



# Viewing guca1a\_mb\_2-185H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	50.63		4 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.60%	Goal: <1%
	Ramachandran outliers	2	1.10%	Goal: <0.05%
	Ramachandran favored	174	95.60%	Goal: >98%
	MolProbity score <sup>^</sup>	2.48		48 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.58%	Goal: 0
	Bad backbone bonds:	0 / 1518	0.00%	Goal: 0%
	Bad backbone angles:	12 / 2046	0.59%	Goal: <0.1%

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

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

<sup>^</sup> 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
		Avg: 71.52	Clashscore: 50.63	Outliers: 2 of 182	Poor rotamers: 1 of 167	Outliers: 1 of 173	Outliers: 0 of 184	Outliers: 12 of 184
2	GLY	37.74	-	-	-	-	-	-
3	ASN	206.79	-	Allowed (0.07%) General / -72.2,-161.0	12.7% ( <i>m</i> -20) chi angles: 292.1,15.8	0.096Å	-	OUTLIER(S) worst is CA-CB-CG: 4.586 σ
4	VAL	58.77	0.509Å O with 4 VAL HG12	Allowed (0.42%) Isoleucine or valine / -79.6,67.5	95.1% ( <i>t</i> ) chi angles: 175.9	0.102Å	-	-
5	MET	72.45	0.76Å HE1 with 13 LEU HD11	Favored (36.06%) General / -99.2,118.5	92% ( <i>mtp</i> ) chi angles: 294.1,184.5,73.7	0.106Å	-	-
			0.42Å	Favored	41.6% ( <i>mm</i> -40)			

6	GLU	78.68	O with 10 VAL HG23	(15.34%) General / -79.3,171.3 Favored (91.31%) Glycine / -60.4,-36.5 Favored (97.99%) General / -62.0,-41.3 Favored (94.32%) General / -64.7,-39.8 Favored (79.43%) Isoleucine or valine / -62.0,-37.9 Favored (99.5%) General / -63.1,-42.1 Favored (97.57%) General / -63.9,-40.9 Favored (88.86%) General / -64.4,-37.8 Favored (73.83%) General / -62.6,-32.8 Favored (59.64%) General / -82.5,-7.6 Favored (52.62%) General / -68.6,146.9 Favored (51.68%) General / -65.6,148.5 Favored	chi angles: 289.2,281.5,302.8 - 93.4% ( <i>mttt</i> ) chi angles: 289.7,171.5,172.9,181 87.3% ( <i>p</i> ) chi angles: 67.6 95% ( <i>t</i> ) chi angles: 176.8 63% ( <i>mm-40</i> ) chi angles: 293.4,286.2,355.3 79.3% ( <i>mm-40</i> ) chi angles: 294.3,296.3,340.5 85.4% ( <i>mt</i> ) chi angles: 296,180.4 94.2% ( <i>p</i> ) chi angles: 65 90.9% ( <i>p</i> ) chi angles: 65.2 86.8% ( <i>m</i> ) chi angles: 301.2 77.8% ( <i>tt0</i> ) chi angles: 180,188.3,9	0.113Å - 0.083Å 0.088Å 0.073Å 0.096Å 0.103Å 0.088Å 0.074Å 0.069Å 0.055Å 0.089Å	-	-
7	GLY	18.54	-			-	-	-
8	LYS	30.66	-			-	-	-
9	SER	26.11	0.438Å OG with 5 MET HB3			-	-	-
10	VAL	33.12	0.501Å HG11 with 177 THR HA			-	-	-
11	GLU	74.22	-			-	-	-
12	GLU	64.74	-			-	-	-
13	LEU	40.79	0.76Å HD11 with 5 MET HE1			-	-	-
14	SER	90.46	-			-	-	-
15	SER	52.78	-			-	-	-
16	THR	42	0.454Å HG22 with 17 GLU N			-	-	-
17	GLU	79.01	0.624Å HG2 with 19 HIS H			-	-	-

