Viewing c1qtnf5_mb_69-112H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	24.01		23rd percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.				
Protein Geometry	Poor rotamers	3	10.34%	Goal: <1%	
	Ramachandran outliers	0	0.00%	Goal: <0.05%	
	Ramachandran favored	42	100.00%	Goal: >98%	
	MolProbity score^	2.64		39th percentile* (N=27675, 0Å - 99Å)	
	Cβ deviations >0.25Å	0	0.00%	Goal: 0	
	Bad backbone bonds:	0 / 308	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.

* 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: 86.29	Clashscore: 24.01	Outliers: 0 of 42	Poor rotamers: 3 of 29	Outliers: 0 of 34	Outliers: 0 of 44	Outliers: 1 of 44
69		GLY	3.48	-	-	-	-	-	-
70		ARG	155.13	-	Favored (81.58%) Pre-proline / -72.2,138.8	9.7% (*ptp85*) chi angles: 58.8,191.5,74.6,96	0.067Å	-	-
71		PRO	142.1	-	Favored (45.35%) Trans-proline / -66.5,-28.3	87.7% (*Cg_exo*) chi angles: 331.3	0.151Å	-	-
72		GLY	91.12	-	Favored (37.42%) Glycine / 93.0,163.7	-	-	-	-
				0.828Å	Favored				

73	LEU	134.84	H with 73 LEU HD13	(83.18%) Pre-proline / -72.9,142.6	0% chi angles: 55.4,298.8	0.064Å	-	-
74	PRO	57.69	-	Favored (25.09%) Trans-proline / -79.2,154.2	75.6% (*Cg_exo*) chi angles: 333.6	0.078Å	-	-
75	GLY	27.91	-	Favored (49.72%) Glycine / -83.8,172.1	-	-	-	-
76	PRO	71.57	-	Favored (25.55%) Trans-proline / -73.4,137.4	72.9% (*Cg_exo*) chi angles: 332.4	0.096Å	-	-
77	ARG	161.44	0.422Å HB3 with 77 ARG NH1	Favored (17.34%) General / -166.1,166.0	29.4% (*mtm105*) chi angles: 296.9,186.7,305.5,88	0.151Å	-	-
78	GLY	25.76	-	Favored (34.87%) Glycine / -74.7,146.1	-	-	-	-
79	ASP	82.26	-	Favored (36.98%) Pre-proline / -84.0,165.8	47.3% (*p-10*) chi angles: 61.5,348.9	0.073Å	-	-
80	PRO	130.92	-	Favored (28.32%) Trans-proline / -78.6,157.1	9.4% (*Cg_endo*) chi angles: 12.7	0.097Å	-	-
81	GLY	20.42	-	Favored (35.98%) Glycine / -83.3,158.4	-	-	-	-
82	PRO	65.81	-	Favored (20.02%) Trans-proline / -80.6,152.4	15.6% (*Cg_endo*) chi angles: 16.6	0.081Å	-	-
83	ARG	83.91	-	Favored (36.2%) General / -77.2,148.0	82.3% (*mtt85*) chi angles: 287.5,181.8,170.7,84.6	0.07Å	-	-
84	GLY	30.78	-	Favored (14.18%) Glycine / -123.6,-174.4	-	-	-	-
				Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
85		GLU	77.67	0.445Å HG2 with 86 ALA N	(38.48%) General / -72.1,157.0	45.6% (*tt0*) chi angles: 180.1,185.2,45.7	0.097Å	-	-
86		ALA	41.86	0.445Å N with 85 GLU HG2	Favored (22.77%) General / -77.1,166.8	-	0.092Å	-	-
87		GLY	97.58	-	Favored (4.05%) Glycine / 116.6,127.6	-	-	-	-
88		PRO	76.88	-	Favored (55.83%) Trans-proline / -63.7,156.7	75% (*Cg_endo*) chi angles: 29.6	0.06Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 86.29	Clashscore: 24.01	Outliers: 0 of 42	Poor rotamers: 3 of 29	Outliers: 0 of 34	Outliers: 0 of 44	Outliers: 1 of 44
89		ALA	38.19	-	Favored (35.89%) General / -77.5,147.2	-	0.091Å	-	-
90		GLY	87.66	0.436Å HA2 with 91 PRO HD2	Favored (3.09%) Glycine / -178.9,137.1	-	-	-	-
91		PRO	157.76	0.436Å HD2 with 90 GLY HA2	Favored (11.31%) Trans-proline / -79.3,-18.1	18.9% (*Cg_endo*) chi angles: 18	0.163Å	-	-
92		THR	123.08	-	Favored (55.9%) General / -65.0,145.8	14% (*t*) chi angles: 189.9	0.051Å	-	-
93		GLY	23.11	-	Favored (46.67%) Glycine / -84.7,171.1	-	-	-	-
94		PRO	77.54	-	Favored (18.45%) Trans-proline / -80.5,148.7	10.3% (*Cg_endo*) chi angles: 13.4	0.164Å	-	-
95		ALA	53.69	-	Favored (84.26%) General / -67.1,-37.7	-	0.087Å	-	-

