



# Viewing RPGR\_mb\_769-953-FFX1FH-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0.72		99 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	28	16.87%	Goal: <1%
	Ramachandran outliers	16	8.74%	Goal: <0.05%
	Ramachandran favored	117	63.93%	Goal: >98%
	MolProbity score^	2.55		44 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	2.27%	Goal: 0
	Bad backbone bonds:	0 / 1470	0.00%	Goal: 0%
	Bad backbone angles:	37 / 1968	1.88%	Goal: <0.1%

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

\* 100<sup>th</sup> percentile is the best among structures of comparable resolution; 0<sup>th</sup> percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

<sup>^</sup> 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:				Clashscore: 119.21	Outliers: 16 of 183	Poor rotamers: 28 of 166	Outliers: 4 of 176	Outliers: 0 of 185	Outliers: 32 of 185
769	GLU	30.45	-	-	Favored (42.99%) General / -146.0,159.6	7.5% ( <i>tp</i> 10) chi angles: 164.1,40.7,27	0.047Å	-	-
770	THR	44.13	-	-	Favored (8.75%) Pre-proline / -144.2,85.7	26.2% ( <i>p</i> ) chi angles: 50.6	0.05Å	-	-
771	LYS	103.07	-	-	Favored (13.06%) Trans-proline / -49.0,145.9	33.5% ( <i>mmtm</i> ) chi angles: 292.4,296,160.1,294.4	0.045Å	-	-
772	PRO	100.49	-	-	Allowed (0.37%) Isoleucine or valine /	21.5% ( <i>Cg_exo</i> ) chi angles: 324.3	0.06Å	-	-
773	ILE	124.94	-	-		4.4% ( <i>tp</i> ) chi angles: 197.3,82.5	0.227Å	-	-

				-77.6,68.3				
			Favored (4.02%)					
774	ILE	129.38	-	Isoleucine or valine / -51.9,142.8	9.2% ( <i>tp</i> ) chi angles: 186.7,69.5	0.096Å	-	-
			Favored (18.72%)					
775	SER	80.37	-	General / -50.4,127.9	3.6% ( <i>t</i> ) chi angles: 202.2	0.051Å	-	-
			Favored (2.92%)					
776	LYS	109.74	-	General / -93.0,58.3	47.4% ( <i>mmtm</i> ) chi angles: 306.3,304.4,183.9,293.3	0.147Å	-	OUTLIER(S) worst is C-N- CA: 5.739 $\sigma$
			OUTLIER (0.04%)					
777	SER	71.11	-	General / 170.1,-178.4	48.4% ( <i>t</i> ) chi angles: 179.6	0.093Å	-	-
			Favored (2.92%)					
778	MET	105.33	-	General / -114.3,-176.5	19.7% ( <i>ptm</i> ) chi angles: 63.1,162.7,285.7	0.088Å	-	-
			Favored (5.78%)					
779	ALA	48.26	-	General / -45.9,137.3	-	0.084Å	-	-
			Favored (7.93%)					
780	LYS	133.13	-	General / -103.6,-36.4	1.9% ( <i>mptt</i> ) chi angles: 317.2,95.9,190.5,183.6	0.098Å	-	-
			Allowed (0.08%)					
781	TYR	138.49	-	General / -164.9,42.1	29.6% ( <i>t80</i> ) chi angles: 197,266	0.046Å	-	-
			Favored (7.74%)					
782	ASP	164.26	-	General / -131.5,177.1	7.2% ( <i>m-20</i> ) chi angles: 316.7,300.3	0.063Å	-	-
			Favored (21.12%)					
783	PHE	328.55	-	General / -77.4,-47.0	14.4% ( <i>m-85</i> ) chi angles: 311.7,128.7	0.11Å	-	-
			Allowed (1.73%)					
784	LYS	146.91	-	General / -146.4,-163.4	23.7% ( <i>mtp</i> ) chi angles: 307.8,193.1,75.1,56.7	0.168Å	-	-
			Favored (50.1%)					
785	CYS	49.44	-	General / -114.5,138.9	56.6% ( <i>m</i> ) chi angles: 306	0.077Å	-	OUTLIER(S) worst is C-N- CA: 4.395 $\sigma$

