

Viewing RPGRIP1_mb_621-757Hmulti.table

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All-Atom				1 st percentile* (N=1784, all resolutions)		
Contacts	Clashscore is the number	of serious	steric ove	laps (> 0.4 Å) per 1000 atoms.		
	Poor rotamers	3	2.61%	Goal: <1%		
	Ramachandran outliers	1	0.74%	Goal: <0.05%		
II I	Ramachandran favored	97.04%		Goal: >98%		
Protein Geometry	MolProbity score [^]	2.79		32 nd percentile* (N=27675, 0Å - 99Å)		
	Cβ deviations >0.25Å	0	0.00%	Goal: 0		
	Bad backbone bonds:	0 / 1123	0.00%	Goal: 0%		
	Bad backbone angles:	23 / 1530	1.50%	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: 81.34	Clashscore: 68.62	Outliers: 1 of 135	Poor rotamers: 3 of 115	Outliers: 0 of 128		
621	1	LEU	38.1	0.76Å CD1 with 755 ARG HA	-	63.3% (<i>mt</i>) chi angles: 291.8,182.3	0.064Å	-	-
622		HIS	116.2	0.718Å HE1 with 756 PHE HB3	Favored (41.83%) General / -70.9,154.4	0.3% chi angles: 24.2,83.4	0.037Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.441 σ
623	(GLN	69.75	-	Favored (14.99%) General / -62.1,122.2	61% (<i>mm-40</i>) chi angles: 298.4,282.2,339.3	0.118Å	-	-
624	. (GLY	20.13	-	Favored (39.92%) Glycine / 167.2,179.0	-	-	-	-

^{* 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.

625	GLU 93.64	0.816Å HG3 with 685 GLU OE2	Favored (38.57%) General / -73.0,156.7	1.8% (<i>mp0</i>) chi angles: 281.9,47,70.7	0.079Å	-	-
626	ASN 52.63	0.744Å HA with 757 PRO HD2	Favored (52.34%) General / -127.7,140.0	97.6% (<i>m-20</i>) chi angles: 291.5,342.1	0.145Å	-	-
627	LEU 56.09	0.899Å HB2 with 757 PRO HG3	Favored (44.21%) General / -118.3,123.0	44% (<i>tp</i>) chi angles: 182,68.6	0.104Å	-	-
628	PHE 132.53	0.782Å CE2 with 754 LEU HD21	Favored (30.31%) General / -103.9,115.3	49% (<i>t80</i>) chi angles: 189.1,270.8	0.078Å	-	-
629	GLU 64.34	0.632Å HG2 with 681 GLN HB3	Favored (45.82%) General / -116.7,143.3	79.5% (<i>mt-10</i>) chi angles: 300,162.9,339	0.161Å	-	-
630	LEU 55.14	0.74Å HD21 with 628 PHE CE1	Favored (13.77%) General / -136.2,116.7	82.3% (<i>mt</i>) chi angles: 296.3,181.4	0.094Å	-	-
631	HIS 80.09	0.535Å HB3 with 751 TRP CE2	Favored (56.18%) General / -112.3,128.2	13.5% (<i>t-80</i>) chi angles: 183.7,305.6	0.128Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.346 σ
632	ILE 93.48	0.407Å CD1 with 750 TYR HB3	Favored (48.64%) Isoleucine or valine / -109.9,115.0	43.4% (<i>mm</i>) chi angles: 298.2,296.2	0.077Å	-	-
633	HIS 94.51	-	Favored (3.91%) General / -66.8,-59.0	9.7% (<i>t60</i>) chi angles: 198.7,96.8	0.06Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.437 σ
634	GLN 61.67	0.827Å CG with 675 LEU HD23	Favored (2.68%) General / -174.2,175.4	91.4% (<i>mt-30</i>) chi angles: 294.8,178.8,306.5	0.219Å	-	-
635	ALA 44.85	-	Favored (44.47%) General / -124.9,125.8	-	0.095Å	-	-
636	PHE 102.54	0.617Å HA with 673 GLN OE1	Favored (17.56%) General /	58.9% (<i>t80</i>) chi angles: 187.1,67.5	0.035Å	-	-