96	GLY 145.31	-	Favored (22.87%) Glycine / 60.6,-120.5	-	-	-	-	-
97	GLU 61.91	-	Favored (34.71%) General / -105.3,117.7	80.2% (*mt-10*) chi angles: 296.3,160.8,346.6	0.093Å	-	-
98	CYS 69.5	-	Favored (51.08%) General / -117.0,139.1	31% (*p*) chi angles: 63.8	0.099Å	-	-
99	SER 68.21	-	Favored (3.64%) General / -65.0,-59.9	48.5% (*t*) chi angles: 179.5	0.058Å	-	-
100	VAL 105.5	0.523Å HB with 101 PRO HD2	Favored (8.09%) Pre-proline / -149.5,170.2	34.4% (*m*) chi angles: 298.8	0.091Å	-	-
101	PRO 78.2	0.523Å HD2 with 100 VAL HB	Favored (41.04%) Trans-proline / -73.9,148.7	15.7% (*Cg_endo*) chi angles: 16.6	0.113Å	-	-
102	PRO 67.69	-	Favored (21.74%) Trans-proline / -78.5,146.3	62.8% (*Cg_exo*) chi angles: 334.2	0.107Å	-	-
103	ARG 140.8	-	Favored (21.73%) General / -123.2,115.4	65.2% (*mtp85*) chi angles: 290,192.2,70.6,87.1	0.092Å	-	-
104	SER 199.89	-	Favored (2.27%) General / -161.4,-169.3	73.3% (*m*) chi angles: 295.4	0.122Å	-	-
105	ALA 128.07	-	Favored (15.29%) General / -95.0,103.4	-	0.095Å	-	-
106	PHE 109.09	0.469Å CD2 with 107 SER N	Favored (3.69%) General / -173.9,171.4	39.3% (*t80*) chi angles: 194,74.3	0.096Å	-	OUTLIER(S) worst is CA-CB-CG: 7.294 σ
107	SER 72.78	0.469Å N with 106 PHE CD2	Favored (24.86%) General / -106.6,151.6	48.3% (*t*) chi angles: 179.6	0.114Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
108		ALA	32.78	-	Favored (44.02%) General / -149.0,158.2	-	0.094Å	-	-
			Avg: 86.29	Clashscore: 24.01	Outliers: 0 of 42	Poor rotamers: 3 of 29	Outliers: 0 of 34	Outliers: 0 of 44	Outliers: 1 of 44
109		LYS	117.9	0.528Å HD3 with 109 LYS N	Favored (19.92%) General / -93.1,151.3	0.1% chi angles: 283.2,61,86.7,287.3	0.077Å	-	-
110		ARG	105.97	0.561Å HB2 with 110 ARG NH1	Favored (26.9%) General / -107.4,150.3	0.3% chi angles: 187.9,70.7,78.2,272.4	0.098Å	-	-
111		SER	78.01	-	Favored (42.72%) General / -69.9,153.8	94.4% (*p*) chi angles: 63.4	0.074Å	-	-
112		GLU	75.06	-	-	19.4% (*pt-20*) chi angles: 60.6,179.1,37.4	0.101Å	-	-

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