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All-Atom Contacts	Clashscore, all atoms:	6.55		89 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	1.79%	Goal: <1%
	Ramachandran outliers	2	3.33%	Goal: <0.05%
	Ramachandran favored	52	86.67%	Goal: >98%
	MolProbity score [^]	2.18		66 th percentile * (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 538	0.00%	Goal: 0%
	Bad backbone angles:	1 / 722	0.14%	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: 50.81	Clashscore: 6.55	Outliers: 2 of 60	Poor rotamers: 1 of 56	Outliers: 0 of 62	Outliers: 0 of 62	Outliers: 1 of 62
A 34	SER	50	-	-	59.8% (<i>m</i>) chi angles: 299.2	0.06Å	-	-
A 35	ALA	50	-	Favored (36.42%) Pre-proline / -110.2,147.5	-	0.114Å	-	-
A 36	PRO	50	-	OUTLIER (0%) Trans-proline / 15.2,-77.9	24.5% (<i>Cg_exo</i>) chi angles: 342.6	0.202Å	-	OUTLIER(S) worst is CA-N- CD: 4.897 σ
A 37	ARG	50	-	Favored (24.03%) General / 56.7,34.1	55.9% (<i>mmm-85</i>) chi angles: 295.5,298.1,293.1,278.1	0.032Å	-	-
A 38	LYS	50	-	Favored (13.76%) General /	30.8% (<i>mtp</i>) chi angles: 293.4,183.6,65.7,64.2	0.111Å	-	-

				-101.9,161.3				
A 39	GLN	50	-	OUTLIER (0%) General / 125.6,147.1	52.8% (<i>tt0</i>) chi angles: 183,178.9,60.8	0.067Å	-	-
A 40	ARG	50	-	Favored (50.89%) General / -109.2,124.4	8.3% (<i>tpt180</i>) chi angles: 178.9,62.9,203.2,293.6	0.056Å	-	-
A 41	ARG	50	-	Favored (23.05%) General / -72.5,166.2	0.1% chi angles: 285.8,80.9,74.6,165.1	0.063Å	-	-
A 42	GLU	50	-	Allowed (1.17%) General / -94.6,-63.5	33.9% (<i>tt0</i>) chi angles: 186.1,185.4,275.5	0.035Å	-	-
A 43	ARG	50	-	Favored (32.56%) General / -153.0,153.3	11.1% (<i>tpt85</i>) chi angles: 210.6,76.5,178.2,82.3	0.117Å	-	-
A 44	THR	50	-	Favored (5.27%) General / -107.4,-40.8	10.1% (<i>t</i>) chi angles: 184	0.054Å	-	-
A 45	THR	50	-	Favored (29.27%) General / -103.6,146.0	18.4% (<i>m</i>) chi angles: 310.9	0.068Å	-	-
A 46	PHE	50	-	Favored (56.72%) General / -67.2,143.0	96.8% (<i>m-85</i>) chi angles: 294.3,270.7	0.021Å	-	-
A 47	THR	50	-	Favored (16.73%) General / -96.2,155.5	8% (<i>t</i>) chi angles: 179.4	0.092Å	-	-
A 48	ARG	50	-	Favored (5.37%) General / -43.8,-42.2	30.2% (<i>tpt180</i>) chi angles: 173.4,54.5,180.2,170.6	0.031Å	-	-
A 49	SER	50	-	Favored (97.25%) General / -63.7,-43.2	33.3% (<i>t</i>) chi angles: 183.6	0.019Å	-	-
A 50	GLN	50	0.459Å CD with A 78 LEU HD11	Favored (76.17%) General / -68.1,-44.5	79.7% (<i>mt-30</i>) chi angles: 287.6,168.7,7.4	0.023Å	-	-

