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All-Atom Contacts	Clashscore, all atoms:	79.75		0th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	4.84%	Goal: <1%
	Ramachandran outliers	3	4.23%	Goal: <0.05%
	Ramachandran favored	63	88.73%	Goal: >98%
	MolProbity score^	3.47		9th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	3.08%	Goal: 0
	Bad backbone bonds:	1 / 575	0.17%	Goal: 0%
	Bad backbone angles:	18 / 785	2.29%	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: 106.65	Clashscore: 79.75	Outliers: 3 of 71	Poor rotamers: 3 of 62	Outliers: 2 of 65	Outliers: 1 of 73	Outliers: 16 of 73
915		ASP	31.38	-	-	56.3% (*m-20*) chi angles: 289.4,307.1	0.08Å	-	OUTLIER(S) worst is CA-CB-CG: 4.286 σ
916		SER	112.98	-	Favored (73.85%) General / -64.7,-48.7	68.5% (*m*) chi angles: 297	0.112Å	-	-
917		PHE	135.68	-	Favored (46.82%) General / -125.7,151.3	84% (*t80*) chi angles: 177.9,71.5	0.066Å	-	OUTLIER(S) worst is CA-CB-CG: 4.634 σ
918		PHE	39.44	-	Favored (47.9%) General / -120.3,144.2	26.1% (*p90*) chi angles: 51.9,80.3	0.052Å	-	OUTLIER(S) worst is CA-CB-CG: 6.292 σ

919	GLU	39.7	-	Favored (50.59%) General / -131.9,153.1	71.1% (*mt-10*) chi angles: 296.6,170.8,23	0.155Å	-	-
920	ARG	113.71	-	Favored (55.16%) General / -112.2,132.0	19% (*mtp180*) chi angles: 293.2,184.6,74.5,132.2	0.082Å	-	-
921	GLU	72.76	-	Favored (48.09%) General / -72.1,138.8	25.4% (*pt-20*) chi angles: 59.1,185.1,9.4	0.062Å	-	-
922	HIS	67.39	-	Favored (74.63%) Pre-proline / -77.9,147.8	69% (*m80*) chi angles: 285.8,81.4	0.101Å	-	OUTLIER(S) worst is CD2-NE2-CE1: 4.487 σ
923	PRO	67.13	-	Favored (25.82%) Trans-proline / -79.4,158.3	11.8% (*Cg_endo*) chi angles: 14.9	0.091Å	-	-
924	GLY	17.11	-	Favored (53.81%) Glycine / -75.0,162.5	-	-	-	-
925	TRP	111.94	-	Favored (37.68%) General / -77.3,145.1	19.4% (*m-90*) chi angles: 293.1,280.8	0.161Å	-	-
926	VAL	96.14	0.599Å HG11 with 929 VAL HG21	Favored (24.23%) Pre-proline / -121.0,133.9	8.6% (*p*) chi angles: 59.9	0.086Å	-	-
927	PRO	124.36	-	Favored (26.33%) Trans-proline / -76.4,145.0	72.5% (*Cg_exo*) chi angles: 333.8	0.133Å	-	-
928	GLY	25.79	-	Favored (89.15%) Glycine / 83.8,3.8	-	-	-	-
929	VAL	61.17	0.741Å HG21 with 934 LEU HD11	Favored (2.52%) Isoleucine or valine / -103.7,93.2	73.2% (*t*) chi angles: 173.9	0.07Å	-	-
930	CYS	43.93	-	Favored (57.28%) General / -73.8,-44.0	88.1% (*m*) chi angles: 293	0.085Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
931		VAL	64.18	0.585Å HG12 with 932 LYS N	Favored (15.19%) Isoleucine or valine / -114.4,157.0	62.8% (t) chi angles: 180	0.114Å	-	-
