

## Viewing clrn1\_mb\_29-99H-multi.table

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All-Atom	Clashscore, all atoms:	84.47		0 <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	2	3.51%	Goal: <1%		
	Ramachandran outliers	0	0.00%	Goal: <0.05%		
	Ramachandran favored	65	94.20%	Goal: >98%		
Protein Geometry	MolProbity score <sup>^</sup>	3.20		16 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)		
	Cβ deviations >0.25Å	1	1.61%	Goal: 0		
	Bad backbone bonds:	0 / 561	0.00%	Goal: 0%		
	Bad backbone angles:	12 / 757	1.59%	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	<b>Bond angles</b>
			Avg: 92.83	Clashscore: 84.47	Outliers: 0 of 69	Poor rotamers: 2 of 57	Outliers: 1 of 62	Outliers: 0 of 71	Outliers: 11 of 71
2	9	GLY	7.49	-	-	-	-	-	-
3	0	THR	82.18	0.989Å HG22 with 32 LEU H	Favored (85.67%) Pre-proline / -75.2,151.2	94.4% ( <i>m</i> ) chi angles: 300	0.109Å	-	-
3	1	PRO	76.56	0.538Å N with 30 THR HG22	Favored (37.35%) Trans-proline / -67.8,-27.6	8.5% ( <i>Cg_endo</i> ) chi angles: 10.5	0.117Å	-	-
3.	2	LEU	77	0.989Å H with 30 THR HG22	Favored (82.52%) General / -68.1,-38.7	5.4% ( <i>mp</i> ) chi angles: 293.7,63.4	0.074Å	-	-
3	3	TRP	87.42	-	Favored (93.16%)	84.4% (t90)	0.084Å	-	-

<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.

			General / -61.9,-45.6	chi angles: 175.1,87			
34	ILE 34.1	0.751Å O with 37 THR HG22	Favored (81.83%) Isoleucine or valine / -64.2,-38.2	95.5% ( <i>mt</i> ) chi angles: 297.6,169.2	0.058Å	-	-
35	LYS 70.24	-	Favored (91.48%) General / -62.1,-39.2	79.8% (tttt) chi angles: 190.4,165.9,178,181	0.065Å	-	-
36	ALA 34.88	-	Favored (97.72%) General / -63.2,-43.6	-	0.081Å	-	-
37	THR 97.22	0.751Å HG22 with 34 ILE O	Favored (92.27%) General / -65.4,-39.5	10.1% ( <i>t</i> ) chi angles: 192.6	0.055Å	-	-
38	VAL 44.88	0.69Å HG23 with 34 ILE O	Favored (91.14%) Isoleucine or valine /-64.1,-47.2	97.8% ( <i>t</i> ) chi angles: 178.4	0.064Å	-	-
39	LEU 46.73	0.446Å CD2 with 86 PHE CE2	Favored (99.11%) General / -62.3,-42.2	64% ( <i>mt</i> ) chi angles: 294.4,183.8	0.089Å	-	-
40	CYS 31.24	-	Favored (98.09%) General / -62.9,-43.7	91.8% ( <i>m</i> ) chi angles: 293.5	0.086Å	-	-
41	LYS 140.65	0.653Å HG3 with 37 THR O	Favored (63.58%) General / -67.1,-49.9	6.3% ( <i>mtpm?</i> ) chi angles: 299.6,161.9,71.5,289.6	0.087Å	-	-
42	THR 87.3	-	Favored (3.41%) General / -65.6,-60.0	88.7% ( <i>m</i> ) chi angles: 302.1	0.059Å	-	-
43	GLY 93.43	0.446Å CA with 51 GLY HA2	Favored (28.36%) Glycine / 61.1,-122.0	-	-	-	-
44	ALA 244.51	0.764Å O with 49 ALA HB3	Favored (48.67%) General / -119.1,141.5	-	0.118Å	-	-
45	LEU 275.53	0.683Å CD2 with 93 ILE HG12	Favored (5.51%) General / -106.0,95.0	56.2% ( <i>tp</i> ) chi angles: 179.7,66	0.124Å	-	-

