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All-Atom Contacts	Clashscore, all atoms:	0		100 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	2	2.82%	Goal: <1%
	Ramachandran outliers	3	3.61%	Goal: <0.05%
	Ramachandran favored	71	85.54%	Goal: >98%
	MolProbity score^	1.49		95 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	1.30%	Goal: 0
	Bad backbone bonds:	0 / 664	0.00%	Goal: 0%
	Bad backbone angles:	3 / 885	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.

[^] 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: 83.21	Clashscore: 0	Outliers: 3 of 83	Poor rotamers: 2 of 71	Outliers: 1 of 77	Outliers: 0 of 85	Outliers: 3 of 85
42	SER	58.57	-	-	-	85.3% (p) chi angles: 68.2	0.044Å	-	-
43	PRO	92.83	-	-	Favored (3.05%) Trans-proline / -88.3,178.3	68.2% (Cg_endo) chi angles: 33.7	0.044Å	-	-
44	SER	161.22	-	-	Allowed (0.18%) General / 65.3,-177.4	5.2% (p) chi angles: 87.4	0.156Å	-	-
45	LEU	92.84	-	-	Favored (46.12%) General / -139.9,157.2	4.6% (mp) chi angles: 297.5,97	0.062Å	-	-
46	GLN	92.23	-	-	Favored (21.2%) General / -105.5,153.8	48.8% (mt-30) chi angles: 285.1,197.9,8.1	0.084Å	-	-

47	CYS	48.11	-	Favored (38.57%) General / -71.2,129.3	42.6% (t) chi angles: 178.2	0.067Å	-	-
48	ARG	187.67	-	Favored (68.39%) General / -65.8,-27.6	40.8% (mtp180) chi angles: 301.5,191.2,81.8,222.5	0.161Å	-	-
49	VAL	99.5	-	Favored (10.78%) Isoleucine or valine / -81.0,-54.2	29.4% (t) chi angles: 186.2	0.063Å	-	-
50	CYS	91.39	-	Favored (8.42%) General / -124.5,9.3	20.2% (p) chi angles: 69.8	0.092Å	-	-
51	GLY	36.1	-	Favored (4.12%) Glycine / 85.6,-49.2	-	-	-	-
52	ASP	50.76	-	Allowed (0.4%) General / -38.5,139.4	30.5% (t0) chi angles: 199.1,22.8	0.105Å	-	-
53	SER	48.05	-	Favored (14.22%) General / -47.7,130.2	49.6% (m) chi angles: 300.4	0.038Å	-	-
54	SER	47.77	-	Favored (42.28%) General / -70.4,154.1	9% (t) chi angles: 193.2	0.05Å	-	-
55	SER	105.31	-	Allowed (1.2%) General / -93.5,46.5	31.2% (t) chi angles: 173.4	0.112Å	-	-
56	GLY	35.48	-	Favored (43.06%) Glycine / 59.7,-147.6	-	-	-	-
57	LYS	137.92	-	Favored (34.42%) General / -80.8,129.2	20.9% (tptp) chi angles: 192.8,71.1,151.1,61	0.129Å	-	-
58	HIS	65.55	-	Favored (3.22%) General / -168.6,142.9	88.8% (m-70) chi angles: 302,299.9	0.156Å	-	OUTLIER(S) worst is CA- CB-CG: 7.171 σ
				Favored (4.32%)	19.3% (m-85)			

