.0,111.8	Favored (48.8%) <i>t</i> chi angles: 181.7	0.03Å	Favored (68.141%) beta sheet	-	-	-	
A 158	SER	0.95	Favored (16.18%) General / -94.1,104.1	Favored (5.2%) <i>m</i> chi angles: 281.1	0.10Å	Favored (69.861%) beta sheet	-	-	-	
A 159	PHE	0.97	Favored (33.77%) General / -77.8,128.3	Favored (88.7%) <i>m-80</i> chi angles: 294.3,282.4	0.10Å	Favored (26.935%)	-	-	-	
A 160	CYS	1	Favored (5.16%) General / -126.1,-17.8	Favored (17.8%) <i>p</i> chi angles: 57.2	0.06Å	Favored (17.408%)	-	-	-	
A 161	TYR	0.99	Favored (30.97%) General / -143.5,142.0	Favored (89.1%) <i>t80</i> chi angles: 179.4,80.3	0.07Å	Favored (27.85%)	-	-	-	
A 162	MET	0.98	Favored (49.62%) General / -127.7,133.6	Favored (44.1%) <i>ttm</i> chi angles: 177.1,169,282.2	0.05Å	Favored (40.474%)	-	-	-	
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non-Trans: 0 of 298

A 163	HIS	0.96	Favored (36.19%) General / -79.9,133.2	Favored (56.6%) <i>t70</i> chi angles: 184.4,55.3	0.03Å	Favored (26.853%)	-	OUTLIER(S) worst is ND1- CG-CD2: 4.8 σ	-
A 164	HIS	0.95	Favored (2.59%) General / -123.0,-38.6	Favored (19%) <i>m90</i> chi angles: 279.5,62.4	0.10Å	Favored (7.775%)	-	OUTLIER(S) worst is ND1- CG-CD2: 4.2 σ	-
A 165	MET	0.92	Favored (27.64%) General / -162.0,160.4	Allowed (1.5%) <i>ptm</i> chi angles: 49.8,177.9,251.8	0.04Å	Favored (17.991%)	-	-	-
A 166	GLU	0.88	Favored (37.87%) General / -101.3,138.8	Favored (15.8%) <i>mp0</i> chi angles: 293.4,63,47.6	0.11Å	Favored (46.87%)	-	-	-
A 167	LEU	0.89	Favored (19.84%) Pre-Pro / -99.9,162.8	Favored (44.7%) <i>mt</i> chi angles: 285.1,164.1	0.03Å	Favored (35.703%)	-	-	-
A 168	PRO	0.85	Favored (69.58%) Trans-Pro / -58.4,-24.6	Favored (55.2%) <i>Cg_exo</i> chi angles: 328.1,36.2,333.2	0.05Å	Favored (57.618%)	-	-	-
A 169	THR	0.85	Favored (35.77%) General / -88.7,7.0	Favored (17.6%) <i>p</i> chi angles: 49.4	0.04Å	Favored (43.518%)	-	-	-
A 170	GLY	0.89	Favored (85.43%) Glycine / 81.8,9.5	-	-	Favored (83.319%)	-	-	-
A 171	VAL	0.93	Allowed (1.42%) Ile or Val / -95.6,169.3	Favored (28.1%) <i>m</i> chi angles: 300.9	0.08Å	Favored (36.933%)	-	-	-
A 172	HIS	0.93	Favored (37.03%) General / -119.0,152.1	Favored (52.1%) <i>m90</i> chi angles: 303.7,93	0.04Å	Favored (47.041%) beta sheet	-	OUTLIER(S) worst is CA- CB-CG: 4.6 σ	-
A 173	ALA	0.98	Favored (43.09%) General / -140.4,149.8	-	0.06Å	Favored (37.509%) beta sheet	-	-	-
A 174	GLY	1	Favored (33.18%) Glycine / -169.3,-169.9	-	-	Favored (51.429%) beta sheet	-	-	-