46	LEU 222.68	1.017Å HB2 with 91 LYS HD3	Allowed (0.36%) General / -125.6,-103.0	2.5% (tm?) chi angles: 191.7,293.8	0.137Å	-	-
47	VAL 131.42	0.866Å HG13 with 46 LEU HD12	Allowed (1.39%) Isoleucine or valine /-71.4,170.0	28.3% (m) chi angles: 296.7	0.112Å	-	-
48	ASN 187.13	-	Allowed (0.42%) General / -57.2,107.4	19.9% ( <i>m120</i> ) chi angles: 285.5,99.1	0.084Å	-	OUTLIER(S) worst is CA-CB-CG: $5.257 \sigma$
# Al	t Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	<b>Bond angles</b>
	Avg: 92.83	Clashscore: 84.47	Outliers: 0 of 69	Poor rotamers: 2 of 57	Outliers: 1 of 62	Outliers: 0 of 71	Outliers: 11 of 71
49	ALA 252.61	0.764Å HB3 with 44 ALA O	Favored (49.01%) General / -133.7,155.8	-	0.116Å	-	-
50	SER 205.95	0.723Å O with 53 GLU HG2	Favored (34.89%) General / -139.9,162.6	68.3% ( <i>m</i> ) chi angles: 296.9	0.115Å	-	-
51	GLY 71.2	0.446Å HA2 with 43 GLY CA	Favored (71.1%) Glycine / -62.0,-28.8	-	-	-	-
52	GLN 61.22	-	Favored (71.29%) General / -58.1,-35.3	74.4% ( <i>mt-30</i> ) chi angles: 301.8,180.8,42	0.084Å	-	-
53	GLU 139.88	0.723Å HG2 with 50 SER O	Favored (74.74%) General / -69.0,-34.1	5.4% ( <i>pt-20</i> ) chi angles: 83.2,163,303	0.157Å	-	-
54	LEU 156.62	0.647Å HD11 with 56 LYS HG2	Favored (48.39%) General / -101.6,126.5	37.1% ( <i>tp</i> ) chi angles: 186.1,57.7	0.112Å	-	-
55	ASP 66.54	-	Favored (58.72%) General / -75.8,-29.3	84.1% ( <i>m-20</i> ) chi angles: 290.8,330.8	0.062Å	-	OUTLIER(S) worst is CA-CB-CG: $5.334 \sigma$
56	LYS 141.88	0.647Å HG2 with 54 LEU HD11	Favored (68.42%) General / -58.2,-32.5	22.1% ( <i>mmmt</i> ) chi angles: 292.5,306.6,308.8,164	0.079Å	-	-

57	PHE 54.38	0.797Å HA with 83 PHE CZ	Favored (96.91%) General / -60.6,-42.6	64.2% ( <i>m-85</i> ) chi angles: 286.5,81.5	0.106Å	-	OUTLIER(S) worst is CA-CB- CG: 5.391 σ
58	MET 61.09	-	Favored (99.39%) General / -62.1,-42.6	27.1% (ttt) chi angles: 178.6,180.9,174.2	0.098Å	-	-
59	GLY 24.37	0.483Å O with 62 GLN HG2	Favored (97.36%) Glycine / -64.5,-42.8	-	-	-	-
60	GLU 87.31	-	Favored (82.58%) General / -67.2,-36.9	33.3% ( <i>tt0</i> ) chi angles: 188.5,174.5,292.4	0.06Å	-	-
61	MET 49.52	0.416Å O with 65 LEU HG	Favored (96.68%) General / -63.8,-43.3	47.1% ( <i>ttp</i> ) chi angles: 191.4,167.6,67.9	0.063Å	-	-
62	GLN 134.1	0.499Å O with 65 LEU HB2	Favored (77.84%) General / -66.6,-34.4	16.8% ( <i>pt20</i> ) chi angles: 64.5,180.1,51.6	0.085Å	-	OUTLIER(S) worst is CB-CG- CD: 4.233 σ
63	TYR 101.2	0.768Å HA with 66 PHE CD1	Favored (99.27%) General / -63.2,-42.8	38.8% ( <i>t80</i> ) chi angles: 164.3,80.1	0.093Å	-	-
64	GLY 30.42	0.535Å O with 67 HIS HB3	Favored (87.22%) Glycine / -61.6,-34.1	-	-	-	-
65	LEU 57.26	0.499Å HB2 with 62 GLN O	Favored (85.74%) General / -60.1,-39.3	87.2% ( <i>mt</i> ) chi angles: 299.7,179.8	0.154Å	-	-
66	PHE 46.27	0.768Å CD1 with 63 TYR HA	Favored (82.87%) General / -59.0,-39.7	77.3% ( <i>m-85</i> ) chi angles: 288,85.7	0.177Å	-	-
67	HIS 104.68	0.793Å HD2 with 69 GLU HG2	Favored (70.62%) General / -58.6,-33.9	63.6% ( <i>t60</i> ) chi angles: 187.5,83	0.093Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.461 σ
68	GLY 21.94	-	Favored (44.59%) Glycine / 103.3,6.6	-	-	-	-

