

## Viewing c1qtnf5\_mb\_69-112\_FFX1Hmulti.table

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All-Atom	Clashscore, all atoms: 0			100 <sup>th</sup> percentile* (N=1784, all resolutions)		
Contacts	Clashscore is the number	of serio	us steric o	verlaps (> 0.4 Å) per 1000 atoms.		
	Poor rotamers	0	0.00%	Goal: <1%		
	Ramachandran outliers	0	0.00%	Goal: <0.05%		
II I	Ramachandran favored	35	83.33%	Goal: >98%		
Protein Geometry	MolProbity score <sup>^</sup>	1.19		99 <sup>th</sup> percentile <sup>*</sup> (N=27675, 0Å - 99Å)		
acometry	Cβ deviations >0.25Å	0	0.00%	Goal: 0		
	Bad backbone bonds: 0 / 3		0.00%	Goal: 0%		
	Bad backbone angles:	1 / 419	0.24%	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:	Clashscore:	Outliers: 0 of	Poor rotamers: 0 of	Outliers:	Outliers:	Outliers: 1
		86.29	0	42	29	0 of 34	0 of 44	of 44
69	GLY	3.48	-	-	-	-	-	_
70	ARG	155.13	-	Favored (83.34%) Pre-proline / -58.1,130.3	75% (ttt180) chi angles: 175.2,172.3,175.3,171.7	0.071Å	-	-
71	PRO	142.1	-	Favored (7.24%) Trans-proline / -73.4,-33.2	91.2% ( <i>Cg_exo</i> ) chi angles: 329.9	0.07Å	-	-
72	GLY	91.12	-	Allowed (0.44%) Glycine / 147.0,-108.5	-	-	-	-
				Favored				

<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.

LEU 134.84	-	(37.65%) Pre-proline / -136.4,165.2	4.8% ( <i>mp</i> ) chi angles: 284.9,91.8	0.051Å	-	-
PRO 57.69	-	Favored (10.51%) Trans-proline / -82.4,139.8	19.6% ( <i>Cg_exo</i> ) chi angles: 344.9	0.089Å	-	-
GLY 27.91	-	Favored (18.33%) Glycine / -70.8,129.1	<del>-</del>	-	-	-
PRO 71.57	-	Favored (6.71%) Trans-proline / -58.6,119.5	1.3% ( <i>Cg_exo</i> ) chi angles: 321.3	0.051Å	-	-
ARG 161.44	-	Favored (3.72%) General / -157.1,-171.7	10.9% (mtm105) chi angles: 313,185,306.9,78	0.086Å	-	-
GLY 25.76	-	Favored (5.58%) Glycine / -80.0,121.8	-	-	-	-
ASP 82.26	-	Favored (30.19%) Pre-proline / -71.2,167.4	15.3% ( <i>p-10</i> ) chi angles: 56,310	0.043Å	-	-
PRO 130.92	-	Allowed (0.9%) Trans-proline / -81.9,95.8	95.7% ( <i>Cg_endo</i> ) chi angles: 32.6	0.018Å	-	-
GLY 20.42	-	Favored (5.66%) Glycine / -57.4,166.3	-	-	-	-
PRO 65.81	-	Favored (26.38%) Trans-proline / -77.9,149.9	29.1% ( <i>Cg_endo</i> ) chi angles: 37.4	0.043Å	-	-
ARG 83.91	-	Favored (5.22%) General / -69.9,110.9	66% (ttp85) chi angles: 189.1,190.2,63.3,85.1	0.063Å	-	-
GLY 30.78	-	Favored (46.66%) Glycine / -65.3,157.8 Favored	-	-	-	-
	PRO 57.69  GLY 27.91  PRO 71.57  ARG 161.44  GLY 25.76  ASP 82.26  PRO 130.92  GLY 20.42  PRO 65.81  ARG 83.91	PRO 57.69 -  GLY 27.91 -  PRO 71.57 -  ARG 161.44 -  GLY 25.76 -  ASP 82.26 -  PRO 130.92 -  GLY 20.42 -  PRO 65.81 -  ARG 83.91 -	Pre-proline / -136.4,165.2 Favored (10.51%) Trans-proline / -82.4,139.8 Favored (118.33%) Glycine / -70.8,129.1 Favored (6.71%) Trans-proline / -58.6,119.5 Favored (6.71%) General / -157.1,-171.7 Favored (5.58%) Glycine / -70.8,129.1 Favored (6.71%) Trans-proline / -58.6,119.5 Favored (30.72%) General / -157.1,-171.7 Favored (5.58%) Glycine / -80.0,121.8 Favored (30.19%) Pre-proline / -71.2,167.4 Allowed (0.9%) Trans-proline / -71.2,167.4 Allowed (0.9%) Trans-proline / -57.4,166.3 Favored (6.71%) Favored (3.72%) General / -61.9,110.9 Favored (46.66%) Glycine / -77.9,149.9 Favored (46.66%) Glycine / -69.9,110.9 Favored (46.66%) Glycine / -69.9,110.9 Favored	PRO 57.69 - 136.4,165.2 Favored (10.51%)	PRO 57.69 - Pre-proline / 136.4165.2 Favored (10.51%)   19.6% (Cg_exo) chi angles: 344.9   0.089Å   19.6% (Cg_exo) chi angles: 344.9   19.6% (Cg_exo) chi angles: 321.3   19.6% (Cg_exo) chi angles: 32.6   19.6% (Cg_exo) chi ang	PRO 57.69 - (10.51%)