786	ASP	56.02	-	Allowed (1.1%) General / -45.5,146.2	0.3% chi angles: 325.1,343.2	0.074Å	-	OUTLIER(S) worst is CA- CB-CG: 6.422 σ
787	ARG	101.2	-	Allowed (0.06%) General / -174.0,88.1	3.3% ( <i>ptm-85</i> ) chi angles: 37.6,170,297.6,289.5	0.104Å	-	-
788	LEU	52.64	-	Favored (35.77%) General / -89.2,129.7	2.7% ( <i>mt</i> ) chi angles: 329,176.7	0.055Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 119.21				Clashscore: 0.72	Outliers: 16 of 183	Poor rotamers: 28 of 166	Outliers: 4 of 176	Outliers: 0 of 185	Outliers: 32 of 185
789	SER	85.68	-	Favored (40.14%) General / -95.9,125.0	7% ( <i>t</i> ) chi angles: 196.9	0.018Å	-	OUTLIER(S) worst is C-N- CA: 4.221 σ	
790	GLU	77.7	-	Allowed (0.43%) General / -45.7,112.2	3.2% ( <i>mp0</i> ) chi angles: 308,91.8,293.4	0.069Å	-	-	
791	ILE	176.33	-	Favored (3.59%) Pre-proline / -149.6,174.3	0.7% chi angles: 236.8,82.7	0.175Å	-	-	
792	PRO	224.27	-	Favored (80.53%) Trans-proline / -59.4,-26.0	10% ( <i>Cg_exo</i> ) chi angles: 322.8	0.089Å	-	-	
793	GLU	233.48	-	Favored (9.63%) General / -135.2,175.4	1.8% ( <i>mm-40</i> ) chi angles: 257.3,299.3,356.5	0.043Å	-	-	
794	GLU	94.01	-	Favored (45.97%) General / -66.3,151.9	4.6% ( <i>tt0</i> ) chi angles: 206.9,204.9,247.2	0.036Å	-	OUTLIER(S) worst is C-N- CA: 5.596 σ	
795	LYS	95.2	-	Favored (2.67%) General / -167.8,137.7	7.3% ( <i>mtmp?</i> ) chi angles: 283.1,177.1,299.8,90.3	0.162Å	-	-	
796	GLU	83.5	-	Favored (44.7%) General / -142.0,157.7	7.3% ( <i>tp10</i> ) chi angles: 184.7,53.4,284.1	0.066Å	-	OUTLIER(S) worst is C-N- CA: 4.862 σ	
797	GLY	24.04	-	Allowed (0.23%) Glycine /	-	-	-	-	

-168.2,52.0

798	ALA	40.59	-	Favored (8.11%) General / -45.3,130.4	-	0.04Å	-	-
799	GLU	131.23	-	Allowed (0.3%) General / -142.7,-150.2	0.3% chi angles: 204.4,238.8,42.7	0.181Å	-	-
800	ASP	227.39	-	Favored (2.48%) General / -100.4,-173.7	65.6% ( <i>m</i> -20) chi angles: 302.1,133.5	0.206Å	-	-
801	SER	110.17	-	Favored (2.36%) General / -75.2,75.9	92.2% ( <i>p</i> ) chi angles: 67	0.083Å	-	-
802	LYS	130.69	-	OUTLIER (0.03%) General / -155.8,-111.4	12.3% ( <i>pttp</i> ) chi angles: 44.1,202.8,183.8,75.1	0.255Å	-	OUTLIER(S) worst is C- CA-CB: 4.189 σ
803	GLY	43.89	-	OUTLIER (0.05%) Glycine / 171.9,-14.2	-	-	-	-
804	ASN	60.2	-	Allowed (1.02%) General / -67.2,-179.7	14.7% ( <i>p</i> -10) chi angles: 66.5,299.3	0.06Å	-	-
805	GLY	45.91	-	Favored (16.81%) Glycine / 107.2,-153.5	-	-	-	-
806	ILE	123.04	-	Allowed (0.8%) Isoleucine or valine / -112.3,-177.2	1.2% ( <i>tt</i> ) chi angles: 225.6,180.1	0.175Å	-	-
807	GLU	115.6	-	Allowed (0.09%) General / 178.3,140.2	11.5% ( <i>pt</i> -20) chi angles: 57.2,187.4,253	0.114Å	-	-
808	GLU	128.81	-	Favored (7.6%) General / -134.3,177.6	24.4% ( <i>mm</i> -40) chi angles: 315.4,311.2,313.8	0.085Å	-	-

# Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles

Avg: Clashscore: Outliers: 16 of Poor rotamers: 28 of Outliers: Outliers: Outliers: 32