59	TYR	70.8	-	General / 62.9,47.8	chi angles: 315.7,285.7	0.113Å	-	-	
60	GLY	31.53	-	Allowed (0.5%) Glycine / 69.0,-65.2	-	-	-	-	
61	ILE	121.12	-	OUTLIER (0.01%) Isoleucine or valine / -74.7,-149.9	4.9% (<i>pt</i>) chi angles: 64.8,146.6	0.224Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 83.21	Clashscore: 0	Outliers: 3 of 83	Poor rotamers: 2 of 71	Outliers: 1 of 77	Outliers: 0 of 85	Outliers: 3 of 85
62	TYR	66.98	-	Favored (37.13%) General / -128.0,124.4	85.6% (<i>m-85</i>) chi angles: 302.5,274	0.094Å	-	-	
63	ALA	36.59	-	Favored (26.04%) General / -148.1,142.3	-	0.078Å	-	-	
64	CYS	43.82	-	Favored (17.78%) General / -73.8,169.2	13.9% (<i>p</i>) chi angles: 76.1	0.048Å	-	-	
65	ASN	51.38	-	Favored (72.06%) General / -61.9,-31.7	91% (<i>m-20</i>) chi angles: 294.4,340.4	0.117Å	-	-	
66	GLY	29.4	-	Favored (73.17%) Glycine / -69.0,-28.3	-	-	-	-	
67	CYS	48.5	-	Favored (20.22%) General / -88.3,-29.7	67.1% (<i>m</i>) chi angles: 287.6	0.137Å	-	-	
68	SER	86.96	-	Favored (93.76%) General / -62.2,-45.3	97.3% (<i>p</i>) chi angles: 64	0.145Å	-	-	
69	GLY	29	-	Favored (36.27%) Glycine / -76.2,-37.8	-	-	-	-	
70	PHE	63.4	-	Favored (86.45%) General /	67.1% (<i>t80</i>) chi angles: 171.2,84.3	0.041Å	-	-	

				-59.1,-47.1					
				Favored					
71	PHE	71.7	-	(64.85%)	81.6% (<i>t80</i>)	0.046Å	-	-	
				General /	chi angles: 182,71.7				
				-68.5,-48.2					
				Favored					
72	LYS	92.03	-	(77.91%)	56.6% (<i>tttp</i>)	0.133Å	-	-	
				General /	chi angles:				
				-58.1,-49.1	180.1,171.8,180.7,71.3				
				Favored					
73	ARG	135.75	-	(69.13%)	15.6% (<i>ptm180</i>)	0.262Å	-	-	
				General /	chi angles:				
				-70.3,-31.7	70.6,186.7,295.5,166.6				
				Favored					
74	SER	106.86	-	(78.02%)	72.6% (<i>m</i>)	0.089Å	-	-	
				General /	chi angles: 293.6				
				-69.4,-38.5					
				Favored					
75	VAL	52.99	-	(9.94%)	70.6% (<i>t</i>)	0.162Å	-	-	
				Isoleucine or	chi angles: 173.3				
				valine /					
				-85.4,-35.6					
				Favored					
76	ARG	90.49	-	(59.31%)	35.9% (<i>tpt85</i>)	0.203Å	-	-	
				General /	chi angles:				
				-76.0,-18.3	189,57.3,185.9,70.5				
				Favored					
77	ARG	124.69	-	(20.85%)	0%	0.154Å	-	-	
				General /	chi angles:				
				-106.4,-3.6	252.6,309.2,318.3,221.5				
				Favored					
78	ARG	68.72	-	(5.53%)	93.7% (<i>mtt180</i>)	0.194Å	-	-	
				General /	chi angles:				
				58.9,53.8	296.8,188.3,175.3,194.7				
				Favored					
79	LEU	120.54	-	(4.82%)	3.3% (<i>mm?</i>)	0.067Å	-	-	
				General /	chi angles: 287.7,310.1				
				-79.0,87.1					
				Allowed					
80	ILE	97.42	-	(1.05%)	88.8% (<i>mt</i>)	0.083Å	-	-	
				Isoleucine or	chi angles: 299.8,172.8				
				valine /					
				-82.2,76.6					
				Favored					
81	TYR	82.89	-	(33.55%)	58.2% (<i>m-85</i>)	0.054Å	-	-	
				General /	chi angles: 306.3,288.5				
				-54.1,140.0					

