Viewing gucy2d_sm_584-810_1H-multi.table

When finished, you should [close this window] .   *Hint: Use File | Save As... to save a copy of this page.*

All-Atom Contacts	Clashscore, all atoms:	208.45		0th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.51%	Goal: <1%
	Ramachandran outliers	10	4.44%	Goal: <0.05%
	Ramachandran favored	204	90.67%	Goal: >98%
	MolProbity score^	3.30		13th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	12	5.61%	Goal: 0
	Bad backbone bonds:	76 / 1846	4.12%	Goal: 0%
	Bad backbone angles:	87 / 2502	3.48%	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: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 584		LEU	99.99	1.085Å HB2 with A 689 ARG HB2	-	23.7% (*tp*) chi angles: 186.3,52.1	0.4Å	OUTLIER(S) worst is CA--CB: 12.115 σ	OUTLIER(S) worst is CD1-CG-CD2: 7.49 σ
A 585		GLN	50	0.662Å HG3 with A 689 ARG HE	Favored (67.91%) General / -59.5,-29.6	86.4% (*mt-30*) chi angles: 293.9,180.4,297.1	0.028Å	-	-
A 586		GLU	50	-	Favored (32.99%) General / -87.5,-17.1	54.2% (*mt-10*) chi angles: 296.1,182.6,296.7	0.032Å	-	-
A				1.17Å	Favored (17.52%)	86.4% (*mt*)			

587	LEU	50	HD13 with A 685 HIS CD2	General / -85.7,107.3	chi angles: 302.3,177.6	0.027Å	-	-
A 588	ARG	50	-	Favored (5.2%) General / -130.7,100.2	15.2% (*mtp85*) chi angles: 324.8,179.1,81.9,109	0.084Å	-	-
A 589	HIS	50	0.85Å O with A 592 VAL HG22	Favored (20.17%) General / -157.1,146.3	59.9% (*t-80*) chi angles: 183.7,276.6	0.043Å	OUTLIER(S) worst is CG--ND1: 4.376 σ	-
A 590	GLU	50	-	Favored (64.96%) General / -56.4,-32.6	54.4% (*mm-40*) chi angles: 292.1,289,0.4	0.038Å	-	-
A 591	ASN	50	0.447Å OD1 with A 652 LYS HE3	Favored (10.22%) General / -104.3,25.4	35.7% (*m120*) chi angles: 296.9,109.6	0.022Å	-	-
A 592	VAL	50	0.85Å HG22 with A 589 HIS O	Favored (56.97%) Isoleucine or valine / -122.1,137.0	33.5% (*m*) chi angles: 299.6	0.072Å	-	-
A 593	ALA	50	-	Favored (12.8%) General / -52.5,124.1	-	0.061Å	-	-
A 594	LEU	50	-	Favored (4.06%) General / -70.1,108.3	64.3% (*tp*) chi angles: 179.3,61.6	0.019Å	-	-
A 595	TYR	50	0.927Å CD1 with A 584 LEU HD23	Favored (51.9%) General / -68.6,135.7	85.5% (*t80*) chi angles: 181.1,73.4	0.09Å	-	-
A 596	LEU	50	-	Favored (5.57%) General / -125.6,178.6	94% (*mt*) chi angles: 294,176.6	0.053Å	-	-
A 597	GLY	50	0.569Å HA2 with A 607 PRO O	Favored (14.42%) Glycine / -135.3,142.9	-	-	-	-
A 598	LEU	99.99	1.1Å O with A 607 PRO HD2	Favored (26.05%) General / -150.5,145.5	97.4% (*mt*) chi angles: 298.3,177.5	0.036Å	-	-
			1.302Å	Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 599		PHE	99.99	CD2 with A 606 GLY HA3	(15.77%) General / -160.6,147.9	99.6% (*m-85*) chi angles: 297.2,96.6	0.044Å	-	-
A 600		LEU	99.99	-	Favored (7.26%) General / -124.9,101.8	97.5% (*mt*) chi angles: 296.6,176.7	0.065Å	-	-
A 601		ALA	99.99	-	Favored (65.78%) General / -55.1,-36.5	-	0.03Å	-	-
A 602		ARG	99.99	-	Favored (72.9%) General / -61.9,-32.5	99.7% (*mtt180*) chi angles: 294.1,182.5,178.6,179.9	0.026Å	-	-
A 603		GLY	99.99	-	Favored (28.82%) Glycine / -111.2,7.5	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 604		ALA	99.99	-	Favored (25.11%) General / 58.7,38.3	-	0.026Å	-	-
A 605		GLU	99.99	-	Favored (42.39%) General / -128.1,156.7	85.5% (*tt0*) chi angles: 187,178.5,350.5	0.061Å	-	-
A 606		GLY	99.99	1.302Å HA3 with A 599 PHE CD2	Favored (10.5%) Glycine / 174.8,153.9	-	-	-	-
A 607		PRO	99.99	1.137Å HA with A 608 ALA C	OUTLIER (0.04%) Trans-proline / -112.8,151.3	0.1% chi angles: 48.3	0.2Å	OUTLIER(S) worst is CA--CB: 5.978 σ	OUTLIER(S) worst is CA-N-CD: 6.292 σ
A 608		ALA	50	1.137Å C with A 607 PRO HA	Favored (10.05%) General / -47.1,127.1	-	0.2Å	-	OUTLIER(S) worst is C-CA-CB: 4.253 σ
A 609		ALA	50	0.913Å HA with A	Favored (5.62%) General /	-	0.034Å	-	-