	119.21	0.72	183	166	4 of 176	0 of 185	of 185
809	GLN 68.38	-	Allowed (0.11%) General / -149.0,-141.1	0.1% chi angles: 201.5,102.7,138.6	0.145Å	-	OUTLIER(S) worst is CB- CG-CD: 4.226 $\sigma$
810	GLU 120.45	-	Allowed (0.4%) General / -80.6,-161.6	20.8% ( <i>mt-10</i> ) chi angles: 294.3,206,29.9	0.198Å	-	-
811	VAL 53.13	-	Favored (11.53%) Isoleucine or valine / -107.2,148.4	83.5% ( <i>t</i> ) chi angles: 174.8	0.096Å	-	-
812	GLU 90.96	-	Allowed (0.19%) General / -96.3,-132.5	0.6% chi angles: 192.9,235.8,48.7	0.18Å	-	-
813	ALA 58.95	-	Favored (8.33%) General / -124.1,-0.9	-	0.039Å	-	-
814	ASN 214.41	-	Favored (7.95%) General / -140.6,177.5	0.1% chi angles: 97.9,105.9	0.104Å	-	-
815	GLU 117.57	-	Favored (12.92%) General / -94.6,-33.6	34.5% ( <i>mt-10</i> ) chi angles: 302.8,191.2,225.2	0.091Å	-	-
816	GLU 91.77	-	Favored (40.17%) General / -77.3,140.9	17% ( <i>mt-10</i> ) chi angles: 289.7,206,39.7	0.053Å	-	-
817	ASN 122.8	-	Favored (6.65%) General / -168.2,153.3	6.8% ( <i>p30</i> ) chi angles: 65.2,96.1	0.022Å	-	-
818	VAL 143.42	-	Favored (11.82%) Isoleucine or valine / -52.6,137.9	12.5% ( <i>p</i> ) chi angles: 65.7	0.08Å	-	-
819	LYS 166.87	-	Favored (2.85%) General / -138.1,13.6	0.9% chi angles: 263.3,85.7,194.2,79.2	0.08Å	-	-
820	VAL 112.83	-	Favored (10.67%) Isoleucine or valine /	55.8% ( <i>t</i> ) chi angles: 169.5	0.1Å	-	OUTLIER(S) worst is C-N- CA: 4.729 $\sigma$

-62.4,148.4

821	HIS	274.48	-	OUTLIER (0.04%) General / -162.5,-35.4	62.3% ( <i>m80</i> ) chi angles: 299.4,74.7	0.171Å	-	OUTLIER(S) worst is CA- CB-CG: 5.963 $\sigma$
822	GLY	132.17	-	Favored (5.36%) Glycine / 97.6,126.3	-	-	-	-
823	GLY	97.8	-	Allowed (1.59%) Glycine / 142.2,120.5	-	-	-	-
824	ARG	246.92	-	Allowed (0.33%) General / -45.9,152.9	23.4% ( <i>ttp-105</i> ) chi angles: 199.1,197.4,70.7,252.3	0.066Å	-	-
825	LYS	270.35	-	Favored (2.31%) General / -61.4,112.8	67.9% ( <i>mttm</i> ) chi angles: 298,182.5,185.4,302.7	0.035Å	-	-
826	GLU	211.5	-	Favored (36.65%) General / -70.4,-50.6	0.2% chi angles: 210.8,309.5,103.7	0.122Å	-	-
827	LYS	141.48	-	Allowed (0.18%) General / -148.8,-53.5	40.6% ( <i>mmtm</i> ) chi angles: 299.6,298.2,166.4,295.5	0.129Å	-	-
828	THR	191.19	-	Favored (2.07%) General / -105.7,-172.3	69.7% ( <i>p</i> ) chi angles: 57.6	0.094Å	-	OUTLIER(S) worst is C-N- CA: 5.084 $\sigma$

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Avg: 119.21				Clashscore: 0.72	Outliers: 16 of 183	Poor rotamers: 28 of 166	Outliers: 4 of 176	Outliers: 0 of 185	Outliers: 32 of 185
829	GLU	243.72	-	Allowed (1.65%) General / -75.9,62.9	11.4% ( <i>mp0</i> ) chi angles: 289.6,51.7,39.8	0.104Å	-	-	-
830	ILE	168.54	-	Favored (33.93%) Isoleucine or valine / -127.8,146.2	18.1% ( <i>tt</i> ) chi angles: 194.5,166.3	0.106Å	-	-	-
831	LEU	129.64	-	Favored (26.22%) General /	5.5% ( <i>mp</i> ) chi angles: 295.7,88.2	0.039Å	-	OUTLIER(S) worst is C-N-	