637	LEU 92.95	0.758Å HB3 with 641 ALA HB3	-100.4,155.9 Favored (17.08%) General / -123.6,165.5	5.8% (<i>mp</i>) chi angles: 292.9,64.8	0.09Å	-	-
638	THR 114.84	0.497Å HG23 with 640 ALA N	Favored (8.48%) General / -94.8,171.9	14% (<i>t</i>) chi angles: 186.7	0.08Å	-	-
639	SER 70.56	-	Favored (69.47%) General / -57.8,-34.4	40.4% (<i>t</i>) chi angles: 176.8	0.105Å	-	-
640	ALA 44.87	0.551Å O with 644 GLN HG3	Favored (77.23%) General / -64.4,-48.0	-	0.08Å	-	-
# Al	lt Res High E	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
	Avg: 81.34	Clashscore: 68.62	Outliers: 1 of 135	Poor rotamers: 3 of 115		Outliers:	Outliers: 23 of 137
641	ALA 58.54	0.758Å HB3 with 637 LEU HB3	Favored (90.53%) General / -64.9,-38.3	-	0.104Å	-	-
642	LEU 141.39	-	Favored (72.29%) General / -60.5,-50.8	22.6% (<i>tp</i>) chi angles: 192.6,60.7	0.052Å	-	-
643	ALA 43.44	-	Favored (75.2%) General / -69.6,-41.9	-	0.071Å	-	-
644	GLN 75.48	0.551Å HG3 with 640 ALA O	Favored (67.06%) General / -62.7,-23.3	29.1% (<i>mt-30</i>) chi angles: 290.1,176,130.5	0.041Å	-	-
645	ALA 55.96	-	Favored (72.9%) General / -54.8,-43.6	-	0.081Å	-	-
646	GLY 45.12	-	Favored (7.22%) Glycine / 118.5,12.7	-	-	-	-
647	ASP 64.91	-	Favored (18.66%)	65.7% (m-20)	0.019Å	-	OUTLIER(S) worst is CA-

			General / 60.8,28.9	chi angles: 295.2,305.1			CB-CG: 6.067 σ
648	THR 108.4	0.422Å O with 650 PRO HD3	Favored (46.84%) General / -132.1,136.0	15.3% (<i>t</i>) chi angles: 187.8	0.065Å	-	-
649	GLN 73.46	0.609Å HB3 with 670 VAL HG12	Favored (3.96%) Pre-proline / -61.3,111.2	46.9% (<i>mt-30</i>) chi angles: 293,168.8,266.5	0.059Å	-	-
650	PRO 83.32	0.436Å HD2 with 649 GLN HA	Favored (49.91%) Trans-proline / -67.5,139.7	59% (<i>Cg_endo</i>) chi angles: 26.8	0.075Å	-	-
651	THR 110.27	0.935Å HG22 with 670 VAL HG22	Favored (43.74%) General / -118.6,122.9	68.7% (p) chi angles: 63.2	0.086Å	-	-
652	THR 44.26	0.439Å HG22 with 705 GLN HA	Favored (27.94%) General / -142.0,165.3	50.7% (p) chi angles: 65.8	0.092Å	-	-
653	PHE 67.73	0.518Å HE1 with 706 ALA HB2	Favored (33.57%) General / -150.0,151.6	26.8% (<i>p90</i>) chi angles: 61.7,283.3	0.092Å	-	-
654	CYS 51.54	0.925Å HB2 with 701 LEU HD11	Favored (23.31%) General / -116.9,158.8	19.4% (<i>p</i>) chi angles: 54.6	0.065Å	-	-
655	THR 124.52	0.625Å O with 701 LEU HD12	Favored (27.14%) General / -149.2,145.5	8.7% (t) chi angles: 179.9	0.046Å	-	-
656	TYR 67.33	-	Favored (25.78%) General / -154.4,168.7	44.9% (<i>p90</i>) chi angles: 58.3,84.6	0.076Å	-	-
657	SER 73.86	0.935Å HB2 with 663 THR HG22	Favored (37.15%) General / -139.8,144.1	41.3% (t) chi angles: 177.3	0.118Å	-	-
658	PHE 60.88	0.666Å CD2 with 659 TYR HB2	Favored (48.68%) General / -122.2,144.9	84.4% (<i>t80</i>) chi angles: 179.9,83.1	0.116Å	-	OUTLIER(S) worst is CA- CB-CG: 4.534 σ
		0.667Å	Favored	43.4% (<i>t80</i>)			