			606 GLY O	-77.6,99.1				
A 610	LEU	50	0.918Å O with A 610 LEU HD23	Favored (38.08%) General / -102.2,11.6	9.1% (*tt*) chi angles: 184.4,157.8	0.071Å	-	-
A 611	TRP	50	-	Favored (53.64%) General / -112.9,124.9	46.5% (*m0*) chi angles: 295.5,357.1	0.041Å	-	-
A 612	GLU	50	0.615Å OE1 with A 613 GLY HA2	Favored (14.47%) General / -56.2,150.3	56.6% (*mm-40*) chi angles: 290.5,289,358.1	0.065Å	-	-
A 613	GLY	50	0.615Å HA2 with A 612 GLU OE1	Favored (3.27%) Glycine / -106.0,38.5	-	-	-	-
A 614	ASN	50	-	Favored (4.34%) General / -121.9,37.6	26.9% (*m120*) chi angles: 305.2,104.5	0.02Å	-	-
A 615	LEU	50	0.739Å HB3 with A 691 LEU HB3	Favored (9.71%) General / -50.9,123.7	68.4% (*mt*) chi angles: 300.4,184.1	0.069Å	-	-
A 616	ALA	50	0.914Å H with A 691 LEU HD12	Favored (27.57%) General / -153.8,149.6	-	0.09Å	-	-
A 617	VAL	50	0.634Å HB with A 690 LEU HA	Favored (62.23%) Isoleucine or valine / -107.7,129.2	8.9% (*p*) chi angles: 60.2	0.094Å	-	-
A 618	VAL	50	0.904Å HG21 with A 607 PRO HG3	Favored (67.76%) Isoleucine or valine / -110.5,126.7	48.8% (*t*) chi angles: 182.6	0.06Å	-	-
A 619	SER	50	-	Favored (16.9%) General / -134.6,169.7	47.7% (*t*) chi angles: 179.9	0.075Å	-	-
A 620	GLU	50	-	Favored (3.36%) General / -58.8,163.4	17.4% (*pt-20*) chi angles: 63.8,178.3,333.4	0.049Å	-	-

A 621		HIS	50	-	Favored (52.79%) General / -109.4,125.8	81.9% (*t60*) chi angles: 184.4,62.2	0.063Å	OUTLIER(S) worst is CG--ND1: 4.389 σ	-
A 622		CYS	50	0.713Å SG with A 673 ILE HD12	Favored (26.53%) General / -104.7,113.1	75.3% (*m*) chi angles: 298.7	0.067Å	-	-
A 623		THR	50	-	Favored (60.93%) General / -72.7,-23.8	68.7% (*p*) chi angles: 62	0.073Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 624		ARG	50	-	Favored (56.84%) General / -90.9,1.6	87.2% (*mtt-85*) chi angles: 293.5,185.4,184.1,290.7	0.06Å	-	-
A 625		GLY	50	-	Favored (49.79%) Glycine / 64.4,-152.4	-	-	-	-
A 626		SER	50	-	Favored (46.52%) General / -67.5,151.9	75.2% (*p*) chi angles: 70.6	0.034Å	-	-
A 627		LEU	50	0.728Å HD22 with A 680 LEU HD11	Favored (72.6%) General / -68.0,-32.3	54.5% (*tp*) chi angles: 179.5,58	0.057Å	-	-
A 628		GLN	99.99	-	Favored (36.48%) General / -61.6,-54.9	7.9% (*tp-100*) chi angles: 182.5,61.3,262.3	0.04Å	-	-
A 629		ASP	50	-	Favored (79.53%) General / -62.0,-35.7	61.9% (*m-20*) chi angles: 294.1,302.9	0.03Å	-	-
A 630		LEU	50	0.594Å O with A 633 GLN HG2	Favored (89.37%) General / -65.5,-38.3	51.3% (*tp*) chi angles: 181.2,57.8	0.012Å	-	-
A 631		LEU	50		Favored (61.84%) General /	76.3% (*mt*) chi angles: 296.4,182.8	0.028Å		

A 631	LEU	50	-	General / -75.0,-36.7	chi angles: 296.4,182.8	0.029A	-	-
A 632	ALA	50	-	Favored (36.68%) General / -90.1,-13.0	-	0.014Å	-	-
A 633	GLN	99.99	1.092Å HE21 with A 635 GLU HB3	Favored (68.83%) General / -64.1,-27.0	20.3% (pt20) chi angles: 60.9,180,65.3	0.01Å	-	-
A 634	ARG	99.99	0.633Å HG2 with A 634 ARG O	Favored (6.13%) General / 61.6,14.6	60.9% (ttm-85) chi angles: 180.4,183.4,297.2,274.1	0.068Å	-	-
A 635	GLU	99.99	1.092Å HB3 with A 633 GLN HE21	Allowed (0.47%) General / -81.1,25.3	88.1% (tt0) chi angles: 179.7,179.6,5.7	0.068Å	-	-
A 636	ILE	99.99	1.084Å HA with A 637 LYS HB3	Favored (12.48%) Isoleucine or valine / -68.7,147.0	22.8% (pt) chi angles: 70.5,166.7	0.382Å	-	OUTLIER(S) worst is N-CA-CB: 4.755 σ
A 637	LYS	50	1.089Å HE3 with A 635 GLU O	OUTLIER (0.01%) General / 124.7,-33.4	40.9% (ttmt) chi angles: 186,180.6,296.2,178.9	0.166Å	-	-
A 638	LEU	50	0.441Å H with A 636 ILE HB	Favored (19.81%) General / -126.4,115.5	23% (mt) chi angles: 312.9,173.6	0.107Å	-	-
A 639	ASP	50	0.803Å OD1 with A 642 PHE CD2	Favored (13.11%) General / -90.4,166.7	30.8% (p-10) chi angles: 64.4,337.4	0.02Å	-	-
A 640	TRP	50	1.017Å CZ2 with A 777 PRO HG3	Favored (62.96%) General / -52.9,-39.5	76.3% (t-105) chi angles: 179.8,255.6	0.038Å	-	-
A 641	MET	50	-	Favored (94.33%) General / -64.6,-39.8	28% (ttt) chi angles: 182.4,178.7,179.9	0.028Å	-	-
A 642	PHE	99.99	0.803Å CD2 with A 639 ASP OD1	Favored (71.21%) General / -68.9,-45.4	20.8% (m-30) chi angles: 293.7,331.2	0.025Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 643		LYS	50	0.961A HB3 with A 739 VAL HG22	Favored (75.43%) General / -65.5,-33.2	54.4% (*mtmt*) chi angles: 290,182.8,297.9,179.1	0.041Å	-	-
			Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 644		SER	50	0.574Å C with A 809 ASN HD21	Favored (68.84%) General / -71.1,-32.2	72.6% (*m*) chi angles: 295.6	0.009Å	-	-
A 645		SER	50	0.431Å N with A 809 ASN HD21	Favored (73.77%) General / -70.6,-36.9	75.1% (*m*) chi angles: 294.8	0.027Å	-	-
A 646		LEU	50	0.558Å HD21 with A 678 PHE O	Favored (97.52%) General / -61.9,-41.1	93.4% (*mt*) chi angles: 293.4,176.6	0.038Å	-	-
A 647		LEU	99.99	0.956Å HD11 with A 739 VAL HG11	Favored (95.78%) General / -62.1,-44.9	86.6% (*mt*) chi angles: 293.4,178.7	0.064Å	-	-
A 648		LEU	50	0.993Å HD12 with A 651 ILE HD11	Favored (91.75%) General / -60.6,-40.5	50.9% (*tp*) chi angles: 183.3,64.7	0.048Å	-	-
A 649		ASP	50	-	Favored (93.81%) General / -61.6,-45.5	92% (*m-20*) chi angles: 292.8,336.5	0.06Å	-	-
A 650		LEU	50	0.584Å C with A 650 LEU HD23	Favored (86.5%) General / -66.9,-38.5	7.8% (*tt*) chi angles: 177.4,156.2	0.026Å	-	-
A 651		ILE	50	1.107Å HB with A 802 PHE CE1	Allowed (0.63%) Isoleucine or valine / -56.2,-63.4	35.8% (*pt*) chi angles: 67.2,173.2	0.208Å	-	OUTLIER(S) worst is C-CA-CB: 4.585 σ
A 652		LYS	50	1.183Å HA with A 802 PHE CE2	Allowed (1.37%) General / -38.1,-50.4	55.6% (*mtmt*) chi angles: 295.2,181.5,296,177.2	0.323Å	-	-
A 653		GLY	50		Favored (92.49%)				