-87.3,117.6

CA: 5.171  $\sigma$ 

832	SER	75.85	-	Favored (8.51%) General / -75.0,175.1	11.7% ( <i>t</i> ) chi angles: 191.3	0.046Å	-	-
833	ASP	61.26	-	Favored (54.18%) General / -74.7,-7.7	5.7% ( <i>m-20</i> ) chi angles: 297,19.3	0.069Å	-	-
834	ASP	77.16	-	Favored (74.32%) General / -65.0,-32.5	0.3% chi angles: 317.6,22.6	0.103Å	-	OUTLIER(S) worst is CA- CB-CG: 6.664 $\sigma$
835	LEU	126.33	-	Favored (11.95%) General / 64.3,32.9	8.9% ( <i>mp</i> ) chi angles: 269.6,55.1	0.219Å	-	-
836	THR	136.89	-	Allowed (0.16%) General / -94.8,-131.4	40% ( <i>p</i> ) chi angles: 53.6	0.214Å	-	OUTLIER(S) worst is C-N- CA: 4.103 $\sigma$
837	ASP	87.44	-	OUTLIER (0.02%) General / -49.2,171.0	6.9% ( <i>p-10</i> ) chi angles: 51.2,296.3	0.039Å	-	-
838	LYS	95.86	-	Favored (2.8%) General / -129.3,-172.7	1.9% ( <i>mptt</i> ) chi angles: 308.5,111.6,192.2,184.4	0.109Å	-	-
839	ALA	83.64	-	Favored (2.92%) General / -148.8,98.9	-	0.059Å	-	-
840	GLU	143.01	-	Favored (3.31%) General / -126.0,-27.3	38.1% ( <i>tt0</i> ) chi angles: 197.2,185,28	0.069Å	-	-
841	ASP	173.67	-	Favored (4.35%) General / -81.8,-55.9	10.1% ( <i>t70</i> ) chi angles: 192.1,294.3	0.051Å	-	-
842	HIS	142.1	-	Favored (2.52%) General / 75.6,-3.7	10.3% ( <i>m80</i> ) chi angles: 320.2,89.9	0.191Å	-	-
843	GLU	211.91	-	Allowed (0.35%) General / -115.8,-135.3	2.6% ( <i>tm-20</i> ) chi angles: 220.8,297.4,320	0.178Å	-	OUTLIER(S) worst is C- CA-CB: 4.031 $\sigma$

Favored

844	PHE	195.61	-	(48.83%) General / -70.6,-8.1 Allowed	27.5% ( <i>p90</i> ) chi angles: 74.6,267.2	0.146Å	-	-
845	SER	123.16	-	(0.07%) General / 77.3,75.5 Favored	5.5% ( <i>t</i> ) chi angles: 198.8	0.196Å	-	-
846	LYS	113.15	-	(14.82%) General / -89.9,-36.9 Favored	0% chi angles: 66.4,274.3,159.3,194.7	0.194Å	-	-
847	THR	77.96	-	(2.93%) General / -157.1,113.2 Favored	23.9% ( <i>p</i> ) chi angles: 49.9	0.1Å	-	-
848	GLU	134.74	-	(11.32%) General / -163.7,149.4 Favored	8.3% ( <i>pt-20</i> ) chi angles: 47.6,162.7,7	0.064Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 119.21				Clashscore: 0.72	Outliers: 16 of 183	Poor rotamers: 28 of 166	Outliers: 4 of 176	Outliers: 0 of 185	Outliers: 32 of 185
849	GLU	152.81	-	Favored (53.56%) General / -65.6,134.6	5.1% ( <i>mt-10</i> ) chi angles: 282.4,221,138.2	0.099Å	-	-	
850	LEU	146.78	-	Allowed (1.15%) General / -129.7,-161.8	18.3% ( <i>mt</i> ) chi angles: 313.5,170.1	0.113Å	-	-	
851	LYS	160.24	-	Favored (15.2%) General / -158.1,141.4	20.1% ( <i>ttmm</i> ) chi angles: 187.8,169.9,280.8,289.1	0.041Å	-	OUTLIER(S) worst is C-N- CA: 4.24 σ	
852	LEU	112.79	-	Allowed (0.97%) General / -117.6,-67.7	1.5% ( <i>mp</i> ) chi angles: 247.6,64.6	0.105Å	-	-	
853	GLU	139.77	-	Favored (12.64%) General / -112.5,-17.6	0% chi angles: 218.8,319.1,85.8	0.2Å	-	-	
854	ASP	276.61	-	Allowed (0.41%) General / -174.2,133.4	0.4% chi angles: 231.2,221.3	0.052Å	-	-	
				Allowed					



