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All-Atom Contacts	Clashscore, all atoms:	6.09	90 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	10.00%	Goal: <1%
	Ramachandran outliers	2	5.71%	Goal: <0.05%
	Ramachandran favored	26	74.29%	Goal: >98%
	MolProbity score^	2.89		27 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 277	0.00%	Goal: 0%
	Bad backbone angles:	5 / 375	1.33%	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: 52.70	Clashscore: 6.09	Outliers: 2 of 35	Poor rotamers: 3 of 30	Outliers: 0 of 32	Outliers: 0 of 37	Outliers: 4 of 37
A 148	ASP	50	-	-	1% chi angles: 310,17.1	0.093Å	-	-
A 149	HIS	50	-	OUTLIER (0.03%) General / -174.6,83.0	40% (t-80) chi angles: 175.8,275	0.025Å	-	-
A 150	ASP	50	-	Allowed (1.1%) General / -122.5,-65.5	11% (m-20) chi angles: 315.1,319.1	0.105Å	-	-
A 151	GLU	50	-	Favored (41.79%) General / -80.0,-23.1	0.5% chi angles: 260.7,282.2,240.1	0.125Å	-	-
A			0.404Å	Favored	51.8% (t)			

152	CYS	50	HB3 with A 165 ASP OD1	(18.03%) General / -78.6,2.8 Favored (9.33%)	chi angles: 179.9	0.156Å	-	-
A 153	ALA	50	-	General / -102.4,-34.0 Favored (56.51%)	-	0.07Å	-	-
A 154	SER	50	-	General / -82.6,-13.4 Allowed (1.36%)	6.6% (<i>t</i>) chi angles: 197.3	0.126Å	-	-
A 155	SER	50	-	Pre-proline / 38.5,70.2 Favored (8.49%)	54.4% (<i>p</i>) chi angles: 73.8	0.185Å	-	-
A 156	PRO	50	-	Trans-proline / -79.7,67.8 Allowed (1.87%)	92% (<i>Cg_endo</i>) chi angles: 32.1	0.03Å	-	-
A 157	CYS	50	-	General / -107.2,83.7 Favored (58.39%)	85.2% (<i>m</i>) chi angles: 295.5	0.034Å	-	-
A 158	GLN	50	-	General / -63.1,137.9 Favored (14.64%)	8.1% (<i>mt-30</i>) chi angles: 291.8,143.4,226.6	0.061Å	-	-
A 159	ASN	50	-	General / 59.8,25.6 Favored (57.89%)	43.1% (<i>m-80</i>) chi angles: 306.1,283.3	0.036Å	-	-
A 160	GLY	50	-	Glycine / 81.9,23.3 Favored (3.77%)	-	-	-	-
A 161	ALA	50	0.462Å HB2 with A 183 CYS SG	General / -52.9,152.8 Favored (49.55%)	-	0.063Å	-	-
A 162	VAL	50	-	Isoleucine or valine / -100.6,120.0 Favored (17.65%)	98.8% (<i>t</i>) chi angles: 176.6	0.051Å	-	-
A 163	CYS	50	-	General / -88.8,159.6 Allowed (1.73%)	4% (<i>p</i>) chi angles: 45.4	0.04Å	-	-
A 164	GLN	50	-	General / -163.5,119.6 Favored (53.12%)	19.1% (<i>tp60</i>) chi angles: 172.4,62.6,90.7	0.078Å	-	-
A 165	ASP	50	0.404Å OD1 with A	General /	4.1% (<i>m-20</i>) chi angles:	0.025Å	-	-

				152 CYS HB3	-61.8,145.3	314.5,91.7			
A 166	GLY	50	-	Favored (22.33%) Glycine / -151.2,-174.7	-	-	-	-	-
A 167	ILE	50	-	Favored (78.24%) Isoleucine or valine / -64.6,-36.7	43.6% (<i>pt</i>) chi angles: 62.5,175.3	0.224Å	-	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
				Avg: 52.70	Clashscore: 6.09	Outliers: 2 of 35	Poor rotamers: 3 of 30	Outliers: 0 of 32	Outliers: 0 of 37
A 168	ASP	50	-	Allowed (0.89%) General / -100.3,51.2	20.2% (<i>p-10</i>) chi angles: 56,325.8	0.136Å	-	OUTLIER(S) worst is CA-CB- CG: 4.267 σ	-
A 169	GLY	50	-	Allowed (1.81%) Glycine / 86.1,-80.0	-	-	-	-	-
A 170	TYR	50	-	Favored (2.2%) General / -176.5,161.5	20.1% (<i>p90</i>) chi angles: 74.7,283	0.099Å	-	-	-
A 171	SER	50	-	Favored (7.22%) General / -135.2,178.2	15% (<i>t</i>) chi angles: 190	0.049Å	-	-	-
A 172	CYS	50	0.409Å HB3 with A 161 ALA HB1	Favored (6.21%) General / -116.5,174.2	81.4% (<i>m</i>) chi angles: 300.8	0.022Å	-	-	-
A 173	PHE	50	-	Favored (46.57%) General / -106.1,122.6	90.9% (<i>m-85</i>) chi angles: 302.2,98	0.04Å	-	-	-
A 174	CYS	50	-	Favored (58.4%) General / -61.9,138.9	20.4% (<i>m</i>) chi angles: 312	0.063Å	-	-	-
A 175	VAL	50	-	Favored (72.35%) Pre-proline / -78.2,160.9	27% (<i>m</i>) chi angles: 296.2	0.107Å	-	-	-
A 176	PRO	50	-	Favored (16.61%) Trans-proline / -57.3,-14.7	18.4% (<i>Cg_exo</i>) chi angles: 324	0.073Å	-	-	-
A 177	GLY	50	-	Favored (52.5%) Glycine / -97.4,-11.2	-	-	-	-	-

A 178	TYR	99.99	-	Favored (2.57%) General / -136.3,-170.0	73.4% (<i>m-85</i>) chi angles: 298.4,260.5	0.04Å	-	-
A 179	GLN	50	-	Allowed (0.08%) General / -146.3,-133.9	3.3% (<i>tp-100</i>) chi angles: 207.5,59.9,196.3	0.209Å	-	OUTLIER(S) worst is CB-CG- CD: 4.989 σ
A 180	GLY	50	-	Favored (51.86%) Glycine / 65.8,-150.7	-	-	-	-
A 181	ARG	50	-	Favored (13.93%) General / -102.4,-23.7	10.1% (<i>tpt180</i>) chi angles: 195.1,74.4,172.3,209	0.04Å	-	-
A 182	HIS	50	-	Favored (5.55%) General / -128.6,3.8	20.5% (<i>m80</i>) chi angles: 313.9,86.7	0.1Å	-	-
A 183	CYS	50	0.462Å SG with A 161 ALA HB2	OUTLIER (0.02%) General / 81.5,66.8	60.9% (<i>m</i>) chi angles: 304	0.196Å	-	OUTLIER(S) worst is N-CA- CB: 4.147 σ
A 184	ASP	99.99	-	-	0% chi angles: 345.4,70	0.05Å	-	OUTLIER(S) worst is CA-CB- CG: 6.172 σ

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