



Viewing guca1a_mb_2-185-FFX1FH-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0.34	99 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	15	8.98%	Goal: <0.3%
	Favored rotamers	138	82.63%	Goal: >98%
	Ramachandran outliers	1	0.55%	Goal: <0.05%
	Ramachandran favored	159	87.36%	Goal: >98%
	MolProbity score^	1.96		78 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	3	1.73%	Goal: 0
	Bad bonds:	0 / 1518	0.00%	Goal: 0%
	Bad angles:	15 / 2046	0.73%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 3	0.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	1 / 183	0.55%	Goal: 0

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

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

[^] MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: Clashscore: 0.34 Outliers: 1 of 182 Poor rotamers: 15 of 167 Outliers: 3 of 173 Outliers: 0 of 184 Outliers: 15 of 184 Non-Trans: 1 of 183									
2	GLY	37.74	-	-	-	-	-	-	-
3	ASN	206.79	-	OUTLIER (0.01%) General / -44.7,170.2	Favored (63.1%) <i>m</i> -40 chi angles: 283,281.2	0.12Å	-	-	-
4	VAL	58.77	-	Favored (3.58%) Ile or Val / -57.1,120.5	Favored (66.5%) <i>t</i> chi angles: 171.7	0.05Å	-	-	-
5	MET	72.45	-	Favored (4.32%) General / -142.6,104.0	Favored (40.3%) <i>mtp</i> chi angles: 280.8,159.6,62.9	0.05Å	-	-	-
6	GLU	78.68	-	Favored (24.59%) General / -57.9,148.8	Favored (5.6%) <i>tm</i> -30 chi angles: 182.9,288.5,310.8	0.12Å	-	-	-
				Favored					

7	GLY	18.54	-	(86.84%) Glycine / -55.9,-45.3	-	-	-	-	-
8	LYS	30.66	-	Favored (74.48%) General / -69.0,-33.9	Favored (15.9%) <i>tptp</i> chi angles: 188.8,65.5,182.1,69.9	0.13Å	-	-	-
9	SER	26.11	-	Favored (79.68%) General / -62.5,-35.5	Favored (4.1%) <i>p</i> chi angles: 86.1	0.20Å	-	-	-
10	VAL	33.12	-	Favored (89.34%) Ile or Val / -64.8,-40.5	Favored (45%) <i>t</i> chi angles: 168.7	0.09Å	-	-	-
11	GLU	74.22	-	Favored (62.15%) General / -55.9,-53.0	Allowed (0.7%) <i>tm</i> - 30 chi angles: 191.4,299.7,287.7	0.05Å	-	-	-
12	GLU	64.74	-	Favored (65.1%) General / -73.7,-35.4	Favored (81.3%) <i>mt</i> - 10 chi angles: 296.6,172,16.5	0.09Å	-	-	-
13	LEU	40.79	-	Favored (72.6%) General / -69.6,-33.4	Favored (65.5%) <i>mt</i> chi angles: 295.9,167	0.12Å	-	-	-
14	SER	90.46	-	Favored (47.15%) General / -79.8,-20.0	Favored (82.9%) <i>p</i> chi angles: 62.4	0.19Å	-	-	-
15	SER	52.78	-	Favored (37.1%) General / -82.0,-21.2	Favored (57.6%) <i>m</i> chi angles: 293.1	0.10Å	-	-	-
16	THR	42	-	Favored (2.4%) General / -70.6,103.1	Favored (43.7%) <i>m</i> chi angles: 294	0.06Å	-	-	-
17	GLU	79.01	-	Allowed (1.3%) General / -43.1,140.9	Favored (3.2%) <i>tm</i> - 30 chi angles: 194.2,289,302.3	0.09Å	-	-	-
18	CYS	79.59	-	Favored (65.84%) General / -55.6,-35.4	Favored (10.1%) <i>m</i> chi angles: 311.3	0.12Å	-	-	-
19	HIS	41.77	-	Favored (58.65%) General / -84.3,-9.2	Favored (51%) <i>m90</i> chi angles: 304.1,79	0.21Å	-	-	-
20	GLN	33.54	-	Favored (64.05%) General / -73.5,-40.5	Favored (11.6%) <i>mm-40</i> chi angles: 313.4,311.5,280.2	0.12Å	-	-	-
				Favored	Favored (94.4%)	OUTLIER(S)			