18	CYS	79.59	-	(85.86%) General / -62.3,-37.5	67.8% ( <i>m</i> ) chi angles: 287.8	0.123Å	-	-
19	HIS	41.77	0.624Å H with 17 GLU HG2	Favored (83.52%) General / -58.3,-41.0	57.8% ( <i>t-80</i> ) chi angles: 182,266.7	0.081Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.444 σ
20	GLN	33.54	-	Favored (99.74%) General / -63.0,-42.3	99.1% ( <i>mm-40</i> ) chi angles: 294.3,301,313.9	0.072Å	-	-
21	TRP	49.93	0.479Å NE1 with 84 LEU HD21	Favored (90.27%) General / -65.0,-44.2	96.2% ( <i>m95</i> ) chi angles: 293,92.6	0.09Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 71.52	Clashscore: 50.63	Outliers: 2 of 182	Poor rotamers: 1 of 167	Outliers: 1 of 173	Outliers: 0 of 184	Outliers: 12 of 184
22	TYR	60.06	0.471Å CE2 with 26 MET HG3	Favored (84.94%) General / -66.6,-43.4	44.8% ( <i>t80</i> ) chi angles: 192.9,77.7	0.044Å	-	-
23	LYS	101.8	-	Favored (97.59%) General / -63.6,-40.7	19.1% ( <i>ptmt</i> ) chi angles: 67.6,174.3,303.7,172.3	0.066Å	-	-
24	LYS	56.02	-	Favored (97.25%) General / -62.9,-44.0	46.9% ( <i>tttp</i> ) chi angles: 180.1,168.5,169.1,79.3	0.09Å	-	-
25	PHE	76.44	0.875Å HE1 with 34 LEU HG	Favored (69.83%) General / -61.3,-51.2	87.5% ( <i>t80</i> ) chi angles: 174.5,77.7	0.075Å	-	-
26	MET	42.08	0.471Å HG3 with 22 TYR CE2	Favored (91.73%) General / -65.2,-38.8	93.9% ( <i>mmm</i> ) chi angles: 294.2,298.9,280.9	0.066Å	-	-
27	THR	28.09	-	Favored (81.96%) General / -64.2,-46.9	89.2% ( <i>m</i> ) chi angles: 300.9	0.072Å	-	-
28	GLU	56.37	-	Favored (70.69%) General / -71.6,-38.9	87.6% ( <i>mt-10</i> ) chi angles: 293.6,180.9,13.4	0.061Å	-	-

29	CYS 108.85	0.481Å SG with 25 PHE CE1	Favored (48.5%) Pre-proline / -123.3,93.0	23.3% ( <i>p</i> ) chi angles: 56.1	0.061Å	-	-
30	PRO 62.46	-	Favored (69.2%) Trans-proline / -63.7,-24.3	20% ( <i>Cg_endo</i> ) chi angles: 19.2	0.108Å	-	-
31	SER 30.37	-	Favored (65.09%) General / -67.9,-22.7	99.8% ( <i>p</i> ) chi angles: 64.5	0.079Å	-	-
32	GLY 19.58	-	Favored (70.32%) Glycine / 83.2,16.1	-	-	-	-
33	GLN 48.16	-	Favored (49.98%) General / -137.3,154.9	94.2% ( <i>mt-30</i> ) chi angles: 297.7,177.4,316.4	0.128Å	-	-
34	LEU 70.77	0.875Å HG with 25 PHE HE1	Favored (40.15%) General / -131.3,128.6	67.4% ( <i>mt</i> ) chi angles: 287.5,176.9	0.149Å	-	-
35	THR 41.35	0.774Å HG22 with 70 TYR CE1	Favored (9.26%) General / -84.1,175.8	75.2% ( <i>p</i> ) chi angles: 61.7	0.108Å	-	-
36	LEU 41.11	0.447Å HD13 with 60 PHE CB	Favored (95.77%) General / -63.5,-39.9	59.1% ( <i>tp</i> ) chi angles: 179.4,59.7	0.075Å	-	-
37	TYR 47.05	-	Favored (89.93%) General / -62.7,-46.0	72.6% ( <i>t80</i> ) chi angles: 185.8,79.8	0.084Å	-	-
38	GLU 43.65	-	Favored (76.2%) General / -66.4,-33.7	89.1% ( <i>mt-10</i> ) chi angles: 289.3,177.2,331.2	0.056Å	-	-
39	PHE 106.78	0.484Å CE1 with 45 LEU HD22	Favored (95.26%) General / -60.4,-44.9	32.7% ( <i>t80</i> ) chi angles: 174.4,276.5	0.099Å	-	-
40	ARG 93.33	0.528Å HA with 45 LEU HB2	Favored (98.08%) General / -63.5,-43.2	40.6% ( <i>mtp180</i> ) chi angles: 295.7,180.4,74.8,156.5	0.074Å	-	-

41	GLN	41.77	-		Favored (92.01%) General / -65.7,-41.7	30.1% ( <i>mt</i> -30) chi angles: 296,180,134.2	0.063Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	
		Avg: 71.52	Clashscore: 50.63	Outliers: 2 of 182	Poor rotamers: 1 of 167	Outliers: 1 of 173	Outliers: 0 of 184	Outliers: 12 of 184	
42	PHE	67.03	-	Favored (74.56%) General / -60.9,-50.1	84.4% ( <i>t80</i> ) chi angles: 181.4,81.6	0.093Å	-	-	
43	PHE	97.62	0.823Å CB with 45 LEU HD13	Favored (49.13%) General / -77.8,-26.0	79.6% ( <i>m</i> -85) chi angles: 289.9,281.3	0.136Å	-	OUTLIER(S) worst is CA- CB-CG: 8.609 σ	
44	GLY	48.7	-	Favored (26.1%) Glycine / 90.5,25.3	-	-	-	OUTLIER(S) worst is C-N- CA: 4.649 σ	
45	LEU	182.48	0.823Å HD13 with 43 PHE CB	Favored (59.33%) General / -81.3,-6.8	6.8% ( <i>mp</i> ) chi angles: 280.5,49.5	0.191Å	-	-	
46	LYS	219.01	-	Favored (21.72%) General / -70.3,165.7	13.9% ( <i>mmmm</i> ) chi angles: 294.6,294.2,295.9,303.7	0.108Å	-	-	
47	ASN	117.38	-	Favored (28.71%) General / 51.3,44.7	5.8% ( <i>p</i> -10) chi angles: 61.1,277.4	0.147Å	-	-	
48	LEU	48.34	0.508Å HG with 45 LEU O	Favored (13.45%) General / -89.6,166.7	84.8% ( <i>mt</i> ) chi angles: 295.7,180.3	0.081Å	-	-	
49	SER	30.94	-	Favored (12.91%) Pre-proline / -67.2,168.0	98.2% ( <i>p</i> ) chi angles: 64.2	0.095Å	-	-	
50	PRO	66.07	-	Favored (67.7%) Trans-proline / -61.6,-37.6	82.3% ( <i>Cg_exo</i> ) chi angles: 330.8	0.185Å	-	-	
51	SER	27.74	-	Favored (65.21%) General /	47.2% ( <i>t</i> ) chi angles: 180.2	0.093Å	-	-	

