Viewing LCA5_MB_107-211_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0.55		99th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	4	4.04%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	99	96.12%	Goal: >98%
	MolProbity score$^\wedge$	1.41		97th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.95%	Goal: 0
	Bad backbone bonds:	0 / 892	0.00%	Goal: 0%
	Bad backbone angles:	4 / 1185	0.34%	Goal: <0.1%

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.

$^\wedge$ 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: 103.07	Clashscore: 0.55	Outliers: 0 of 103	Poor rotamers: 4 of 99	Outliers: 1 of 105	Outliers: 0 of 105	Outliers: 4 of 105
107		ALA	8.61	-	-	-	0.102Å	-	-
108		ARG	84.31	-	Favored (71.02%) General / -71.0,-34.1	47.5% (*tpt85*) chi angles: 182,65.3,192.1,92.6	0.128Å	-	-
109		LEU	62.92	-	Favored (85.12%) General / -62.0,-47.4	8.3% (*mp*) chi angles: 284.9,71	0.105Å	-	-
110		LEU	67.55	-	Favored (71.84%) General / -54.1,-45.8	37.5% (*tp*) chi angles: 186.5,58.8	0.078Å	-	-
					Favored	0.2%			

111	LYS	112.83	-	(70.32%) General / -61.9,-29.6	chi angles: 186.4,75.5,282.6,283.6	0.205Å	-	-
112	ILE	129.27	-	Favored (18.52%) Isoleucine or valine / -80.3,-38.8	0.1% chi angles: 209.9,277.3	0.226Å	-	-
113	ASN	65.21	-	Favored (77.86%) General / -68.3,-35.5	34.2% (m120) chi angles: 299.7,119.7	0.127Å	-	-
114	GLU	78.07	-	Favored (82.11%) General / -66.5,-44.6	7.1% (pt-20) chi angles: 58.7,203.2,257.3	0.169Å	-	-
115	LEU	40.07	-	Favored (76.12%) General / -61.0,-35.2	85.2% (mt) chi angles: 299.9,180.3	0.183Å	-	-
116	GLN	83.98	-	Favored (54.56%) General / -77.0,-27.6	8.6% (tp60) chi angles: 185.5,60.2,100.7	0.093Å	-	-
117	ASN	74.22	-	Favored (23.18%) General / -79.1,-43.9	6.1% (t30) chi angles: 193.4,89.3	0.065Å	-	-
118	GLU	71.35	-	Favored (93.33%) General / -65.4,-40.5	4.6% (pt-20) chi angles: 78.5,204.8,52	0.161Å	-	-
119	VAL	88.98	-	Favored (65.4%) Isoleucine or valine / -65.5,-33.7	33.5% (m) chi angles: 299.7	0.226Å	-	-
120	SER	67.3	-	Favored (87.92%) General / -66.8,-40.5	55.6% (m) chi angles: 299.7	0.089Å	-	-
121	GLU	99.61	-	Favored (82.25%) General / -67.3,-36.8	11.6% (tm-20) chi angles: 186.5,291.2,325.7	0.124Å	-	-
122	LEU	154.81	-	Favored (51.8%) General / -54.1,-31.4	96.4% (mt) chi angles: 296.9,174.9	0.131Å	-	-
				Favored	90.9% (mt-30)			