A 175	THR	1	Favored (15.29%) General / -120.8,165.4	Favored (76.2%) <i>p</i> chi angles: 61.2	0.05Å	Favored (33.462%)	-	-	-
A 176	ASP	0.99	Favored (4.14%) General / -73.3,179.0	Favored (23%) <i>p0</i> chi angles: 57.5,31.5	0.13Å	Favored (36.596%)	-	-	-
A 177	LEU	0.98	Favored (10.75%) General / -84.9,10.8	Favored (2.8%) <i>mm</i> chi angles: 275,287.1	0.12Å	CaBLAM Disfavored (4.076%)	-	-	-
A 178	GLU	0.95	Favored (38.27%) General / -99.2,-1.8	Favored (20.8%) <i>mt-10</i> chi angles: 292.4,199.4,120.2	0.04Å	Favored (12.757%)	-	-	-
A 179	GLY	0.99	Favored (75.63%)	-	-	Favored (88.459%)	-	-	-

Glycine / 84.8,12.0

A 180	ASN	0.98		Favored (35.85%) General / -91.1,125.3	Favored (59.1%) <i>t0</i> chi angles: 186.1,336.3	0.06Å	Favored (31.483%)	-	-	-
A 181	PHE	0.98		Favored (39.39%) General / -55.9,141.3	Favored (5.8%) <i>m-80</i> chi angles: 267.5,89.6	0.14Å	Favored (23.233%)	-	-	-
A 182	TYR	0.98		Favored (23.74%) General / -84.8,117.3	Favored (67.8%) <i>m-80</i> chi angles: 288.3,283.9	0.05Å	Favored (6.617%)	-	-	-
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non-Trans: 0 of 298
A 183	GLY	0.98		Favored (43.82%) Glycine / 90.4,179.4	-	-	Favored (39.77%)	-	-	-
A 184	PRO	0.96		Favored (2.31%) Trans-Pro / -89.1,59.7	Favored (38.1%) <i>Cg_endo</i> chi angles: 34.1,321.8,27.4	0.08Å	CaBLAM Outlier (0.329%)	-	-	-
A 185	PHE	0.95		Favored (41.07%) General / -120.9,150.4	Favored (51%) <i>m-80</i> chi angles: 303.7,296.5	0.07Å	Favored (23.371%)	-	-	-
A 186	VAL	0.94		Favored (33.87%) Ile or Val / -128.8,146.6	Favored (30.8%) <i>m</i> chi angles: 296.8	0.03Å	Favored (45.428%)	-	-	-
A 187	ASP	0.93		Favored (5.66%) General / -80.1,66.6	Favored (9.1%) <i>p0</i> chi angles: 48.6,351.7	0.20Å	CaBLAM Disfavored (2.662%)	-	OUTLIER(S) worst is CA-CB-CG: 4.2 σ	-
A 188	ARG	0.82		Favored (35.2%) General / -159.6,161.6	Allowed (1.1%) <i>ptt-90</i> chi angles: 49.8,218.4,195.8,239	0.10Å	Favored (7.871%)	-	-	-
A 189	GLN	0.8		Favored (7.87%) General / -84.2,92.2	OUTLIER (0.1%) chi angles: 50.4,141.2,183.4	0.12Å	CaBLAM Disfavored (4.643%)	-	-	-
A 190	THR	0.8		Allowed (1.88%) General / -108.0,-171.5	Favored (54.8%) <i>p</i> chi angles: 64.9	0.04Å	Favored (21.502%)	-	-	-
A 191	ALA	0.73		Favored (6.41%) General / -88.3,16.4	-	0.10Å	CaBLAM Disfavored (2.213%)	-	-	-
A 192	GLN	0.78		Favored (40.43%) General / -57.9,144.1	Favored (17.6%) <i>pt0</i> chi angles: 64.6,192.4,320	0.09Å	Favored (13.378%)	-	-	-
A 193	ALA	0.84		Favored (46.82%) General / -139.5,152.3	-	0.09Å	Favored (34.983%)	-	-	-
