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All-Atom Contacts	Clashscore, all atoms:	9.17	76 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	2	2.41%	Goal: <0.05%
	Ramachandran favored	72	86.75%	Goal: >98%
	MolProbity score^	2.46		50 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	2.60%	Goal: 0
	Bad backbone bonds:	0 / 664	0.00%	Goal: 0%
	Bad backbone angles:	5 / 885	0.56%	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: 9.17	Outliers: 2 of 83	Poor rotamers: 2 of 71	Outliers: 2 of 77	Outliers: 0 of 85	Outliers: 5 of 85
42	SER	58.57	-	-	-	60.2% (p) chi angles: 56.1	0.034Å	-	-
43	PRO	92.83	-	-	Favored (33.41%) Trans-proline / -74.4,145.0 OUTLIER (0.01%) General / 39.9,-153.5	30.4% (Cg_endo) chi angles: 21.3	0.029Å	-	-
44	SER	161.22	-	-	Favored (15.24%) General / -106.7,160.7	59.8% (p) chi angles: 72.7	0.319Å	-	-
45	LEU	92.84	-	-	Favored (43.03%) General / -113.6,144.3	6.8% (mp) chi angles: 288.1,79.1	0.039Å	-	-
46	GLN	92.23	-	-	-	98.7% (mt-30) chi angles: 293,180,335	0.062Å	-	-

47	CYS	48.11	-	Favored (27.06%) General / -71.2,125.5	40.6% (t) chi angles: 177.6	0.074Å	-	-
48	ARG	187.67	0.589Å O with 107 LYS HE3	Favored (60.92%) General / -74.3,-16.9	84.6% (mtp180) chi angles: 293,180,65,185	0.186Å	-	-
49	VAL	99.5	-	Favored (22.31%) Isoleucine or valine / -75.9,-50.7	96.9% (t) chi angles: 176.1	0.137Å	-	-
50	CYS	91.39	0.458Å HA with 92 VAL O	Favored (3.34%) General / -132.5,-4.3	21.1% (p) chi angles: 69.2	0.119Å	-	-
51	GLY	36.1	-	Favored (48.72%) Glycine / 93.5,-20.1	-	-	-	-
52	ASP	50.76	0.854Å HA with 94 LYS HD3	Allowed (0.1%) General / -45.8,157.8	10.3% (t0) chi angles: 208.9,342.4	0.112Å	-	OUTLIER(S) worst is CA- CB-CG: 4.661 σ
53	SER	48.05	-	Favored (27.11%) General / -64.9,126.2	72% (m) chi angles: 295.6	0.036Å	-	-
54	SER	47.77	-	Favored (45.39%) General / -73.8,144.7	21.6% (t) chi angles: 188.1	0.052Å	-	OUTLIER(S) worst is C-N- CA: 4.217 σ
55	SER	105.31	-	Allowed (1.1%) General / -95.2,45.6	21% (t) chi angles: 169.9	0.12Å	-	-
56	GLY	35.48	-	Favored (52.16%) Glycine / 69.2,-161.5	-	-	-	-
57	LYS	137.92	-	Favored (43.67%) General / -73.7,136.4	0.9% chi angles: 197.5,68.8,119.6,74.8	0.064Å	-	-
58	HIS	65.55	-	Favored (3.73%) General / -155.0,114.7	73.8% (m-70) chi angles: 289.8,305.6	0.06Å	-	-