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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		Avg: 83.21	Clashscore: 0	Outliers: 3 of 83	Poor rotamers: 2 of 71	Outliers: 1 of 77	Outliers: 0 of 85	Outliers: 3 of 85
82	ARG 112.35	-	Favored (20.45%) General / -85.9,156.6	77.8% (<i>ttt180</i>) chi angles: 181.5,174.6,172.2,175.7	0.056Å	-	-	
83	CYS 44.78	-	Favored (10.35%) General / -132.4,174.3	6.3% (<i>t</i>) chi angles: 200.1	0.046Å	-	-	
84	GLN 47.29	-	Favored (9.27%) General / -112.0,-25.7	39% (<i>mt-30</i>) chi angles: 295.3,174.4,247.3	0.056Å	-	-	
85	VAL 62.05	-	Favored (4.45%) Isoleucine or valine / -99.5,152.8	98.9% (<i>t</i>) chi angles: 176.5	0.114Å	-	-	
86	GLY 70.6	-	Favored (3.07%) Glycine / -76.7,51.7	-	-	-	-	
87	ALA 237.84	-	OUTLIER (0.03%) General / 64.8,-79.3	-	0.172Å	-	-	
88	GLY 85.11	-	Favored (70.38%) Glycine / -65.1,-24.5	-	-	-	-	
89	MET 141.5	-	Favored (73.12%) General / -64.5,-31.8	0.5% chi angles: 310.2,81.9,204.1	0.127Å	-	-	
90	CYS 64.94	-	Favored (76.32%) Pre-proline / -83.6,121.2	63.3% (<i>m</i>) chi angles: 303	0.054Å	-	-	
91	PRO 93.41	-	Favored (20.97%) Trans-proline / -80.0,150.9	42.2% (<i>Cg_endo</i>) chi angles: 36.1	0.016Å	-	-	
92	VAL 121.31	-	Allowed (1.17%) Isoleucine or valine / -134.7,17.6	22.8% (<i>m</i>) chi angles: 302.7	0.097Å	-	-	
93	ASP 65.88	-	OUTLIER (0.02%) General /	7.7% (<i>p-10</i>) chi angles: 58.6,283.4	0.23Å	-	OUTLIER(S) worst is C-CA-CB: 4.271	

-81.8,-124.6

 σ

94	LYS	116.85	-	Favored (2.1%) General / -133.1,-21.5	68.7% (<i>tttt</i>) chi angles: 205.3,183.3,186.9,179.4	0.049Å	-	-
95	ALA	59.74	-	Allowed (1.09%) General / -95.4,41.9	-	0.057Å	-	-
96	HIS	75.92	-	Favored (22.75%) General / -154.6,145.7	26.9% (<i>m-70</i>) chi angles: 319.6,287.9	0.101Å	-	-
97	ARG	128.79	-	Favored (39.99%) General / -74.7,149.4	99.8% (<i>mtt180</i>) chi angles: 294.1,180.4,180.3,178.5	0.065Å	-	-
98	ASN	58.56	-	Favored (21.42%) General / 58.2,42.8	2.3% (<i>m-20</i>) chi angles: 304.4,18.1	0.07Å	-	-
99	GLN	74.68	-	Favored (57.82%) General / -62.5,136.3	33% (<i>mt-30</i>) chi angles: 295.5,185.9,119.2	0.041Å	-	-
100	CYS	72.61	-	Favored (13.97%) General / -66.2,120.9	50.4% (<i>t</i>) chi angles: 179.5	0.027Å	-	-
101	GLN	78.03	-	Favored (65.3%) General / -73.1,-33.0	27.9% (<i>mp0</i>) chi angles: 301.8,84.7,348.9	0.093Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
Avg:			Clashscore:	Outliers: 3 of	Poor rotamers: 2 of	Outliers:	Outliers:	Outliers: 3
83.21			0	83	71	1 of 77	0 of 85	of 85
102	ALA	43.32	-	Favored (75.56%) General / -69.4,-35.2	-	0.107Å	-	-
103	CYS	94.69	-	Favored (16.9%) General / -89.1,-34.0	14.5% (<i>p</i>) chi angles: 75	0.17Å	-	-
104	ARG	82.35	-	Favored (77.75%) General / -55.7,-46.4	54.2% (<i>ttt180</i>) chi angles: 181.8,184.6,168.2,207.7	0.067Å	-	-