A 194	ALA	0.85		Favored (52.81%) General / -59.4,132.0	-	0.07Å	Favored (39.853%)	-	-	-

A 195	GLY	0.84		Favored (30.6%) Glycine / -72.6,-177.1	-	-	Favored (41.644%)	-	-	-
A 196		THR	0.83	Favored (55.23%) General / -59.6,141.3	Favored (21.3%) <i>p</i> chi angles: 50.9	0.09Å	Favored (11.398%)	-	-	-
A 197		ASP	0.86	Favored (42.76%) General / -126.2,154.8	Favored (11.5%) <i>t70</i> chi angles: 201.9,45.5	0.04Å	Favored (64.783%)	-	-	-
A 198		THR	0.92	Favored (38.12%) General / -126.2,157.5	Favored (2.7%) <i>p</i> chi angles: 42.9	0.07Å	Favored (33.724%)	-	-	-
A 199		THR	0.96	Favored (45.75%) General / -72.4,135.2	Favored (90.5%) <i>m</i> chi angles: 298.8	0.04Å	Favored (24.862%)	-	-	-
A 200		ILE	0.96	Allowed (1.32%) Ile or Val / -78.7,90.7	Favored (9.9%) <i>mt</i> chi angles: 309.4,157.5	0.08Å	Favored (43.73%) beta sheet	-	-	-
A 201		THR	0.99	Favored (73.58%) General / -55.4,-42.2	Favored (33.7%) <i>m</i> chi angles: 306.2	0.05Å	Favored (47.933%)	-	-	-
A 202		VAL	0.99	Favored (86.02%) Ile or Val / -60.6,-40.9	Favored (9.8%) <i>p</i> chi angles: 64.1	0.13Å	Favored (89.283%) alpha helix	-	-	-
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non-Trans: 0 of 298
A 203		ASN	0.94	Favored (76.53%) General / -69.7,-40.1	Favored (31%) <i>m-40</i> chi angles: 289.7,7.5	0.04Å	Favored (92.334%) alpha helix	-	-	-
A 204		VAL	0.96	Favored (94.63%) Ile or Val / -59.7,-45.3	Favored (76.3%) <i>t</i> chi angles: 178.2	0.05Å	Favored (90.843%) alpha helix	-	-	-
A 205		LEU	0.97	Favored (98.94%) General / -62.2,-42.0	Favored (75.5%) <i>mt</i> chi angles: 291.1,166.2	0.04Å	Favored (95.85%) alpha helix	-	-	-
A 206		ALA	0.98	Favored (88.64%) General / -58.4,-44.0	-	0.06Å	Favored (98.178%) alpha helix	-	-	-
A 207		TRP	0.92	Favored (86.41%) General / -65.6,-37.3	Favored (82.9%) <i>t60</i> chi angles: 183,83.3	0.17Å	Favored (83.347%) alpha helix	-	-	-
A 208		LEU	0.96	Favored (87.61%) General / -63.1,-37.5	Favored (94.8%) <i>mt</i> chi angles: 297.3,174.6	0.11Å	Favored (93.295%) alpha helix	-	-	-
A 209		TYR	0.96	Favored (97.37%)	Favored (28.2%) <i>m-80</i>	0.09Å	Favored (86.057%)	-	-	-

				General / -61.4,-41.6	chi angles: 279.1,111.1	alpha helix				
A 210	ALA	0.96		Favored (84.96%) General / -58.5,-41.3	-	0.03Å	Favored (88.673%) alpha helix	-	-	-
A 211	ALA	0.95		Favored (96.5%) General / -61.3,-44.9	-	0.08Å	Favored (94.334%) alpha helix	-	-	-
A 212	VAL	0.94		Favored (98.26%) Ile or Val / -62.4,-43.5	Favored (82.6%) <i>t</i> chi angles: 176.8	0.14Å	Favored (94.629%) alpha helix	-	-	-