21	TRP	49.93	-	(76.14%) General / -60.9,-35.3	<i>m100</i> chi angles: 294.9,91	0.10Å	-	worst is CE3- CD2-CG: 4.2 σ	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles	Cis Peptides
		Avg: 71.52	Clashscore: 0.34	Outliers: 1 of 182	Poor rotamers: 15 of 167	Outliers: 3 of 173	Outliers: 0 of 184	Outliers: 15 of 184	Non- Trans: 1 of 183
22	TYR	60.06	-	Favored (79.55%) General / -57.2,-41.5	Favored (4.9%) <i>t80</i> chi angles: 176.6,27.4	0.08Å	-	-	-
23	LYS	101.8	-	Favored (94.92%) General / -62.7,-39.8	Favored (2.5%) <i>tptp</i> chi angles: 183,65.6,221.3,70.4	0.16Å	-	-	-
24	LYS	56.02	-	Favored (63%) General / -53.7,-51.5	Favored (39.8%) <i>tttm</i> chi angles: 187.7,188.5,178.1,293.8	0.12Å	-	-	-
25	PHE	76.44	-	Favored (66.04%) General / -52.5,-48.6	Allowed (1.3%) <i>t80</i> chi angles: 183.9,119.2	0.09Å	-	OUTLIER(S) worst is CA- CB-CG: 5.0 σ	-
26	MET	42.08	-	Allowed (0.12%) General / -74.4,20.2	Favored (56.6%) <i>mmm</i> chi angles: 303.6,316.5,290.1	0.09Å	-	-	-
27	THR	28.09	-	Favored (5.9%) General / -122.9,-20.2	OUTLIER (0.1%) chi angles: 331.2	0.13Å	-	-	-
28	GLU	56.37	-	Favored (4.34%) General / -121.1,-30.5	Favored (58.9%) <i>mt-10</i> chi angles: 295,174.7,33.6	0.03Å	-	-	-
29	CYS	108.85	-	Favored (50.96%) Pre-Pro / -83.2,132.2	Favored (7.8%) <i>p</i> chi angles: 77.7	0.09Å	-	-	-
30	PRO	62.46	-	Favored (2.62%) Trans-Pro / -94.7,3.9	Favored (2.9%) <i>Cg_endo</i> chi angles: 40.9	0.04Å	-	-	-
31	SER	30.37	-	Favored (12.87%) General / -112.3,-16.9	Favored (5.2%) <i>p</i> chi angles: 46.9	0.03Å	-	-	-
32	GLY	19.58	-	Allowed (1.41%) Glycine / 99.8,-46.4	-	-	-	-	-
33	GLN	48.16	-	Favored (22.05%) General / -108.4,154.3	Favored (34.9%) <i>mt0</i> chi angles: 300.4,182.5,253.5	0.07Å	-	OUTLIER(S) worst is NE2- CD-OE1: 4.5 σ	-

34	LEU	70.77	-	Favored (35.5%) General / -92.9,122.6	Favored (75.8%) <i>mt</i> chi angles: 287.3,168.2	0.06Å	-	-	-
35	THR	41.35	-	Favored (4.92%) General / -64.3,169.0	Favored (47.8%) <i>p</i> chi angles: 55.8	0.06Å	-	-	-
36	LEU	41.11	-	Allowed (1.38%) General / -39.3,-45.3	Favored (69.9%) <i>tp</i> chi angles: 177.3,59.8	0.04Å	-	-	-
37	TYR	47.05	-	Favored (11.52%) General / -87.3,-44.3	Favored (54.3%) <i>t80</i> chi angles: 181.1,94.2	0.10Å	-	-	-
38	GLU	43.65	-	Favored (38.91%) General / -81.4,-21.4	Favored (79.2%) <i>mm-30</i> chi angles: 291.7,304.5,321	0.20Å	-	-	-
39	PHE	106.78	-	Favored (95.59%) General / -60.0,-43.0	Favored (59.6%) <i>t80</i> chi angles: 175.4,269.7	0.03Å	-	-	-
40	ARG	93.33	-	Favored (92.17%) General / -65.0,-38.8	Favored (39.7%) <i>mtt180</i> chi angles: 303,169.4,183.7,208.5	0.07Å	-	-	-
41	GLN	41.77	-	Favored (88.24%) General / -66.7,-41.2	OUTLIER (0.3%) chi angles: 305.3,234.2,119.8	0.10Å	-	OUTLIER(S) worst is C-N- CA: 4.0 σ	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash > 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> <div>Cis Peptides</div> </div>									
<div> <div>Avg: 71.52</div> <div>Clashscore: 0.34</div> <div>Outliers: 1 of 182</div> <div>Poor rotamers: 15 of 167</div> <div>Outliers: 3 of 173</div> <div>Outliers: 0 of 184</div> <div>Outliers: 15 of 184</div> <div>Non-Trans: 1 of 183</div> </div>									
42	PHE	67.03	-	Favored (85.44%) General / -58.5,-41.5	Favored (52.2%) <i>t80</i> chi angles: 180,94.2	0.06Å	-	-	-
43	PHE	97.62	-	Favored (21.51%) General / -100.6,-9.9	Favored (29.6%) <i>m-80</i> chi angles: 281.2,296.2	0.07Å	-	-	-
44	GLY	48.7	-	Favored (50.1%) Glycine / 80.7,27.6	-	-	-	-	-
45	LEU	182.48	-	Favored (66.86%) General / -72.2,-32.4	Favored (4.6%) <i>mp</i> chi angles: 276.9,73.9	0.06Å	-	-	-
Favored					Favored (3.5%)				