A 51	LEU	50	-	Favored (42.36%) General / -63.8,-54.0	68.8% (<i>mt</i>) chi angles: 286.5,169.6	0.043Å	-	-	
A 52	GLU	50	-	Favored (6.85%) General / -45.1,-40.4	10.1% (<i>tm-20</i>) chi angles: 178.9,289.7,326.1	0.055Å	-	-	
A 53	GLU	50	0.544Å OE2 with A 72 VAL HA	Favored (5.39%) General / -79.2,-55.0	59.7% (<i>tt0</i>) chi angles: 181.8,175.3,328.8	0.023Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.81	Clashscore: 6.55	Outliers: 2 of 60	Poor rotamers: 1 of 56	Outliers: 0 of 62	Outliers: 0 of 62	Outliers: 1 of 62
A 54	LEU	50	-	Favored (31.87%) General / -47.9,-46.5	81.7% (<i>mt</i>) chi angles: 288.6,171.2	0.051Å	-	-	
A 55	GLU	50	-	Favored (83.97%) General / -67.8,-40.5	33.1% (<i>mt-10</i>) chi angles: 302.5,192.7,275.3	0.045Å	-	-	
A 56	ALA	50	-	Favored (67.68%) General / -55.6,-37.0	-	0.02Å	-	-	
A 57	LEU	50	-	Favored (45.92%) General / -78.9,-32.2	43.7% (<i>tp</i>) chi angles: 185.2,60	0.066Å	-	-	
A 58	PHE	50	-	Favored (61.83%) General / -73.3,-27.9	63.9% (<i>t80</i>) chi angles: 183.4,65.9	0.039Å	-	-	
A 59	ALA	50	-	Favored (57.57%) General / -76.9,-32.6	-	0.026Å	-	-	
A 60	LYS	50	-	Favored (13.1%) General / -87.1,-42.4	21.9% (<i>ptmt</i>) chi angles: 58.8,180.9,290.2,181.6	0.065Å	-	-	
A 61	THR	50	-	Favored (4.48%) General /	12.2% (<i>t</i>) chi angles: 185.4	0.087Å	-	-	

A 62	GLN	50	-	-149.4,111.0 Favored (71.75%) General / -63.7,-30.7	84.4% (<i>mt-30</i>) chi angles: 296.7,180.9,297.5	0.023Å	-	-
A 63	TYR	50	-	Favored (12.87%) Pre-proline / -117.8,78.8	56.7% (<i>m-85</i>) chi angles: 286.3,79.1	0.059Å	-	-
A 64	PRO	50	-	Favored (15.98%) Trans-proline / -67.0,168.9	98.6% (<i>Cg_endo</i>) chi angles: 30.5	0.033Å	-	-
A 65	ASP	50	-	Favored (5.77%) General / -99.5,175.7	40.9% (<i>t0</i>) chi angles: 190.3,25.4	0.076Å	-	-
A 66	VAL	50	0.401Å O with A 70 GLU HG3	Favored (39.33%) Isoleucine or valine / -53.7,-39.6	34.6% (<i>m</i>) chi angles: 298.6	0.062Å	-	-
A 67	TYR	50	-	Favored (80.72%) General / -64.8,-46.7	97.5% (<i>m-85</i>) chi angles: 294.4,274.2	0.011Å	-	-
A 68	ALA	50	-	Favored (73.41%) General / -63.7,-49.4	-	0.022Å	-	-
A 69	ARG	50	-	Favored (91%) General / -59.4,-42.1	92% (<i>mtm-85</i>) chi angles: 285.1,193.3,288.3,278.9	0.053Å	-	-
A 70	GLU	50	0.401Å HG3 with A 66 VAL O	Favored (90.39%) General / -64.3,-44.8	47.7% (<i>mt-10</i>) chi angles: 289.4,187.6,44.9	0.058Å	-	-
A 71	GLU	50	-	Favored (3.49%) General / -55.7,-60.4	41.2% (<i>tt0</i>) chi angles: 182.5,173.3,311.3	0.023Å	-	-
A 72	VAL	50	0.571Å O with A 76 ILE HG12	Favored (2.07%) Isoleucine or valine / -52.6,-58.8	53.5% (<i>t</i>) chi angles: 170.3	0.061Å	-	-
A 73	ALA	50	-	Favored (6.52%) General / -50.8,-27.0	-	0.046Å	-	-