123		GLN	136.61	-	(15.66%) General / -70.2,-3.2	chi angles: 293.8,178,353.3	0.077Å	-	-
124		VAL	41.13	-	Favored (45.22%) Isoleucine or valine / -57.9,-33.1	31.4% (*m*) chi angles: 300.8	0.17Å	-	-
125		LYS	98.27	-	Favored (71.11%) General / -64.1,-30.0	31.6% (*mmmt*) chi angles: 294.3,300.2,294.9,173.2	0.16Å	-	-
126		LEU	86.24	-	Favored (96.58%) General / -63.2,-40.1	83.5% (*mt*) chi angles: 300.4,174.1	0.079Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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127		ALA	29.02	-	Favored (79.49%) General / -67.0,-35.2	-	0.097Å	-	-
128		GLU	67.32	-	Favored (16.73%) General / -75.1,-50.3	1% chi angles: 175.4,284.2,284.6	0.096Å	-	-
129		LEU	128.04	-	Favored (70.92%) General / -62.0,-30.4	47.6% (*mt*) chi angles: 299.4,165.5	0.137Å	-	-
130		LEU	71.15	-	Favored (63.73%) General / -69.5,-23.8	28% (*tp*) chi angles: 190.3,64.8	0.081Å	-	-
131		LYS	157.45	-	Favored (51.17%) General / -77.8,-30.2	55.2% (*mttp*) chi angles: 300.6,171.4,181.8,71.6	0.079Å	-	-
132		GLU	43.43	-	Favored (44.86%) General / -77.7,-39.5	11.9% (*tp10*) chi angles: 182.2,38.7,31.4	0.177Å	-	-
133		ASN	200.7	-	Favored (2.6%) General / -64.3,111.4	51.6% (*t-20*) chi angles: 193.1,350.5	0.028Å	-	-
134		LYS	268.55	-	Favored (24.31%)	40.5% (*mmtm*) chi angles:	0.04Å	-	-

				General / -86.7,115.7	302.4,293.9,176.8,276.3			
135	SER	130.23	-	Allowed (0.1%) General / -33.7,136.9	37% (*t*) chi angles: 182.2	0.031Å	-	-
136	LEU	154.71	-	Favored (65.59%) General / -57.4,-31.2	1.6% (*tm?*) chi angles: 201.8,280.8	0.073Å	-	-
137	LYS	74.5	-	Favored (72.68%) General / -62.0,-32.2	32.6% (*mmmt*) chi angles: 293.9,294.2,294.4,181.6	0.132Å	-	-
138	ARG	65.55	-	Favored (60.89%) General / -75.1,-30.4	49.3% (*tpt85*) chi angles: 183.3,64.8,191.3,88.3	0.13Å	-	-
139	LEU	50.03	-	Favored (96.89%) General / -64.2,-41.8	14.5% (*tp*) chi angles: 191.1,77.4	0.085Å	-	-
140	GLN	36.61	-	Favored (85.58%) General / -58.2,-42.1	57.9% (*tt0*) chi angles: 188,186.4,8.1	0.099Å	-	-
141	TYR	88.06	-	Favored (74.66%) General / -65.8,-32.9	66.4% (*t80*) chi angles: 187.2,71.8	0.16Å	-	-
142	ARG	131.81	-	Favored (55.3%) General / -76.8,-27.6	25.3% (*ptt85*) chi angles: 78.5,158.9,195.2,74.7	0.235Å	-	-
143	GLN	85.83	-	Favored (35.01%) General / -82.4,-23.0	31.6% (*tp60*) chi angles: 190.6,55.5,81.3	0.116Å	-	-
144	GLU	62.87	-	Favored (79.46%) General / -68.8,-40.4	6.4% (*pt-20*) chi angles: 82,192.7,59.3	0.119Å	-	-
145	LYS	83.06	-	Favored (61.5%) General / -75.2,-34.1	43.8% (*mmtt*) chi angles: 309.6,308.6,176.1,206.8	0.181Å	-	-
146	ALA	38.46	-	Favored (82.24%) General /	-	0.118Å	-	-