52	ALA	27.57	O with 56 VAL HG23	0.512Å Favored (95.03%) General / -63.9,-39.8	-	0.074Å	-	-
53	SER	22.24	-	Favored (94.34%) General / -63.5,-39.4	48% (t) chi angles: 179.7	0.087Å	-	-
54	GLN	60.54	O with 57 GLU HG2	0.666Å Favored (94.44%) General / -64.0,-39.6	35.7% (tp60) chi angles: 183,76.1,12.9	0.101Å	-	-
55	TYR	122.6	HD2 with 183 LEU HD21	0.569Å Favored (99.23%) General / -63.2,-42.4	71.7% (t80) chi angles: 173.2,85.3	0.064Å	-	-
56	VAL	36.53	HG23 with 52 ALA O	0.512Å Favored (96.05%) Isoleucine or valine / -61.7,-42.9	93.7% (t) chi angles: 175.7	0.079Å	-	-
57	GLU	76.95	HG2 with 54 GLN O	0.666Å Favored (94.64%) General / -64.5,-43.3	15.9% (pt-20) chi angles: 65.2,176.5,301	0.1Å	-	-
58	GLN	42.08	HA with 61 GLU OE2	0.767Å Favored (78.16%) General / -66.3,-34.5	95.8% (mt-30) chi angles: 294.1,181,316.6	0.072Å	-	-
59	MET	80.86	HG3 with 63 PHE HE2	0.749Å Favored (95.79%) General / -64.9,-40.9	30.5% (tpp) chi angles: 191.1,62.9,50.1	0.033Å	-	-
60	PHE	52.13	CE1 with 71 ILE HG12	0.725Å Favored (88.32%) General / -60.0,-46.8	81.3% (t80) chi angles: 179.8,84.3	0.104Å	-	-
61	GLU	97.24	OE2 with 58 GLN HA	0.767Å Favored (83.02%) General / -64.2,-36.1	8.8% (pt-20) chi angles: 52.5,197.8,296.5	0.093Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 71.52	Clashscore: 50.63	Outliers: 2 of 182	Poor rotamers: 1 of 167	Outliers: 1 of 173	Outliers: 0 of 184	Outliers: 12 of 184
62	THR	125.96	-	Favored (95.7%)	66.3% (p)	0.107Å	-	-

			General / -63.9,-40.1	chi angles: 57.2			
63	PHE 142.52	0.749Å HE2 with 59 MET HG3	Favored (63.62%) General / -71.5,-28.0	78.6% ( <i>m-85</i> ) chi angles: 293.4,287.2	0.096Å	-	OUTLIER(S) worst is CA- CB-CG: 8.164 σ
64	ASP 84.33	0.479Å O with 67 LYS HE3	Allowed (1.87%) General / -74.1,86.0	63.8% ( <i>t0</i> ) chi angles: 185,2.4	0.113Å	-	-
65	PHE 131.03	0.711Å HD2 with 75 GLU HG2	Favored (74.28%) General / -60.8,-50.2	97% ( <i>m-85</i> ) chi angles: 294.5,271.2	0.07Å	-	OUTLIER(S) worst is CA- CB-CG: 6.168 σ
66	ASN 96.49	-	Favored (60.72%) General / -73.7,-19.8	49% ( <i>p30</i> ) chi angles: 60.8,2.9	0.155Å	-	-
67	LYS 162.37	0.479Å HE3 with 64 ASP O	Favored (6.19%) General / 68.2,29.3	23.8% ( <i>mmt</i> ) chi angles: 300.5,302.2,163.2,45.9	0.067Å	-	-
68	ASP 100	-	Favored (57.72%) General / -76.2,-20.1	55.3% ( <i>p-10</i> ) chi angles: 61,356.7	0.118Å	-	-
69	GLY 39.39	-	Favored (35.4%) Glycine / 107.2,0.1	-	-	-	-
70	TYR 67.61	0.774Å CE1 with 35 THR HG22	Favored (44.16%) General / -131.6,157.2	98.2% ( <i>m-85</i> ) chi angles: 297,271.4	0.151Å	-	-
71	ILE 117.24	0.725Å HG12 with 60 PHE CE1	Favored (24.1%) Isoleucine or valine / -109.0,107.9	36% ( <i>mm</i> ) chi angles: 298.6,293.5	0.182Å	-	-
72	ASP 77.19	-	Favored (6.9%) General / -85.9,-179.9	42.1% ( <i>p30</i> ) chi angles: 58.1,15.8	0.07Å	-	-
73	PHE 130.99	0.497Å CZ with 74 MET CE	Favored (85.5%) General / -62.0,-37.6	40.6% ( <i>p90</i> ) chi angles: 54.8,273.3	0.131Å	-	-
		0.497Å	Favored (80.27%)	2.2% ( <i>mpt?</i> )			