46	LYS 219.01	-	(2.57%) General / -41.9,124.2	<i>mmmm</i> chi angles: 284,297.6,307.7,310.3	0.12Å	-	-	-
47	ASN 117.38	-	Favored (5.34%) General / 45.9,57.2	Allowed (0.3%) <i>p0</i> chi angles: 51.9,250.7	0.19Å	-	OUTLIER(S) worst is CA- CB-CG: 5.1 σ	-
48	LEU 48.34	-	Allowed (0.15%) General / -92.6,-134.6	Favored (25.5%) <i>mt</i> chi angles: 310.9,176.7	0.18Å	-	-	-
49	SER 30.94	-	Favored (45.68%) Pre-Pro / -67.7,163.8	Favored (94.8%) <i>p</i> chi angles: 63.3	0.06Å	-	-	-
50	PRO 66.07	-	Favored (88.17%) Trans-Pro / -60.3,-36.3	Favored (16.2%) <i>Cg_exo</i> chi angles: 325.1	0.06Å	-	-	-
51	SER 27.74	-	Favored (98.35%) General / -61.6,-42.1	Favored (68.6%) <i>p</i> chi angles: 58.7	0.13Å	-	-	-
52	ALA 27.57	-	Favored (79.02%) General / -63.0,-48.4	-	0.06Å	-	-	-
53	SER 22.24	-	Favored (84.61%) General / -65.8,-36.8	Allowed (0.9%) <i>t</i> chi angles: 205.9	0.20Å	-	-	-
54	GLN 60.54	-	Favored (80.86%) General / -65.5,-35.4	Favored (10.7%) <i>tp40</i> chi angles: 180.4,62.8,100.8	0.10Å	-	-	-
55	TYR 122.6	-	Favored (69.38%) General / -70.4,-31.9	Favored (14.4%) <i>t80</i> chi angles: 180.5,42.9	0.08Å	-	-	-
56	VAL 36.53	-	Favored (85.23%) Ile or Val / -62.7,-39.6	Favored (42.8%) <i>t</i> chi angles: 168.3	0.10Å	-	-	-
57	GLU 76.95	-	Favored (94.84%) General / -60.1,-44.5	Favored (13.4%) <i>mm-30</i> chi angles: 309.5,317.5,314.3	0.12Å	-	-	-
58	GLN 42.08	-	Favored (59.2%) General / -76.1,-18.3	OUTLIER (0.2%) chi angles: 282.8,258.6,244	0.07Å	-	-	-
59	MET 80.86	-	Favored (23.74%) General / -87.4,-25.6	Favored (32.7%) <i>tpp</i> chi angles: 181.9,51.4,59	0.08Å	-	-	-
			Favored					

60	PHE	52.13	-	(90.87%) General / -66.1,-40.6	Favored (79.4%) <i>t80</i> chi angles: 183,84.3	0.13Å	-	-	-
61	GLU	97.24	-	Favored (75.59%) General / -57.6,-38.9	Favored (3.6%) <i>pt0</i> chi angles: 69.1,206.7,238.3	0.13Å	-	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash > 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> <div>Cis Peptides</div> </div>									
<div> <div>Avg: 71.52</div> <div>Clashscore: 0.34</div> <div>Outliers: 1 of 182</div> <div>Poor rotamers: 15 of 167</div> <div>Outliers: 3 of 173</div> <div>Outliers: 0 of 184</div> <div>Outliers: 15 of 184</div> <div>Non-Trans: 1 of 183</div> </div>									
62	THR	125.96	-	Favored (2.58%) General / -69.9,3.6	OUTLIER (0.1%) chi angles: 30.6	0.18Å	-	-	-
63	PHE	142.52	-	Favored (7.8%) General / -123.7,-10.7	Favored (19.8%) <i>m-10</i> chi angles: 304.3,323.2	0.07Å	-	-	-
64	ASP	84.33	-	Favored (4.37%) General / -98.9,89.6	Favored (55.6%) <i>t0</i> chi angles: 190,347.9	0.07Å	-	-	-
65	PHE	131.03	-	Favored (23.5%) General / -86.6,-28.2	Favored (9.5%) <i>m-80</i> chi angles: 313.1,311.3	0.12Å	-	-	-
66	ASN	96.49	-	Favored (52.32%) General / -83.5,-14.4	Allowed (1.2%) <i>m-40</i> chi angles: 282,239	0.12Å	-	-	-
67	LYS	162.37	-	Allowed (1.24%) General / 71.0,37.5	Favored (13.3%) <i>mmtp</i> chi angles: 316.3,294.2,167,62.8	0.13Å	-	-	-
68	ASP	100	-	Favored (14.73%) General / -108.9,-13.5	Favored (47.3%) <i>p0</i> chi angles: 69,354.7	0.16Å	-	OUTLIER(S) worst is CA-CB-CG: 4.6 σ	-
69	GLY	39.39	-	Favored (58.45%) Glycine / 95.3,8.8	-	-	-	-	-
70	TYR	67.61	-	Favored (2.43%) General / -134.8,-169.8	OUTLIER (0.1%) chi angles: 316.6,242.1	0.05Å	-	-	-
71	ILE	117.24	-	Allowed (1.13%) Ile or Val / -147.3,115.6	Favored (24.6%) <i>mm</i> chi angles: 306.6,293.4	0.06Å	-	-	-
72	ASP	77.19	-	Favored (27.02%) General / -72.7,164.1	OUTLIER (0.1%) chi angles: 150.5,253	0.12Å	-	OUTLIER(S) worst is CA-CB-CG: 4.4 σ	-