932		LYS	193.59	0.899Å HB3 with 955 GLU HB2	Favored (4.66%) General / -93.1,73.8	45.1% (mtmt) chi angles: 295.1,173.8,274.2,188.5	0.085Å	-	-
933		ASN	242.14	0.415Å CG with 954 TYR CE2	Allowed (1.67%) General / -146.7,86.6	39.8% (t30) chi angles: 179.6,14.6	0.133Å	-	OUTLIER(S) worst is CA-CB-CG: 4.829 σ
934		LEU	163.35	0.93Å HD21 with 955 GLU HG3	Favored (3.87%) General / -75.4,-57.5	1.6% (mm?) chi angles: 298.2,297.7	0.1Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 106.65	Clashscore: 79.75	Outliers: 3 of 71	Poor rotamers: 3 of 62	Outliers: 2 of 65	Outliers: 1 of 73	Outliers: 16 of 73
935		VAL	142.6	0.436Å HG13 with 934 LEU C	Allowed (0.17%) Isoleucine or valine / -162.1,176.0	35.3% (m) chi angles: 298.1	0.13Å	-	-
936		LYS	152.68	0.534Å C with 936 LYS HD3	Favored (20.32%) General / -144.8,131.8	11.5% (tmtt?) chi angles: 176.7,287.9,183.2,178.8	0.09Å	-	-
937		ILE	155.62	1.034Å HG22 with 987 VAL HA	Allowed (0.39%) Isoleucine or valine / -159.7,172.0	44.7% (pt) chi angles: 62.3,167.3	0.146Å	OUTLIER(S) worst is C--N: 4.08 σ	OUTLIER(S) worst is C-N-CA: 6.101 σ
938		PHE	285.97	0.86Å CG with 949 LEU HB2	OUTLIER (0%) General / 135.3,-146.0	5.2% (m-85) chi angles: 264.6,77.9	0.415Å	-	OUTLIER(S) worst is CA-CB-CG: 12.66 σ
939		GLU	170.31	0.732Å HB3 with 984 SER O	Allowed (1%) Pre-proline / -172.5,176.0	5.8% (pm0) chi angles: 55.3,263.9,355.3	0.159Å	-	OUTLIER(S) worst is CA-C-N: 7.041 σ
940		PRO	178.5	0.438Å HD2 with 985 GLY CA	Favored (3.94%) Trans-proline / -80.0,-177.6	68.1% (Cg_exo) chi angles: 333.9	0.046Å	-	-
941		CYS	156.49	0.412Å HB3 with 942 GLY H	OUTLIER (0%) General / -60.4,-139.9	64.5% (m) chi angles: 286.9	0.139Å	-	-

942	GLY	234.19	0.715Å O with 944 PRO HD3	Favored (12.84%) Glycine / 102.8,-136.4	-	-	-	OUTLIER(S) worst is N-CA-C: 4.096 σ
943	ARG	315.36	0.472Å HD3 with 943 ARG N	Favored (65.68%) Pre-proline / -99.9,115.3	0.4% chi angles: 289.5,57.4,58.8,92	0.139Å	-	-
944	PRO	241.01	0.715Å HD3 with 942 GLY O	Allowed (1.2%) Trans-proline / -85.5,110.5	52.8% (Cg_exo) chi angles: 336.4	0.236Å	-	-
945	ALA	94.34	0.887Å HB1 with 971 THR HG21	Favored (49.73%) General / -75.7,-42.8	-	0.124Å	-	-
946	VAL	101.38	1.042Å HG11 with 949 LEU HD11	Favored (20.19%) Isoleucine or valine / -143.2,147.6	97.1% (t) chi angles: 178.3	0.108Å	-	-
947	ASP	141.2	0.671Å HB3 with 944 PRO HB3	Favored (39.01%) General / -140.6,160.9	55.9% (p-10) chi angles: 62.1,355.6	0.099Å	-	-
948	ARG	191.32	-	Favored (16.11%) General / 51.7,35.8	83.7% (mtm180) chi angles: 291.5,187.6,296.4,173.6	0.065Å	-	-