74	MET	137.17	O with 77 VAL HG22	General / -64.8,-46.8	chi angles: 303.4,76.2,165.8	0.171Å	-	-
75	GLU	59.39	0.711Å HG2 with 65 PHE HD2	Favored (73.2%) General / -67.1,-32.2	95.3% ( <i>mt-10</i> ) chi angles: 292.4,168.9,342.8	0.057Å	-	-
76	TYR	70.45	-	Favored (72.76%) General / -62.2,-50.2	83.7% ( <i>t80</i> ) chi angles: 182.6,73.3	0.061Å	-	-
77	VAL	38.49	0.497Å HG22 with 74 MET O	Favored (81.22%) Isoleucine or valine / -67.4,-38.7	27.4% ( <i>m</i> ) chi angles: 295.9	0.058Å	-	-
78	ALA	24.82	0.459Å N with 77 VAL HG23	Favored (99.69%) General / -63.0,-41.9	-	0.095Å	-	-
79	ALA	31.01	0.497Å CB with 63 PHE CD1	Favored (99.28%) General / -63.2,-42.9	-	0.101Å	-	-
80	LEU	54.52	-	Favored (74.62%) General / -64.2,-32.9	66.7% ( <i>mt</i> ) chi angles: 290.6,180.3	0.09Å	-	-
81	SER	88.71	-	Favored (76.03%) General / -61.1,-35.0	79.1% ( <i>p</i> ) chi angles: 70.1	0.08Å	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash &gt; 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> </div>								
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82	LEU	77.17	0.594Å HD21 with 94 TRP CB	Favored (34.21%) General / -76.0,-45.6	55.3% ( <i>mt</i> ) chi angles: 288.2,180.2	0.089Å	-	-
83	VAL	56.83	0.513Å HG12 with 176 LEU HB2	Favored (77.91%) Isoleucine or valine / -70.1,-44.6	92.4% ( <i>t</i> ) chi angles: 178	0.052Å	-	-
84	LEU	103.71	0.479Å HD21 with 21 TRP NE1	Favored (22.63%) General / -79.4,165.9	6.9% ( <i>mp</i> ) chi angles: 286,55.2	0.083Å	-	-



85	LYS	46.56	-	Favored (57.66%) General / -66.3,138.5	93% ( <i>mttt</i> ) chi angles: 289.1,168.6,178.8,178.1	0.08Å	-	-
86	GLY	24.94	-	Favored (7.47%) Glycine / -162.4,-154.2	-	-	-	-
87	LYS	74.6	0.505Å HD2 with 87 LYS N	Favored (39.88%) General / -93.5,129.0	9.9% ( <i>mptt</i> ) chi angles: 299.9,70.1,180.6,178.5	0.112Å	-	-
88	VAL	27.79	-	Favored (74.22%) Isoleucine or valine / -63.9,-35.7	93.3% ( <i>t</i> ) chi angles: 175.7	0.08Å	-	-
89	GLU	40.47	-	Favored (89.54%) General / -60.4,-46.6	37.8% ( <i>mt-10</i> ) chi angles: 296.6,167.2,290.1	0.137Å	-	-
90	GLN	48.79	0.425Å NE2 with 94 TRP CH2	Favored (78.05%) General / -69.3,-37.8	26.3% ( <i>mt-30</i> ) chi angles: 296.9,180,186.8	0.063Å	-	-
91	LYS	49.49	-	Favored (73.08%) General / -63.0,-31.9	92.8% ( <i>mttt</i> ) chi angles: 292.2,167.9,179.9,179.9	0.115Å	-	-
92	LEU	65.48	0.989Å HD21 with 157 ILE HA	Favored (94.06%) General / -59.6,-43.0	20.2% ( <i>tp</i> ) chi angles: 194,59	0.013Å	-	-
93	ARG	111.36	-	Favored (87.5%) General / -66.9,-39.7	63.8% ( <i>mtp85</i> ) chi angles: 293.7,176.7,81.5,84.4	0.066Å	-	-
94	TRP	64.65	0.594Å CB with 82 LEU HD21	Favored (92.06%) General / -65.8,-40.8	49% ( <i>m0</i> ) chi angles: 295.3,336.8	0.009Å	-	-
95	TYR	67.55	0.575Å OH with 174 LEU HB2	Favored (93.56%) General / -64.6,-39.4	33.5% ( <i>m-85</i> ) chi angles: 277.4,86.8	0.106Å	-	-
96	PHE	97.52	0.422Å CE2 with 153 LEU HA	Favored (94.24%) General / -59.9,-44.5	33.5% ( <i>t80</i> ) chi angles: 180.6,279.3	0.078Å	-	OUTLIER(S) worst is CA- CB-CG: 4.233 σ