73	PHE	130.99	-	Favored (69.42%) General / -71.0,-32.6	Favored (21.7%) <i>p90</i> chi angles: 48.4,266.3	0.16Å	-	-	-
74	MET	137.17	-	Favored (63.08%) General / -72.4,-44.0	Favored (40.3%) <i>mtm</i> chi angles: 305,171.1,286.6	0.13Å	-	-	-
75	GLU	59.39	-	Favored (65.54%) General / -53.4,-50.2	Favored (48.1%) <i>mt-10</i> chi angles: 295.7,189.2,302	0.11Å	-	-	-
76	TYR	70.45	-	Favored (63.8%) General / -51.7,-47.8	Favored (17.3%) <i>t80</i> chi angles: 171.2,96.6	0.07Å	-	-	-
77	VAL	38.49	-	Favored (41.39%) Ile or Val / -70.1,-29.9	Favored (11.2%) <i>m</i> chi angles: 306.5	0.30Å	-	-	-
78	ALA	24.82	-	Favored (77.53%) General / -69.4,-40.2	-	0.07Å	-	-	-
79	ALA	31.01	-	Favored (98.87%) General / -62.0,-42.1	-	0.02Å	-	-	-
80	LEU	54.52	-	Favored (70.11%) General / -64.6,-29.1	Favored (89.3%) <i>mt</i> chi angles: 291.4,173.7	0.10Å	-	-	-
81	SER	88.71	-	Favored (64.11%) General / -57.0,-30.4	Favored (12.4%) <i>p</i> chi angles: 81.5	0.18Å	-	-	-

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Avg: 71.52				Clashscore: 0.34	Outliers: 1 of 182	Poor rotamers: 15 of 167	Outliers: 3 of 173	Outliers: 0 of 184	Outliers: 15 of 184	Non-Trans: 1 of 183
82	LEU	77.17	-		Favored (12.2%) General / -93.8,-36.6	Favored (65%) <i>mt</i> chi angles: 304.4,178.6	0.08Å	-	-	-
83	VAL	56.83	-		Favored (66.88%) Ile or Val / -72.2,-40.9	Favored (85.4%) <i>t</i> chi angles: 177.6	0.13Å	-	-	-
84	LEU	103.71	-		Favored (6.89%) General / -87.1,178.5	OUTLIER (0.1%) chi angles: 279.1,32	0.06Å	-	-	-
					Favored (29.55%)	Favored (3.7%) <i>mptt</i>				