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
653 GLY	50	-	(92.49%) Glycine / -60.7,-47.2	-	-	-	-
A 654 ILE	99.99	0.76Å HG22 with A 798 MET HG3	Favored (81.18%) Isoleucine or valine / -66.1,-38.1	64.5% (*mt*) chi angles: 298,180.2	0.038Å	-	-
A 655 ARG	99.99	0.698Å O with A 659 HIS CD2	Favored (88.01%) General / -61.8,-38.4	71.4% (*ttp85*) chi angles: 181.6,177.9,62.5,86.3	0.057Å	-	-
A 656 TYR	50	-	Favored (75.79%) General / -67.0,-46.1	68% (*t80*) chi angles: 169.8,79	0.021Å	-	-
A 657 LEU	50	1.258Å HD21 with A 685 HIS NE2	Favored (89.5%) General / -62.3,-38.5	63.3% (*mt*) chi angles: 293.4,183.4	0.019Å	OUTLIER(S) worst is CG--CD2: 5.186 σ	OUTLIER(S) worst is CB-CG-CD2: 6.688 σ
A 658 HIS	50	-	Favored (63.77%) General / -69.3,-17.9	9.2% (*m170*) chi angles: 276.8,209.2	0.045Å	OUTLIER(S) worst is CD2--NE2: 4.421 σ	-
A 659 HIS	50	0.698Å CD2 with A 655 ARG O	Favored (38.62%) General / -100.3,11.8	95.9% (*m-70*) chi angles: 292.6,289.1	0.013Å	OUTLIER(S) worst is CD2--NE2: 5.556 σ	-
A 660 ARG	99.99	-	Favored (4.3%) General / -128.9,-15.6	61.2% (*ttm-85*) chi angles: 188.5,175.8,295.2,270.5	0.034Å	-	-
A 661 GLY	99.99	-	Favored (39.33%) Glycine / 164.2,-178.9	-	-	-	-
A 662 VAL	99.99	0.889Å HB with A 663 ALA HB2	Allowed (0.53%) Isoleucine or valine / -65.0,173.3	12% (*m*) chi angles: 307.3	0.205Å	-	OUTLIER(S) worst is C-N-CA: 5.512 σ
A 663 ALA	50	0.889Å HB2 with A 662 VAL HB	OUTLIER (0.01%) General / 165.5,123.3	-	0.106Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 65.20	Clashscore: 208.45		Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227