855	VAL	127.6	-	(1.03%) Isoleucine or valine / -158.5,130.6	4.3% ( <i>p</i> ) chi angles: 77.6	0.092Å	-	-
856	ASP	54.72	-	Favored (32.3%) General / -139.4,134.4	0.3% chi angles: 323.4,166.3	0.076Å	-	OUTLIER(S) worst is CA- CB-CG: 7.222 σ
857	GLU	60.13	-	Favored (15.59%) General / -105.9,160.0	77.2% ( <i>mm-40</i> ) chi angles: 298.3,299.9,130.8	0.052Å	-	-
858	GLU	83.86	-	Favored (6.97%) General / -139.6,110.8	25.9% ( <i>tt0</i> ) chi angles: 182.6,194.9,291.2	0.075Å	-	-
859	ILE	47.64	-	Favored (27.33%) Isoleucine or valine / -104.8,138.9	96.6% ( <i>mt</i> ) chi angles: 292.5,169.8	0.077Å	-	-
860	ASN	73.34	-	Favored (4.7%) General / -91.3,-176.9	34.2% ( <i>p-10</i> ) chi angles: 74.4,357.2	0.145Å	-	-
861	ALA	56.72	-	Favored (50.88%) General / -73.6,-7.2	-	0.09Å	-	-
862	GLU	70.05	-	Favored (35.4%) General / -83.8,-19.2	41.2% ( <i>mt-10</i> ) chi angles: 305.4,178.2,289.7	0.089Å	-	-
863	ASN	143.42	-	Allowed (0.06%) General / 84.0,32.4	5.3% ( <i>m120</i> ) chi angles: 311.4,152.9	0.128Å	-	OUTLIER(S) worst is CA- CB-CG: 5.458 σ
864	VAL	49.2	-	Favored (10.71%) Isoleucine or valine / -110.0,156.9	1.2% ( <i>t</i> ) chi angles: 130	0.118Å	-	-
865	GLU	120.67	-	Favored (17.72%) General / -76.7,116.8	0% chi angles: 29.8,49.7,98.2	0.074Å	-	-
866	SER	96.54	-	Favored (2.48%) General / -104.9,-54.5	21% ( <i>t</i> ) chi angles: 188.4	0.093Å	-	-

Favored (13%)      38% (*mttp*)

867	LYS	85.7	-	General / -152.8,175.3	chi angles: 315.8,186.2,195.4,71.8	0.091Å	-	-
868	LYS	128.34	-	Favored (16.79%) General / -146.5,170.5	0.1% chi angles: 66.9,70.9,170.5,159.5	0.064Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 119.21				Clashscore: 0.72	Outliers: 16 of 183	Poor rotamers: 28 of 166	Outliers: 4 of 176	Outliers: 0 of 185
869	LYS	178.12	-	Favored (34.02%) General / -129.0,160.0	0% chi angles: 35.2,66.7,71,172.1	0.181Å	-	-
870	THR	117.49	0.414Å O with 871 VAL HB	Allowed (0.13%) General / 55.3,-163.6	9.1% (p) chi angles: 43.9	0.329Å	-	OUTLIER(S) worst is C-N- CA: 4.916 σ
871	VAL	106.02	0.414Å HB with 870 THR O	OUTLIER (0%) Isoleucine or valine / 176.8,-134.5	9.6% (p) chi angles: 71.2	0.343Å	-	OUTLIER(S) worst is C- CA-CB: 5.054 σ
872	GLY	38.34	-	Favored (2.97%) Glycine / -136.6,27.3	-	-	-	-
873	ASP	112.24	-	Allowed (0.63%) General / -153.7,46.5	0.7% chi angles: 322.8,251.7	0.035Å	-	OUTLIER(S) worst is CA- CB-CG: 4.797 σ
874	ASP	75.39	-	OUTLIER (0.03%) General / 58.7,-12.2	10.9% (m-20) chi angles: 304.4,1.5	0.202Å	-	-
875	GLU	117.93	-	Allowed (0.43%) General / -71.1,67.0	35.6% (tt0) chi angles: 189.2,171.3,268.6	0.059Å	-	-
876	SER	104.43	-	Allowed (0.66%) General / -81.7,41.7	37.3% (t) chi angles: 182.2	0.068Å	-	-
877	VAL	157.28	-	Favored (63.77%) Pre-proline / -123.3,152.2	4.9% (p) chi angles: 76.5	0.134Å	-	-
878	PRO	133.53	-	Allowed (1.56%) Trans-proline /	76.4% (Cg_endo) chi angles: 29.7	0.03Å	-	-