85	LYS	46.56	-	General / -61.4,127.0	chi angles: 277.7,81.1,170.5,192.7	0.11Å	-	-	-
86	GLY	24.94	-	Favored (27.46%) Glycine / -143.0,160.0	-	-	-	-	-
87	LYS	74.6	-	Favored (21.88%) General / -64.1,124.5	Favored (11%) <i>mtpt</i> chi angles: 289.3,183.5,68.4,206.4	0.07Å	-	-	-
88	VAL	27.79	-	Favored (59.26%) Ile or Val / -62.0,-33.6	Favored (47%) <i>t</i> chi angles: 169	0.17Å	-	-	-
89	GLU	40.47	-	Favored (8.02%) General / -44.0,-45.7	Favored (47.1%) <i>mt-10</i> chi angles: 293.7,169.2,38.7	0.12Å	-	-	-
90	GLN	48.79	-	Favored (14.27%) General / -96.1,-29.1	Favored (7%) <i>mt0</i> chi angles: 295.9,157.3,226.4	0.12Å	-	-	-
91	LYS	49.49	-	Favored (68.48%) General / -59.9,-29.7	Favored (39.5%) <i>mttt</i> chi angles: 300.8,206.8,186,187.7	0.15Å	-	-	-
92	LEU	65.48	-	Favored (63.62%) General / -55.0,-34.6	Favored (19.2%) <i>tp</i> chi angles: 189.6,55.4	0.08Å	-	-	-
93	ARG	111.36	-	Favored (13.25%) General / -101.0,-27.5	Favored (54.8%) <i>mtp85</i> chi angles: 302.3,182.2,73.3,98.3	0.10Å	-	-	-
94	TRP	64.65	-	Favored (71.89%) General / -71.2,-36.2	Favored (26.7%) <i>m-10</i> chi angles: 301,323.8	0.14Å	-	-	-
95	TYR	67.55	-	Favored (71.61%) General / -66.9,-31.2	Favored (21.7%) <i>m-80</i> chi angles: 277.4,114.3	0.16Å	-	-	-
96	PHE	97.52	-	Favored (71.76%) General / -54.9,-49.2	Favored (14%) <i>t80</i> chi angles: 171.5,278.2	0.08Å	-	-	-
97	LYS	61.19	-	Favored (70.26%) General / -63.7,-29.0	OUTLIER (0.3%) chi angles: 187,67.5,234.4,78.7	0.11Å	-	-	-
98	LEU	65.53	-	Favored (89.33%) General / -65.9,-38.7	Favored (7.9%) <i>tp</i> chi angles: 192.9,78.5	0.08Å	-	-	-
				Favored					

99	TYR	73.33	-	(27.12%) General / -87.1,-20.4	Favored (24.1%) <i>m</i> - 80 chi angles: 304.4,310.5	0.14Å	-	-	-
100	ASP	59.66	-	Favored (30.51%) General / -98.2,141.9	OUTLIER (0%) chi angles: 117.2,66.1	0.12Å	-	-	-
101	VAL	43.68	-	Favored (57.67%) Ile or Val / -70.8,-34.8	Favored (64.5%) <i>t</i> chi angles: 179.4	0.20Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 71.52			Clashscore: 0.34	Outliers: 1 of 182	Poor rotamers: 15 of 167	Outliers: 3 of 173	Outliers: 0 of 184	Outliers: 15 of 184	Non-Trans: 1 of 183
102	ASP	69.69	-	Allowed (0.15%) General / -157.4,7.0	Favored (10.3%) <i>m</i> - 30 chi angles: 280.6,299.4	0.07Å	-	-	-
103	GLY	28.48	-	Allowed (1.6%) Glycine / 111.0,38.0	-	-	-	-	-
104	ASN	81.69	-	Favored (73.6%) General / -68.6,-44.8	Favored (9.9%) <i>p</i> 0 chi angles: 50.2,10.8	0.14Å	-	-	-
105	GLY	37.74	-	Favored (8.56%) Glycine / 122.2,-17.2	-	-	-	-	-
106	CYS	90.08	-	Allowed (1.64%) General / -128.2,-166.6	Favored (30%) <i>p</i> chi angles: 61.1	0.06Å	-	-	-
107	ILE	50.61	-	Favored (37.2%) Ile or Val / -139.9,134.3	Favored (21.1%) <i>mt</i> chi angles: 297,153.2	0.06Å	-	-	-
108	ASP	57.68	-	Favored (9.19%) General / -87.3,173.5	Allowed (0.7%) <i>p</i> 0 chi angles: 76.7,54.2	0.22Å	-	OUTLIER(S) worst is CA- CB-CG: 4.1 σ	-
109	ARG	69.57	-	Favored (83.98%) General / -61.1,-37.8	Favored (38.2%) <i>t</i> tt- 90 chi angles: 191.4,191.5,171.4,269.4	0.10Å	-	-	-
110	ASP	35.71	-	Favored (15.36%) General / -110.1,-5.4	Favored (3.3%) <i>m</i> - 30 chi angles: 292.3,22.6	0.31Å	-	-	-
111	GLU	38.73	-	Favored (72.23%) General /	Favored (36.4%) <i>mt</i> - 10 chi angles:	0.10Å	-	-	Twisted nonPRO omega=