949	LEU	90.87	1.042Å HD11 with 946 VAL HG11	Favored (30.12%) General / -81.2,147.1	32.7% (mt) chi angles: 292.1,188.2	0.148Å	-	-
950	ASN	69.71	-	Favored (9.61%) General / -142.1,116.6	69.7% (m-80) chi angles: 295,285.6	0.164Å	-	OUTLIER(S) worst is CA-CB-CG: 4.304 σ
951	ILE	100.8	0.559Å HG21 with 953 PHE HE1	Favored (13.98%) Isoleucine or valine / -145.0,155.7	18.4% (tt) chi angles: 194.7,167.2	0.076Å	-	-
952	THR	40.35	0.497Å CG2 with 954 TYR CE1	Favored (48.89%) General / -122.8,144.9	92.3% (m) chi angles: 300.4	0.1Å	-	-
953	PHE	72.75	0.559Å HE1 with 951	Favored (51.29%) General /	60.7% (m-85)	0.153Å	-	OUTLIER(S) worst is CA-CB-CG: 4.552

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					General / -126.4,143.1	chi angles: 288.6,78.7			CB-CG: 4.332 σ
954		TYR	90.22	0.693Å CD1 with 957 GLN HG3	Favored (47.45%) General / -139.2,152.6	31.5% (*m-85*) chi angles: 295.2,72.5	0.25Å	-	OUTLIER(S) worst is CB-CA-C: 4.003 σ
			Avg: 106.65	Clashscore: 79.75	Outliers: 3 of 71	Poor rotamers: 3 of 62	Outliers: 2 of 65	Outliers: 1 of 73	Outliers: 16 of 73
955		GLU	67.97	0.93Å HG3 with 934 LEU HD21	Favored (67.75%) General / -66.1,-27.0	93.2% (*mt-10*) chi angles: 292.8,181.3,6.6	0.058Å	-	-
956		ASN	115.65	-	Favored (80.46%) General / -68.3,-41.6	0.4% chi angles: 197.7,164.9	0.055Å	-	-
957		GLN	91.41	0.693Å HG3 with 954 TYR CD1	Favored (46.65%) General / -67.3,151.9	24.2% (*mt-30*) chi angles: 288.7,190.5,163.2	0.141Å	-	-
958		ILE	117.47	0.614Å O with 958 ILE HG13	Favored (43.52%) Isoleucine or valine / -127.6,116.5	43.8% (*pt*) chi angles: 61.7,167.3	0.057Å	-	-
959		THR	112.89	-	Favored (31.05%) General / -127.8,160.7	13.9% (*t*) chi angles: 190	0.086Å	-	-
960		ALA	29.87	-	Favored (54.67%) General / -123.6,137.8	-	0.094Å	-	-
961		PHE	64.91	-	Favored (16.15%) General / -97.7,104.2	61.6% (*m-85*) chi angles: 304,83.1	0.172Å	-	OUTLIER(S) worst is CA-CB-CG: 6.592 σ
962		LEU	98.2	0.556Å N with 962 LEU HD12	Favored (21.83%) General / -68.3,164.0	5.4% (*mp*) chi angles: 293.4,62.5	0.069Å	-	-
963		GLY	100.93	0.432Å O with 964 HIS HB2	Favored (50.43%) Glycine / -84.5,-174.6	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
964		HIS	157.09	0.432Å HB2 with 963 GLY O	OUTLIER (0.01%) General / 98.0,112.8	40.7% (*m170*) chi angles: 291.7,148.9	0.108Å	-	OUTLIER(S) worst is CD2-NE2-CE1: 4.42 σ
965		ASN	94.26	-	Favored (40.43%) General / -74.1,150.6	17.3% (*t30*) chi angles: 185.1,79.4	0.09Å	-	OUTLIER(S) worst is CA-CB-CG: 4.689 σ
966		GLY	20.66	-	Favored (40.87%) Glycine / -178.8,169.4	-	-	-	-