					-82.0,106.0				
879	THR	134.33	-		Favored (30.38%) General / -98.2,116.4	39.3% ( <i>p</i> ) chi angles: 53.4	0.066Å	-	-
880	GLY	40.52	-		Favored (13.06%) Glycine / -64.5,174.8	-	-	-	-
881	TYR	68.15	-		Allowed (0.43%) General / -122.6,-99.4	93.7% ( <i>m-85</i> ) chi angles: 300.6,278.2	0.14Å	-	OUTLIER(S) worst is C-N- CA: 5.26 $\sigma$
882	HIS	145.98	-	0.484Å CE1 with 902 LYS HE2	OUTLIER (0%) General / 126.0,142.2	0% chi angles: 83,332.3	0.185Å	-	OUTLIER(S) worst is CA- CB-CG: 5.944 $\sigma$
883	SER	51.11	-		OUTLIER (0%) General / -34.8,72.8	4% ( <i>m</i> ) chi angles: 316.2	0.072Å	-	-
884	LYS	194.56	-		OUTLIER (0%) General / 169.8,23.4	4% ( <i>ptmm?</i> ) chi angles: 53,212,288.9,285.4	0.202Å	-	-
885	THR	182.51	-		Favored (6.6%) General / 52.0,57.3	70.9% ( <i>p</i> ) chi angles: 64	0.211Å	-	-
886	GLU	127.08	-		Favored (2.54%) General / -152.8,100.6	31.9% ( <i>tt0</i> ) chi angles: 194.6,179.6,89.1	0.11Å	-	-
887	GLY	48.14	-		Favored (44.87%) Glycine / -57.8,141.3	-	-	-	-
888	ALA	73.32	-		Allowed (1.32%) General / -102.0,-166.7	-	0.112Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
Avg:				Clashscore:	Outliers: 16 of	Poor rotamers: 28 of	Outliers:	Outliers:	Outliers: 32
119.21				0.72	183	166	4 of 176	0 of 185	of 185

889	GLU	99.22	-		Favored (7.27%) General / -45.4,133.7	36.2% ( <i>mt-10</i> ) chi angles: 309,192.5,131.6	0.055Å	-	-
890	ARG	216.01	-		Favored (5.47%) General / -157.4,-175.6	5.3% ( <i>ptm-85</i> ) chi angles: 61.8,164.7,286.6,262.2	0.089Å	-	-

891	THR 123.15	-	Favored (15.19%) General / -71.0,119.5	53.6% ( <i>m</i> ) chi angles: 294.3	0.035Å	-	-
892	ASN 85.67	-	Favored (25.09%) General / -75.6,123.2	0.8% chi angles: 292.4,212	0.076Å	-	OUTLIER(S) worst is CA- CB-CG: 7.676 σ
893	ASP 93.97	-	OUTLIER (0.01%) General / -42.9,-18.7	3.8% ( <i>m-20</i> ) chi angles: 314.3,344.3	0.102Å	-	OUTLIER(S) worst is CA- CB-CG: 4.093 σ
894	ASP 149.83	-	Favored (45.34%) General / -92.7,7.0	26.1% ( <i>p-10</i> ) chi angles: 62.5,151.3	0.157Å	-	OUTLIER(S) worst is C-N- CA: 4.252 σ
895	SER 225.64	-	OUTLIER (0%) General / 102.1,34.2	19.7% ( <i>t</i> ) chi angles: 188.8	0.222Å	-	-
896	SER 158.96	-	Favored (4.56%) General / -148.5,110.4	92.3% ( <i>p</i> ) chi angles: 63	0.076Å	-	-
897	ALA 85.46	-	Favored (14.21%) General / -80.4,108.7	-	0.023Å	-	-
898	GLU 103.48	-	Favored (32.91%) General / -156.8,156.2	0.3% chi angles: 28.3,71.8,16.2	0.099Å	-	-
899	THR 137.32	-	Favored (53.94%) General / -63.9,133.8	27.3% ( <i>p</i> ) chi angles: 50.8	0.085Å	-	-
900	ILE 169.45	-	OUTLIER (0.03%) Isoleucine or valine / -155.4,10.9	0% chi angles: 207.2,262.2	0.148Å	-	-
901	GLU 81.63	-	Favored (10.33%) General / -52.3,145.8	14.4% ( <i>tp10</i> ) chi angles: 185.4,44.3,3.2	0.083Å	-	OUTLIER(S) worst is C-N- CA: 4.631 σ
902	LYS 165.45	0.484Å HE2 with 882 HIS CE1	Allowed (0.56%) General / -91.0,-158.6	0% chi angles: 76.3,315.1,186.1,198.2	0.207Å	-	-

