Viewing clrn1_mb_29-99_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0		100th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	5.26%	Goal: <1%
	Ramachandran outliers	1	1.45%	Goal: <0.05%
	Ramachandran favored	57	82.61%	Goal: >98%
	MolProbity score^	1.75		87th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 561	0.00%	Goal: 0%
	Bad backbone angles:	5 / 757	0.66%	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.

^ 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: 92.83	Clashscore: 0	Outliers: 1 of 69	Poor rotamers: 3 of 57	Outliers: 0 of 62	Outliers: 0 of 71	Outliers: 5 of 71
29		GLY	7.49	-	-	-	-	-	-
30		THR	82.18	-	Allowed (1.06%) Pre-proline / -47.5,153.2	8.9% (*m*) chi angles: 313.8	0.08Å	-	-
31		PRO	76.56	-	Favored (32.23%) Trans-proline / -68.7,-27.0	32.4% (*Cg_endo*) chi angles: 21.8	0.121Å	-	-
32		LEU	77	-	Favored (89.22%) General / -63.2,-37.9	11% (*mp*) chi angles: 277.3,65.8	0.105Å	-	-
					Favored				OUTLIER(S)

33	TRP	87.42	-	(87.05%) General / -64.6,-37.3	61.8% (*t90*) chi angles: 170,89.7	0.131Å	-	worst is CE3-CD2-CG: 4.19 σ
34	ILE	34.1	-	Favored (98.99%) Isoleucine or valine / -62.6,-44.0	76.6% (*mt*) chi angles: 298.3,177.4	0.107Å	-	-
35	LYS	70.24	-	Favored (88.12%) General / -63.2,-37.7	48.3% (*tttt*) chi angles: 204.8,197,181.6,192	0.197Å	-	-
36	ALA	34.88	-	Favored (94.04%) General / -60.0,-42.4	-	0.093Å	-	-
37	THR	97.22	-	Favored (91.59%) General / -64.5,-38.6	2.2% (*p*) chi angles: 38.4	0.179Å	-	-
38	VAL	44.88	-	Favored (93.44%) Isoleucine or valine / -60.5,-43.1	40.4% (*t*) chi angles: 166.5	0.074Å	-	-
39	LEU	46.73	-	Favored (71.37%) General / -57.6,-36.1	14.3% (*mt*) chi angles: 309,193.8	0.16Å	-	-
40	CYS	31.24	-	Favored (47.55%) General / -87.8,-11.6	66.2% (*m*) chi angles: 302.2	0.162Å	-	-
41	LYS	140.65	-	Favored (5.58%) General / -128.0,-5.8	7.9% (*tptp*) chi angles: 189.9,64.1,223.8,73.7	0.153Å	-	-
42	THR	87.3	-	OUTLIER (0.03%) General / -77.1,-92.7	19.8% (*m*) chi angles: 289.8	0.18Å	-	-
43	GLY	93.43	-	Favored (2.59%) Glycine / 79.1,-71.7	-	-	-	-
44	ALA	244.51	-	Allowed (0.64%) General / -168.7,115.6	-	0.066Å	-	-
45	LEU	275.53	-	Favored (6.23%) General / -93.0,88.7	41.1% (*tp*) chi angles: 183.2,56.1	0.041Å	-	-
46	LEU	222.68	-	Allowed (0.49%)	44.1% (*tp*)	0.082Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					General / -136.2,-69.0	chi angles: 180.9,69			