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A 74	LEU	50	-	Favored (19.48%) General / -87.2,-33.1	74.3% (<i>mt</i>) chi angles: 290.9,166.4	0.028Å	-	-
A 75	LYS	50	0.405Å HE3 with A 53 GLU OE1	Allowed (0.83%) General / -75.5,-66.0	57.9% (<i>tttp</i>) chi angles: 176.9,172.4,162,62.4	0.056Å	-	-
A 76	ILE	50	0.812Å HD12 with A 78 LEU HD12	Favored (2.73%) Isoleucine or valine / -59.9,-11.1	29.1% (<i>pt</i>) chi angles: 60.8,180	0.056Å	-	-
A 77	ASN	50	-	Allowed (1.77%) General / 66.0,48.4	64.4% (<i>m-80</i>) chi angles: 301.3,288.2	0.036Å	-	-
A 78	LEU	50	0.812Å HD12 with A 76 ILE HD12	Favored (66.92%) Pre-proline / -125.8,149.8	62.5% (<i>mt</i>) chi angles: 293.3,183.5	0.083Å	-	-
A 79	PRO	50	-	Favored (55.99%) Trans-proline / -65.2,138.4	59.2% (<i>Cg_endo</i>) chi angles: 26.8	0.029Å	-	-
A 80	GLU	50	-	Favored (2.1%) General / -47.5,-28.1	13.5% (<i>tm-20</i>) chi angles: 185.3,287.8,331.1	0.076Å	-	-
A 81	SER	50	-	Favored (13.32%) General / -59.9,-57.3	40.9% (<i>t</i>) chi angles: 181.3	0.006Å	-	-
A 82	ARG	50	-	Favored (52.22%) General / -50.8,-39.1	10.2% (<i>mmm180</i>) chi angles: 287.7,275.2,287.9,199.5	0.063Å	-	-
A 83	VAL	50	-	Favored (16.33%) Isoleucine or valine / -61.9,-56.6	57.6% (<i>t</i>) chi angles: 180.6	0.041Å	-	-
A 84	GLN	50	-	Favored (70.75%) General / -55.4,-40.0 Allowed	5.1% (<i>tp60</i>) chi angles: 178.5,61.9,317.3	0.04Å	-	-

A 85	VAL	50	-	(0.68%) Isoleucine or valine / -65.0,-64.6	83.7% (t) chi angles: 179	0.053Å	-	-
A 86	TRP	50	-	Favored (4.97%) General / -44.1,-40.6	85.4% (t90) chi angles: 182.7,93	0.027Å	-	-
A 87	PHE	50	-	Favored (98.32%) General / -61.1,-43.8	10.8% (m-85) chi angles: 273.7,66.2	0.017Å	-	-
A 88	LYS	50	-	Favored (11.13%) General / -68.2,-55.8	34.6% (ttpt) chi angles: 171.2,163.6,58.8,174.2	0.076Å	-	-
A 89	ASN	50	-	Favored (72.96%) General / -58.5,-35.9	1.6% (m-80) chi angles: 277.8,227.1	0.038Å	-	-
A 90	ARG	50	-	Allowed (1.63%) General / -70.9,-61.8	26.8% (tpt180) chi angles: 185.6,62.5,180.5,186.4	0.024Å	-	-
A 91	ARG	50	-	Favored (72.15%) General / -58.5,-35.3	12.8% (ttp180) chi angles: 201.7,206.6,72.8,162.7	0.053Å	-	-
A 92	ALA	50	-	Favored (8.24%) General / -52.6,-24.3	-	0.034Å	-	-
A 93	LYS	50	-	Favored (75.31%) General / -58.4,-37.5	84.7% (tttt) chi angles: 177.3,185.6,177.3,172.7	0.051Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 50.81	Clashscore: 6.55	Outliers: 2 of 60	Poor rotamers: 1 of 56	Outliers: 0 of 62	Outliers: 0 of 62	Outliers: 1 of 62
A 94	CYS	50	-	Allowed (0.2%) General / -42.2,-28.6	22.7% (p) chi angles: 68.3	0.027Å	-	-
A 95	ARG	99.99	-	-	36.3% (ttm180) chi angles: 187.9,166,295.1,182.1	0.088Å	-	-

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