-58.1,-50.8 285.3,188.4,299.5 146.91

112	LEU	123.82	-	Favored (72.93%) General / -62.6,-50.0	OUTLIER (0.1%) chi angles: 204.3,303.3	0.07Å	-	-	-
113	LEU	104.3	-	Favored (81.57%) General / -56.8,-46.4	Allowed (1.2%) <i>tp</i> chi angles: 201.1,85.6	0.06Å	-	-	-
114	THR	104.04	-	Favored (63.88%) General / -69.8,-47.2	Favored (94.9%) <i>m</i> chi angles: 300.9	0.12Å	-	-	-
115	ILE	54.8	-	Favored (15.4%) Ile or Val / -77.4,-26.5	Favored (72.3%) <i>mt</i> chi angles: 297.3,163.2	0.18Å	-	-	-
116	ILE	137.19	-	Favored (40.75%) Ile or Val / -66.6,-27.6	OUTLIER (0.2%) chi angles: 219.3,80.8	0.23Å	-	-	-
117	GLN	45.09	-	Favored (33.69%) General / -83.1,-21.2	Favored (29.1%) <i>mt0</i> chi angles: 283.2,183,100.3	0.08Å	-	-	-
118	ALA	44.51	-	Favored (34.11%) General / -62.8,-54.8	-	0.02Å	-	-	-
119	ILE	115.36	-	Favored (9.99%) Ile or Val / -83.4,-19.0	OUTLIER (0%) chi angles: 71.8,218.1	0.16Å	-	-	-
120	ARG	107.23	0.43Å O with 124 PRO HD2	Favored (23.43%) General / 56.3,45.2	Favored (15.3%) <i>mmt180</i> chi angles: 290.9,287.3,158.4,168.5	0.14Å	-	-	-
121	ALA	55.97	-	Favored (62.28%) General / -55.1,-32.9	-	0.11Å	-	OUTLIER(S) worst is C-N- CA: 4.3 σ	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 71.52				Clashscore: 0.34	Outliers: 1 of 182	Poor rotamers: 15 of 167	Outliers: 3 of 173	Outliers: 0 of 184	Outliers: 15 of 184	Non-Trans: 1 of 183
122	ILE	72.75	-	Allowed (1.24%) Ile or Val / -43.5,-39.7	Favored (6.1%) <i>pt</i> chi angles: 47.4,169.3	0.10Å	-	-	-	-
123	ASN	73.62	-	Allowed (0.19%) Pre-Pro / -102.7,-17.6	Favored (3.4%) <i>m110</i> chi angles: 304.5,158.9	0.13Å	-	OUTLIER(S) worst is CA- CB-CG: 6.5 σ	-	-
				Favored	Favored (18.7%)					

124	PRO	134.28	0.43Å HD2 with 120 ARG O	(3.12%) Trans-Pro / -93.7,-2.6	<i>Cg_endo</i> chi angles: 37.1	0.04Å	-	-	-
125	CYS	109.17	-	Favored (79.71%) General / -56.2,-46.2	Favored (47.4%) <i>t</i> chi angles: 179.5	0.06Å	-	-	-
126	SER	128.28	-	Allowed (0.07%) General / -152.1,-136.6	Favored (2.9%) <i>t</i> chi angles: 198.5	0.14Å	-	-	-
127	ASP	52.7	-	Allowed (0.57%) General / -50.5,158.8	Allowed (1.3%) <i>m-30</i> chi angles: 309.3,56.8	0.05Å	-	-	-
128	THR	94.38	-	Allowed (0.75%) General / -67.7,5.9	Favored (2.6%) <i>t</i> chi angles: 198.4	0.17Å	-	-	-
129	THR	55.16	-	Favored (3.63%) General / -95.9,83.2	Favored (68.5%) <i>p</i> chi angles: 58.8	0.04Å	-	-	-
130	MET	78.4	-	Favored (3.96%) General / -168.2,144.8	Favored (2.6%) <i>mtp</i> chi angles: 272,209.4,82.4	0.12Å	-	-	-
131	THR	32.99	-	Favored (3.7%) General / -104.1,-178.6	OUTLIER (0%) chi angles: 12.3	0.17Å	-	-	-
132	ALA	20.45	-	Favored (18.22%) General / -88.7,-31.9	-	0.09Å	-	OUTLIER(S) worst is C-N- CA: 4.4 σ	-
133	GLU	71.46	-	Favored (17.43%) General / -50.8,-55.3	Favored (2.9%) <i>mp0</i> chi angles: 304.6,87.7,297.8	0.08Å	-	-	-
134	GLU	37.01	-	Favored (93.09%) General / -59.4,-43.1	OUTLIER (0.2%) chi angles: 334.1,80.7,98.2	0.21Å	-	OUTLIER(S) worst is N- CA-CB: 4.5 σ	-
135	PHE	47.09	-	Favored (32.59%) General / -55.8,-55.4	Favored (48.6%) <i>t80</i> chi angles: 184.7,95.9	0.08Å	-	-	-
136	THR	42.97	-	Favored (72.85%) General / -66.1,-31.8	Favored (15.6%) <i>m</i> chi angles: 310.1	0.17Å	-	-	-
137	ASP	32.46	-	Favored (59.29%) General / -78.8,-14.4	Favored (23.4%) <i>m-30</i> chi angles: 307,328.6	0.22Å	-	-	-
				Favored					