			65.20	208.45	225	196	214	of 227	of 227
A 664	HIS	50	1.193Å CD2 with A 704 GLU HB3	Favored (3.01%) General / -107.9,89.5	22.1% (*t-160*) chi angles: 189.6,194.8	0.045Å	OUTLIER(S) worst is CG-- CD2: 12.195 σ	OUTLIER(S) worst is CD2- NE2-CE1: 12.118 σ
A 665	GLY	50	1.147Å C with A 705 ASP HB2	Favored (13.26%) Glycine / -86.5,-33.6	-	-	OUTLIER(S) worst is C--N: 16.678 σ	OUTLIER(S) worst is C-N- CA: 5.229 σ
A 666	ARG	99.99	1.493Å CA with A 666 ARG CG	Allowed (0.06%) General / -51.0,-9.9	13.8% (*mmt-85*) chi angles: 326.6,281.8,206.3,276.7	0.888Å	OUTLIER(S) worst is CA-- C: 40.87 σ	OUTLIER(S) worst is O-C- N: 23.065 σ
A 667	LEU	50	0.963Å N with A 704 GLU CA	Favored (47.89%) General / -57.3,130.8	21.5% (*tp*) chi angles: 164.9,61	0.248Å	OUTLIER(S) worst is N-- CA: 13.216 σ	OUTLIER(S) worst is N-CA- C: 6.291 σ
A 668	LYS	50	1.115Å HE2 with A 703 ALA HB2	Favored (7.19%) General / -168.4,154.7	35.1% (*pttt*) chi angles: 63.2,187.2,191.2,204.8	0.019Å	-	-
A 669	SER	50	-	Favored (69.68%) General / -60.0,-31.2	57.8% (*p*) chi angles: 55.6	0.078Å	-	-
A 670	ARG	99.99	-	Favored (67.92%) General / -64.1,-25.1	99.5% (*mtt180*) chi angles: 290.4,183.8,178.2,178.7	0.022Å	-	-
A 671	ASN	50	0.831Å ND2 with A 703 ALA CB	Favored (30.91%) General / -84.1,-23.1	6.2% (*m-20*) chi angles: 274.8,26.9	0.023Å	-	OUTLIER(S) worst is CA- CB-CG: 4.243 σ
A 672	CYS	50	-	Favored (31%) General / -83.2,142.7	75% (*m*) chi angles: 298.6	0.03Å	-	-
A 673	ILE	50	0.713Å HD12 with A 622 CYS SG	Favored (17.17%) Isoleucine or valine / -115.3,150.8	34.2% (*pt*) chi angles: 60.4,178.1	0.051Å	-	-
A 674	VAL	50	-	Favored (59.17%) Isoleucine or valine / -127.7,136.9	23% (*t*) chi angles: 187.3	0.106Å	-	-
A	ASP	50	0.941Å CG with A	Allowed (1.82%)	27.9% (*p-10*)	0.019Å		

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 675		ASP	50	CG with A 679 VAL HG22 (1.82 %)	General / -96.5,-169.0	27.9 % (p-70) chi angles: 72.7,348	0.019Å	-	-
A 676		GLY	50	-	Favored (98.44%) Glycine / -62.6,-39.9	-	-	-	-
A 677		ARG	50	-	Favored (5.14%) General / -84.9,14.2	96.4% (mtt-85) chi angles: 294.6,180.6,178.2,273.9	0.034Å	-	-
A 678		PHE	99.99	0.558Å O with A 646 LEU HD21	Favored (12.11%) General / 65.3,24.5	97.2% (m-85) chi angles: 293.9,274.3	0.028Å	-	-
A 679		VAL	50	0.941Å HG22 with A 675 ASP CG	Favored (16.58%) Isoleucine or valine / -80.6,140.5	32.9% (m) chi angles: 300.2	0.043Å	-	-
A 680		LEU	50	0.728Å HD11 with A 627 LEU HD22	Favored (51.57%) General / -112.4,136.7	8.3% (tt) chi angles: 183,159.5	0.071Å	-	-
A 681		LYS	50	0.417Å N with A 680 LEU HD23	Favored (50.48%) General / -130.5,141.9	83.6% (mttt) chi angles: 304.4,190.5,179.3,191.5	0.041Å	-	-
A 682		ILE	50	0.943Å HD12 with A 657 LEU HD11	Favored (38.56%) Isoleucine or valine / -79.5,125.2	31.2% (pt) chi angles: 62.7,179.5	0.07Å	-	-
A 683		THR	50	0.517Å O with A 687 HIS CD2	Favored (9.81%) General / -88.4,14.3	80.9% (p) chi angles: 61.3	0.069Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 684		ASP	50	-	Favored (70.83%) General / -58.5,-51.2	38.1% (t70) chi angles: 183,58.3	0.065Å	-	-
A 685		HIS	99.99	1.258Å NE2 with A	Favored (85.79%)	60.9% (m170)	0.055Å	OUTLIER(S) worst is CD2--	OUTLIER(S) worst is CD2-

	HIS 99.99	NE2 with A 657 LEU HD21	(85.7 %) General / -63.7,-37.0	60.9 % (m170) chi angles: 298.3,166.6	0.033Å	worst is CD2 NE2: 13.407 σ	worst is CD2 NE2-CE1: 18.006 σ
A 686	GLY 50	-	Favored (98.58%) Glycine / -62.4,-43.8	-	-	-	-
A 687	HIS 99.99	0.888Å O with A 696 VAL HG11	Favored (78.07%) General / -69.4,-38.9	96.8% (m-70) chi angles: 293.5,280.5	0.024Å	OUTLIER(S) worst is CD2-- NE2: 4.673 σ	OUTLIER(S) worst is CB- CG-CD2: 4.166 σ
A 688	GLY 99.99	-	Favored (67.44%) Glycine / -63.6,-23.9	-	-	-	-
A 689	ARG 99.99	1.085Å HB2 with A 584 LEU HB2	Favored (19.14%) General / -110.1,1.8	39.2% (tpt85) chi angles: 188.4,65.4,182,70.7	0.448Å	OUTLIER(S) worst is CA-- CB: 14.566 σ	OUTLIER(S) worst is C-CA- CB: 6.949 σ
A 690	LEU 99.99	0.964Å HD22 with A 696 VAL HG21	Favored (50.2%) General / -68.7,134.7	6.9% (tt) chi angles: 183.3,163.7	0.072Å	-	-
A 691	LEU 99.99	0.914Å HD12 with A 616 ALA H	Favored (80.9%) General / -65.1,-35.4	82.1% (mt) chi angles: 294.8,180.4	0.011Å	-	-
A 692	GLU 99.99	0.817Å N with A 690 LEU HD23	Favored (2.96%) General / -76.1,75.1	67.9% (mt-10) chi angles: 308,181.5,332.5	0.037Å	-	-
A 693	ALA 99.99	0.838Å O with A 697 LEU HG	Favored (98.04%) General / -63.7,-42.5	-	0.029Å	-	-
A 694	GLN 99.99	1.026Å O with A 698 PRO HD3	Favored (82.99%) General / -63.7,-47.0	93.3% (mt-30) chi angles: 295.2,183.9,330.9	0.028Å	-	OUTLIER(S) worst is CA-C- O: 4.055 σ
A 695	LYS 99.99	0.797Å C with A 698 PRO HD2	Favored (58.31%) General / -75.8,-28.4	99.6% (mttt) chi angles: 294.6,182.4,177.9,180.3	0.06Å	-	-
A 696	VAL 99.99	1.264Å O with A 697 LEU N	Favored (21.69%) Isoleucine or valine / -79.6,-41.0	58.2% (t) chi angles: 180.7	0.16Å	OUTLIER(S) worst is C--O: 27.667 σ	OUTLIER(S) worst is CA-C- N: 5.786 σ
		1.264Å	Favored				OUTLIER(S)