659	TYR	78.28	HB3 with 661 PHE CE2	(16.99%) General / 54.5,32.6	chi angles: 193.2,77	0.061Å	-	-
660	ASP	47.8	-	Favored (27.67%) General / 51.6,45.7	60.6% (<i>t0</i>) chi angles: 188.4,0.5	0.065Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 81.34	Clashscore: 68.62	Outliers: 1 of 135	Poor rotamers: 3 of 115		Outliers: 0 of 137	Outliers: 23 of 137
661	PHE	71.15	0.667Å CE2 with 659 TYR HB3	Favored (5.1%) General / -97.0,179.0	39.1% (<i>m-85</i>) chi angles: 280.6,288.4	0.152Å	-	OUTLIER(S) worst is CA- CB-CG: 4.664 σ
662	GLU	77.3	-	Favored (57.63%) General / -59.7,135.3	36.4% (<i>tt0</i>) chi angles: 180.1,184.3,297	0.091Å	-	-
663	THR	100.09	0.935Å HG22 with 657 SER HB2	Favored (34.68%) General / -79.3,144.0	58.9% (<i>p</i>) chi angles: 62.6	0.072Å	-	-
664	HIS	37.23	-	Favored (49.57%) General / -113.6,138.9	67.5% (<i>t60</i>) chi angles: 183.5,85.1	0.113Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.49 σ
665	CYS	78.71	-	Favored (45.09%) General / -98.5,130.4	19.4% (<i>p</i>) chi angles: 54.6	0.062Å	-	-
666	THR	45.77	0.823Å HG21 with 654 CYS SG	Favored (92.69%) Pre-proline / -68.6,155.6	67.6% (p) chi angles: 59.4	0.05Å	-	-
667	PRO	82.06	-	Favored (19.55%) Trans-proline / -68.1,129.5	16.9% (<i>Cg_endo</i>) chi angles: 16.9	0.138Å	-	-
668	LEU	99.99	0.577Å N with 668 LEU HD12	Favored (35.96%) General / -80.5,140.3	4.4% (<i>mp</i>) chi angles: 297.3,65.4	0.067Å	-	-
669	SER	34.99	-	Favored (26.41%) General / -150.8,146.5	73.7% (<i>m</i>) chi angles: 293.9	0.082Å	-	-