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			Avg: 103.07	Clashscore: 0.55	Outliers: 0 of 103	Poor rotamers: 4 of 99	Outliers: 1 of 105	Outliers: 0 of 105	Outliers: 4 of 105
147		LEU	97.11	-	Favored (95.09%) General / -62.9,-44.8	1.8% (*tt*) chi angles: 212.2,169.4	0.105Å	-	-
148		ASN	103.11	-	Favored (60.36%) General / -75.4,-13.0	18.6% (*p30*) chi angles: 67,66.2	0.266Å	-	OUTLIER(S) worst is CA-CB-CG: 4.944 σ
149		LYS	141.9	-	Favored (59.13%) General / -80.3,-13.5	27.7% (*mmmt*) chi angles: 291.2,306.5,306.6,177.9	0.188Å	-	-
150		PHE	141.53	-	Favored (17.79%) General / -88.6,-33.0	83.7% (*m-85*) chi angles: 295.9,106.5	0.108Å	-	-
151		GLU	36.65	-	Favored (93.06%) General / -63.8,-44.5	89.6% (*mt-10*) chi angles: 293.8,163.2,349	0.1Å	-	-
152		ASP	99.63	-	Favored (68.83%) General / -72.3,-38.2	54% (*p-10*) chi angles: 61.4,354.8	0.248Å	-	OUTLIER(S) worst is CA-CB-CG: 6.005 σ
153		ALA	31.93	-	Favored (83.25%) General / -57.1,-45.8	-	0.077Å	-	-
154		GLU	103.22	-	Favored (72.66%) General / -69.1,-44.3	10.2% (*tm-20*) chi angles: 188.1,293.2,322.4	0.129Å	-	-
155		ASN	37.84	-	Favored (68.47%) General / -54.4,-40.6	7.5% (*m-80*) chi angles: 266.8,270.5	0.122Å	-	-
156		GLU	62.92	-	Favored (70.9%) General / -71.6,-38.5	53.2% (*mm-40*) chi angles: 280.2,304.6,322.6	0.169Å	-	-
					Favored (70.91%)	6.7% (*tt*)			

-67.7,-37.4

157	ILE	89.77	-	Isoleucine or valine / -67.2,-34.7	chi angles: 208,176.3	0.223Å	-	-
158	SER	70.92	-	Favored (67.03%) General / -66.3,-49.5	1.6% (*t*) chi angles: 207	0.057Å	-	-
159	GLN	111.92	-	Favored (78.4%) General / -66.0,-34.6	3.8% (*pp0?*) chi angles: 79.3,76.2,26.8	0.203Å	-	-
160	LEU	91.79	-	Favored (70.98%) General / -59.4,-51.2	5.9% (*tt*) chi angles: 195.9,166.6	0.054Å	-	-
161	ILE	84.48	-	Favored (76.3%) Isoleucine or valine / -71.0,-40.4	11.9% (*tt*) chi angles: 200,175.1	0.233Å	-	-
162	PHE	68.67	-	Favored (39.92%) General / -77.8,-40.6	73.7% (*m-85*) chi angles: 286.6,87	0.174Å	-	-
163	ARG	217.95	-	Favored (2.4%) General / -111.9,-174.1	94.1% (*mtm-85*) chi angles: 294.3,189.3,291.3,270.6	0.104Å	-	-
164	HIS	269.07	0.406Å NE2 with 165 ASN O	Favored (23.02%) General / -93.7,147.4	83.8% (*t60*) chi angles: 175.6,75.9	0.138Å	-	-
165	ASN	201.03	0.406Å O with 164 HIS NE2	Favored (3.21%) General / -123.4,-175.5	12.7% (*m-80*) chi angles: 312.8,275.2	0.089Å	-	-
166	ASN	78.75	-	Favored (13.65%) General / -96.9,-29.6	86.4% (*m-20*) chi angles: 296.3,335.1	0.083Å	-	OUTLIER(S) worst is C-N-CA: 5.267 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 103.07	Clashscore: 0.55	Outliers: 0 of 103	Poor rotamers: 4 of 99	Outliers: 1 of 105	Outliers: 0 of 105	Outliers: 4 of 105
167		GLU	90.5	-	Favored (25.46%) General / -83.2,-35.4	21.5% (*mp0*) chi angles: 312.3,76.6,353.7	0.068Å	-	OUTLIER(S) worst is CB-CG-CD: 5.026 σ
					Favored				