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 697		LEU	50	1.264Å N with A 696 VAL O	Favored (3.08%) Pre-proline / -59.0,-27.0	93.7% (*mt*) chi angles: 293.2,176.2	0.062Å	OUTLIER(S) worst is C--O: 4.262 σ	-
A 698		PRO	50	1.026Å HD3 with A 694 GLN O	OUTLIER (0.04%) Trans-proline / -86.7,-45.6	89.5% (*Cg_endo*) chi angles: 31.9	0.054Å	OUTLIER(S) worst is N--CD: 8.758 σ	OUTLIER(S) worst is N-CD-CG: 5.683 σ
A 699		GLU	50	0.782Å HG2 with A 702 ARG NH2	Favored (8.95%) Pre-proline / -67.5,-35.8	87.2% (*mt-10*) chi angles: 301.4,183.7,338.2	0.028Å	-	-
A 700		PRO	99.99	1.053Å O with A 666 ARG HB2	Allowed (0.1%) Trans-proline / -63.3,-62.5	24.1% (*Cg_exo*) chi angles: 324.6	0.214Å	OUTLIER(S) worst is N--CD: 19.138 σ	OUTLIER(S) worst is N-CA-CB: 8.274 σ
A 701		PRO	99.99	1.121Å HA with A 666 ARG HG3	Favored (55.3%) Trans-proline / -66.4,-19.9	45.3% (*Cg_exo*) chi angles: 326.3	0.338Å	OUTLIER(S) worst is C--O: 25.425 σ	OUTLIER(S) worst is O-C-N: 23.724 σ
A 702		ARG	99.99	0.971Å HH12 with A 698 PRO HB2	Favored (11.4%) General / -82.4,-48.2	94.7% (*mtm-85*) chi angles: 293.2,190.3,298.6,268.6	0.134Å	OUTLIER(S) worst is N--CA: 4.251 σ	-
A 703		ALA	99.99	1.357Å C with A 704 GLU N	OUTLIER (0%) General / -47.8,-90.8	-	0.846Å	OUTLIER(S) worst is C--N: 31.615 σ	OUTLIER(S) worst is C-CA-CB: 16.348 σ
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 704		GLU	99.99	1.404Å C with A 705 ASP N	OUTLIER (0.01%) General / -17.3,-57.5	7.7% (*pt-20*) chi angles: 45.2,192.1,316.7	0.968Å	OUTLIER(S) worst is CA--CB: 39.736 σ	OUTLIER(S) worst is N-CA-CB: 12.57 σ
A 705		ASP	99.99	1.404Å N with A 704 GLU C	Allowed (0.13%) General / -150.6,-42.4	8% (*t70*) chi angles: 181.6,294.5	1.015Å	OUTLIER(S) worst is CA--CB: 11.082 σ	OUTLIER(S) worst is C-CA-CB: 11.221 σ
A 706		GLN	99.99	0.793Å HA with A 709 THR HG21	Favored (5.99%) General / -108.6,-37.2	94.7% (*mt-30*) chi angles: 297.4,182.1,329.5	0.273Å	-	-
A 707		LEU	99.99	1.082Å HD12 with A 668 LYS HD2	Favored (23.6%) General / -103.8,151.0	2.7% (*mt*) chi angles: 327.6,164.7	0.333Å	OUTLIER(S) worst is CB--CG: 9.189 σ	OUTLIER(S) worst is N-CA-CB: 5.956 σ