A 213	ILE	0.91		Favored (80.12%) Ile or Val / -59.6,-39.7	Favored (98.5%) <i>mt</i> chi angles: 292.9,168.1	0.10Å	Favored (91.855%)	-	-	-
A 214	ASN	0.89		Favored (6.72%) General / -87.2,15.0	Favored (2.8%) <i>m110</i> chi angles: 280.9,52.9	0.03Å	Favored (16.383%)	-	-	-
A 215	GLY	0.9		Favored (52.71%) Glycine / 101.2,5.4	-	-	Favored (71.99%)	-	-	-
A 216	ASP	0.86		Favored (48.99%) General / -109.2,123.3	Favored (26.4%) <i>t0</i> chi angles: 197.3,357.1	0.05Å	Favored (8.116%)	-	-	-
A 217	ARG	0.84		Favored (7.27%) General / -126.0,7.0	Favored (35.6%) <i>mtp85</i> chi angles: 281.3,181,71.8,102.5	0.08Å	Favored (7.355%)	-	-	-
A 218	TRP	0.86		Favored (70.03%) General / -60.8,-30.5	Favored (34.3%) <i>p-90</i> chi angles: 73.6,261	0.16Å	Favored (39.588%)	-	-	-
A 219	PHE	0.95		Favored (55.97%) General / -91.0,2.9	Favored (26%) <i>p90</i> chi angles: 52.8,79.9	0.05Å	Favored (32.432%)	-	-	-
A 220	LEU	0.93		Favored (38.92%) General / -74.3,154.4	Favored (57.4%) <i>mt</i> chi angles: 300,184.4	0.08Å	Favored (28.208%)	-	-	-
A 221	ASN	0.84		Favored (4.75%) General / -135.2,-177.7	Favored (31.7%) <i>p0</i> chi angles: 66.9,31.5	0.23Å	Favored (28.125%)	-	-	-
A 222	ARG	0.77		Favored (39.48%) General / -97.0,10.4	Favored (47.2%) <i>ptt90</i> chi angles: 67.8,171.3,176.6,94	0.07Å	Favored (7.796%)	-	-	-
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non- Trans: 0 of 298
A 223	PHE	0.88		Favored (15.14%) General / -106.1,160.7	Favored (67.2%) <i>m-80</i> chi angles: 302.2,290.7	0.09Å	Favored (22.576%)	-	-	-
A 224	THR	0.9		Favored (4.85%)	Favored (12.8%) <i>t</i> chi angles: 187.3	0.11Å	Favored (51.2%)	-	-	-

				General / -121.0,178.1						
A 225	THR	0.92		Favored (31.98%) General / -152.2,152.2	Favored (8.3%) <i>t</i> chi angles: 183.9	0.02Å	Favored (37.104%) beta sheet	-	-	-
A 226	THR	0.91		Favored (28.07%) General / -75.5,162.7	Favored (35.7%) <i>p</i> chi angles: 68.5	0.17Å	Favored (51.57%)	-	-	-
A 227	LEU	0.91		Favored (84.04%) General / -59.7,-39.3	Favored (26.4%) <i>tp</i> chi angles: 186.4,54.9	0.04Å	Favored (61.001%)	-	-	-
A 228	ASN	0.89		Favored (72.47%) General / -60.0,-50.8	Favored (12.3%) <i>t0</i> chi angles: 187.2,79.8	0.04Å	Favored (84.394%) alpha helix	-	-	-
A 229	ASP	0.91		Favored (69.32%) General / -68.4,-30.4	Favored (82.2%) <i>m-30</i> chi angles: 290.5,332.4	0.03Å	Favored (70.804%) alpha helix	-	-	-
A 230	PHE	0.93		Favored (74.69%) General / -61.2,-50.0	Favored (71.5%) <i>t80</i> chi angles: 173.6,69.9	0.05Å	Favored (64.251%) alpha helix	-	-	-