47		VAL	131.42	-	Allowed (0.13%) Isoleucine or valine / -90.2,-168.4	33.4% (*m*) chi angles: 299.7	0.148Å	-	-
48		ASN	187.13	-	Favored (6.1%) General / -88.4,61.4	49.3% (*t30*) chi angles: 186.5,10.8	0.048Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 92.83	Clashscore: 0	Outliers: 1 of 69	Poor rotamers: 3 of 57	Outliers: 0 of 62	Outliers: 0 of 71	Outliers: 5 of 71
49		ALA	252.61	-	Favored (20.98%) General / -74.5,167.8	-	0.043Å	-	-
50		SER	205.95	-	Favored (43.1%) General / -146.6,159.7	20.9% (*m*) chi angles: 305.4	0.064Å	-	-
51		GLY	71.2	-	Favored (74.69%) Glycine / -70.3,-17.9	-	-	-	-
52		GLN	61.22	-	Favored (57.81%) General / -90.6,-3.0	0.2% chi angles: 250.7,296.6,163.7	0.063Å	-	OUTLIER(S) worst is CB-CG-CD: 5.262 σ
53		GLU	139.88	-	Favored (3.88%) General / -104.6,-48.2	0.3% chi angles: 149.9,288.1,309	0.118Å	-	-
54		LEU	156.62	-	Favored (8.24%) General / -81.1,99.0	61.7% (*tp*) chi angles: 181.5,62.5	0.077Å	-	OUTLIER(S) worst is C-N-CA: 4.342 σ
55		ASP	66.54	-	Allowed (0.81%) General / -40.9,-37.5	22.4% (*p-10*) chi angles: 62.7,325.4	0.063Å	-	-
56		LYS	141.88	-	Favored (62.76%) General / -56.5,-30.3	39.4% (*mmtm*) chi angles: 313.2,304,177.9,283.5	0.166Å	-	-
57		PHE	54.38	-	Favored (86.05%) General / -61.8,-37.9	42.6% (*m-85*) chi angles: 281.1,103.5	0.085Å	-	-
58		MET	61.09	-	Favored (46.25%) General /	14.6% (*mmt*) chi angles: 307.4,312,183.1	0.134Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-78.4,-25.9				
59		GLY	24.37	-	Favored (96.26%) Glycine / -59.8,-40.1	-	-	-	-
60		GLU	87.31	-	Favored (81.58%) General / -67.5,-43.2	3.9% (tm-20) chi angles: 197.4,300.2,306.9	0.04Å	-	-
61		MET	49.52	-	Favored (89.37%) General / -59.4,-41.4	19% (ttp) chi angles: 203.7,160.5,65.1	0.085Å	-	-
62		GLN	134.1	-	Favored (44.77%) General / -78.7,-26.1	9.7% (pt20) chi angles: 70.9,191.7,126.2	0.209Å	-	-
63		TYR	101.2	-	Favored (79.26%) General / -57.7,-40.4	10.8% (t80) chi angles: 182,108.5	0.061Å	-	-
64		GLY	30.42	-	Favored (71.68%) Glycine / -58.0,-49.8	-	-	-	-
65		LEU	57.26	-	Favored (70.26%) General / -54.1,-43.2	88.6% (mt) chi angles: 299.3,174.3	0.105Å	-	-
66		PHE	46.27	-	Favored (72.61%) General / -60.7,-33.3	16% (m-30) chi angles: 302.6,158.6	0.132Å	-	-
67		HIS	104.68	-	Favored (54.18%) General / -94.8,4.1	1.7% (p80) chi angles: 89.6,74.1	0.199Å	-	OUTLIER(S) worst is CA-CB-CG: 5.556 σ
68		GLY	21.94	-	Favored (64.25%) Glycine / 78.8,23.4	-	-	-	-

