

Viewing abca4_mb_915-987-FFX1Hmulti.table

When finished, you should close this window .

Hint: Use File | Save As... to save a copy of this page.

All-Atom	Clashscore, all atoms: 0.9			99 th percentile* (N=1784, all resolutions)			
Contacts	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.						
	Poor rotamers	7	11.29%	Goal: <1%			
	Ramachandran outliers	3	4.23%	Goal: <0.05%			
III I	Ramachandran favored	55	77.46%	Goal: >98%			
Protein Geometry	MolProbity score [^]	2.34		56 th percentile* (N=27675, 0Å - 99Å)			
	Cβ deviations >0.25Å	0	0.00%	Goal: 0			
	Bad backbone bonds:	0 / 575	0.00%	Goal: 0%			
	Bad backbone angles:	11 / 785	1.40%	Goal: <0.1%			

In the two column results, the left column gives the raw count, right column gives the percentage.

[^] 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: 0.9	Outliers: 3 of 71	Poor rotamers: 7 of 62	Outliers: 0 of 65	Outliers: 0 of 73	Outliers: 11 of 73
915	5	ASP	31.38	-	-	0.8% chi angles: 306.2,209.4	0.152Å	-	-
916	Ó	SER	112.98	-	Favored (72.01%) General / -61.9,-31.7	35.6% (<i>m</i>) chi angles: 303.6	0.097Å	-	-
917	7	PHE	135.68	-	Favored (9.96%) General / -130.4,174.3	42.3% (<i>t80</i>) chi angles: 185.3,59.5	0.092Å	-	-
918	3	PHE	39.44	-	Favored (40.05%) General / -156.4,162.2	55.4% (<i>p90</i>) chi angles: 62.3,89.8	0.028Å	-	-
					Favored	5% (<i>tp10</i>)			OUTLIER(S)

^{* 100&}lt;sup>th</sup> 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.

919	GLU 39.7	-	(40.37%) General / -155.5,160.2	chi angles: 174.2,58,299.4	0.11Å	-	worst is C-N-CA: 4.968σ
920	ARG 113.71	0.425Å CZ with 921 GLU OE2	Favored (37.89%) General / -107.3,141.9	29.8% (<i>tpt180</i>) chi angles: 170.4,66.1,175.6,162.9	0.142Å	-	-
921	GLU 72.76	0.425Å OE2 with 920 ARG CZ	Favored (55.98%) General / -60.8,142.4	1.7% (pm0) chi angles: 79.1,304.3,321.3	0.099Å	-	-
922	HIS 67.39	-	Favored (25.65%) Pre-proline / -116.4,89.1	12.3% (<i>m80</i>) chi angles: 280.6,54.8	0.056Å	-	-
923	PRO 67.13	-	Favored (12.29%) Trans-proline / -83.7,147.8	66.4% (<i>Cg_endo</i>) chi angles: 33.8	0.056Å	-	-
924	GLY 17.11	-	Favored (50.75%) Glycine / -68.5,161.4	-	-	-	-
925	TRP 111.94	-	Favored (50.3%) General / -69.4,135.4	0.4% chi angles: 330.3,277.3	0.088Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.352 σ
926	VAL 96.14	-	Favored (84.46%) Pre-proline / -73.1,130.6	94.9% (<i>t</i>) chi angles: 175.9	0.054Å	-	-
927	PRO 124.36	-	Favored (8.79%) Trans-proline / -50.9,121.8	0.1% chi angles: 318.2	0.048Å	-	-
928	GLY 25.79	-	Favored (76.84%) Glycine / 88.0,-8.8	-	-	-	-
929	VAL 61.17	-	Allowed (0.74%) Isoleucine or valine /-86.2,70.7	65.8% (<i>t</i>) chi angles: 171.4	0.156Å	-	-
930	CYS 43.93	-	Favored (57.73%) General / -76.0,-38.1	82.9% (<i>m</i>) chi angles: 300.7	0.107Å	-	-
931	VAL 64.18	-	Favored (28.75%) Isoleucine or valine	74.5% (t) chi angles: 172.1	0.054Å	-	-