A 231	ASN	0.9		Favored (97.99%) General / -61.1,-44.0	Favored (26%) <i>m-40</i> chi angles: 272.9,328.5	0.10Å	Favored (78.714%) alpha helix	-	-	-
A 232	LEU	0.91		Favored (69.24%) General / -55.9,-37.6	Favored (29.2%) <i>mt</i> chi angles: 282.1,170.3	0.02Å	Favored (67.732%) alpha helix	-	-	-
A 233	VAL	0.91		Favored (17.53%) Ile or Val / -78.1,-51.6	Favored (76.8%) <i>t</i> chi angles: 178.2	0.03Å	Favored (44.752%) alpha helix	-	-	-
A 234	ALA	0.88		Favored (90.9%) General / -63.5,-38.4	-	0.10Å	Favored (74.739%) alpha helix	-	-	-
A 235	MET	0.84		Favored (64.05%) General / -66.1,-16.6	Favored (53.3%) <i>mtt</i> chi angles: 291.6,173.4,194.5	0.06Å	Favored (63.717%) three-ten	-	OUTLIER(S) worst is CG- SD-CE: 7.3 σ	-
A 236	LYS	0.84		Favored (69.19%) General / -67.6,-29.8	OUTLIER (0%) chi angles: 212.4,279.8,128.6,292.7	0.12Å	Favored (64.509%) three-ten	-	-	-
A 237	TYR	0.89		Favored (22.57%) General / -101.5,17.5	Favored (80.6%) <i>m-80</i> chi angles: 289.8,264.8	0.04Å	Favored (25.82%)	-	-	-
A 238	ASN	0.87		Favored (3.43%) General / 69.3,32.8	Favored (46.1%) <i>t0</i> chi angles: 197.7,49.6	0.15Å	Favored (8.722%)	-	-	-
A 239	TYR	0.94		Favored (24.96%) General / -92.4,144.8	Favored (5.9%) <i>m-80</i> chi angles: 271,54.4	0.04Å	Favored (26.116%)	-	-	-
A 240	GLU	0.89		Favored (86.87%)	Favored (64.9%) <i>tp30</i>	0.08Å	Favored (35.089%)	-	-	-

				Pre-Pro / -58.8,139.1	chi angles: 185.6,61.3,21.6					
A 241		PRO	0.9	Favored (23.7%) Trans-Pro / -50.8,128.2	Favored (78.9%) <i>Cg_exo</i> chi angles: 329.1,39.3,327.3	0.11Å	Favored (69.122%)	-	-	-
A 242		LEU	0.94	Favored (36.75%) General / -92.8,124.3	Favored (11.2%) <i>tp</i> chi angles: 195.8,70.8	0.05Å	Favored (58.994%) beta sheet	-	-	-
#	Alt	Res	High B	Ramachandran	Rotamer	C β deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non- Trans: 0 of 298
A 243		THR	0.92	Favored (8.74%) General / -105.9,169.0	Favored (58.5%) <i>p</i> chi angles: 64.4	0.05Å	Favored (22.044%)	-	-	-
A 244		GLN	0.87	Favored (86.96%) General / -60.5,-39.2	Favored (74.7%) <i>tp40</i> chi angles: 184,56,44.9	0.10Å	Favored (61.701%)	-	-	-
A 245		ASP	0.91	Favored (75.14%) General / -55.5,-42.8	Favored (33%) <i>m-30</i> chi angles: 284.5,9.5	0.08Å	Favored (80.627%) alpha helix	-	-	-
A 246		HIS	0.87	Favored (89.01%) General / -65.5,-38.2	Favored (4.6%) <i>m-70</i> chi angles: 303,341.9	0.09Å	Favored (92.426%) alpha helix	-	-	-
A 247		VAL	0.91	Favored (99.61%) Ile or Val / -62.0,-44.9	Favored (49.5%) <i>t</i> chi angles: 169.3	0.06Å	Favored (78.25%) alpha helix	-	-	-