97	LYS	61.19	-	Favored (83.23%) General / -62.1,-37.0	51.3% ( <i>mttm</i> ) chi angles: 290,167.9,168.5,287.1	0.116Å	-	-
98	LEU	65.53	-	Favored (85%) General / -64.0,-46.3	20.2% ( <i>tp</i> ) chi angles: 180.2,76.2	0.134Å	-	-
99	TYR	73.33	0.812Å HA with 115 ILE HD12	Favored (87.9%) General / -64.3,-37.5	69.2% ( <i>m-85</i> ) chi angles: 290.1,287.8	0.103Å	-	-
100	ASP	59.66	-	Allowed (1.03%) General / -72.2,84.8	52.2% ( <i>t0</i> ) chi angles: 184.1,14.4	0.105Å	-	-
101	VAL	43.68	-	Favored (81.11%) Isoleucine or valine / -61.5,-50.2	92.5% ( <i>t</i> ) chi angles: 178	0.055Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 71.52	Clashscore: 50.63	Outliers: 2 of 182	Poor rotamers: 1 of 167	Outliers: 1 of 173	Outliers: 0 of 184	Outliers: 12 of 184
102	ASP	69.69	-	Favored (63.66%) General / -71.8,-28.5	57.8% ( <i>p-10</i> ) chi angles: 61.7,359.3	0.151Å	-	-
103	GLY	28.48	-	Favored (59.14%) Glycine / 87.2,17.5	-	-	-	-
104	ASN	81.69	-	Favored (62.33%) General / -71.5,-18.2	50.5% ( <i>p30</i> ) chi angles: 61.7,1.4	0.12Å	-	-
105	GLY	37.74	-	Favored (38.66%) Glycine / 106.1,1.3	-	-	-	-
106	CYS	90.08	-	Favored (48.56%) General / -137.3,156.2	25.6% ( <i>p</i> ) chi angles: 57.8	0.07Å	-	-
107	ILE	50.61	-	Favored (44.25%) Isoleucine or valine / -108.0,113.6	87.2% ( <i>mt</i> ) chi angles: 299.2,168.5	0.123Å	-	-

108	ASP	57.68	0.643Å OD1 with 111 GLU HG3	Favored (9.68%) General / -89.7,171.4	21.2% ( <i>p30</i> ) chi angles: 58.2,32.7	0.108Å	-	-
109	ARG	69.57	-	Favored (98.22%) General / -60.9,-42.6	65.4% ( <i>ttt180</i> ) chi angles: 179.7,194.3,175.4,188.2	0.133Å	-	-
110	ASP	35.71	0.542Å O with 114 THR HG23	Favored (97.38%) General / -63.9,-42.4	1.1% ( <i>m-20</i> ) chi angles: 292.4,43.3	0.088Å	-	OUTLIER(S) worst is CA- CB-CG: 4.791 σ
111	GLU	38.73	0.643Å HG3 with 108 ASP OD1	Favored (93.22%) General / -64.8,-43.4	83.9% ( <i>mt-10</i> ) chi angles: 294.5,179.8,324.2	0.054Å	-	-
112	LEU	123.82	0.591Å O with 112 LEU HD13	Favored (99.53%) General / -62.4,-42.5	0.6% chi angles: 193.7,308.7	0.164Å	-	-
113	LEU	104.3	0.77Å O with 116 ILE HG22	Favored (95.32%) General / -64.6,-42.7	1.6% ( <i>tm?</i> ) chi angles: 194.8,297.9	0.057Å	-	-
114	THR	104.04	0.542Å HG23 with 110 ASP O	Favored (76.33%) General / -63.6,-48.7	61.3% ( <i>p</i> ) chi angles: 62.7	0.072Å	-	-
115	ILE	54.8	0.812Å HD12 with 99 TYR HA	Favored (81.74%) Isoleucine or valine / -67.3,-38.9	96.4% ( <i>mt</i> ) chi angles: 295.2,168.8	0.061Å	-	-
116	ILE	137.19	0.77Å HG22 with 113 LEU O	Favored (87.66%) Isoleucine or valine / -61.2,-41.0	7.5% ( <i>tp</i> ) chi angles: 204.5,67.3	0.04Å	-	-
117	GLN	45.09	0.545Å HG3 with 113 LEU HD13	Favored (85.28%) General / -67.1,-42.0	39.1% ( <i>mt-30</i> ) chi angles: 294.7,183.1,249.2	0.159Å	-	-
118	ALA	44.51	-	Favored (85.29%) General / -60.8,-47.7	-	0.086Å	-	-
119	ILE	115.36	0.576Å HD12 with 173 SER OG	Favored (16.2%) Isoleucine or valine / -75.0,-17.6	49% ( <i>pt</i> ) chi angles: 62.6,170.8	0.158Å	-	-