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			Avg: 92.83	Clashscore: 0	Outliers: 1 of 69	Poor rotamers: 3 of 57	Outliers: 0 of 62	Outliers: 0 of 71	Outliers: 5 of 71
69		GLU	77.73	-	Favored (5.37%) General / -56.9,157.8	6.2% (tp10) chi angles: 192.7,45.6,271.5	0.075Å	-	-
					Favored (3.36%)				

70	GLY	22.01	-	Glycine / -84.5,69.3	-	-	-	-
71	VAL	124.74	-	Favored (49.9%) Isoleucine or valine / -57.4,-35.6	4.1% (*p*) chi angles: 78.1	0.22Å	-	-
72	ARG	82.01	-	Allowed (0.24%) General / -59.3,-1.7	35.4% (*ptt-85*) chi angles: 62.7,189.8,179.1,278.2	0.064Å	-	-
73	GLN	165.26	-	Allowed (0.25%) General / -147.0,-69.0	0.9% chi angles: 185.4,291.9,110.7	0.096Å	-	-
74	CYS	56.93	-	Favored (84.49%) General / -64.8,-36.5	51.5% (*t*) chi angles: 181.7	0.104Å	-	-
75	GLY	29.76	-	Favored (72.99%) Glycine / -68.0,-20.7	-	-	-	-
76	LEU	48.67	-	Favored (57.17%) General / -75.0,-8.7	57.5% (*mt*) chi angles: 307.3,176.6	0.126Å	-	-
77	GLY	25.4	-	Favored (5.25%) Glycine / -99.8,-33.5	-	-	-	-
78	ALA	33.63	-	Favored (86.96%) General / -59.8,-47.1	-	0.091Å	-	-
79	ARG	113.67	-	Favored (88.17%) Pre-proline / -58.9,-50.4	37.6% (*mtp180*) chi angles: 264.6,172.5,64.9,185	0.135Å	-	-
80	PRO	118.65	-	Favored (8.07%) Trans-proline / -82.8,-15.8	93.7% (*Cg_endo*) chi angles: 30.3	0.061Å	-	-
81	PHE	72.48	-	Favored (15.07%) General / -105.8,-15.0	10.1% (*m-30*) chi angles: 309.8,145	0.166Å	-	-
82	ARG	129.05	-	Favored (22.73%) General / -85.1,-32.5	83.2% (*mtp180*) chi angles: 296.7,174.8,71.5,190.2	0.11Å	-	-
83	PHE	111.98	-	Favored (17.86%) General /	34.8% (*m-85*) chi angles: 278.9,79.4	0.056Å	-	OUTLIER(S) worst is CA-CB-CG: 4.415 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-81.9,111.2				
84		SER	80.88	-	Favored (56.52%) General / -54.9,-29.6	19.2% (*m*) chi angles: 306.5	0.1Å	-	-
85		PHE	67.59	-	Favored (72.56%) General / -64.0,-31.4	3.3% (*m-30*) chi angles: 319.6,135.6	0.123Å	-	-
86		PHE	145.48	-	Favored (2.4%) Pre-proline / -75.5,-37.5	7.2% (*t80*) chi angles: 200,287.1	0.138Å	-	-
87		PRO	217.42	-	Favored (70.83%) Trans-proline / -68.5,154.9	62.7% (*Cg_exo*) chi angles: 327.3	0.072Å	-	-
88		ASP	48.72	-	Favored (78.73%) General / -60.4,-36.7	1.4% (*m-20*) chi angles: 304.2,59.5	0.071Å	-	-

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			Avg: 92.83	Clashscore: 0	Outliers: 1 of 69	Poor rotamers: 3 of 57	Outliers: 0 of 62	Outliers: 0 of 71	Outliers: 5 of 71
89		LEU	47.56	-	Favored (49.55%) General / -78.6,-4.6	49.2% (*mt*) chi angles: 308.2,181.4	0.079Å	-	-
90		LEU	181.7	-	Allowed (0.58%) General / -113.9,-79.0	3.6% (*mm?*) chi angles: 275.3,286.5	0.065Å	-	-
91		LYS	88.75	-	Allowed (0.35%) General / -154.6,10.1	10% (*mmmt*) chi angles: 265.5,308.4,308.9,173.7	0.084Å	-	-
92		ALA	47.76	-	Favored (22.03%) General / -159.6,152.8	-	0.073Å	-	-
93		ILE	103.64	-	Favored (45.44%) Pre-proline / -114.1,155.4	38.5% (*pt*) chi angles: 56,170.8	0.065Å	-	-
94		PRO	80.21	-	Favored (19.78%) Trans-proline / -75.4,136.6	83.8% (*Cg_endo*) chi angles: 31.4	0.032Å	-	-

95	VAL	50.56	-	Allowed (0.34%) Isoleucine or valine / -67.2,98.0	99.2% (*t*) chi angles: 176.4	0.05Å	-	-
96	SER	86.99	-	Allowed (0.75%) General / -50.9,158.0	24.1% (*t*) chi angles: 186.2	0.044Å	-	-
97	ILE	147.09	-	Favored (8.91%) Isoleucine or valine / -70.7,152.2	87.8% (*mt*) chi angles: 295.8,165.9	0.086Å	-	-
98	HIS	35.7	-	Favored (35.35%) General / -144.4,148.9	50.9% (*t-80*) chi angles: 180.4,279.5	0.105Å	-	-
99	VAL	7.53	-	-	68.7% (*t*) chi angles: 171.7	0.052Å	-	-

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