A 248		ASP	0.9	Favored (87.05%) General / -58.2,-42.8	Favored (98.7%) <i>m-30</i> chi angles: 287.6,348.4	0.03Å	Favored (77.97%) alpha helix	-	-	-
A 249		ILE	0.93	Favored (50.27%) Ile or Val / -58.4,-34.3	Favored (68.4%) <i>mt</i> chi angles: 290.3,161.8	0.13Å	Favored (73.63%) alpha helix	-	-	-
A 250		LEU	0.95	Favored (24.74%) General / -79.4,1.6	Favored (68.9%) <i>mt</i> chi angles: 289.1,165.7	0.04Å	Favored (39.331%) alpha helix	-	-	-
A 251		GLY	0.93	Favored (8.93%) Glycine / -47.8,-56.2	-	-	Favored (57.038%) alpha helix	-	-	-
A 252		PRO	0.92	Favored (44.14%) Trans-Pro / -56.3,-44.7	Favored (59.1%) <i>Cg_exo</i> chi angles: 328.4,38.8,328.6	0.07Å	Favored (98.617%) alpha helix	-	-	-
A 253		LEU	0.93	Favored (94.3%) General / -65.0,-40.1	Favored (82.2%) <i>mt</i> chi angles: 289.4,169.1	0.07Å	Favored (95.454%) alpha helix	-	-	-
A 254		SER	0.92	Favored (86.75%) General / -61.1,-47.3	Favored (44.1%) <i>t</i> chi angles: 178.8	0.03Å	Favored (85.59%) alpha helix	-	-	-
A		ALA	0.92	Favored	-	0.01Å	Favored	-	-	-

255				(99.31%) General / -63.1,-41.1			(94.044%) alpha helix			
A 256		GLN	0.86	Favored (98.74%) General / -61.1,-42.5	Favored (16.6%) <i>tt0</i> chi angles: 164.7,164,13	0.10Å	Favored (70.43%) alpha helix	-	-	-
A 257		THR	0.92	Favored (22.33%) General / -91.3,-20.0	Favored (36.5%) <i>p</i> chi angles: 54.1	0.11Å	Favored (35.892%)	-	-	-
A 258		GLY	0.93	Favored (84.72%) Glycine / 77.5,12.2	-	-	Favored (77.369%)	-	-	-
A 259		ILE	0.91	Favored (43.21%) Ile or Val / -108.3,113.2	Favored (38.5%) <i>mt</i> chi angles: 299.6,157.6	0.08Å	Favored (23.548%) beta sheet	-	-	-
A 260		ALA	0.93	Favored (25.44%) General / -57.3,147.5	-	0.06Å	Favored (27.301%)	-	-	-
A 261		VAL	0.95	Favored (83.36%) Ile or Val / -57.6,-43.3	Favored (81.8%) <i>t</i> chi angles: 177.9	0.06Å	Favored (56.287%)	-	-	-
A 262		LEU	0.94	Favored (71.95%) General / -67.3,-31.6	Favored (95.3%) <i>mt</i> chi angles: 296.5,176.4	0.18Å	Favored (77.933%) alpha helix	-	-	-
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non- Trans: 0 of 298
A 263		ASP	0.94	Favored (94.93%) General / -64.8,-42.5	Favored (30.8%) <i>m-30</i> chi angles: 297.7,357.7	0.05Å	Favored (80.968%) alpha helix	-	-	-
A 264		MET	0.94	Favored (87.78%) General / -63.4,-37.6	Favored (36.3%) <i>tpp</i> chi angles: 193.9,61,85.6	0.12Å	Favored (87.288%) alpha helix	-	-	-
A 265		CYS	0.98	Favored (82.57%) General / -61.0,-37.5	Favored (83.9%) <i>m</i> chi angles: 294	0.04Å	Favored (83.259%) alpha helix	-	-	-