168	ILE 137.62	-	(24.41%) Isoleucine or valine / -138.9,152.5	20.6% (*tt*) chi angles: 190.7,166.9	0.097Å	-	-
169	THR 221.78	-	Allowed (0.5%) General / -62.3,177.3	6.3% (*t*) chi angles: 195.2	0.186Å	-	-
170	ALA 203.33	-	Favored (49.75%) General / -71.2,145.3	-	0.044Å	-	-
171	LEU 152.86	-	Favored (23.3%) General / -84.0,-36.2	96.2% (*mt*) chi angles: 296.8,174.8	0.105Å	-	-
172	LYS 143.83	-	Allowed (0.14%) General / -97.9,-114.6	91% (*mttt*) chi angles: 296.4,170.7,180.9,168.5	0.165Å	-	-
173	GLU 100.92	-	Favored (84.72%) General / -67.2,-42.0	30.3% (*mm-40*) chi angles: 270.1,295.4,301.3	0.181Å	-	-
174	ARG 98.94	-	Favored (70.52%) General / -66.1,-30.1	66.2% (*ttt180*) chi angles: 193.8,185.1,170.7,177.6	0.23Å	-	-
175	LEU 119.45	-	Favored (25.52%) General / -81.0,-39.6	64.9% (*tp*) chi angles: 178.7,63.6	0.075Å	-	-
176	ARG 166.19	-	Favored (92.96%) General / -61.8,-39.8	20.2% (*tpp85*) chi angles: 180.2,60.7,66.9,75.8	0.141Å	-	-
177	LYS 82.5	-	Favored (57.44%) General / -76.4,-30.0	45.3% (*mmtm*) chi angles: 299.4,290.9,174.3,292.8	0.138Å	-	-
178	SER 42	-	Favored (7.99%) General / -72.3,-55.0	18% (*p*) chi angles: 81	0.176Å	-	-
179	GLN 83.92	-	Favored (3.62%) General / -41.4,-52.0	53.5% (*tt0*) chi angles: 181.6,189.2,33	0.036Å	-	-
			Favored	11.2% (*tt0*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
180		GLU	32.13	-	(85.95%) General / -64.3,-37.0	chi angles: 186.4,210.9,325.5	0.062Å	-	-
181		LYS	127.36	-	Favored (27.57%) General / -84.4,-27.4	41.1% (*mmtm*) chi angles: 305,292.9,168.4,290.8	0.124Å	-	-
182		GLU	41.77	-	Favored (88.56%) General / -66.7,-41.2	23.9% (*mt-10*) chi angles: 291.3,148.2,26.1	0.039Å	-	-
183		ARG	192.05	-	Allowed (0.7%) General / -107.1,53.3	8% (*ptm-85*) chi angles: 61.6,164.2,294.9,276.2	0.144Å	-	-
184		ALA	66.36	-	Favored (86.83%) General / -58.0,-45.3	-	0.083Å	-	-
185		THR	254.91	-	Favored (2%) General / -158.2,106.9	41.5% (*p*) chi angles: 54.3	0.062Å	-	-
186		GLU	107.08	-	Favored (70.49%) General / -61.0,-30.7	22% (*mp0*) chi angles: 300.6,88.2,328.6	0.089Å	-	-

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187		LYS	53.31	-	Favored (66.27%) General / -55.5,-36.0	63.8% (*tttp*) chi angles: 183.4,171.1,172.2,59.3	0.127Å	-	-
188		ARG	84.12	-	Favored (91.53%) General / -61.5,-39.6	39.6% (*mmt180*) chi angles: 291.1,294.9,179.8,181.7	0.178Å	-	-
189		VAL	82.48	-	Favored (39.83%) Isoleucine or valine / -74.0,-34.6	7.8% (*p*) chi angles: 73.8	0.211Å	-	-
190		LYS	116.9	-	Favored (89.09%) General / -64.7,-37.9	15% (*ttmm*) chi angles: 180.7,151.2,293.3,302.3	0.185Å	-	-
191		ASP	39.9	-	Favored (79.75%)	68.5% (*m-20*) chi angles: 298.7,346.6	0.12Å	-	-

