

Viewing myoc_mb_118-153_FFX1Hmulti.table

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All-Atom	Clashscore, all atoms: 0			100 th percentile* (N=1784, all resolutions)			
Contacts	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.						
	Poor rotamers	4	11.76%	Goal: <1%			
	Ramachandran outliers	0	0.00%	Goal: <0.05%			
	Ramachandran favored	32	94.12%	Goal: >98%			
Protein Geometry	MolProbity score [^] 1.71			89 th percentile* (N=27675, 0Å - 99Å)			
Geometry	Cβ deviations >0.25Å	0	0.00%	Goal: 0			
	Bad backbone bonds:	0/305	0.00%	Goal: 0%			
	Bad backbone angles:	0 / 408	0.00%	Goal: <0.1%			

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

[^] 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	$\begin{array}{c} C\beta \\ \text{deviation} \end{array}$	Bond lengths	Bond angles
		Avg: 64.56	Clashscore: 0	Outliers: 0 of 34	Poor rotamers: 4 of 34	Outliers: 0 of 35	Outliers: 0 of 36	Outliers: 0 of 36
118	GLN	58.14	-	-	4.7% (mm100) chi angles: 310.5,316.4,85.3	0.213Å	-	-
119) ARG	106.4	-	Favored (65.92%) General / -67.9,-26.3	48.3% (<i>tpt85</i>) chi angles: 178,55.7,181.1,76.6	0.16Å	-	-
120) GLU	83.98	-	Favored (93.57%) General / -64.5,-39.3	0.6% chi angles: 73,314.4,319.6	0.166Å	-	-
121	LEU	86.56	-	Favored (74.78%) General / -65.4,-32.9	90.6% (<i>mt</i>) chi angles: 291.7,170.3	0.118Å	-	-

^{* 100&}lt;sup>th</sup> 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.

122	GLY 29.83	-	Favored (95.74%) Glycine / -60.4,-39.1	-	-	-	-
123	THR 37.43	-	Favored (82.95%) General / -65.6,-45.5	0.2% chi angles: 334.2	0.174Å	-	-
124	LEU 44.11	-	Favored (65.9%) General / -53.8,-40.0	38.1% (<i>tp</i>) chi angles: 186.6,59.8	0.073Å	-	-
125	ARG 98.77	-	Favored (91.02%) General / -65.6,-39.0	0.1% chi angles: 267.9,268.9,52.3,261.4	0.165Å	-	-
126	ARG 125.68	-	Favored (52.08%) General / -77.8,-21.2	4.3% (<i>tpm_</i> ?) chi angles: 186.9,55.6,262.7,198.6	0.117Å	-	-
127	GLU 36.64	-	Favored (49.86%) General / -77.5,-24.6	24.5% (<i>mt-10</i>) chi angles: 295.5,150.4,29.8	0.07Å	-	-
128	ARG 36.71	-	Favored (20.94%) General / -81.2,-42.4	17.1% (mmm180) chi angles: 279.1,301.6,310.5,169.9	0.088Å	-	-
129	ASP 27.61	-	Favored (65.4%) General / -52.8,-42.8	76.9% (<i>m-20</i>) chi angles: 295.8,323.4	0.112Å	-	-
130	GLN 81.49	-	Favored (75.72%) General / -62.8,-33.7	23.9% (<i>pt20</i>) chi angles: 66.3,190.2,346.9	0.137Å	-	-
131	LEU 79.4	-	Favored (58.78%) General / -75.8,-38.0	28.5% (<i>mt</i>) chi angles: 311.7,174.5	0.07Å	-	-
132	GLU 28.53	-	Favored (47.99%) General / -78.0,-24.6	30.4% (<i>mt-10</i>) chi angles: 294,147.7,356.5	0.103Å	-	-
133	THR 95.88	-	Favored (6.71%) General / -78.9,-53.8	56.7% (<i>p</i>) chi angles: 56.2	0.141Å	-	-
134	GLN 49.98	-	Favored (4.92%) General / -43.6,-42.0	28.7% (<i>mt-30</i>) chi angles: 281.5,179.3,117.6	0.131Å	-	-

135	THR	26.13	-	Allowed (0.64%) General / -35.6,-51.1	67.3% (<i>m</i>) chi angles: 296.5	0.127Å	-	-
136	ARG	136.81	-	Favored (12.48%) General / -113.2,-16.9	8.5% (<i>tpt180</i>) chi angles: 168.5,58.1,211.7,180.3	0.146Å	-	-
137	GLU	77.64	-	Favored (61.94%) General / -70.6,-47.1	39.6% (<i>tt0</i>) chi angles: 175.8,182.5,59.1	0.095Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	$\begin{array}{c} C\beta \\ \text{deviation} \end{array}$	Bond lengths	Bond angles
		Avg: 64.56	Clashscore: 0	Outliers: 0 of 34	Poor rotamers: 4 of 34	Outliers: 0 of 35	Outliers: 0 of 36	Outliers: 0 of 36
138	LEU	88.95	-	Favored (60.4%) General / -75.2,-29.2	5.6% (<i>mp</i>) chi angles: 271.8,44.4	0.127Å	-	-
139	GLU	76	-	Favored (59.63%) General / -78.2,-14.0	13.4% (<i>tm-20</i>) chi angles: 187.3,272.2,322.3	0.188Å	-	-
140	THR	29	-	Favored (76.67%) General / -67.0,-45.8	88.8% (<i>m</i>) chi angles: 300.9	0.133Å	-	-
141	ALA	27.38	-	Favored (99.63%) General / -62.2,-43.1	-	0.089Å	-	-
142	TYR	131.74	-	Favored (8.05%) General / -70.4,-55.8	42.1% (<i>t80</i>) chi angles: 178.5,57.8	0.088Å	-	-
143	SER	71.03	-	Favored (98.3%) General / -63.5,-40.9	0.5% chi angles: 255.8	0.157Å	-	-
144	ASN	33.02	-	Favored (69.36%) General / -61.4,-51.3	5.4% (<i>m-20</i>) chi angles: 291.7,25.8	0.149Å	-	-
145	LEU	35.19	-	Favored (71.52%) General / -61.7,-31.4	96.3% (<i>mt</i>) chi angles: 297.6,175	0.1 <i>7</i> 1Å	-	-
146	LEU	44.57	-	Favored (65.49%) General / -56.4,-33.2	84.8% (<i>mt</i>) chi angles: 292.6,178.7	0.118Å	-	-

147	ARG 109.53	-	Favored (11.17%) General / -96.7,-34.9	12.8% (<i>mmt-85</i>) chi angles: 322.1,316.6,197.2,278	0.113Å	-	-
148	ASP 29.29	-	Favored (75.36%) General / -66.0,-33.2	10.3% (<i>m-20</i>) chi angles: 313.1,330.4	0.109Å	-	-
149	LYS 115.04	-	Favored (74.18%) General / -59.0,-36.0	2% (tmtm?) chi angles: 180,263.3,151.8,277	0.142Å	-	-
150	SER 67.13	-	Favored (54.13%) General / -85.0,-12.1	46.9% (<i>m</i>) chi angles: 302.2	0.114Å	-	-
151	VAL 22.74	-	Favored (65.03%) Isoleucine or valine / -60.8,-35.5	55.8% (<i>t</i>) chi angles: 170.7	0.14Å	-	-
152	LEU 72.67	-	Allowed (1.42%) General / -127.1,73.3	3.5% (<i>tt</i>) chi angles: 202.9,175.5	0.045Å	-	-
153	GLU 23.33	-	-	4.5% (<i>tp10</i>) chi angles: 201,75.8,93.8	0.076Å	-	-

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