

## Viewing myoc\_mb\_118-153Hmulti.table

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All-Atom	Clashscore, all atoms: 39.34			8 <sup>th</sup> percentile* (N=1784, all resolutions)			
Contacts	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.						
	Poor rotamers	0	0.00%	Goal: <1%			
	Ramachandran outliers	0	0.00%	Goal: <0.05%			
	Ramachandran favored	34	100.00%	Goal: >98%			
Protein Geometry	MolProbity score <sup>^</sup>	2.07		72 <sup>nd</sup> percentile* (N=27675, 0Å - 99Å)			
	Cβ deviations >0.25Å	0	0.00%	Goal: 0			
	Bad backbone bonds:	0/305	0.00%	Goal: 0%			
	Bad backbone angles:	2 / 408	0.49%	Goal: <0.1%			

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

<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:	Clashscore:	Outliers: 0 of	Poor rotamers: 0 of	Outliers:		
		64.56	39.34	34	34	0 of 35	0 of 36	of 36
118	B GLN	58.14	0.797Å N with 121 LEU HD23	-	40% (tt0) chi angles: 192.1,182.1,310.2	0.057Å	-	-
119	) ARG	106.4	0.571Å H with 118 GLN HG2	Favored (89.12%) General / -65.1,-37.9	80.3% ( <i>mtp85</i> ) chi angles: 294.1,175.2,63.6,89.1	0.062Å	-	-
120	) GLU	83.98	-	Favored (98.41%) General / -61.4,-43.7	40.8% ( <i>mm-40</i> ) chi angles: 293.5,276.4,0.5	0.125Å	-	-
121	LEU	86.56	0.797Å HD23 with 118 GLN N	Favored (72.77%) General / -65.8,-31.7	2.4% ( <i>mm</i> ?) chi angles: 289.8,292.3	0.065Å	-	-

<sup>\* 100&</sup>lt;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.

122	GLY 29.83	-	Favored (60.48%) Glycine / -56.6,-31.6	-	-	-	-
123	THR 37.43	-	Favored (70.8%) General / -58.7,-34.0	91.2% ( <i>m</i> ) chi angles: 300.6	0.077Å	-	-
124	LEU 44.11	-	Favored (86.84%) General / -58.8,-46.8	54.5% ( <i>tp</i> ) chi angles: 180.1,66.4	0.093Å	-	-
125	ARG 98.77	-	Favored (85%) General / -64.0,-36.8	25.2% ( <i>mtp-105</i> ) chi angles: 292,184.1,77.4,260.3	0.085Å	-	-
126	ARG 125.68	-	Favored (97.57%) General / -62.8,-40.5	37.6% (ttm180) chi angles: 185.1,167.5,302.2,169.7	0.07Å	-	-
127	GLU 36.64	0.692Å O with 130 GLN HG2	Favored (96.42%) General / -61.5,-44.8	42.8% ( <i>mt-10</i> ) chi angles: 293.8,176.1,84.9	0.111Å	-	-
128	ARG 36.71	-	Favored (95.59%) General / -61.0,-41.0	85.8% ( <i>mtt-85</i> ) chi angles: 283.3,188.9,173.5,270.3	0.134Å	-	-
129	ASP 27.61	0.681Å O with 133 THR HG23	Favored (95.27%) General / -62.5,-40.0	96.5% ( <i>m-20</i> ) chi angles: 291.4,344.4	0.075Å	-	OUTLIER(S) worst is CA- CB-CG: 5.328 σ
130	GLN 81.49	0.887Å HG3 with 131 LEU HD22	Favored (95.42%) General / -64.8,-41.8	10.7% ( <i>pt20</i> ) chi angles: 69.1,171.5,26.6	0.124Å	-	-
131	LEU 79.4	0.887Å HD22 with 130 GLN HG3	Favored (97.39%) General / -64.1,-41.0	3.4% ( <i>mm</i> ?) chi angles: 285,292.7	0.089Å	-	-
132	GLU 28.53	-	Favored (99.28%) General / -63.2,-41.9	97.7% ( <i>mt-10</i> ) chi angles: 295.3,171.5,354.6	0.069Å	-	-
133	THR 95.88	0.681Å HG23 with 129 ASP O	Favored (91.06%) General / -64.7,-44.2	47% (p) chi angles: 66.3	0.085Å	-	-
			Favored				