120	ARG	107.23	0.514Å HD2 with 55 TYR CD1	Favored (12.56%) General / 60.7,43.3	99.9% ( <i>mtt180</i> ) chi angles: 293.7,181.2,180.4,175.7	0.081Å	-	-
121	ALA	55.97	0.517Å HB3 with 116 ILE CD1	Favored (73.21%) General / -63.1,-31.9	-	0.074Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 71.52	Clashscore: 50.63	Outliers: 2 of 182	Poor rotamers: 1 of 167	Outliers: 1 of 173	Outliers: 0 of 184	Outliers: 12 of 184
122	ILE	72.75	-	Favored (46.23%) Isoleucine or valine / -62.9,-29.1	47.7% ( <i>pt</i> ) chi angles: 62.4,169.5	0.061Å	-	-
123	ASN	73.62	0.753Å HB3 with 182 ARG NH1	Favored (25.01%) Pre-proline / -58.8,-34.6	2.8% ( <i>m120</i> ) chi angles: 291.9,183.7	0.088Å	-	OUTLIER(S) worst is CA- CB-CG: 4.521 $\sigma$
124	PRO	134.28	0.506Å HG2 with 121 ALA O	Favored (23.45%) Trans-proline / -73.8,-10.7	4% ( <i>Cg_endo</i> ) chi angles: 6.8	0.26Å	-	-
125	CYS	109.17	0.568Å SG with 130 MET HG3	Allowed (0.96%) General / -54.6,-64.0	35.9% ( <i>t</i> ) chi angles: 188.5	0.038Å	-	-
126	SER	128.28	0.501Å HB2 with 125 CYS O	OUTLIER (0%) General / 157.6,-107.4	47.3% ( <i>t</i> ) chi angles: 180.1	0.171Å	-	-
127	ASP	52.7	-	Favored (50.31%) General / -57.7,140.9	93.6% ( <i>m-20</i> ) chi angles: 289.8,337.7	0.091Å	-	OUTLIER(S) worst is CA- CB-CG: 4.449 $\sigma$
128	THR	94.38	0.454Å HG23 with 129 THR N	Favored (71.27%) General / -59.9,-33.0	12% ( <i>t</i> ) chi angles: 185.3	0.078Å	-	-
129	THR	55.16	0.687Å O with 130 MET HG2	OUTLIER (0.01%) General / -59.1,89.0	86.5% ( <i>m</i> ) chi angles: 301.3	0.066Å	-	-
130	MET	78.4	0.835Å CE with 130 MET HA	Allowed (0.11%) General / -173.9,101.9	1.1% ( <i>mmp</i> ) chi angles: 278.1,283.2,65.5	0.129Å	-	-

131	THR	32.99	0.687Å HB with 134 GLU HG3	Favored (26.88%) General / -80.6,155.4	92.7% ( <i>m</i> ) chi angles: 300.3	0.074Å	-	-
132	ALA	20.45	0.544Å N with 131 THR HG22	Favored (98.28%) General / -62.9,-40.6	-	0.093Å	-	-
133	GLU	71.46	0.633Å H with 131 THR HG22	Favored (87.96%) General / -66.7,-39.5	1.5% ( <i>mp0</i> ) chi angles: 288,82,288.2	0.069Å	-	-
134	GLU	37.01	0.687Å HG3 with 131 THR HB	Favored (84.26%) General / -65.1,-45.7	96.6% ( <i>mt-10</i> ) chi angles: 293.7,173.4,0.9	0.123Å	-	-
135	PHE	47.09	0.824Å CZ with 169 THR HG21	Favored (96.16%) General / -64.2,-40.5	83% ( <i>t80</i> ) chi angles: 181.8,82.2	0.067Å	-	OUTLIER(S) worst is CA- CB-CG: 5.832 σ
136	THR	42.97	-	Favored (97.49%) General / -63.8,-42.9	87.5% ( <i>m</i> ) chi angles: 301.1	0.051Å	-	-
137	ASP	32.46	-	Favored (93.6%) General / -63.5,-39.1	90.7% ( <i>m-20</i> ) chi angles: 290.9,350	0.109Å	-	-
138	THR	94.5	0.816Å HG22 with 135 PHE O	Favored (88.49%) General / -65.8,-38.2	5.2% ( <i>t</i> ) chi angles: 197.4	0.079Å	-	-
139	VAL	45.8	1.074Å HG13 with 143 ILE HD12	Favored (82.87%) Isoleucine or valine / -57.9,-48.9	58.8% ( <i>t</i> ) chi angles: 170.9	0.079Å	-	-
140	PHE	132.11	0.439Å CE2 with 151 LEU HG	Favored (91.91%) General / -65.6,-39.8	57% ( <i>m-85</i> ) chi angles: 282.7,87.8	0.061Å	-	OUTLIER(S) worst is CA- CB-CG: 7.742 σ
141	SER	38.57	-	Favored (85.75%) General / -58.8,-47.1	68.1% ( <i>m</i> ) chi angles: 296.9	0.091Å	-	-

# Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles  
 Avg: Clashscore: Outliers: 2 of Poor rotamers: 1 of Outliers: Outliers: Outliers: 12

		71.52	50.63	182	167	1 of 173	0 of 184	of 184
142	LYS	143.46	-	Favored (7.04%) General / -74.1,-54.8	55.6% ( <i>tp</i> ) chi angles: 187.2,70.5,176.6,179.8	0.068Å	-	-
143	ILE	183.07	1.074Å HD12 with 139 VAL HG13	Favored (25.09%) Isoleucine or valine / -78.1,-39.4	73.8% ( <i>mt</i> ) chi angles: 303.1,171.7	0.083Å	-	-
144	ASP	83.73	-	Favored (3.37%) General / -76.8,85.3	47% ( <i>t0</i> ) chi angles: 193.5,354	0.078Å	-	-
145	VAL	103.11	0.692Å HG22 with 155 GLU OE2	Favored (80.41%) Isoleucine or valine / -59.5,-50.3	28.9% ( <i>m</i> ) chi angles: 295.2	0.059Å	-	-
146	ASN	75.15	0.6Å N with 145 VAL HG23	Favored (66.48%) General / -70.8,-30.1	37.5% ( <i>p-10</i> ) chi angles: 57.2,346.8	0.146Å	-	-
147	GLY	32.31	-	Favored (57.04%) Glycine / 84.4,21.2	-	-	-	-
148	ASP	79.07	-	Favored (60.35%) General / -73.3,-22.4	53.3% ( <i>p-10</i> ) chi angles: 59.2,357.7	0.115Å	-	-
149	GLY	32.59	-	Favored (53.13%) Glycine / 98.7,9.3	-	-	-	-
150	GLU	52.64	-	Favored (52.28%) General / -132.2,149.9	67.4% ( <i>mt-10</i> ) chi angles: 297.8,169.6,319.4	0.118Å	-	-
151	LEU	59.55	0.439Å HG with 140 PHE CE2	Favored (38.86%) General / -112.1,119.6	81.1% ( <i>mt</i> ) chi angles: 294.5,180.5	0.128Å	-	-
152	SER	30.06	-	Favored (18.92%) General / -81.0,168.2	95.6% ( <i>p</i> ) chi angles: 63.7	0.094Å	-	-
153	LEU	98.52	0.553Å HD23 with 157 ILE HG23	Favored (96.08%) General / -63.4,-40.0	1.6% ( <i>tt</i> ) chi angles: 196,186.6	0.068Å	-	-

154	GLU	67.01	0.638Å O with 158 GLU HG2	Favored (92.25%) General / -64.2,-44.3	92.5% ( <i>mt-10</i> ) chi angles: 286,185.7,355	0.105Å	-	-
155	GLU	35.14	0.692Å OE2 with 145 VAL HG22	Favored (95.63%) General / -63.8,-40.0	62.1% ( <i>mt-10</i> ) chi angles: 292.3,179.5,306.2	0.058Å	-	-
156	PHE	64.58	0.625Å O with 160 VAL HG23	Favored (39.09%) General / -61.6,-54.7	69.7% ( <i>t80</i> ) chi angles: 187,75.8	0.068Å	-	-
157	ILE	92.98	0.989Å HA with 92 LEU HD21	Favored (97.94%) Isoleucine or valine / -63.9,-44.3	44.7% ( <i>pt</i> ) chi angles: 63,167.9	0.061Å	-	-
158	GLU	82.39	0.675Å N with 157 ILE HG13	Favored (69.03%) General / -64.9,-49.8	33% ( <i>mm-40</i> ) chi angles: 301.4,292.2,9.3	0.119Å	-	-
159	GLY	30.19	-	Favored (91.99%) Glycine / -66.4,-43.7	-	-	-	-
160	VAL	38.86	0.678Å CG1 with 167 LEU HA	Favored (80.32%) Isoleucine or valine / -65.3,-37.5	89.1% ( <i>t</i> ) chi angles: 177.8	0.064Å	-	-
161	GLN	57.57	0.634Å HG3 with 157 ILE O	Favored (72.93%) General / -66.6,-31.9	73.8% ( <i>mt-30</i> ) chi angles: 296,177.6,58.3	0.036Å	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash &gt; 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> </div>								
Avg: 71.52			Clashscore: 50.63	Outliers: 2 of 182	Poor rotamers: 1 of 167	Outliers: 1 of 173	Outliers: 0 of 184	Outliers: 12 of 184
162	LYS	126.89	0.583Å HG2 with 158 GLU O	Favored (75.18%) General / -70.2,-37.7	46.7% ( <i>mmtm</i> ) chi angles: 300.3,299.8,177.9,289.6	0.062Å	-	-
163	ASP	62.13	-	Favored (51.51%) General / -110.2,124.4	21.7% ( <i>t0</i> ) chi angles: 193.6,317.8	0.059Å	-	-
164	GLN	39.51	-	Favored (89.68%) General /	98.5% ( <i>mt-30</i> ) chi angles:	0.07Å	-	-