85	GLU 77.67	-	(33.19%) General / -67.8,158.1	2.4% ( <i>mm-40</i> ) chi angles: 257.6,319.8,330.1	0.154Å	-	-
86	ALA 41.86	-	Allowed (1.3%) General / -85.4,46.5	-	0.054Å	-	-
87	GLY 97.58	-	Favored (16.99%) Glycine / -103.6,159.1	-	-	-	-
88	PRO 76.88	-	Favored (3.12%) Trans-proline / -82.9,79.0	31.9% ( <i>Cg_endo</i> ) chi angles: 37.2	0.039Å	-	-
#	Alt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	<b>C</b> β <b>deviation</b>	Bond lengths	<b>Bond angles</b>
	Avg: 86.29	Clashscore: 0	Outliers: 0 of 42	Poor rotamers: 0 of 29	Outliers: 0 of 34	Outliers: 0 of 44	Outliers: 1 of 44
89	ALA 38.19	-	Favored (38.93%) General / -53.7,136.8	-	0.048Å	-	-
90	GLY 87.66	-	Favored (38.64%) Glycine / -178.0,-177.7	-	-	-	-
91	PRO 157.76	-	Favored (3.01%) Trans-proline / -89.8,10.8	5.9% ( <i>Cg_endo</i> ) chi angles: 41.1	0.037Å	-	-
92	THR 123.08	-	Favored (27.96%) General / -81.5,151.1	12.8% ( <i>t</i> ) chi angles: 185.9	0.081Å	-	-
93	GLY 23.11	-	Favored (33.13%) Glycine / -97.5,-171.0	-	-	-	-
94	PRO 77.54	-	Favored (14.55%) Trans-proline / -83.6,159.8	25.5% ( <i>Cg_endo</i> ) chi angles: 37.9	0.064Å	-	-
95	ALA 53.69	-	Favored (51.47%) General / -78.9,-19.6	-	0.102Å	-	-

96	GLY 145.31	-	Favored (38.18%) Glycine / 67.8,-169.4	-	-	-	OUTLIER(S) worst is C-N- CA: 4.264 σ
97	GLU 61.91	-	Allowed (0.75%) General / -75.0,56.1	2.3% ( <i>mp0</i> ) chi angles: 321.5,89.5,300.7	0.063Å	-	-
98	CYS 69.5	-	Favored (4.86%) General / -79.5,66.2	24.8% ( <i>p</i> ) chi angles: 57	0.115Å	-	-
99	SER 68.21	-	Favored (76.5%) General / -59.8,-36.3	64.9% ( <i>p</i> ) chi angles: 56.9	0.101Å	-	-
100	VAL 105.5	-	Favored (2.07%) Pre-proline / -97.4,94.7	11.3% ( <i>m</i> ) chi angles: 287.9	0.108Å	-	-
101	PRO 78.2	-	Favored (3.52%) Trans-proline / -76.9,112.8	37.3% ( <i>Cg_endo</i> ) chi angles: 23	0.038Å	-	-
102	PRO 67.69	-	Favored (24.96%) Trans-proline / -48.6,138.4	12.6% ( <i>Cg_exo</i> ) chi angles: 323.2	0.063Å	-	-
103	ARG 140.8	-	Favored (51.67%) General / -127.6,141.3	17.2% (mmt85) chi angles: 310.4,301.8,174,103.8	0.066Å	-	-
104	SER 199.89	-	Allowed (1.92%) General / -161.5,-168.1	11.2% ( <i>t</i> ) chi angles: 191.5	0.076Å	-	-
105	ALA 128.07	-	Favored (10.51%) General / -84.2,70.1	-	0.033Å	-	-
106	PHE 109.09	-	Favored (19.9%) General / -165.3,163.7	59.6% ( <i>t80</i> ) chi angles: 189.1,73.3	0.05Å	-	-
107	SER 72.78	-	Favored (5.34%) General /	8.1% ( <i>t</i> ) chi angles: 195.1	0.078Å	-	-

108	ALA 32.78	-	-72.7,176.6 Allowed (0.92%) General / -169.2,125.9	-	0.083Å	-	-
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#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	<b>Bond angles</b>
		Avg:	Clashscore:	Outliers: 0 of	Poor rotamers: 0 of	Outliers:	Outliers:	Outliers: 1
		86.29	0	42	29	0 of 34	0 of 44	of 44
109	) LYS	117.9	-	Favored (6.42%) General / -76.1,104.0	27.4% ( <i>tptp</i> ) chi angles: 178.8,60.9,184.4,63.6	0.048Å	-	-
110	) ARC	G 105.97	-	Allowed (1.83%) General / -55.2,161.4	50.7% ( <i>ptt85</i> ) chi angles: 61,170.5,183.9,80	0.049Å	-	-
111	I SER	78.01	-	Favored (13.79%) General / -66.0,165.2	44.9% (p) chi angles: 54.1	0.028Å	-	-
112	2 GLU	J 75.06	-	-	80.7% ( <i>mm-40</i> ) chi angles: 299,292.2,330.7	0.101Å	-	-

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