A 266		ALA	0.95	Favored (99.52%) General / -63.0,-41.5	-	0.07Å	Favored (89.928%) alpha helix	-	-	-
A 267		SER	0.97	Favored (95.03%) General / -60.1,-44.2	Favored (21.3%) <i>m</i> chi angles: 304.4	0.08Å	Favored (98.603%) alpha helix	-	-	-
A 268		LEU	0.96	Favored (99.42%) General / -63.0,-41.1	Favored (18.3%) <i>tp</i> chi angles: 181.4,49.7	0.06Å	Favored (85.948%) alpha helix	-	-	-
A 269		LYS	0.91	Favored (85.12%) General / -57.5,-45.3	Favored (26.7%) <i>ttmt</i> chi angles: 178.1,191.3,295.4,178.3	0.05Å	Favored (85.692%) alpha helix	-	-	-

A 270	GLU	0.9	Favored (96.25%) General / -63.6,-43.6	Favored (43.3%) <i>tt0</i> chi angles: 181.9,175,315.3	0.06Å	Favored (87.469%) alpha helix	-	-	-	
A 271	LEU	0.93	Favored (87.28%) General / -60.0,-39.9	Favored (85%) <i>mt</i> chi angles: 290.2,169.5	0.08Å	Favored (76.184%) alpha helix	-	-	-	
A 272	LEU	0.94	Favored (77.28%) General / -66.7,-45.9	Favored (94.4%) <i>mt</i> chi angles: 296.5,174	0.04Å	Favored (72.864%) alpha helix	-	-	-	
A 273	GLN	0.89	Favored (87.8%) General / -66.7,-39.0	Favored (87.5%) <i>mt0</i> chi angles: 286.7,167.7,342.5	0.02Å	Favored (57.269%) alpha helix	-	-	-	
A 274	ASN	0.9	Favored (14.13%) General / -112.5,-4.7	Favored (3.1%) <i>m110</i> chi angles: 293.3,183.2	0.04Å	Favored (32.208%)	-	-	-	
A 275	GLY	0.92	Favored (40.44%) Glycine / 69.9,-172.2	-	-	Favored (48.081%)	-	-	-	
A 276	MET	0.88	Favored (24.7%) General / -97.2,-11.1	Allowed (0.7%) <i>ttm</i> chi angles: 236.9,179.1,270.7	0.06Å	CaBLAM Outlier (0.321%)	-	-	-	
A 277	ASN	0.86	Favored (16.52%) General / 47.4,48.3	Allowed (1.1%) <i>p0</i> chi angles: 82.2,281	0.42Å	CaBLAM Disfavored (3.548%)	-	-	-	
A 278	GLY	0.87	Favored (90.2%) Glycine / 81.4,5.2	-	-	Favored (69.939%)	-	-	-	
A 279	ARG	0.83	Favored (13.58%) General / -102.5,161.6	Allowed (1%) <i>mtp180</i> chi angles: 306.2,156.3,109.1,170.6	0.05Å	Favored (35.376%)	-	-	-	
A 280	THR	0.89	Favored (35.66%) General / -123.8,156.6	Favored (47.6%) <i>p</i> chi angles: 55.7	0.07Å	Favored (52.483%)	-	-	-	
A 281	ILE	0.92	Favored (56.93%) Ile or Val / -126.3,120.6	Favored (66.1%) <i>mt</i> chi angles: 302.2,175.8	0.03Å	Favored (12.508%)	-	-	-	
A 282	LEU	0.92	Favored (17.11%) General / 56.4,30.5	Favored (38.8%) <i>mt</i> chi angles: 283.9,164.5	0.21Å	Favored (25.217%)	-	-	-	
#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 0.91	Outliers: 0 of 297	Poor rotamers: 8 of 258	Outliers: 3 of 275	Outliers: 2 of 295	Outliers: 0 of 299	Outliers: 14 of 299	Non-Trans: 0 of 298