903	LYS	88.99	-	OUTLIER (0.03%) General / -157.4,-108.8	5.8% ( <i>ttpm?</i> ) chi angles: 196.8,176,84.1,280.8	0.181Å	-	-
904	GLU	86.38	-	Favored (17.9%) General / -86.7,-37.6	0% chi angles: 79.1,294.5,66.1	0.144Å	-	-
905	LYS	262.48	-	Favored (6.64%) General / -50.4,145.2	36.5% ( <i>mtpt</i> ) chi angles: 287.4,153.2,50.7,188.8	0.171Å	-	-
906	ALA	109.67	-	Allowed (1.78%) General / -93.4,30.2	-	0.037Å	-	-
907	ASN	65.57	-	Favored (39.81%) General / -145.3,152.4	11.1% ( <i>m120</i> ) chi angles: 295.6,156.6	0.136Å	-	OUTLIER(S) worst is CA- CB-CG: 7.874 σ
908	LEU	85.65	-	Allowed (0.11%) General / -35.8,140.4	33.1% ( <i>tp</i> ) chi angles: 168.8,60.2	0.127Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 119.21				Clashscore: 0.72	Outliers: 16 of 183	Poor rotamers: 28 of 166	Outliers: 4 of 176	Outliers: 0 of 185	Outliers: 32 of 185
909	GLU	100.08	-	Allowed (0.72%) General / -109.5,-72.5	1.2% ( <i>tt0</i> ) chi angles: 196.9,128.2,119.8	0.13Å	-	-	
910	GLU	80.96	-	Favored (42.72%) General / -123.1,150.9	56.3% ( <i>mt-10</i> ) chi angles: 293.1,180.4,222.8	0.074Å	-	-	
911	ARG	125.72	-	Favored (14.69%) General / -151.5,132.9	5.3% ( <i>ttp180</i> ) chi angles: 157.1,140.4,60.7,180.3	0.082Å	-	-	
912	ALA	93.01	-	Allowed (1.43%) General / -101.9,39.7	-	0.065Å	-	-	
913	ILE	202.9	-	Favored (12.11%) Isoleucine or valine / -80.1,-19.6	5.4% ( <i>tt</i> ) chi angles: 205.9,183.5	0.176Å	-	-	
				Allowed					

914	CYS 166.49	-	(1.8%) General / -137.2,-165.7	9.2% ( <i>t</i> ) chi angles: 196.5	0.101Å	-	-
915	GLU 165.41	-	Favored (74.65%) General / -63.8,-33.0	3.7% ( <i>mm-40</i> ) chi angles: 288.4,259.1,301.5	0.034Å	-	-
916	TYR 287.77	-	Favored (6.04%) General / 62.4,46.1	10.3% ( <i>t80</i> ) chi angles: 203.7,71.3	0.119Å	-	OUTLIER(S) worst is C-N- CA: 4.731 $\sigma$
917	ASN 184.53	-	OUTLIER (0%) General / 126.4,91.5	20.6% ( <i>t-20</i> ) chi angles: 170.2,260.2	0.113Å	-	-
918	GLU 106.74	-	Favored (8.12%) General / -81.1,98.7	49% ( <i>mt-10</i> ) chi angles: 278.2,177.3,208.3	0.07Å	-	-
919	ASN 119.63	-	Favored (63.12%) Pre-proline / -105.3,109.3	3% ( <i>p30</i> ) chi angles: 50.9,96.8	0.119Å	-	OUTLIER(S) worst is CA- CB-CG: 5.762 $\sigma$
920	PRO 159.98	-	Allowed (0.22%) Trans-proline / -70.8,20.1	65.4% ( <i>Cg_exo</i> ) chi angles: 327.5	0.046Å	-	-
921	LYS 152.75	-	Allowed (1.64%) General / 68.1,43.0	27.5% ( <i>mmtt</i> ) chi angles: 323.1,310.1,165.8,202.2	0.207Å	-	-
922	GLY 31.11	-	OUTLIER (0.06%) Glycine / 178.8,-27.2	-	-	-	-
923	TYR 59.13	-	Favored (2.87%) General / -140.6,-169.8	25.2% ( <i>p90</i> ) chi angles: 71.4,102.7	0.083Å	-	-
924	MET 91.94	-	Favored (42.5%) General / -153.2,161.4	13.9% ( <i>ptp</i> ) chi angles: 46.3,178.6,60.2	0.032Å	-	OUTLIER(S) worst is C-N- CA: 4.049 $\sigma$
925	LEU 76.91	-	Favored (55.46%) General / -109.8,128.7	29% ( <i>mt</i> ) chi angles: 311.6,174.3	0.057Å	-	-
926	ASP 109.66	-	Favored (41.41%) General /	33.5% ( <i>m-20</i> ) chi angles: 305.1,343.7	0.086Å	-	-