59	TYR	70.8	-	Favored (2.75%) General / 67.5,39.9	10.9% (<i>m</i> -85) chi angles: 319.1,286.8	0.173Å	-	-	
60	GLY	31.53	-	Favored (4.09%) Glycine / 94.4,-35.7	-	-	-	-	
61	ILE	121.12	-	Allowed (0.18%) Isoleucine or valine / -115.1,-160.0	2.4% (<i>pt</i>) chi angles: 66.9,139.2	0.25Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 83.21	Clashscore: 9.17	Outliers: 2 of 83	Poor rotamers: 2 of 71	Outliers: 2 of 77	Outliers: 0 of 85	Outliers: 5 of 85
62	TYR	66.98	-	Favored (37.23%) General / -115.5,119.8	73.3% (<i>m</i> -85) chi angles: 301.3,289.3	0.057Å	-	-	
63	ALA	36.59	-	Favored (29.97%) General / -146.2,144.5	-	0.072Å	-	-	
64	CYS	43.82	-	Favored (7.41%) General / -66.1,169.1	31.5% (<i>p</i>) chi angles: 64.1	0.063Å	-	-	
65	ASN	51.38	-	Favored (72.55%) General / -56.5,-38.9	3.9% (<i>m</i> 120) chi angles: 299.3,54.7	0.128Å	-	-	
66	GLY	29.4	-	Favored (95.27%) Glycine / -64.1,-37.9	-	-	-	-	
67	CYS	48.5	-	Favored (20.52%) General / -90.5,-24.8	91.9% (<i>m</i>) chi angles: 289.9	0.142Å	-	-	
68	SER	86.96	-	Favored (64.08%) General / -74.0,-38.4	95.5% (<i>p</i>) chi angles: 66.7	0.114Å	-	-	
69	GLY	29	-	Favored (54.53%) Glycine / -74.9,-33.7	-	-	-	-	
				Favored					

Favored

70	PHE	63.4	-	(86.92%) General / -67.0,-39.2	83.6% (<i>t80</i>) chi angles: 181.1,82.5	0.092Å	-	-
71	PHE	71.7	-	Favored (40.4%) General / -65.4,-53.6	41.7% (<i>t80</i>) chi angles: 188.3,61.6	0.062Å	-	-
72	LYS	92.03	0.699Å HG2 with 118 VAL HG12	Favored (85.35%) General / -63.9,-36.9	63.7% (<i>tttp</i>) chi angles: 183,180,180,65	0.201Å	-	-
73	ARG	135.75	-	Favored (68.76%) General / -63.3,-26.4	8.1% (<i>ptm105</i>) chi angles: 78.7,192.8,290.8,110	0.219Å	-	-
74	SER	106.86	-	Favored (11.23%) General / -89.3,-43.0	38.3% (<i>m</i>) chi angles: 303.3	0.068Å	-	-
75	VAL	52.99	-	Favored (24.09%) Isoleucine or valine / -76.9,-49.1	66.6% (<i>t</i>) chi angles: 171.5	0.185Å	-	-
76	ARG	90.49	0.595Å HD2 with 119 GLN HG3	Favored (69.19%) General / -60.5,-29.7	53.6% (<i>tpt85</i>) chi angles: 183,65,180,85	0.164Å	-	-
77	ARG	124.69	-	Favored (36.06%) General / -101.0,-0.7	29.9% (<i>mmm180</i>) chi angles: 298,292,295,174.9	0.094Å	-	-
78	ARG	68.72	-	Favored (13.56%) General / 56.6,50.1	99.7% (<i>mtt180</i>) chi angles: 293,180,180,180.1	0.125Å	-	-
79	LEU	120.54	-	Favored (37.22%) General / -79.8,138.3	3.2% (<i>mm?</i>) chi angles: 288,295.6	0.142Å	-	-
80	ILE	97.42	-	Favored (38.02%) Isoleucine or valine / -116.5,112.1	4.9% (<i>mp</i>) chi angles: 298.3,93.9	0.032Å	-	-
81	TYR	82.89	-	Favored (45.31%) General / -98.9,130.4	14.1% (<i>m-85</i>) chi angles: 317.7,290.2	0.063Å	-	-

[Clash >](#)[C \$\beta\$](#) [Bond](#)[Bond](#)