A 283	GLY	0.89	Favored (81.65%) Glycine / 80.5,-1.5	-	-	Favored (78.261%)	-	-	-	
A 284	SER	0.84	Favored (29.34%) General / -101.0,144.9	Favored (26.4%) <i>t</i> chi angles: 184.2	0.04Å	Favored (26.955%)	-	-	-	
A 285	ALA	0.85	Favored (56.4%)	-	0.12Å	Favored (44.156%)	-	-	-	

General / -92.4,-2.3

A 286	LEU	0.86	Favored (36.45%) General / -132.8,160.6	Favored (87.9%) <i>mt</i> chi angles: 295.2,170.8	0.08Å	Favored (17.297%)	-	-	-
A 287	LEU	0.91	Favored (28.41%) General / -82.6,122.7	Favored (63.4%) <i>mt</i> chi angles: 302,172.3	0.04Å	Favored (28.362%)	-	-	-
A 288	GLU	0.89	Favored (33.72%) General / -90.0,135.3	Favored (9.1%) <i>tp30</i> chi angles: 172.9,64.2,253	0.12Å	Favored (46.09%) beta sheet	-	-	-
A 289	ASP	0.95	Favored (10.23%) General / -121.4,8.6	Favored (3.1%) <i>p0</i> chi angles: 83.5,345.6	0.23Å	Favored (17.537%)	-	OUTLIER(S) worst is CA- CB-CG: 6.7 σ	-
A 290	GLU	0.92	Favored (9.01%) General / -106.0,27.0	Favored (23.5%) <i>mt-10</i> chi angles: 298.8,194.9,289.9	0.02Å	CaBLAM Disfavored (2.116%)	-	-	-
A 291	PHE	0.94	Favored (42.76%) General / -117.0,121.9	Favored (97.6%) <i>m-80</i> chi angles: 294,271.5	0.14Å	Favored (16.633%)	-	-	-
A 292	THR	0.96	Favored (51.5%) Pre-Pro / -74.9,165.7	Favored (27.7%) <i>p</i> chi angles: 70.2	0.15Å	Favored (28.445%)	-	-	-
A 293	PRO	0.97	Favored (48.52%) Trans-Pro / -49.8,-39.3	Favored (86.4%) <i>Cg_exo</i> chi angles: 330.5,36.9,329.8	0.10Å	Favored (80.646%)	-	-	-
A 294	PHE	0.92	Favored (88.34%) General / -63.6,-45.9	Favored (60.1%) <i>t80</i> chi angles: 177.4,91.2	0.07Å	Favored (81.23%) alpha helix	-	-	-
A 295	ASP	0.91	Favored (94.18%) General / -61.0,-40.6	Favored (76.2%) <i>m-30</i> chi angles: 297.1,326.8	0.09Å	Favored (86.641%) alpha helix	-	-	-
A 296	VAL	0.94	Favored (98.42%) Ile or Val / -62.8,-45.6	Favored (66.4%) <i>t</i> chi angles: 179.2	0.09Å	Favored (95.228%) alpha helix	-	-	-
A 297	VAL	0.9	Favored (84.9%) Ile or Val / -61.3,-40.1	Favored (50.9%) <i>t</i> chi angles: 169.5	0.13Å	Favored (96.7%) alpha helix	-	-	-
A 298	ARG	0.78	Favored (81.09%) General / -62.0,-36.3	OUTLIER (0%) chi angles: 137.3,147.7,111.8,120.3	0.19Å	Favored (73.134%) alpha helix	-	-	-
A 299	GLN	0.82	Favored (31.09%) General / -102.3,-1.4	Favored (3.1%) <i>tt0</i> chi angles: 201.3,184,139	0.06Å	Favored (29.512%)	-	-	-
A 300	CYS	0.83	Allowed (1.73%) General / -107.3,-60.1	Favored (71.9%) <i>m</i> chi angles: 287.5	0.07Å	-	-	-	-
A 301	SER	0.71	-	Favored (34.8%) <i>t</i> chi angles: 182.5	0.09Å	-	-	-	-