138	THR	94.5	-	(13.01%) General / -93.1,16.4 Allowed	Favored (50.7%) <i>p</i> chi angles: 65.6	0.15Å	-	-	-
139	VAL	45.8	-	(0.63%) Ile or Val / -107.6,-73.0 Favored	Favored (46.8%) <i>t</i> chi angles: 169	0.10Å	-	-	-
140	PHE	132.11	-	(63.18%) General / -53.0,-39.3 Allowed	Favored (11.3%) <i>m</i> - 80 chi angles: 280.9,63	0.10Å	-	-	-
141	SER	38.57	-	(0.42%) General / -63.2,1.9 Favored	Favored (34.2%) <i>m</i> chi angles: 302.4	0.06Å	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 71.52				Clashscore: 0.34	Outliers: 1 of 182	Poor rotamers: 15 of 167	Outliers: 3 of 173	Outliers: 0 of 184	Outliers: 15 of 184	Non-Trans: 1 of 183
142	LYS	143.46	-		Favored (4.18%) General / -130.5,-5.8 Favored	Favored (44.3%) <i>mttt</i> chi angles: 300.9,156.5,181.5,169.4	0.07Å	-	-	-
143	ILE	183.07	-		(3.66%) Ile or Val / -112.8,-40.7 Favored	Favored (3.4%) <i>mt</i> chi angles: 301.8,195	0.15Å	-	-	-
144	ASP	83.73	-		(56.35%) General / -68.0,140.8 Favored	Favored (42.6%) <i>t0</i> chi angles: 182.3,16.8	0.03Å	-	-	-
145	VAL	103.11	-		(11.24%) Ile or Val / -115.3,-4.3 Favored	Favored (18.9%) <i>m</i> chi angles: 302.8	0.15Å	-	-	-
146	ASN	75.15	-		(4.15%) General / -114.3,-38.3 Favored	Allowed (0.8%) <i>m</i> - 40 chi angles: 321.6,276	0.05Å	-	-	-
147	GLY	32.31	-		(9.21%) Glycine / 104.4,21.6 Favored	-	-	-	-	-
148	ASP	79.07	-		(10.66%) General / -118.8,-5.3 Favored	Favored (65.4%) <i>m</i> - 30 chi angles: 301,319	0.07Å	-	-	-
149	GLY	32.59	-		(3.24%) Glycine / 88.5,-37.9 Allowed	-	-	-	-	-
150	GLU	52.64	-		(1.91%) General / Favored	Favored (28.7%) <i>mt</i> - 10 chi angles:	0.07Å	-	-	-

-69.4,103.0 287,192.8,46.2

151	LEU	59.55	-	Favored (2.36%) General / -74.4,93.1	Favored (13%) <i>mt</i> chi angles: 312.6,185.5	0.09Å	-	-	-
152	SER	30.06	-	Favored (8.04%) General / -59.7,159.9	Favored (74.8%) <i>p</i> chi angles: 71.3	0.04Å	-	-	-
153	LEU	98.52	-	Favored (71.45%) General / -54.0,-45.2	Allowed (1%) <i>tt</i> chi angles: 208.9,175.3	0.05Å	-	-	-
154	GLU	67.01	-	Favored (68.45%) General / -72.4,-35.5	Favored (28.7%) <i>mm-30</i> chi angles: 305,314.2,306.3	0.14Å	-	-	-
155	GLU	35.14	-	Favored (87.56%) General / -66.8,-39.2	Favored (24.7%) <i>mt-10</i> chi angles: 288.4,163.9,283.5	0.07Å	-	-	-
156	PHE	64.58	-	Favored (73.53%) General / -54.9,-43.7	Favored (42.9%) <i>t80</i> chi angles: 183,97.9	0.08Å	-	-	-
157	ILE	92.98	-	Favored (73.69%) Ile or Val / -61.0,-36.7	Allowed (1.8%) <i>pt</i> chi angles: 76.5,188.7	0.29Å	-	-	-
158	GLU	82.39	-	Favored (19.32%) General / -87.9,-31.7	Favored (27%) <i>mm-30</i> chi angles: 280.4,313.3,304.6	0.15Å	-	-	-
159	GLY	30.19	-	Favored (85.26%) Glycine / -68.7,-40.6	-	-	-	-	-
160	VAL	38.86	-	Favored (56.86%) Ile or Val / -62.5,-32.9	Favored (37.6%) <i>t</i> chi angles: 183.9	0.13Å	-	-	-
161	GLN	57.57	-	Favored (59.85%) General / -79.3,-13.1	Favored (28.5%) <i>mt0</i> chi angles: 292.2,182.1,111.6	0.11Å	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 71.52				Clashscore: 0.34	Outliers: 1 of 182	Poor rotamers: 15 of 167	Outliers: 3 of 173	Outliers: 0 of 184	Outliers: 15 of 184	Non-Trans: 1 of 183
162	LYS	126.89	-		Favored (42.15%) General / -79.6,-24.1	Favored (7.2%) <i>mmtm</i> chi angles: 305.3,298.8,154.5,282.4	0.15Å	-	-	-
					Favored					

