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All-Atom Contacts	Clashscore, all atoms:	40.43	8 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	0	0.00%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	31	96.88%	Goal: >98%
	MolProbity score^	2.27		60 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 267	0.00%	Goal: 0%
	Bad backbone angles:	8 / 358	2.23%	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	C β deviation	Bond lengths	Bond angles
			Avg: Clashscore: 71.90 40.43	Outliers: 0 of 32	Poor rotamers: 0 of 30	Outliers: 0 of 30	Outliers: 0 of 34	Outliers: 7 of 34
1143	CYS	30.63	-	-	86.7% (<i>m</i>) chi angles: 292.8	0.052Å	-	-
1144	ASN	76.37	-	Favored (41.63%) General / -73.4,150.7	23.8% (<i>t30</i>) chi angles: 184.6,75.8	0.095Å	-	OUTLIER(S) worst is CA-CB-CG: 5.542 σ
1145	SER	101.47	-	Favored (8.5%) General / 68.0,11.7	75.3% (<i>m</i>) chi angles: 294.4	0.06Å	-	-
1146	ASN	77.38	-	Allowed (0.74%) Pre-proline / 42.8,74.7 Favored	3.2% (<i>m-20</i>) chi angles: 294.6,30	0.075Å	-	OUTLIER(S) worst is CA-CB-CG: 4.866 σ

1147	PRO	84.18	-	(67.11%) Trans-proline / -64.0,-23.9	30.3% (<i>Cg_endo</i>) chi angles: 21.3	0.116Å	-	-
1148	CYS	79.05	-	Favored (23.01%) General / -80.0,119.6	24.1% (<i>m</i>) chi angles: 280.5	0.158Å	-	-
1149	LEU	115.67	0.816Å CD1 with 1173 HIS HB3	Favored (9.6%) General / -97.4,169.7	2% (<i>mp</i>) chi angles: 309.5,76.6	0.073Å	-	-
1150	HIS	74.48	-	Favored (22.06%) General / 55.8,46.6	43.1% (<i>m80</i>) chi angles: 308.8,94.5	0.089Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.463 σ
1151	GLY	23.8	-	Favored (87.31%) Glycine / 82.5,7.6	-	-	-	-
1152	GLY	20.3	-	Favored (54.5%) Glycine / -72.4,162.1	-	-	-	-
1153	ASN	33.21	-	Favored (54.26%) General / -112.8,134.6	32.8% (<i>t-20</i>) chi angles: 191.3,309.5	0.101Å	-	OUTLIER(S) worst is CA- CB-CG: 4.59 σ
1154	CYS	42.88	-	Favored (29.69%) General / -100.2,144.0	47.1% (<i>t</i>) chi angles: 182.7	0.069Å	-	-
1155	GLU	53.11	0.433Å O with 1157 ILE HD12	Favored (53.93%) General / -123.2,132.1	16.5% (<i>tt0</i>) chi angles: 196.6,159.2,58.7	0.086Å	-	-
1156	ASP	48.54	0.557Å C with 1157 ILE HD12	Favored (36.7%) General / -78.4,143.5	33.1% (<i>t0</i>) chi angles: 189.7,31.4	0.09Å	-	-
1157	ILE	101.26	0.826Å HD13 with 1161 TYR HA	Favored (2.75%) Isoleucine or valine / -134.1,-178.7	3.2% (<i>mp</i>) chi angles: 303.2,73.8	0.039Å	-	-
1158	TYR	176.1	0.784Å H with 1157 ILE HG22	Favored (21.4%) General / -88.5,111.1	86.5% (<i>t80</i>) chi angles: 174.2,77.8	0.068Å	-	-

1159	SER	150.74	-		Favored (14.45%) General / 60.4,24.9	38.3% (<i>t</i>) chi angles: 181.9	0.059Å	-	-
1160	SER	104.47	-		Favored (32.48%) General / -155.4,166.8	65.9% (<i>m</i>) chi angles: 298.5	0.134Å	-	-
1161	TYR	148.55	0.826Å HA with 1157 ILE HD13		Favored (46.05%) General / -140.8,156.8	40.7% (<i>p90</i>) chi angles: 70.9,271.1	0.081Å	-	-
1162	HIS	57.62	0.417Å CD2 with 1157 ILE HG12		Favored (44.87%) General / -121.8,148.3	82.1% (<i>m-70</i>) chi angles: 285.6,285.4	0.159Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.42 σ
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 71.90	Clashscore: 40.43	Outliers: 0 of 32	Poor rotamers: 0 of 30	Outliers: 0 of 30	Outliers: 0 of 34	Outliers: 7 of 34
1163	CYS	100.49	0.486Å SG with 1174 CYS SG		Favored (52.91%) General / -122.1,130.1	5.1% (<i>t</i>) chi angles: 202.1	0.158Å	-	-
1164	SER	90.14	-		Favored (44.62%) General / -100.5,133.6	98.1% (<i>p</i>) chi angles: 64.1	0.109Å	-	-
1165	CYS	46.25	-		Favored (50.8%) Pre-proline / -117.6,154.6	63% (<i>m</i>) chi angles: 303.1	0.121Å	-	-
1166	PRO	61.4	-		Favored (34.92%) Trans-proline / -71.1,164.7	73.2% (<i>Cg_exo</i>) chi angles: 332.8	0.066Å	-	-
1167	LEU	41.07	-		Favored (56.89%) General / -59.0,134.4	48.4% (<i>tp</i>) chi angles: 175.3,68.3	0.123Å	-	-
1168	GLY	21.04	-		Favored (69.9%) Glycine / 95.0,-7.8	-	-	-	-
1169	TRP	49.32	-		Favored (37.5%) General / -116.4,150.6	96.3% (<i>m95</i>) chi angles: 294.5,94.6	0.063Å	-	-

1170	SER	75.67	-	Favored (4.34%) General / -149.7,-173.2	73.5% (<i>m</i>) chi angles: 295.3	0.104Å	-	-
1171	GLY	21.21	-	Favored (34.64%) Glycine / 95.5,165.1	-	-	-	-
1172	LYS	56.89	-	Favored (97.27%) General / -63.9,-43.0	74.3% (<i>tttt</i>) chi angles: 188.1,162.4,181.9,167.2	0.072Å	-	OUTLIER(S) worst is C-N- CA: 4.269 σ
1173	HIS	94.62	0.816Å HB3 with 1149 LEU CD1	Favored (59.58%) General / -83.4,-6.8	80.8% (<i>m80</i>) chi angles: 292.3,83.1	0.091Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.423 σ
1174	CYS	72.07	0.486Å SG with 1163 CYS SG	Favored (5.58%) General / 69.6,24.5	52.5% (<i>m</i>) chi angles: 306.7	0.152Å	-	-
1175	GLU	83.27	0.694Å HG2 with 1176 LEU N	Favored (71.58%) General / -71.1,-40.6	17.6% (<i>pm0</i>) chi angles: 75.4,272.2,33.9	0.123Å	-	-
1176	LEU	31.34	0.694Å N with 1175 GLU HG2	-	43% (<i>mt</i>) chi angles: 292.2,186.2	0.109Å	-	-

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