A 708	TRP	50	0.853Å HE3 with A 707 LEU HB2	Favored (8.37%) General / 66.1,12.3	5.5% (*m-90*) chi angles: 292.3,248.6	0.196Å	OUTLIER(S) worst is CD2-- CE3: 4.388 σ	OUTLIER(S) worst is CD2- CE3-CZ3: 5.955 σ
A 709	THR	50	0.912Å HG22 with A 705 ASP O	Favored (50.14%) General / -71.1,138.9	20.6% (*p*) chi angles: 48.5	0.091Å	OUTLIER(S) worst is CB-- CG2: 8.081 σ	-
A 710	ALA	50	0.6Å HA with A 730 PHE CD2	Favored (92.1%) Pre-proline / -65.0,152.0	-	0.068Å	-	-
A 711	PRO	50	-	Favored (29.43%) Trans-proline / -51.6,-46.8	71.5% (*Cg_exo*) chi angles: 327.9	0.041Å	-	-
A 712	GLU	50	1.018Å O with A 717 PRO HD3	Favored (89.56%) General / -62.3,-38.5	26.2% (*pm0*) chi angles: 65.6,274.8,19.2	0.059Å	OUTLIER(S) worst is C--O: 6.329 σ	-
A 713	LEU	99.99	1.034Å O with A 717 PRO HG3	Favored (19.66%) General / -74.0,-1.4	21.8% (*mt*) chi angles: 280.3,181.3	0.106Å	-	-
A 714	LEU	50	0.789Å O with A 717 PRO HG2	Allowed (0.63%) General / -104.3,-75.2	95.9% (*mt*) chi angles: 292.5,174.5	0.021Å	-	-
A 715	ARG	50	0.836Å HH12 with A 719 LEU CD2	Favored (82.36%) General / -67.4,-43.0	51.5% (*tpt85*) chi angles: 183.9,65.7,178,82.8	0.047Å	-	-
A 716	ASP	50	0.993Å HB2 with A 712 GLU O	Favored (55.85%) Pre-proline / -64.4,-40.9	36.3% (*m-20*) chi angles: 306.7,327.9	0.206Å	-	-
A 717	PRO	50	1.034Å HG3 with A 713 LEU O	Favored (52.06%) Trans-proline / -64.4,-35.1	96.5% (*Cg_endo*) chi angles: 32.4	0.068Å	OUTLIER(S) worst is N-- CD: 5.055 σ	OUTLIER(S) worst is CA-N- CD: 4.093 σ
A 718	ALA	50	-	Favored (78.19%) General / -68.0,-35.4	-	0.043Å	-	-
A 719	LEU	50	0.836Å CD2 with A 715 ARG	Favored (72.14%) General /	85.2% (*mt*) chi angles: 291.4,177.4	0.009Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
									HH12	-69.3,-32.8				
A 720		GLU	50	-	Favored (3.49%) General / -157.0,116.9	91.6% (*mt-10*) chi angles: 299.2,184.5,340	0.042Å	-	-
A 721		ARG	50	-	Favored (60.35%) General / -75.4,-16.5	99.7% (*mtt180*) chi angles: 293.6,182.4,177.7,179.2	0.014Å	-	-
A 722		ARG	99.99	-	Favored (27.47%) General / -86.5,-20.9	99.6% (*mtt180*) chi angles: 292.7,183.2,176.8,179.7	0.007Å	-	-
A 723		GLY	99.99	-	Favored (48.22%) Glycine / -70.1,150.0	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 724		THR	99.99	-	Favored (33.58%) General / -113.6,118.1	80.3% (*p*) chi angles: 61.5	0.063Å	-	-
A 725		LEU	99.99	0.975Å HD12 with A 713 LEU HD23	Favored (49.5%) General / -102.8,129.4	68.1% (*mt*) chi angles: 301.1,171	0.053Å	-	-
A 726		ALA	99.99	-	Favored (30.57%) General / -92.5,118.0	-	0.078Å	-	-
A 727		GLY	50	-	OUTLIER (0.03%) Glycine / 177.3,-1.8	-	-	-	-
A 728		ASP	50	0.606Å HB3 with A 664 HIS O	Favored (65.16%) General / -63.8,-19.6	16.9% (*p30*) chi angles: 48.9,12.1	0.095Å	-	-
A 729		VAL	50	-	Favored (77.71%) Isoleucine or valine / -65.0,-36.4	60.4% (*t*) chi angles: 171	0.025Å	-	-

A 730	PHE	50	0.6Å CD2 with A 710 ALA HA	Favored (85.91%) General / -66.4,-43.5	87.3% (*t80*) chi angles: 179.4,82	0.052Å	-	-
A 731	SER	50	-	Favored (79.97%) General / -60.2,-37.4	51.1% (*m*) chi angles: 301.5	0.064Å	-	-
A 732	LEU	50	0.707Å HD11 with A 651 ILE HG22	Favored (78.43%) General / -66.1,-34.6	8.4% (*tt*) chi angles: 183.9,159.5	0.043Å	-	OUTLIER(S) worst is CD1-CG-CD2: 4.133 σ
A 733	ALA	50	0.953Å HB2 with A 787 CYS CB	Favored (83.82%) General / -63.0,-36.5	-	0.091Å	-	-
A 734	ILE	99.99	0.721Å HD12 with A 708 TRP HA	Favored (65.43%) Isoleucine or valine / -71.1,-37.1	63.9% (*mt*) chi angles: 296.7,180.3	0.039Å	-	-
A 735	ILE	50	-	Favored (79.04%) Isoleucine or valine / -69.5,-39.9	77.2% (*mt*) chi angles: 294.9,176.9	0.059Å	-	-
A 736	MET	99.99	0.853Å HE2 with A 733 ALA HA	Favored (72.15%) General / -65.5,-31.2	69.3% (*mtm*) chi angles: 292.8,178.3,297.9	0.01Å	-	-
A 737	GLN	50	0.866Å HG3 with A 784 MET HE1	Favored (70.47%) General / -71.2,-41.4	49.1% (*tt0*) chi angles: 188.5,172.5,55	0.121Å	-	-
A 738	GLU	50	-	Favored (97.76%) General / -61.6,-41.7	45.1% (*mt-10*) chi angles: 290.5,182.9,71.5	0.107Å	-	-
A 739	VAL	50	0.961Å HG22 with A 643 LYS HB3	Favored (69.98%) Isoleucine or valine / -69.5,-36.1	13.3% (*p*) chi angles: 65.2	0.068Å	-	-
A 740	VAL	50	0.899Å HG23 with A 640 TRP CH2	Favored (13.65%) Isoleucine or valine / -80.7,-33.6	7.3% (*p*) chi angles: 56.1	0.034Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 741		CYS	50	0.608Å SG with A 737 GLN O	Favored (11.34%) General / -109.9,-23.5	30.9% (*p*) chi angles: 63.7	0.008Å	-	-
A 742		ARG	50	1.024Å NH1 with A 636 ILE HG21	Favored (14.55%) General / 63.5,25.9	79.1% (*mtp85*) chi angles: 294.1,179.3,60.7,84.4	0.062Å	-	-
A 743		SER	50	0.43Å HB3 with A 748 MET HE1	Favored (24.13%) General / -102.2,149.6	66.4% (*m*) chi angles: 296.4	0.074Å	-	-
			Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 744		ALA	50	-	Favored (73.73%) Pre-proline / -76.7,131.6	-	0.064Å	-	-
A 745		PRO	50	0.734Å O with A 746 TYR CD2	Favored (14.16%) Trans-proline / -69.4,126.9	91.6% (*Cg_endo*) chi angles: 30.2	0.016Å	-	-
A 746		TYR	99.99	0.864Å HA with A 750 GLU OE1	Favored (26.2%) General / 56.7,35.4	54.8% (*p90*) chi angles: 61.9,88.6	0.011Å	-	-
A 747		ALA	99.99	-	Favored (9.06%) General / -124.2,15.2	-	0.05Å	-	-
A 748		MET	99.99	0.518Å HG3 with A 748 MET O	Favored (14.39%) General / -129.4,113.0	23.9% (*ptp*) chi angles: 61.5,180.7,62.7	0.026Å	-	-
A 749		LEU	99.99	1.029Å O with A 749 LEU HD23	Favored (9.18%) General / 57.0,24.1	7.2% (*tt*) chi angles: 182.4,162.2	0.067Å	-	OUTLIER(S) worst is CA-C-O: 4.185 σ
A 750		GLU	99.99	1.07Å HB3 with A 751 LEU HG	Allowed (0.17%) General / -134.1,-137.4	61.1% (*mt-10*) chi angles: 281.9,185.7,322.7	0.057Å	-	-
A		LEU	50	1.07Å	Favored	38.3% (*mt*)	0.061Å		