927	ASP	136.98	-	Allowed (0.37%) General / -150.8,-151.0	6.7% ( <i>t0</i> ) chi angles: 202.4,309.1	0.13Å	-	OUTLIER(S) worst is CA- CB-CG: 5.145 σ
928	ALA	56.6	-	Allowed (0.12%) General / -152.3,-53.0	-	0.069Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 119.21				Clashscore: 0.72	Outliers: 16 of 183	Poor rotamers: 28 of 166	Outliers: 4 of 176	Outliers: 0 of 185
929	ASP	53.89	-	Favored (5.17%) General / -105.0,-43.0	13.7% ( <i>t0</i> ) chi angles: 205.6,28.7	0.214Å	-	-
930	SER	98.55	-	Favored (4.04%) General / -79.2,-174.3	38.6% ( <i>t</i> ) chi angles: 181.8	0.113Å	-	-
931	SER	122.54	-	Allowed (1.39%) General / -142.9,54.1	24.4% ( <i>p</i> ) chi angles: 51.2	0.17Å	-	-
932	SER	131.42	-	Favored (10.18%) General / -83.2,71.6	74% ( <i>m</i> ) chi angles: 295.1	0.03Å	-	-
933	LEU	130.59	-	Favored (5.69%) General / -84.3,60.0	6.3% ( <i>mt</i> ) chi angles: 299.2,147.7	0.106Å	-	-
934	GLU	53.23	-	Favored (21.08%) General / -59.9,124.7	45.1% ( <i>mt-10</i> ) chi angles: 297.9,178,271.8	0.061Å	-	-
935	ILE	105.37	-	Favored (3.97%) Isoleucine or valine / -107.4,166.6	3.5% ( <i>tt</i> ) chi angles: 206.4,149.6	0.2Å	-	-
936	LEU	150.09	-	Favored (18.07%) General / -105.5,-8.5	6% ( <i>mp</i> ) chi angles: 293.5,83.4	0.094Å	-	-
937	GLU	100.38	-	Favored (2.18%) General / 51.0,-130.3	0.2% chi angles: 199.2,235.9,236.7	0.197Å	-	-

938	ASN 147.81	-	Allowed (0.64%) General / -152.2,23.0	0.9% chi angles: 56.9,252	0.077Å	-	-
939	SER 131.16	-	Allowed (0.96%) General / -151.7,-159.0	38.4% ( <i>p</i> ) chi angles: 76.6	0.16Å	-	-
940	GLU 199.01	-	Favored (2.2%) General / -82.5,53.0	46.2% ( <i>mt-10</i> ) chi angles: 297.4,186.4,242.6	0.05Å	-	-
941	THR 141.08	-	Favored (2.06%) General / -167.4,133.0	8.8% ( <i>t</i> ) chi angles: 182.5	0.055Å	-	-
942	THR 59.17	-	Favored (27.66%) Pre-proline / -113.3,93.7	34.5% ( <i>p</i> ) chi angles: 52.2	0.04Å	-	-
943	PRO 95.5	-	Allowed (0.65%) Trans-proline / -69.6,98.0	53% ( <i>Cg_exo</i> ) chi angles: 336.4	0.047Å	-	-
944	SER 41.59	-	Favored (8.57%) General / -55.3,152.3	74% ( <i>m</i> ) chi angles: 295.1	0.027Å	-	-
945	LYS 87.11	-	Allowed (0.83%) General / -157.8,77.8	7% ( <i>ttmt</i> ) chi angles: 189.4,216.1,298.8,148	0.072Å	-	-
946	ASP 50.78	-	Allowed (1.13%) General / -67.4,102.5	3.7% ( <i>m-20</i> ) chi angles: 280.5,90.9	0.034Å	-	-
947	MET 134.99	-	Favored (15.09%) General / -111.0,162.2	0% chi angles: 195.1,222.8,164.7	0.093Å	-	-
948	LYS 77.65	-	Favored (14.57%) General / -139.2,171.2	1.7% ( <i>mptp?</i> ) chi angles: 290.1,88.5,197.3,67.2	0.037Å	-	-

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Avg: 119.21				Clashscore: 0.72	Outliers: 16 of 183	Poor rotamers: 28 of 166	Outliers: 4 of 176	Outliers: 0 of 185	Outliers: 32 of 185



949	LYS 103.24	-	Favored (59.68%) General / -54.9,-31.5	57.7% ( <i>mttp</i> ) chi angles: 298.4,191.1,180.5,72.5	0.122Å	-	-
950	THR 115.54	-	Favored (51.21%) General / -53.2,-33.1	33.7% ( <i>p</i> ) chi angles: 52	0.089Å	-	-
951	LYS 114.73	-	Allowed (1.81%) General / 77.9,12.7	33.9% ( <i>ttpt</i> ) chi angles: 191.8,190.1,63,177.8	0.08Å	-	-
952	LYS 88.96	-	Favored (3.22%) General / -150.2,104.0	0.1% chi angles: 210.6,300.1,92.8,198.1	0.081Å	-	-
953	ILE 125.53	-	-	0% chi angles: 194.8,265.9	0.258Å	-	-

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