105	LEU	111.48	-	Favored (77.86%) General / -60.3,-36.4	2.6% (<i>tm?</i>) chi angles: 187.8,273	0.072Å	-	-
106	LYS	81.83	-	Favored (61.27%) General / -75.0,-31.4	43.3% (<i>mttp</i>) chi angles: 297.9,160.6,184.7,59.1	0.135Å	-	-
107	LYS	74.14	-	Favored (59.23%) General / -74.3,-24.6	30.2% (<i>tttt</i>) chi angles: 199.2,207.2,161.6,187.7	0.165Å	-	-
108	CYS	42.96	-	Favored (81.47%) General / -56.6,-45.4	87.2% (<i>m</i>) chi angles: 292.1	0.098Å	-	-
109	LEU	56.27	-	Favored (75.68%) General / -67.0,-46.0	51.4% (<i>mt</i>) chi angles: 301.8,168.6	0.088Å	-	-
110	GLN	53.5	-	Favored (67.79%) General / -57.7,-32.8	40.8% (<i>tt0</i>) chi angles: 196.6,190.5,21.9	0.053Å	-	-
111	ALA	41.98	-	Favored (59.62%) General / -77.8,-14.4	-	0.051Å	-	-
112	GLY	51.55	-	Favored (7.23%) Glycine / 105.4,24.2	-	-	-	-
113	MET	79.04	-	Favored (3.61%) General / -75.7,96.3	93.1% (<i>mtp</i>) chi angles: 292.7,183.6,76.8	0.103Å	-	-
114	ASN	71.26	-	Favored (6.66%) General / -59.0,159.8	57.6% (<i>t30</i>) chi angles: 187.3,22.8	0.07Å	-	-
115	GLN	105.5	-	Favored (7.84%) General / -95.2,21.5	13.5% (<i>pt20</i>) chi angles: 76,181.3,11.9	0.132Å	-	-
116	ASP	98.54	-	Favored (24.47%) General / -50.2,-54.0	1.8% (<i>p30</i>) chi angles: 41.1,45.9	0.169Å	-	OUTLIER(S) worst is CA- CB-CG: 5.599 σ
117	ALA	45.79	-	Favored (58.5%)	-	0.086Å	-	-

				General / -86.9,-2.3					
				Allowed (1.71%)					
118	VAL	55.86	-	Isoleucine or valine / -87.0,-61.8	98.7% (<i>t</i>) chi angles: 176.4	0.044Å	-	-	
				Favored (6.88%)					
119	GLN	125.44	-	General / -94.4,91.9	3.2% (<i>mt-30</i>) chi angles: 293.5,216.6,238	0.034Å	-	-	
				Favored (3.8%)					
120	ASN	109.31	-	General / -91.9,60.2	21.2% (<i>m120</i>) chi angles: 310.2,109.5	0.047Å	-	-	
				Favored (7.03%)					
121	GLU	304.59	-	General / -161.3,-178.9	3.2% (<i>pt-20</i>) chi angles: 62.4,214.5,296	0.087Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 83.21	Clashscore: 0	Outliers: 3 of 83	Poor rotamers: 2 of 71	Outliers: 1 of 77	Outliers: 0 of 85	Outliers: 3 of 85
				Favored (7.8%)					
122	ARG	69.53	-	General / -77.8,103.5	70.5% (<i>mtm180</i>) chi angles: 293.9,194.5,291.9,184.4	0.059Å	-	-	
				Favored (91.86%)					
123	GLN	74.92	-	Pre-proline / -68.5,130.8	28.8% (<i>mp0</i>) chi angles: 298.2,85,358.2	0.064Å	-	-	
				Favored (8.06%)					
124	PRO	66.89	-	Trans-proline / -86.5,145.2	60.5% (<i>Cg_endo</i>) chi angles: 34.5	0.057Å	-	-	
				Allowed (1.71%)					
125	ARG	87.57	-	General / -60.9,170.0	49.7% (<i>ptt85</i>) chi angles: 71.7,168.4,179.5,81.2	0.078Å	-	-	
				Favored (8.06%)					
126	SER	57.6	-	-	38.5% (<i>m</i>) chi angles: 303.3	0.061Å	-	-	

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