#	Alt Res	High B	0.4Å	Ramachandran	Rotamer	deviation lengths	angles
		Avg: 83.21	Clashscore: 9.17	Outliers: 2 of 83	Poor rotamers: 2 of 71	Outliers: 2 of 77	Outliers: 0 of 85
				Outliers: 5 of 85			
82	ARG	112.35	-	Favored (35.32%) General / -97.2,138.0	79.5% (<i>ttt180</i>) chi angles: 183,180,180,180	0.056Å	-
83	CYS	44.78	-	Favored (35.54%) General / -80.6,131.8	4% (<i>t</i>) chi angles: 204.8	0.047Å	-
84	GLN	47.29	-	Favored (64.84%) General / -69.9,-46.7	37.4% (<i>mt-30</i>) chi angles: 298.9,167.8,253.5	0.073Å	-
85	VAL	62.05	-	Allowed (1.82%) Isoleucine or valine / -72.7,168.6	21.5% (<i>t</i>) chi angles: 188.1	0.093Å	-
86	GLY	70.6	-	Favored (6.35%) Glycine / -69.2,4.4	-	-	-
87	ALA	237.84	-	Allowed (0.13%) General / 80.3,-33.9	-	0.244Å	-
88	GLY	85.11	-	Favored (60.56%) Glycine / -72.3,-34.8	-	-	-
89	MET	141.5	0.409Å O with 91 PRO HD2	Favored (92.13%) General / -64.4,-38.8	68.7% (<i>mtt</i>) chi angles: 293,180,180	0.037Å	-
90	CYS	64.94	-	Favored (2.24%) Pre-proline / -72.9,106.5	98.8% (<i>m</i>) chi angles: 294.4	0.049Å	-
91	PRO	93.41	0.419Å HB3 with 93 ASP OD1	Favored (10.69%) Trans-proline / -78.6,131.9	15.3% (<i>Cg_endo</i>) chi angles: 39.3	0.065Å	-
92	VAL	121.31	0.458Å O with 50 CYS HA	Allowed (0.21%) Isoleucine or valine / -110.5,67.4	16.8% (<i>m</i>) chi angles: 291	0.232Å	-

93	ASP	65.88	0.419Å OD1 with 91 PRO HB3	Favored (5.1%) General / -89.4,-176.6	0% chi angles: 337.8,359.4	0.108Å	-	OUTLIER(S) worst is CA- CB-CG: 7.967 σ
94	LYS	116.85	0.854Å HD3 with 52 ASP HA	Favored (16.12%) General / -90.9,-32.1	88.1% (<i>tttt</i>) chi angles: 183,180,180,180	0.043Å	-	-
95	ALA	59.74	-	Favored (63.03%) General / -71.5,-27.1	-	0.07Å	-	-
96	HIS	75.92	-	Favored (34.27%) General / -95.2,137.4	65.6% (<i>m-70</i>) chi angles: 309.2,301	0.053Å	-	OUTLIER(S) worst is CB- CG-CD2: 4.255 σ
97	ARG	128.79	-	Allowed (0.1%) General / -44.1,154.7	99.7% (<i>mtt180</i>) chi angles: 293,180,180,180	0.052Å	-	-
98	ASN	58.56	-	OUTLIER (0.02%) General / -15.4,109.2	83.3% (<i>m-20</i>) chi angles: 288.6,318.3	0.079Å	-	-
99	GLN	74.68	-	Favored (13.16%) General / -98.1,162.5	9.6% (<i>mt-30</i>) chi angles: 302.4,160.5,141.3	0.062Å	-	-
100	CYS	72.61	-	Favored (8.32%) General / -45.6,132.5	44% (<i>t</i>) chi angles: 178.6	0.033Å	-	-
101	GLN	78.03	-	Favored (80.24%) General / -63.8,-35.3	28.7% (<i>mp0</i>) chi angles: 295,85,0	0.085Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 83.21	Clashscore: 9.17	Outliers: 2 of 83	Poor rotamers: 2 of 71	Outliers: 2 of 77	Outliers: 0 of 85	Outliers: 5 of 85
102	ALA	43.32	-		Favored (59.08%) General / -75.8,-37.6	-	0.075Å	-	-
103	CYS	94.69	-		Favored (21.15%) General / -87.9,-29.0	28.5% (<i>p</i>) chi angles: 61.4	0.118Å	-	-
					Favored				