932	LYS	193.59	-	/ -89.6,115.2 Allowed (0.06%) General / -71.2,38.5	35.2% (<i>mttm</i>) chi angles: 283.8,180.9,153.4,285.2	0.102Å	-	-
933	ASN	242.14	-	Favored (47.46%) General / -101.6,132.0	0.6% chi angles: 193.4,110.7	0.106Å	-	-
934	LEU	163.35	-	Allowed (0.34%) General / -106.9,-134.7	2% (<i>mm</i> ?) chi angles: 299.9,317.8	0.18Å	-	-
# A	lt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 106.65	Clashscore: 0.9	Outliers: 3 of 71	Poor rotamers: 7 of 62	Outliers: 0 of 65	Outliers: 0 of 73	Outliers: 11 of 73
935	VAL	142.6	-	Favored (3.08%) Isoleucine or valine /-92.2,155.7	16.2% (<i>m</i>) chi angles: 290.6	0.072Å	-	OUTLIER(S) worst is C-N-CA: 4.053σ
936	LYS	152.68	-	Allowed (1.72%) General / -110.2,83.2	0% chi angles: 195.5,273.6,88.2,208.6	0.05Å	-	-
937	ILE	155.62	-	Allowed (1.12%) Isoleucine or valine / -90.1,171.3	5.6% (<i>pt</i>) chi angles: 40.8,169.2	0.18Å	-	OUTLIER(S) worst is C-N- CA: 4.154 σ
938	PHE	285.97	-	Allowed (0.25%) General / 76.8,166.6	88.9% (<i>m-85</i>) chi angles: 301.2,101.9	0.151Å	-	-
939	GLU	170.31	-	Favored (71.37%) Pre-proline / -125.1,153.3	9.9% (<i>pt-20</i>) chi angles: 70.6,195.3,262.2	0.08Å	-	-
940	PRO	178.5	-	OUTLIER (0.07%) Trans-proline / -69.9,-60.8	34.4% (<i>Cg_exo</i>) chi angles: 339.9	0.078Å	-	-
941	CYS	156.49	-	Favored (18.66%) General / -140.9,168.9	82.5% (<i>m</i>) chi angles: 299.9	0.063Å	-	-
942	GLY	234.19	-	Allowed (0.23%) Glycine /	-	-	-	-

943	ARG 315.36	-	151.7,-102.8 Allowed (1.94%) Pre-proline / -126.2,46.6	1.4% (mpp_?) chi angles: 303.3,79.3,57.9,76.2	0.046Å	-	-
944	PRO 241.01	-	Favored (14.61%) Trans-proline / -73.2,129.9	3.2% (<i>Cg_exo</i>) chi angles: 354.9	0.062Å	-	-
945	ALA 94.34	-	Favored (68.28%) General / -69.7,-30.6	-	0.1Å	-	-
946	VAL 101.38	-	Favored (21.54%) Isoleucine or valine /-141.4,129.0	49.3% (<i>t</i>) chi angles: 182.5	0.057Å	-	-
947	ASP 141.2	-	Favored (12.74%) General / -82.8,172.6	20.6% (<i>p-10</i>) chi angles: 62.1,319.2	0.081Å	-	-
948	ARG 191.32	-	Allowed (0.08%) General / 64.8,-24.2	72% (<i>mtm180</i>) chi angles: 282.2,163.8,283.4,165	0.216Å	-	OUTLIER(S) worst is CD- NE-CZ: 4.124 σ
949	LEU 90.87	-	Favored (33.89%) General / -53.2,130.2	68% (<i>mt</i>) chi angles: 298.1,184.5	0.06Å	-	-
950	ASN 69.71	-	Favored (2.56%) General / -156.4,109.0	52.3% (<i>m-80</i>) chi angles: 283.9,277.2	0.103Å	-	-
951	ILE 100.8	-	Favored (15.78%) Isoleucine or valine /-148.2,137.4	14% (tt) chi angles: 178,165.5	0.083Å	-	-
952	THR 40.35	-	Favored (28.14%) General / -95.7,142.3	11.3% (<i>m</i>) chi angles: 312.8	0.036Å	-	-
953	PHE 72.75	-	Favored (21.81%) General / -105.6,153.4	52.8% (<i>m-85</i>) chi angles: 283.3,81.4	0.062Å	-	OUTLIER(S) worst is CA- CB-CG: 5.043 σ
954	TYR 90.22	-	Favored (46.51%) General / -138.4,150.4	92.3% (<i>m-85</i>) chi angles: 296.5,85.1	0.088Å	-	-

# A	lt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
	Avg: 106.65	Clashscore: 0.9	Outliers: 3 of 71	Poor rotamers: 7 of 62	Outliers: 0 of 65	Outliers: 0 of 73	Outliers: 11 of 73
955	GLU 67.97	-	Allowed (0.8%) General / -78.5,48.7	72.3% (<i>mt-10</i>) chi angles: 300.6,194.1,342.3	0.083Å	-	OUTLIER(S) worst is CA- CB-CG: 4.088
956	ASN 115.65	-	OUTLIER (0.02%) General / -171.0,2.1	0.1% chi angles: 230.1,117.2	0.037Å	-	-
957	GLN 91.41	-	Favored (29.64%) General / -79.8,152.6	29.2% (<i>mt-30</i>) chi angles: 296.7,192.4,124.7	0.061Å	-	-
958	ILE 117.47	-	Favored (14.22%) Isoleucine or valine / -110.2,147.8	36.2% (<i>pt</i>) chi angles: 55.7,169.5	0.063Å	-	-
959	THR 112.89	-	Allowed (0.84%) General / -172.0,-171.2	14.4% (<i>t</i>) chi angles: 189.6	0.179Å	-	-
960	ALA 29.87	-	Favored (5%) General / -164.8,138.6	-	0.084Å	-	-
961	PHE 64.91	-	Favored (6.34%) General / -81.0,84.8	8.7% (<i>m-30</i>) chi angles: 309.9,149	0.056Å	-	-
962	LEU 98.2	-	Favored (6.79%) General / -47.4,139.3	8.3% (<i>mp</i>) chi angles: 265.9,61.3	0.048Å	-	-
963	GLY 100.93	-	Favored (22.28%) Glycine / -56.4,151.9	-	-	-	OUTLIER(S) worst is C-N- CA: 4.499 σ
964	HIS 157.09	-	OUTLIER (0.01%) General / 97.2,102.7	81% (<i>m80</i>) chi angles: 292.5,84.8	0.17Å	-	OUTLIER(S) worst is N-CA-CB: 4.615σ
965	ASN 94.26	-	Favored (35.6%) General / -125.3,157.9	79.2% (<i>m-20</i>) chi angles: 286.3,354	0.069Å	-	-
966	GLY 20.66	-	Favored (8.45%) Glycine / 124.0,152.7 Allowed	-	-	-	-