				-65.7,-38.6	292.7,180.1,320.9			
165	MET	72.03	-	Favored (92.22%) General / -64.1,-44.5	67.6% ( <i>ttp</i> ) chi angles: 181.5,180,68.9	0.089Å	-	-
166	LEU	48.23	0.402Å HD13 with 143 ILE HD11	Favored (94.14%) General / -64.2,-39.5	87.6% ( <i>mt</i> ) chi angles: 296.8,180.4	0.099Å	-	-
167	LEU	51.48	0.678Å HA with 160 VAL CG1	Favored (83.71%) General / -62.4,-47.5	58.9% ( <i>tp</i> ) chi angles: 180.1,64.8	0.07Å	-	-
168	ASP	100.87	0.508Å O with 172 ARG HB2	Favored (63.83%) General / -62.7,-52.3	87.7% ( <i>m-20</i> ) chi angles: 292.6,350.3	0.157Å	-	-
169	THR	119.7	0.824Å HG21 with 135 PHE CZ	Favored (79.8%) General / -66.0,-45.9	12.8% ( <i>t</i> ) chi angles: 185.9	0.044Å	-	-
170	LEU	87.34	0.569Å N with 169 THR HG23	Favored (61.63%) General / -73.9,-41.8	89.1% ( <i>mt</i> ) chi angles: 297.4,180.4	0.066Å	-	-
171	THR	134.66	0.413Å O with 95 TYR CZ	Favored (15.62%) General / -94.5,-28.2	44.4% ( <i>p</i> ) chi angles: 66.8	0.197Å	-	-
172	ARG	137.96	0.508Å HB2 with 168 ASP O	Favored (30.04%) General / -86.5,-19.1	87.5% ( <i>mtt-85</i> ) chi angles: 304.3,189.1,188.2,281.2	0.066Å	-	-
173	SER	73.94	0.576Å OG with 119 ILE HD12	Favored (63.3%) General / -55.3,-33.6	89.9% ( <i>p</i> ) chi angles: 62.5	0.071Å	-	-
174	LEU	126.4	0.575Å HB2 with 95 TYR OH	Favored (59.71%) General / -80.0,-9.6	64.5% ( <i>mt</i> ) chi angles: 293,183	0.155Å	-	-
175	ASP	50.08	0.48Å HB2 with 178 ARG HG2	Favored (16.51%) General / -53.1,143.9	74.2% ( <i>m-20</i> ) chi angles: 291.1,357.2	0.094Å	-	-
			0.513Å	Favored (95.98%)	61.9% ( <i>tp</i> )			



176	LEU	50.89	HB2 with 83 VAL HG12	General / -60.3,-43.9	chi angles: 180.8,63	0.056Å	-	-
177	THR	37.44	0.501Å HA with 10 VAL HG11	Favored (97.47%) General / -62.8,-40.5	75.4% ( <i>p</i> ) chi angles: 60	0.057Å	-	-
178	ARG	90.52	0.48Å HG2 with 175 ASP HB2	Favored (93.07%) General / -64.8,-39.1	29.2% ( <i>mmt180</i> ) chi angles: 297.6,305.7,175.9,206.9	0.076Å	-	-
179	ILE	51.22	-	Favored (84.87%) Isoleucine or valine / -66.2,-47.4	86.2% ( <i>mt</i> ) chi angles: 299.3,168	0.048Å	-	-
180	VAL	32.33	-	Favored (91.36%) Isoleucine or valine / -64.0,-41.1	88.2% ( <i>t</i> ) chi angles: 175.2	0.073Å	-	-
181	ARG	87.83	-	Favored (93.48%) General / -60.4,-41.2	43.6% ( <i>ttm180</i> ) chi angles: 179.9,180.2,290.9,168	0.113Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 71.52	Clashscore: 50.63	Outliers: 2 of 182	Poor rotamers: 1 of 167	Outliers: 1 of 173	Outliers: 0 of 184	Outliers: 12 of 184
182	ARG	125.8	0.753Å NH1 with 123 ASN HB3	Favored (96.52%) General / -64.0,-43.1	8.3% ( <i>tpm_?</i> ) chi angles: 186.4,66.8,280.8,162.2	0.078Å	-	-	
183	LEU	56.64	0.569Å HD21 with 55 TYR HD2	Favored (43.01%) General / -62.7,-54.2	76.1% ( <i>mt</i> ) chi angles: 292.3,180.2	0.096Å	-	-	
184	GLN	71.91	0.503Å O with 185 ASN HB2	Favored (11.44%) General / -82.6,102.5	3.1% ( <i>tp-100</i> ) chi angles: 191.2,89,233.5	0.131Å	-	-	
185	ASN	83.82	0.503Å HB2 with 184 GLN O	-	9.7% ( <i>m120</i> ) chi angles: 296.3,160.7	0.09Å	-	-	

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