A 751	LEU	50	HG with A 750 GLU HB3	(43.97%) General / -122.3,149.3	58.5% (mt) chi angles: 310.6,178.9	0.061Å	-	-
A 752	THR	50	-	Favored (56.2%) Pre-proline / -85.5,159.2	81.4% (p) chi angles: 61.1	0.078Å	-	-
A 753	PRO	50	-	Favored (21.64%) Trans-proline / -46.6,-44.4	67.7% (Cg_exo) chi angles: 327.7	0.036Å	-	-
A 754	GLU	50	-	Favored (89.13%) General / -63.9,-37.9	12.3% (pt-20) chi angles: 61.1,179.1,61.2	0.003Å	-	-
A 755	GLU	50	1.058Å CD with A 751 LEU HD22	Favored (72.25%) General / -69.9,-33.5	69.3% (tt0) chi angles: 181.8,170.5,20.6	0.024Å	-	-
A 756	VAL	50	-	Favored (88.59%) Isoleucine or valine / -62.4,-48.4	52.9% (t) chi angles: 170.5	0.051Å	-	-
A 757	VAL	50	1.09Å HG12 with A 761 ARG NE	Favored (75.1%) Isoleucine or valine / -55.0,-48.8	91.1% (t) chi angles: 175.4	0.094Å	OUTLIER(S) worst is C--O: 4.453 σ	-
A 758	GLN	50	0.598Å HG2 with A 755 GLU O	Favored (78.06%) General / -67.0,-45.3	18.2% (pt20) chi angles: 64.5,180.2,56.1	0.014Å	-	-
A 759	ARG	50	1.02Å HG2 with A 768 ARG HB2	Favored (2.79%) General / -60.1,-61.2	57.6% (ttm-85) chi angles: 183.2,178.2,294.2,265.1	0.039Å	-	-
A 760	VAL	50	-	Favored (20.53%) Isoleucine or valine / -78.2,-36.0	89.6% (t) chi angles: 177.9	0.052Å	-	-
A 761	ARG	99.99	1.09Å NE with A 757 VAL HG12	Favored (35.56%) General / -79.5,-38.0	16.5% (ptt85) chi angles: 78.3,184.6,152.4,97.2	0.058Å	-	-
A	SER	99.99	0.837Å HB3 with A	Favored (48.42%)	48% (t)	0.104Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
762				765 PRO HG3	Pre-proline / -98.6,123.9	chi angles: 179.7			
A 763		PRO	99.99	1.046Å HG2 with A 764 PRO HD3	Favored (95.74%) Trans-proline / -59.5,-35.4	43.7% (*Cg_endo*) chi angles: 24.4	0.062Å	-	-
			Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 764		PRO	99.99	1.046Å HD3 with A 763 PRO HG2	Favored (4.33%) Trans-proline / -55.9,-54.3	88.1% (*Cg_exo*) chi angles: 331.6	0.043Å	-	OUTLIER(S) worst is N-CD-CG: 4.652 σ
A 765		PRO	99.99	0.837Å HG3 with A 762 SER HB3	Allowed (1.16%) Trans-proline / -82.2,20.0	59.8% (*Cg_endo*) chi angles: 34.5	0.077Å	-	-
A 766		LEU	99.99	1.13Å HD22 with A 768 ARG HD3	OUTLIER (0%) General / 53.0,116.5	6.9% (*tt*) chi angles: 187.9,164.7	0.146Å	OUTLIER(S) worst is CG--CD2: 7.104 σ	OUTLIER(S) worst is CD1-CG-CD2: 10.127 σ
A 767		CYS	50	0.902Å C with A 766 LEU HD23	OUTLIER (0%) General / 33.9,25.6	90.9% (*m*) chi angles: 289.8	0.026Å	-	OUTLIER(S) worst is C-N-CA: 4.571 σ
A 768		ARG	50	1.13Å HD3 with A 766 LEU HD22	Favored (90.7%) Pre-proline / -69.0,124.6	39.6% (*mmt180*) chi angles: 300.5,290.3,178.4,180.9	0.357Å	OUTLIER(S) worst is CA--C: 4.665 σ	OUTLIER(S) worst is C-CA-CB: 5.237 σ
A 769		PRO	50	-	OUTLIER (0.03%) Trans-proline / -116.2,152.4	13.4% (*Cg_endo*) chi angles: 39.6	0.101Å	-	-
A 770		LEU	50	0.726Å HD13 with A 737 GLN OE1	Favored (24.23%) General / -54.4,143.2	85.6% (*mt*) chi angles: 291.7,168.4	0.095Å	-	-
A 771		VAL	50	-	Favored (27.07%) Isoleucine or valine / -79.0,134.8	11.2% (*p*) chi angles: 61.5	0.049Å	-	-
A 772		SER	50	-	Favored (45.55%) General / -102.7,123.0	42.1% (*t*) chi angles: 181.2	0.079Å	-	-