			General / -68.9,-38.9 Favored (62.51%)				
192	THR	101.39	-	General / -74.8,-37.2 Favored (98.04%)	24.1% (*p*) chi angles: 49.9	0.131Å	-	-
193	GLU	87.8	-	General / -61.8,-41.7 Favored (27.74%)	8.5% (*pt-20*) chi angles: 84.4,197,338.2	0.109Å	-	-
194	SER	82.06	-	General / -80.4,-39.8 Favored (17.61%)	78.2% (*p*) chi angles: 59.1	0.164Å	-	-
195	GLU	83.24	-	General / -63.9,-56.1 Favored (41.24%)	7% (*tp10*) chi angles: 163.9,54.9,265	0.102Å	-	-
196	LEU	125.63	-	General / -59.4,-54.9 Favored (53.49%)	3.1% (*tm?*) chi angles: 190.2,279.1	0.094Å	-	-
197	PHE	78.73	-	General / -76.3,-39.6 Favored (70.28%)	2.7% (*t80*) chi angles: 212.9,93.3	0.149Å	-	-
198	ARG	84.22	-	General / -70.7,-32.9 Favored (60.09%)	52.2% (*ttt-85*) chi angles: 193.4,184.9,166.7,286.4	0.136Å	-	-
199	THR	110.02	-	General / -75.7,-11.9 Favored (25.01%)	0.6% chi angles: 214.8	0.178Å	-	-
200	LYS	191.33	-	General / -86.0,-27.3 Favored (7.45%)	12.6% (*tptp*) chi angles: 185.5,64.3,213.9,79.6	0.097Å	-	-
201	PHE	147.37	-	General / -115.7,-26.4 Favored (13.01%)	19.2% (*p90*) chi angles: 71.6,259.5	0.149Å	-	-
202	SER	100.99	-	General / -80.5,173.0 Favored (2.41%)	96.7% (*p*) chi angles: 66.4	0.082Å	-	-
					6.3% (*mp*)			

203		LEU	214.3	-	General / -74.9,90.9	chi angles: 292.2,80.3	0.079Å	-	-
204		GLN	243.53	-	Favored (2.43%) General / -151.3,-166.1	0% chi angles: 230,300.3,261.9	0.12Å	-	-
205		LYS	124.16	-	Favored (22.66%) General / -47.6,-42.0	34.3% (*mtmm*) chi angles: 299.5,174.7,294.8,288.8	0.093Å	-	-
206		LEU	120.52	-	Favored (11.23%) General / -108.3,25.8	56.6% (*mt*) chi angles: 304.6,184.2	0.167Å	-	-

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207		LYS	78.73	-	Favored (2.4%) General / -128.4,-30.1	45% (*tptt*) chi angles: 191.6,67.5,190.3,173.9	0.122Å	-	-
208		GLU	85.9	-	Favored (65.07%) General / -68.5,-25.6	18.8% (*mt-10*) chi angles: 300.8,147,344.8	0.046Å	-	-
209		ILE	81.24	-	Favored (9.35%) Isoleucine or valine / -95.0,-9.6	5.5% (*tt*) chi angles: 209.9,177.7	0.142Å	-	-
210		SER	27.45	-	Favored (8.5%) General / -98.0,-40.3	91.2% (*p*) chi angles: 67.1	0.229Å	-	-
211		GLU	52.65	-	-	1.3% (*mp0*) chi angles: 316.7,99.2,85.7	0.133Å	-	-

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