134	GLN 49.98	0.764Å HE21 with 131 LEU HA	(93.02%) General / -62.9,-45.3	22.5% ( <i>mt-30</i> ) chi angles: 298.8,168.6,131.9	0.08Å	-	-
135	THR 26.13	-	Favored (92.61%) General / -62.6,-45.5	87.8% ( <i>m</i> ) chi angles: 301.1	0.077Å	-	-
136	ARG 136.81	-	Favored (98.89%) General / -63.3,-41.3	52% (ttm-85) chi angles: 183.6,192.4,305.1,273.2	0.084Å	-	-
137	GLU 77.64	-	Favored (85.02%) General / -62.2,-47.3	77.6% ( <i>tt0</i> ) chi angles: 180.1,187.2,11.3	0.1Å	-	-
# <b>A</b>	lt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 64.56	Clashscore: 39.34	Outliers: 0 of 34	Poor rotamers: 0 of 34	Outliers: 0 of 35	Outliers: 0 of 36	Outliers: 2 of 36
138	LEU 88.95	0.585Å HD13 with 134 GLN O	Favored (92.37%) General / -65.5,-42.2	9.5% ( <i>mp</i> ) chi angles: 283.5,62.7	0.101Å	-	-
139	GLU 76	-	Favored (92.24%) General / -63.2,-45.3	70.9% (tt0) chi angles: 179.7,189.8,346.3	0.106Å	-	-
140	THR 29	0.526Å HG22 with 144 ASN ND2	Favored (92.34%) General / -64.6,-43.9	86.7% ( <i>m</i> ) chi angles: 301.2	0.067Å	-	-
141	ALA 27.38	0.632Å O with 145 LEU HG	Favored (98.67%) General / -62.7,-41.0	-	0.088Å	-	-
142	TYR 131.74	-	Favored (86.11%) General / -63.4,-46.5	25.7% ( <i>t80</i> ) chi angles: 198.4,79.8	0.076Å	-	-
143	SER 71.03	-	Favored (91.15%) General / -64.9,-44.0	71.5% ( <i>m</i> ) chi angles: 295.7	0.082Å	-	-
144	ASN 33.02	0.526Å ND2 with 140 THR HG22	Favored (90.03%) General / -66.0,-42.0	96.1% ( <i>m-20</i> ) chi angles: 291.7,333.3	0.095Å	-	OUTLIER(S) worst is CA- CB-CG: 4.776 σ

145	LEU 35.19	0.632Å HG with 141 ALA O	Favored (99.5%) General / -62.5,-43.2	83.2% ( <i>mt</i> ) chi angles: 294.5,180	0.073Å	-	-
146	LEU 44.57	-	Favored (95.84%) General / -64.6,-42.0	45.4% ( <i>mt</i> ) chi angles: 287.2,181.1	0.08Å	-	-
147	ARG 109.53	-	Favored (94.81%) General / -64.9,-42.4	25.4% ( <i>mmt-85</i> ) chi angles: 291.4,322.8,189.3,278.8	0.073Å	-	-
148	ASP 29.29	-	Favored (94.54%) General / -64.2,-39.7	69.5% ( <i>m-20</i> ) chi angles: 294.4,355	0.117Å	-	-
149	LYS 115.04	0.489Å HD3 with 149 LYS O	Favored (97.63%) General / -60.7,-43.7	2.1% ( <i>tmtm?</i> ) chi angles: 195.2,299.9,188.6,308.8	0.096Å	-	-
150	SER 67.13	0.576Å O with 153 GLU HB3	Favored (95.11%) General / -65.0,-40.5	74.5% ( <i>m</i> ) chi angles: 295	0.085Å	-	-
151	VAL 22.74	-	Favored (96.2%) Isoleucine or valine / -60.9,-46.5	92.9% ( <i>t</i> ) chi angles: 175.6	0.09Å	-	-
152	LEU 72.67	0.673Å O with 152 LEU HD23	Favored (98.71%) General / -62.6,-41.0	3.2% ( <i>tt</i> ) chi angles: 187.9,180	0.078Å	-	-
153	GLU 23.33	0.576Å HB3 with 150 SER O	-	33.6% ( <i>tt0</i> ) chi angles: 180.8,190.8,58.2	0.09Å	-	-

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