670	VAL 36.25	0.935Å HG22 with 651 THR HG22	Favored (5.04%) Isoleucine or valine / -92.9,147.9	93.1% (<i>t</i>) chi angles: 178.1	0.072Å	-	-
671	GLY 40.97	0.465Å N with 670 VAL HG12	Favored (11.63%) Glycine / 136.6,169.1	-	-	-	-
672	PRO 169.99	-	Allowed (0.28%) Trans-proline / -74.6,-46.0	51.9% (<i>Cg_exo</i>) chi angles: 335.1	0.171Å	-	-
673	GLN 139.8	0.617Å OE1 with 636 PHE HA	Favored (41.33%) Pre-proline / -135.0,82.9	31.1% (<i>tp60</i>) chi angles: 181.7,80.9,10.9	0.139Å	-	-
674	PRO 77.1	-	Favored (22.32%) Trans-proline / -80.2,163.7	13.2% (<i>Cg_endo</i>) chi angles: 15.8	0.113Å	-	-
675	LEU 70.84	0.827Å HD23 with 634 GLN CG	Favored (7.59%) General / -109.1,98.1	65.2% (<i>mt</i>) chi angles: 288.9,179	0.2Å	-	-
676	TYR 55.87	-	Favored (92.95%) General / -59.5,-42.8	97.1% (<i>m-85</i>) chi angles: 293.5,276.1	0.142Å	-	-
677	ASP 46.2	-	Favored (28.9%) General / 51.6,41.5	75% (<i>m-20</i>) chi angles: 289.2,358.1	0.08Å	-	OUTLIER(S) worst is CA- CB-CG: 4.038 σ
678	PHE 55.18	0.577Å CE2 with 680 SER HB3	Favored (47.37%) General / -100.8,126.8	87.2% (<i>t80</i>) chi angles: 176.8,73.5	0.058Å	-	OUTLIER(S) worst is CA- CB-CG: 4.051 σ
679	THR 46.88	-	Favored (23.79%) General / -123.7,116.9	86.3% (<i>m</i>) chi angles: 302.7	0.09Å	-	-
680	SER 87.33	0.577Å HB3 with 678 PHE CE2	Favored (49.83%) General / -116.5,140.0	25.1% (<i>p</i>) chi angles: 78.6	0.165Å	-	-
# Al	t Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg:	Clashscore:	Outliers: 1 of	Poor rotamers: 3 of		•	Outliers: 23

 $http://molprobity.biochem.duke.edu/viewtable.php? MolProbSID=5 iurpv...6 pr 0 vo 3 t 45 hbc 2 d 1 rb 1 qdv 9 o/raw_data/RPGRIP1_mb_621-757 H-multi.table$

	81.34	68.62	135	115	0 of 128	0 of 137	of 137
681	GLN 55.82	0.632Å HB3 with 629 GLU HG2	Favored (21.25%) General / -150.7,139.9	15.2% (<i>pt20</i>) chi angles: 62.6,180.8,18	0.073Å	-	-
682	TYR 89.63	0.514Å C with 627 LEU HD12	Favored (30.84%) General / -142.7,138.9	3.6% (<i>p90</i>) chi angles: 37.2,88.7	0.036Å	-	OUTLIER(S) worst is CA- CB-CG: 4.831 σ
683	VAL 40.3	0.587Å HG22 with 627 LEU HD13	Favored (19.72%) Isoleucine or valine / -86.7,110.0	76.8% (<i>t</i>) chi angles: 172.8	0.067Å	-	-
684	MET 86.14	0.617Å CE with 661 PHE HZ	Favored (51.41%) General / -127.1,142.8	19.6% (<i>tpp</i>) chi angles: 189.2,59,41	0.102Å	-	-
685	GLU 130.39	0.816Å OE2 with 625 GLU HG3	Favored (16.58%) General / -112.1,107.6	58% (<i>mp0</i>) chi angles: 295.7,77.8,8.1	0.091Å	-	-
686	THR 91.25	0.851Å HG21 with 689 LEU HB2	Favored (2.2%) General / -162.3,120.7	94.7% (<i>m</i>) chi angles: 299.9	0.086Å	-	-
687	ASP 108.83	-	Favored (2.03%) General / -93.1,-59.5	69% (<i>m-20</i>) chi angles: 296.6,352.6	0.045Å	-	OUTLIER(S) worst is CA- CB-CG: 6.403 σ
688	SER 47.82	-	Favored (34.32%) General / -67.7,-52.7	47.2% (<i>t</i>) chi angles: 180.2	0.076Å	-	-
689	LEU 51.68	0.851Å HB2 with 686 THR HG21	Favored (70.63%) General / -64.1,-29.5	52.4% (<i>mt</i>) chi angles: 294.3,185.6	0.067Å	-	-
690	PHE 116.92	0.407Å CE2 with 658 PHE HZ	Favored (54.12%) General / -60.8,-53.7	29.3% (<i>t80</i>) chi angles: 189.1,281	0.086Å	-	OUTLIER(S) worst is CA- CB-CG: 5.078 σ
691	LEU 48.45	-	Favored (92.33%) General / -62.6,-45.6	87.8% (<i>mt</i>) chi angles: 299.1,180	0.11Å	-	-
692	HIS 69.78	-	Favored (76.3%) General /	90% (<i>m-70</i>) chi angles: 289,272.7	0.061Å	-	OUTLIER(S) worst is CD2- NE2-CE1:

			-63.2,-33.8				4.358σ
693	TYR 46.82	0.788Å HA with 696 GLU HG2	Favored (98.77%) General / -60.8,-43.0	35.7% (<i>t80</i>) chi angles: 172.9,274.8	0.085Å	-	-
694	LEU 143.63	0.655Å HD21 with 721 PHE O	Favored (80.75%) General / -56.4,-44.8	43.9% (<i>tp</i>) chi angles: 171.6,67.2	0.137Å	-	-
695	GLN 67.23	-	Favored (30.41%) General / -73.6,-48.7	26.4% (mm100) chi angles: 304.8,296.8,132.8	0.097Å	-	-
696	GLU 86.47	0.788Å HG2 with 693 TYR HA	Favored (84.14%) General / -60.1,-47.9	10.6% (<i>pt-20</i>) chi angles: 58.6,167.3,300.8	0.111Å	-	-
697	ALA 33.03	0.666Å N with 696 GLU HG3	Favored (46.6%) General / -139.7,152.3	-	0.106Å	-	-
698	SER 80.78	0.602Å HB3 with 718 TRP NE1	Favored (12.16%) General / -121.5,168.0	45.8% (t) chi angles: 180.6	0.066Å	-	-
699	ALA 41.79	1.002Å HB3 with 719 ILE HG23	Favored (31.03%) General / -81.8,144.5	-	0.061Å	-	-
700	ARG 111.88	0.64Å HD2 with 700 ARG N	Favored (23.84%) General / -116.9,114.5	0.8% chi angles: 318.7,73.3,179.9,165.4	0.196Å	-	-
# Al	t Res High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
	Avg:	Clashscore:	Outliers: 1 of	Poor rotamers: 3 of			
	81.34	68.62	135	115	0 of 128	0 of 137	of 137
701	LEU 74.18	0.925Å HD11 with 654 CYS HB2	Favored (16.58%) General / -119.4,110.1	25.7% (<i>tp</i>) chi angles: 179.9,74.1	0.175Å	-	-
702	ASP 51.95	-	Favored (33.26%) General / -107.6,145.5	82.2% (<i>m-20</i>) chi angles: 296.9,341.1	0.046Å	-	OUTLIER(S) worst is CA- CB-CG: 6.399 σ
		0.72Å	Favored (51.05%)				