967	ALA 52.95	-	(1.24%) General / 45.5,-127.1	-	0.197Å	-	OUTLIER(S) worst is C-CA-CB: 4.451σ
968	GLY 38.59	-	Favored (70.83%) Glycine / -59.5,-31.5	-	-	-	-
969	LYS 144.85	-	Favored (57.59%) General / -75.4,-8.8	1.7% (mmmp?) chi angles: 257.1,298.7,288.9,66.1	0.143Å	-	-
970	THR 104.31	-	Favored (9.41%) General / -92.5,-43.0	0% chi angles: 11.3	0.159Å	-	-
971	THR 122.39	-	Favored (75.76%) General / -63.1,-33.6	22.4% (p) chi angles: 49.3	0.154Å	-	-
972	THR 114.86	-	Favored (66.36%) General / -52.5,-48.1	25.7% (<i>m</i>) chi angles: 308.6	0.072Å	-	-
973	LEU 90.29	-	Favored (88.99%) General / -66.4,-39.5	8.3% (<i>mp</i>) chi angles: 281.3,54.4	0.102Å	-	-
974	SER 37.34	-	Favored (77.17%) General / -58.1,-38.8	28.9% (<i>m</i>) chi angles: 304.2	0.088Å	-	-
# Al	lt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
	Avg: 106.65	Clashscore 0.9	Outliers: 3 of 71	Poor rotamers: 7 of 62	Outliers: 0 of 65	Outliers: 0 of 73	Outliers: 11 of 73
975	ILE 60.78	-	Favored (48.09%) Isoleucine or valine /-71.9,-33.5	97.9% (<i>mt</i>) chi angles: 296.1,172.6	0.192Å	-	-
976	LEU 159.75	-	Favored (84.3%) General / -63.1,-36.6	21.9% (<i>mt</i>) chi angles: 310.6,187.6	0.137Å	-	-
977	THR 105.3	-	Favored (52.57%) General / -81.2,-16.5	2.8% (<i>m</i>) chi angles: 320.4	0.09Å	-	-
978	GLY 31.23	-	Favored (77.9%) Glycine / 86.1,8.8 Favored	-	-	-	-

979	LEU 78.31	-	(64.58%) General / -72.2,-30.1	50% (<i>tp</i>) chi angles: 175.2,57.5	0.064Å	-	-
980	LEU 80.8	-	Favored (71.74%) Pre-proline / -133.3,149.2	96.7% (<i>mt</i>) chi angles: 295.8,177.4	0.068Å	-	-
981	PRO 89.4	-	Favored (3.5%) Trans-proline / -91.2,168.2	19.3% (<i>Cg_endo</i>) chi angles: 38.7	0.098Å	-	-
982	PRO 169.56	-	Favored (96.81%) Trans-proline / -61.6,143.2	76.9% (<i>Cg_exo</i>) chi angles: 333.3	0.058Å	-	-
983	THR 132.86	-	Favored (38.87%) General / -80.8,-23.9	1.3% (<i>p</i>) chi angles: 88.6	0.18Å	-	-
984	SER 103.74	-	Allowed (0.96%) General / -150.2,-158.9	44.1% (<i>t</i>) chi angles: 178.4	0.137Å	-	-
985	GLY 24.1	-	Favored (20.23%) Glycine / 69.7,-128.0	-	-	-	-
986	THR 98.42	-	Favored (5.89%) General / -138.1,-179.6	32.8% (p) chi angles: 69.1	0.064Å	-	OUTLIER(S) worst is C-N- CA: 4.163 σ
987	VAL 24.55	-	-	97.4% (<i>t</i>) chi angles: 178.3	0.078Å	-	-

About MolProbity | Website for the Richardson Lab | Using ecloud x-H | Internal reference 4.1-537