104	ARG	82.35	-	Favored (85.59%) General / -60.1,-47.5	72.7% (<i>ttt180</i>) chi angles: 192.7,173,179.2,177.8	0.074Å	-	-
105	LEU	111.48	-	Favored (77.51%) General / -69.5,-38.5	2.2% (<i>tm?</i>) chi angles: 193,271.9	0.088Å	-	-
106	LYS	81.83	-	Favored (44.89%) General / -78.8,-24.1	36.7% (<i>mttp</i>) chi angles: 297,161.2,192.2,52.3	0.164Å	-	-
107	LYS	74.14	0.589Å HE3 with 48 ARG O	Favored (64.03%) General / -71.5,-28.6	88.1% (<i>tttt</i>) chi angles: 183,180,180,180	0.209Å	-	-
108	CYS	42.96	-	Favored (27.06%) General / -52.5,-54.8	80.4% (<i>m</i>) chi angles: 299.6	0.144Å	-	-
109	LEU	56.27	-	Favored (83.12%) General / -64.4,-46.5	50.3% (<i>mt</i>) chi angles: 305,171.2	0.094Å	-	-
110	GLN	53.5	-	Favored (63.65%) General / -55.7,-32.8	66% (<i>tt0</i>) chi angles: 183,180,0	0.038Å	-	-
111	ALA	41.98	-	Favored (58.56%) General / -86.6,-7.2	-	0.026Å	-	-
112	GLY	51.55	-	Favored (32.84%) Glycine / 98.7,15.9	-	-	-	-
113	MET	79.04	-	Favored (8.48%) General / -83.1,96.7	85.6% (<i>mtp</i>) chi angles: 301.5,182.8,76.8	0.102Å	-	-
114	ASN	71.26	-	Favored (32.31%) General / -78.8,150.2	26.8% (<i>t-20</i>) chi angles: 201,359.9	0.05Å	-	-
115	GLN	105.5	-	Favored (52.52%) General / -77.2,-26.0	14.7% (<i>pt20</i>) chi angles: 62,180,20	0.155Å	-	-
116	ASP	98.54	-	Favored (71.14%) General /	9% (<i>p30</i>) chi angles: 44.7,10.7	0.083Å	-	OUTLIER(S) worst is CA- CB-CG: 4.919

-56.7,-50.8

 σ

117	ALA	45.79	-	Allowed (1.23%) General / -66.5,2.6	-	0.059Å	-	-
118	VAL	55.86	0.699Å HG12 with 72 LYS HG2	Favored (7.08%) Isoleucine or valine / -85.9,-23.2	58.6% (<i>t</i>) chi angles: 180.8	0.11Å	-	-
119	GLN	125.44	0.595Å HG3 with 76 ARG HD2	Favored (11.03%) General / -130.9,110.1	33.3% (<i>mt-30</i>) chi angles: 291.3,170.6,226.9	0.099Å	-	-
120	ASN	109.31	-	Favored (8.99%) General / -86.3,93.1	33.6% (<i>m120</i>) chi angles: 295,120	0.036Å	-	-
121	GLU	304.59	0.422Å OE2 with 119 GLN HB2	Allowed (0.46%) General / -169.4,-164.6	15% (<i>pt-20</i>) chi angles: 56.7,179.8,316	0.064Å	-	-

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Avg: 83.21				Clashscore: 9.17	Outliers: 2 of 83	Poor rotamers: 2 of 71	Outliers: 2 of 77	Outliers: 0 of 85	Outliers: 5 of 85
122	ARG	69.53	-	-	Favored (24.96%) General / -84.4,119.3	81% (<i>mtm-85</i>) chi angles: 296.8,188.7,307,288.1	0.107Å	-	-
123	GLN	74.92	-	-	Favored (43.3%) Pre-proline / -95.1,109.2	22.8% (<i>mp0</i>) chi angles: 306.8,86.4,354.2	0.031Å	-	-
124	PRO	66.89	-	-	Favored (17%) Trans-proline / -81.7,151.6	87.8% (<i>Cg_endo</i>) chi angles: 31.2	0.037Å	-	-
125	ARG	87.57	-	-	Favored (18.4%) General / -95.5,152.5	54.1% (<i>ptt85</i>) chi angles: 62,180,180,85	0.068Å	-	-
126	SER	57.6	-	-	-	74.4% (<i>m</i>) chi angles: 295	0.065Å	-	-

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