703	ILE 100.62	CG2 with 715 ALA HB3	Isoleucine or valine / -107.8,116.3	19.9% (tt) chi angles: 185.1,169.3	0.055Å	-	-
704	HIS 61.86	-	Favored (35.69%) General / -114.4,149.7	1.4% (<i>p-80</i>) chi angles: 30.7,261.2	0.068Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.329 σ
705	GLN 55.38	0.439Å HA with 652 THR HG22	Favored (36.24%) General / -90.5,127.5	7% (tt0) chi angles: 180.1,176.8,161.1	0.071Å	-	-
706	ALA 46.22	0.518Å HB2 with 653 PHE HE1	Favored (30.78%) General / -102.1,115.5	-	0.091Å	-	-
707	MET 100.62	0.938Å HG3 with 710 GLU H	Favored (11.76%) General / -104.9,164.5	23.9% (<i>ptp</i>) chi angles: 64.5,186,65.8	0.121Å	-	-
708	ALA 30.22	-	Favored (98.9%) General / -62.4,-41.8	-	0.094Å	-	-
709	SER 48.93	-	Favored (8.39%) General / -74.7,-53.9	98.6% (p) chi angles: 64.2	0.066Å	-	-
710	GLU 61.29	0.938Å H with 707 MET HG3	Favored (4.33%) General / -143.0,-175.0	64.6% (tt0) chi angles: 194,167.5,349.9	0.062Å	-	-
711	HIS 82.81	0.557Å H with 710 GLU HG2	Favored (50.94%) General / -129.1,147.5	60.8% (<i>m80</i>) chi angles: 303.9,82.5	0.201Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.469 σ
712	SER 45.61	-	Favored (31.23%) General / -153.9,153.0	98.6% (p) chi angles: 64.6	0.112Å	-	-
713	THR 77.82	-	Favored (28.23%) General / -109.9,114.6	62% (<i>m</i>) chi angles: 303.7	0.077Å	-	-
714	LEU 180.94	0.558Å HD23 with 745 PHE CE1	Favored (29.16%) General / -82.0,-35.1	61.1% (<i>tp</i>) chi angles: 179.9,64	0.081Å	-	-

715	ALA 62.75	0.72Å HB3 with 703 ILE CG2	Favored (43.41%) General / -143.4,158.7	-	0.074Å	-	-
716	ALA 49.31	-	Favored (19.38%) General / -153.3,140.4	-	0.098Å	-	-
717	GLY 22.06	-	Favored (25.27%) Glycine / -141.3,168.9	-	-	-	-
718	TRP 158.33	0.602Å NE1 with 698 SER HB3	Favored (28.67%) General / -113.5,115.9	51.7% (<i>t-105</i>) chi angles: 187.9,270.8	0.14Å	-	-
719	ILE 106.65	1.002Å HG23 with 699 ALA HB3	Favored (43.49%) Isoleucine or valine / -101.0,115.9	20.6% (tt) chi angles: 190.9,166.9	0.101Å	-	-
720	CYS 84.05	0.518Å HB2 with 698 SER OG	Favored (47.35%) General /	49.7% (t) chi angles: 186.4	0.097Å	-	-
			-139.5,152.9				
# Al	t Res High B	Clash > 0.4Å	-139.5,152.9 Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
# A l	Avg:	0.4Å Clashscore:	Ramachandran Outliers: 1 of	Poor rotamers: 3 of	deviation Outliers:	lengths Outliers:	Outliers: 23
# Al		0.4Å	Ramachandran Outliers: 1 of 135		deviation	lengths Outliers:	Outliers: 23 of 137
# Al	Avg:	0.4 Å Clashscore: 68.62 0.714Å	Ramachandran Outliers: 1 of	Poor rotamers: 3 of	deviation Outliers:	lengths Outliers:	Outliers: 23
	Avg: 81.34	0.4Å Clashscore: 68.62 0.714Å HD1 with 752	Ramachandran Outliers: 1 of 135 Favored (25.05%) General /	Poor rotamers: 3 of 115 66.3% (<i>m</i> -85)	deviation Outliers: 0 of 128	lengths Outliers:	Outliers: 23 of 137 OUTLIER(S) worst is CA- CB-CG: 5.959
721	Avg: 81.34 PHE 72.36	0.4Å Clashscore: 68.62 0.714Å HD1 with 752	Ramachandran Outliers: 1 of 135 Favored (25.05%) General / -117.6,115.4 Favored (29.33%) General /	Poor rotamers: 3 of 115 66.3% (<i>m-85</i>) chi angles: 305.5,285.1	deviation Outliers: 0 of 128 0.126Å	lengths Outliers:	Outliers: 23 of 137 OUTLIER(S) worst is CA- CB-CG: 5.959
721 722	Avg: 81.34 PHE 72.36 ASP 109.07	0.4Å Clashscore: 68.62 0.714Å HD1 with 752 MET HE3 - 0.954Å HD2 with 731	Ramachandran Outliers: 1 of 135 Favored (25.05%) General / -117.6,115.4 Favored (29.33%) General / -76.7,-45.4 Favored (74.71%) General /	Poor rotamers: 3 of 115 66.3% (<i>m-85</i>) chi angles: 305.5,285.1 20.3% (<i>p-10</i>) chi angles: 59.5,318.9 91.1% (<i>mtt180</i>) chi angles: 294.9,194.4,180.2,192.5 93.7% (<i>t</i>) chi angles: 175.7	deviation Outliers: 0 of 128 0.126Å 0.067Å	lengths Outliers:	Outliers: 23 of 137 OUTLIER(S) worst is CA- CB-CG: 5.959