# Al	lt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	<b>Bond angles</b>
		Avg: 92.83	Clashscore: 84.47	Outliers: 0 of 69	Poor rotamers: 2 of 57		•	Outliers: 11 of 71
69	GLU	77.73	0.974Å HB3 with 74 CYS HB3	Favored (38.82%) General / -74.6,153.9	5.3% ( <i>mm-40</i> ) chi angles: 288.7,294.2,64.4	0.083Å	-	-
70	GLY	22.01	-	Favored (41.89%) Glycine / -64.8,140.2	-	-	-	-
71	VAL	124.74	0.618Å HG13 with 72 ARG N	Favored (28.85%) Isoleucine or valine / -64.9,-54.5	7.4% (p) chi angles: 57.5	0.056Å	-	-
72	ARG	82.01	0.618Å N with 71 VAL HG13	Favored (63.83%) General / -64.7,-51.2	24% ( <i>ptt-85</i> ) chi angles: 54.9,187,166.2,267.3	0.04Å	-	-
73	GLN	165.26	0.445Å OE1 with 74 CYS HA	Allowed (1.05%) General / -71.9,-63.8	0.7% chi angles: 176.3,263.5,101.4	0.049Å	-	-
74	CYS	56.93	0.974Å HB3 with 69 GLU HB3	Favored (37.31%) General / -74.0,-47.4	53.4% ( <i>t</i> ) chi angles: 180.3	0.118Å	-	-
75	GLY	29.76	-	Favored (97.22%) Glycine / -60.9,-39.6	-	-	-	-
76	LEU	48.67	0.723Å O with 80 PRO HD2	Favored (88.19%) General / -66.8,-40.4	78.1% ( <i>mt</i> ) chi angles: 292.5,180	0.083Å	-	-
77	GLY	25.4	-	Favored (97.44%) Glycine / -64.1,-39.7	-	-	-	-
78	ALA	33.63	-	Favored (88.06%) General / -61.3,-38.8	-	0.093Å	-	-
79	ARG	113.67	0.551Å HB2 with 80 PRO HD2	Favored (92.96%) Pre-proline /	41.8% ( <i>mtp180</i> ) chi angles: 292.4,161.8,51.1,166.8	0.034Å	-	-