967		ALA	52.95	0.605Å O with 971 THR HG23	Favored (95.02%) General / -64.8,-42.3	-	0.097Å	-	-
968		GLY	38.59	0.683Å HA2 with 946 VAL CG2	Favored (91.48%) Glycine / -65.8,-44.7	-	-	-	-
969		LYS	144.85	0.813Å O with 972 THR HG22	Favored (77.97%) General / -65.2,-47.1	0% chi angles: 196.4,293,251.7,52.7	0.061Å	-	-
970		THR	104.31	0.531Å HG23 with 971 THR N	Favored (85.36%) General / -67.2,-41.8	13.2% (*t*) chi angles: 186.2	0.052Å	-	-
971		THR	122.39	0.887Å HG21 with 945 ALA HB1	Favored (81.36%) General / -63.0,-35.8	74.3% (*p*) chi angles: 58.1	0.068Å	-	-
972		THR	114.86	0.916Å HG23 with 973 LEU HD12	Favored (98.53%) General / -63.5,-42.4	7.4% (*t*) chi angles: 193.8	0.066Å	-	-
973		LEU	90.29	0.916Å HD12 with 972 THR HG23	Favored (88.2%) General / -66.8,-40.5	8.7% (*mp*) chi angles: 285.1,64	0.102Å	-	-
974		SER	37.34	0.728Å HB3 with 980 LEU HG	Favored (86.51%) General / -62.6,-37.5	69.8% (*m*) chi angles: 297.2	0.083Å	-	-
			Avg: 106.65	Clashscore: 79.75	Outliers: 3 of 71	Poor rotamers: 3 of 62	Outliers: 2 of 65	Outliers: 1 of 73	Outliers: 16 of 73

975	ILE	60.78	0.65Å HD12 with 938 PHE CZ	Favored (77.95%) Isoleucine or valine / -70.0,-40.0	97.5% (*mt*) chi angles: 297.5,170.4	0.065Å	-	-
976	LEU	159.75	0.732Å HG with 972 THR O	Favored (99.06%) General / -62.1,-43.3	86.7% (*mt*) chi angles: 299.4,180.2	0.14Å	-	-
977	THR	105.3	-	Favored (85.77%) General / -63.7,-37.0	90.7% (*m*) chi angles: 302.3	0.126Å	-	-
978	GLY	31.23	-	Favored (31.29%) Glycine / 109.2,-0.3	-	-	-	-
979	LEU	78.31	-	Favored (91.46%) General / -65.1,-43.6	61.1% (*tp*) chi angles: 179.7,64.2	0.082Å	-	-
980	LEU	80.8	0.728Å HG with 974 SER HB3	Favored (23.91%) Pre-proline / -107.8,129.6	85.3% (*mt*) chi angles: 301,179.5	0.226Å	-	OUTLIER(S) worst is CB-CA-C: 4.025 σ
981	PRO	89.4	-	Favored (12.62%) Trans-proline / -79.5,136.8	10.8% (*Cg_endo*) chi angles: 13.9	0.103Å	-	-
982	PRO	169.56	-	Favored (36.64%) Trans-proline / -72.0,141.4	82.5% (*Cg_exo*) chi angles: 331.9	0.122Å	-	-
983	THR	132.86	-	Favored (77.72%) General / -68.1,-43.8	81.9% (*p*) chi angles: 60.9	0.071Å	-	-
984	SER	103.74	0.732Å O with 939 GLU HB3	Favored (4.14%) General / -140.9,-175.0	65% (*m*) chi angles: 292.5	0.116Å	-	-
985	GLY	24.1	0.832Å HA3 with 938 PHE O	Favored (38.82%) Glycine / 92.9,166.9	-	-	-	-
986	THR	98.42	-	Favored (40.17%) General / 113.2,145.9	14.8% (*t*) chi angles: 188.9	0.092Å	-	-

				-113.2,143.9				
987	VAL	24.55	1.034Å HA with 937 ILE HG22	-	71.5% (*t*) chi angles: 171.9	0.124Å	-	-

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