			General / -60.5,-52.3	chi angles: 187.5,61.3			
726	GLU 103.33	-	Favored (4.74%) General / -78.6,-56.0	84.9% (<i>tt0</i>) chi angles: 183.6,179.7,348.1	0.059Å	-	-
727	THR 60.75	0.636Å HG22 with 728 VAL N	Favored (6.53%) General / -111.2,173.0	47.5% (<i>m</i>) chi angles: 305.1	0.052Å	-	-
728	VAL 120.12	0.636Å N with 727 THR HG22	Favored (6.26%) Isoleucine or valine / -147.4,129.0	30.7% (<i>m</i>) chi angles: 296.9	0.062Å	-	-
729	GLU 78.6	0.515Å HG3 with 728 VAL O	OUTLIER (0%) General / 149.0,-156.6	49.7% (<i>mt-10</i>) chi angles: 272.5,168.4,348.7	0.172Å	-	OUTLIER(S) worst is N-CA- CB: 4.051 σ
730	LYS 122.19	0.554Å HD2 with 730 LYS N	Favored (3.57%) General / -75.5,96.8	11.3% (<i>mptt</i>) chi angles: 295,66.1,180.1,176.9	0.079Å	-	-
731	VAL 111.58	0.954Å HG21 with 723 ARG HD2	Favored (37.3%) Isoleucine or valine / -113.6,111.7	7.7% (p) chi angles: 56.7	0.051Å	-	-
732	HIS 75.19	-	Favored (57.79%) General / -66.5,141.7	42.8% (<i>m80</i>) chi angles: 301.4,113	0.067Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.415 σ
733	GLY 20.13	0.443Å O with 734 LEU HD23	Favored (33.79%) Glycine / -161.6,162.2	-	-	-	-
734	LEU 49.75	0.443Å HD23 with 733 GLY O	Favored (20.16%) General / -136.0,168.0	62.6% (<i>mt</i>) chi angles: 293.8,183.7	0.129Å	-	-
735	ALA 37.22	-	Favored (45.52%) General / -136.7,146.1	-	0.105Å	-	-
736	THR 90.01	-	Favored (17.86%) General / -94.6,153.4 Favored	13.4% (<i>t</i>) chi angles: 186.4	0.08Å	-	-