80	PRO 118.65	0.723Å HD2 with 76 LEU O	-60.2,-48.9 Favored (71.75%) Trans-proline / -62.8,-34.7	11.8% ( <i>Cg_exo</i> ) chi angles: 349	0.259Å	-	-
81	PHE 72.48	-	Favored (26.26%) General / -74.4,-48.7	23.2% ( <i>m-85</i> ) chi angles: 274.4,83.2	0.132Å	-	OUTLIER(S) worst is CA-CB- CG: 6.344 σ
82	ARG 129.05	-	Favored (66.65%) General / -67.4,-48.7	10.2% ( <i>tpt180</i> ) chi angles: 193.9,61.6,167.9,261.3	0.042Å	-	-
83	PHE 111.98	0.797Å CZ with 57 PHE HA	Favored (52.83%) General / -63.4,132.9	72.6% ( <i>m-85</i> ) chi angles: 289.5,81.4	0.091Å	-	OUTLIER(S) worst is CA-CB- CG: 6.252 σ
84	SER 80.88	0.55Å O with 90 LEU HG	Favored (72.69%) General / -68.1,-32.4	68.3% ( <i>m</i> ) chi angles: 296.2	0.074Å	-	-
85	PHE 67.59	0.526Å CD2 with 44 ALA HB2	Favored (93.85%) General / -64.3,-39.4	89% ( <i>m-85</i> ) chi angles: 297.5,83.1	0.077Å	-	OUTLIER(S) worst is CA-CB- CG: 7.445 σ
86	PHE 145.48	0.723Å CD1 with 80 PRO HB3	Favored (8.82%) Pre-proline / -64.2,-33.2	7.2% ( <i>t80</i> ) chi angles: 206.7,272.5	0.085Å	-	OUTLIER(S) worst is CA-CB-CG: $9.593 \sigma$
87	PRO 217.42	1.082Å HB2 with 90 LEU HD23	Favored (85.11%) Trans-proline / -62.8,141.4	79.8% ( <i>Cg_exo</i> ) chi angles: 330.5	0.217Å	-	-
88	ASP 48.72	-	Favored (92.32%) General / -63.6,-38.8	49.4% ( <i>t0</i> ) chi angles: 191.1,8.3	0.105Å	-	OUTLIER(S) worst is CA-CB- CG: 5.628 σ
# <b>A</b> l	t Res High B	Clash > 0.4Å	Ramachandran		Cβ deviation		<b>Bond angles</b>
	Avg: 92.83	Clashscore: 84.47	Outliers: 0 of 69	Poor rotamers: 2 of 57	Outliers: 1 of 62	Outliers: 0 of 71	Outliers: 11 of 71
89	LEU 47.56	-	Favored (77.97%) General / -60.5,-36.3	86.3% ( <i>mt</i> ) chi angles: 296.2,180.3	0.111Å	-	-
90	LEU 181.7	1.082Å HD23 with 87 PRO HB2	Favored (2.22%) General / -78.1,-171.2	3.1% ( <i>mm</i> ?) chi angles: 287.4,293.4	0.076Å	-	-

91	LYS 88.75	1.017Å HD3 with 46 LEU HB2	Favored (93.42%) General / -59.6,-44.6	37.6% (ttmt) chi angles: 193,177,292.7,173.8	0.085Å	-	-
92	ALA 47.76	0.466Å HB3 with 86 PHE HA	Favored (56.04%) General / -68.2,139.6	-	0.084Å	-	-
93	ILE 103.64	0.683Å HG12 with 45 LEU CD2	Favored (73.49%) Pre-proline / -134.9,150.6	36% ( <i>pt</i> ) chi angles: 63.9,165.6	0.127Å	-	-
94	PRO 80.21	-	Favored (39.21%) Trans-proline / -75.5,153.3	7.3% ( <i>Cg_endo</i> ) chi angles: 9.7	0.161Å	-	-
95	VAL 50.56	0.508Å HG12 with 96 SER N	Favored (6.46%) Isoleucine or valine /-75.8,150.7	81% ( <i>t</i> ) chi angles: 174.6	0.073Å	-	-
96	SER 86.99	0.508Å N with 95 VAL HG12	Favored (13.55%) General / -67.4,166.9	89.4% ( <i>p</i> ) chi angles: 65.7	0.094Å	-	-
97	ILE 147.09	0.821Å H with 97 ILE HD13	Favored (57.93%) Isoleucine or valine / -104.7,129.0	0.2% chi angles: 64.6,297.8	0.079Å	-	-
98	HIS 35.7	-	Favored (23.22%) General / -94.6,111.5	92.6% ( <i>m-70</i> ) chi angles: 298.1,272.8	0.102Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.448 σ
99	VAL 7.53	-	-	97.1% ( <i>t</i> ) chi angles: 176.7	0.077Å	-	-

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