163	ASP	62.13	-	(44.37%) General / -125.0,125.7	Favored (14.2%) <i>t0</i> chi angles: 173.2,29.1	0.06Å	-	-	-
164	GLN	39.51	-	Favored (71.94%) General / -65.7,-31.1	Allowed (1%) <i>tt0</i> chi angles: 208,199.4,265.3	0.14Å	-	-	-
165	MET	72.03	-	Favored (86.88%) General / -60.2,-47.2	Favored (9.3%) <i>ttp</i> chi angles: 187,210.8,79.2	0.10Å	-	-	-
166	LEU	48.23	-	Favored (86.81%) General / -58.9,-41.3	Favored (32.1%) <i>mt</i> chi angles: 295.2,186.8	0.13Å	-	-	-
167	LEU	51.48	-	Favored (77.52%) General / -62.5,-34.8	Favored (3.8%) <i>tp</i> chi angles: 208.2,69.7	0.13Å	-	-	-
168	ASP	100.87	-	Favored (41.49%) General / -85.3,-16.0	Favored (65.6%) <i>m-30</i> chi angles: 299.6,309.2	0.14Å	-	-	-
169	THR	119.7	-	Allowed (0.51%) General / -101.3,-79.7	Favored (54.9%) <i>p</i> chi angles: 56.8	0.17Å	-	-	-
170	LEU	87.34	-	Favored (57.95%) General / -50.7,-44.8	Favored (94.8%) <i>mt</i> chi angles: 295.7,173.4	0.11Å	-	-	-
171	THR	134.66	-	Favored (14.73%) General / -100.0,20.2	Favored (5.2%) <i>p</i> chi angles: 44.7	0.23Å	-	-	-
172	ARG	137.96	-	Allowed (0.51%) General / -152.9,29.6	Favored (19.6%) <i>mtm-85</i> chi angles: 267.6,178.2,289.9,290.1	0.09Å	-	-	-
173	SER	73.94	-	Favored (17.18%) General / -82.2,-43.9	Favored (35.6%) <i>p</i> chi angles: 55.5	0.07Å	-	-	-
174	LEU	126.4	-	Favored (45.71%) General / -78.9,-22.5	Favored (16.5%) <i>mt</i> chi angles: 279.6,174.8	0.10Å	-	-	-
175	ASP	50.08	-	Allowed (1.83%) General / -45.2,118.8	Allowed (1.3%) <i>m-30</i> chi angles: 293.3,57	0.03Å	-	OUTLIER(S) worst is C-N- CA: 5.3 σ	-
176	LEU	50.89	-	Allowed (0.08%) General / -36.2,-35.7	Favored (13.4%) <i>tp</i> chi angles: 192.6,55.6	0.11Å	-	-	-

177	THR	37.44	-	Favored (76.23%) General / -58.1,-38.4	Favored (6.1%) <i>p</i> chi angles: 45.2	0.08Å	-	-	-
178	ARG	90.52	-	Favored (68.57%) General / -69.3,-45.9	Favored (31.8%) <i>mmt90</i> chi angles: 302.3,295.3,179.7,79.1	0.05Å	-	-	-
179	ILE	51.22	-	Favored (97.54%) Ile or Val / -63.9,-45.2	Favored (36%) <i>mt</i> chi angles: 301.4,183	0.10Å	-	-	-
180	VAL	32.33	-	Favored (84.67%) Ile or Val / -64.6,-39.2	Favored (18.4%) <i>t</i> chi angles: 164.4	0.18Å	-	-	-
181	ARG	87.83	-	Favored (98.98%) General / -62.0,-42.2	OUTLIER (0.1%) chi angles: 140.2,68.8,203.8,120.2	0.16Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 71.52			Clashscore: 0.34	Outliers: 1 of 182	Poor rotamers: 15 of 167	Outliers: 3 of 173	Outliers: 0 of 184	Outliers: 15 of 184	Non-Trans: 1 of 183
182	ARG	125.8	-	Favored (47.18%) General / -78.2,-23.9	Favored (5.9%) <i>tpm170</i> chi angles: 177.5,69,286.7,172.2	0.15Å	-	-	-
183	LEU	56.64	-	Favored (5.07%) General / -72.2,-56.7	Favored (53.4%) <i>mt</i> chi angles: 289.9,163.4	0.07Å	-	-	-
184	GLN	71.91	-	Favored (2.29%) General / -97.8,73.0	Allowed (1.3%) <i>mt0</i> chi angles: 285.6,138,77.9	0.06Å	-	OUTLIER(S) worst is C-N- CA: 5.3 σ	-
185	ASN	83.82	-	-	Favored (8.1%) <i>m110</i> chi angles: 292.3,162.4	0.15Å	-	OUTLIER(S) worst is CA- CB-CG: 7.2 σ	-

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