737	LEU 73.55	0.503Å C with 738 ILE HD12	(54.4%) General / -119.0,135.8	60.3% (<i>mt</i>) chi angles: 288.6,179.7	0.076Å	-	-
738	ILE 87.79	0.541Å N with 738 ILE HD12	Favored (48.18%) Isoleucine or valine / -123.8,140.1	2.5% (<i>mp</i>) chi angles: 297.3,69.3	0.08Å	-	-
739	GLY 39.66	-	Favored (27.57%) Glycine / -77.0,142.4	-	-	-	-
740	ALA 33.6	-	Favored (79.85%) General / -65.4,-46.5	-	0.106Å	-	-
# A l	It Res High B	Clash > 0.4Å	Ramachandran	Rotamer	$\begin{array}{c} C\beta \\ \text{deviation} \end{array}$	Bond lengths	Bond angles
	Avg: 81.34	Clashscore: 68.62	Outliers: 1 of 135	Poor rotamers: 3 of 115	Outliers: 0 of 128		Outliers: 23 of 137
741	GLY 72.45	-	Favored (99.11%) Glycine / -63.5,-41.9	-	-	-	-
742	GLY 302.96	0.524Å O with 743 GLU HG3	Favored (2.46%) Glycine / 121.1,116.4	-	-	-	-
743	GLU 336.37	0.524Å HG3 with 742 GLY O	Allowed (0.42%) General / -171.5,-165.9	51.3% (<i>mt-10</i>) chi angles: 287.8,180.7,48.8	0.162Å	-	OUTLIER(S) worst is C-N-CA: 10.932σ
744	GLU 170.94	0.45Å H with 743 GLU HB3	Favored (3.12%) General / -89.5,22.0	93.9% (<i>mt-10</i>) chi angles: 292.5,185.3,1.2	0.101Å	-	-
		· · · · · · · · · · · · · · · · ·	Allowed				OUTLIER(S)
745	PHE 115.64	0.558Å CE1 with 714 LEU HD23	(1.96%) General / -43.0,-59.5	49.9% (<i>t80</i>) chi angles: 191.1,83	0.072Å	-	worst is CA- CB-CG: 4.646 σ
745 746	PHE 115.64 GLY 39.67	CE1 with 714	General /		0.072Å -	-	worst is CA-CB-CG: 4.646

		748 LEU N	valine / -119.3,151.6	chi angles: 177			
748	LEU 47.29	0.534Å N with 747 VAL HG12	Favored (49.26%) General / -114.2,139.6	43.2% (<i>tp</i>) chi angles: 186.2,62.5	0.061Å	-	-
749	GLU 76.92	0.426Å CD with 734 LEU HD21	Favored (29.21%) General / -107.0,114.9	35.6% (<i>mm-40</i>) chi angles: 280.7,280.3,353.4	0.109Å	-	-
750	TYR 64.12	0.407Å HB3 with 632 ILE CD1	Favored (32.04%) General / -147.2,164.8	32.9% (<i>p90</i>) chi angles: 57.9,79.9	0.093Å	-	-
751	TRP 66.7	0.535Å CE2 with 631 HIS HB3	Favored (37.88%) General / -145.1,151.0	61.3% (<i>p</i> -90) chi angles: 51.7,265.9	0.068Å	-	-
752	MET 126.29	0.793Å HE1 with 731 VAL HG13	Favored (46.26%) General / -129.0,154.8	0% chi angles: 53.6,290.4,192.3	0.089Å	-	-
753	ARG 135.06	0.537Å HD3 with 629 GLU OE1	Favored (23.25%) General / -152.2,143.4	2.2% (ptm180) chi angles: 58.9,145.4,274.6,205.4	0.152Å	-	-
754	LEU 193.6	0.782Å HD21 with 628 PHE CE2	Favored (11%) General / -135.3,113.2	4.5% (mm?) chi angles: 276.4,295.2	0.191Å	-	-
755	ARG 144.16	0.76Å HA with 621 LEU CD1	Favored (14.24%) General / -149.8,173.0	8.1% (<i>ptm-85</i>) chi angles: 59.2,186.6,294.3,268.2	0.089Å	-	-
756	PHE 109.12	0.718Å HB3 with 622 HIS HE1	Favored (89.99%) Pre-proline / -74.6,125.1	28.4% (<i>t80</i>) chi angles: 162.4,80.8	0.065Å	-	OUTLIER(S) worst is CA- CB-CG: 4.638 σ
757	PRO 61.62	0.899Å HG3 with 627 LEU HB2	-	19.3% (<i>Cg_endo</i>) chi angles: 17.7	0.122Å	-	OUTLIER(S) worst is N-CA- CB: 4.379 σ

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