#	Alt	Res	High	Clash >	Ramachandran	Rotamer	Cβ	Bond	Bond
A 773		MET	50	-	Favored (53.91%) General / -57.6,132.7	36.6% (*mmp*) chi angles: 295.6,295.9,96.6	0.072Å	-	-
A 774		ASP	50	-	Favored (63.09%) General / -61.7,-20.0	36.7% (*t70*) chi angles: 184.2,55.9	0.068Å	-	-
A 775		GLN	50	0.416Å HG2 with A 775 GLN O	Favored (59.76%) General / -80.8,-10.1	53.5% (*tt0*) chi angles: 182.6,180.4,60.1	0.04Å	-	-
A 776		ALA	50	0.434Å HB1 with A 777 PRO HD2	Favored (88.78%) Pre-proline / -73.9,152.4	-	0.019Å	-	-
A 777		PRO	50	1.017Å HG3 with A 640 TRP CZ2	Favored (28.05%) Trans-proline / -60.0,128.9	60.4% (*Cg_endo*) chi angles: 27.2	0.022Å	-	-
A 778		VAL	50	0.754Å O with A 781 ILE HG12	Favored (80.39%) Isoleucine or valine / -61.2,-38.8	11.8% (*p*) chi angles: 61.9	0.034Å	-	-
A 779		GLU	50	0.515Å OE2 with A 808 ILE HD13	Favored (74.21%) General / -68.9,-33.7	11.7% (*pt-20*) chi angles: 57.7,179.1,66.9	0.023Å	-	-
A 780		CYS	50	0.656Å HB3 with A 777 PRO HG2	Favored (55.1%) General / -76.1,-39.5	42.6% (*t*) chi angles: 183.4	0.027Å	-	-
A 781		ILE	50	0.754Å HG12 with A 778 VAL O	Favored (77.35%) Isoleucine or valine / -61.8,-37.1	34.7% (*pt*) chi angles: 65.2,176.5	0.029Å	-	-
A 782		LEU	50	0.539Å C with A 782 LEU HD23	Favored (86.04%) General / -67.3,-40.0	8.9% (*tt*) chi angles: 183,158	0.046Å	-	-
A 783		LEU	50	1.127Å HD13 with A 805 PHE CE1	Favored (99.49%) General / -62.7,-42.2	90.9% (*mt*) chi angles: 293.9,170.5	0.05Å	-	-

		B	**0.4Å**			**deviation**	**lengths**	**angles**
		Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 784	MET	99.99	0.866Å HE1 with A 737 GLN HG3	Favored (67.61%) General / -63.8,-50.8	85.3% (*mtp*) chi angles: 296.2,181.8,60.5	0.031Å	-	-
A 785	LYS	50	-	Favored (80.17%) General / -59.7,-37.9	30.7% (*mtpp*) chi angles: 293.8,181.1,63.7,66.1	0.034Å	-	-
A 786	GLN	50	0.94Å NE2 with A 796 PRO HG3	Favored (72.51%) General / -66.7,-31.7	16.9% (*pt20*) chi angles: 64.3,182.1,51.9	0.019Å	-	-
A 787	CYS	50	0.953Å CB with A 733 ALA HB2	Favored (60.91%) General / -73.9,-18.3	73.6% (*m*) chi angles: 298.3	0.035Å	-	-
A 788	TRP	50	0.661Å NE1 with A 733 ALA HB3	Favored (26.77%) General / -105.7,15.5	50.8% (*m0*) chi angles: 291.1,344.6	0.031Å	OUTLIER(S) worst is NE1--CE2: 4.562 σ	-
A 789	ALA	50	-	Favored (57.4%) General / -62.2,142.9	-	0.065Å	-	-
A 790	GLU	50	0.502Å O with A 792 PRO HD3	Favored (95.23%) General / -62.4,-44.9	58% (*mm-40*) chi angles: 292.6,290.4,358.8	0.037Å	-	-
A 791	GLN	50	0.611Å HB3 with A 794 LEU HD13	Favored (4.51%) Pre-proline / -73.0,108.4	26.2% (*mp0*) chi angles: 297.3,79.5,1.9	0.038Å	-	-
A 792	PRO	50	0.502Å HD3 with A 790 GLU O	Favored (36.69%) Trans-proline / -54.9,-46.0	83.5% (*Cg_exo*) chi angles: 330.9	0.063Å	-	-
A 793	GLU	50	0.594Å HG3 with A 794 LEU HD12	Favored (36.42%) General / -64.9,-11.3	12.3% (*pt-20*) chi angles: 60.6,178.8,62.5	0.046Å	-	-
A 794	LEU	50	0.611Å HD13 with A 791 GLN HB3	Favored (39.81%) General / 87.6,14.5	11.2% (*mp*) chi angles: 278,62.7	0.041Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		HB3		-87.6,-14.5					
A 795		ARG	50	-	Favored (86.76%) Pre-proline / -72.4,144.5	66.9% (*mtt180*) chi angles: 307.5,181.1,185.6,143	0.064Å	-	-
A 796		PRO	50	0.94Å HG3 with A 786 GLN NE2	Favored (49.49%) Trans-proline / -70.5,144.3	90.8% (*Cg_endo*) chi angles: 32	0.043Å	-	-
A 797		SER	50	-	Favored (8.63%) General / -62.3,163.3	90.3% (*p*) chi angles: 62.6	0.085Å	-	-
A 798		MET	99.99	0.823Å O with A 802 PHE CD1	Favored (74%) General / -64.1,-32.4	96.8% (*mmm*) chi angles: 294.3,296.7,295	0.021Å	-	-
A 799		ASP	99.99	0.514Å HA with A 655 ARG HD3	Favored (93.59%) General / -64.8,-39.4	35.5% (*t70*) chi angles: 185.1,54.2	0.04Å	-	-
A 800		HIS	50	-	Favored (83.6%) General / -67.5,-37.9	22.4% (*t-160*) chi angles: 181,199.7	0.046Å	OUTLIER(S) worst is CG--ND1: 4.489 σ	-
A 801		THR	50	0.828Å CG2 with A 805 PHE CE2	Favored (79.01%) General / -62.6,-35.3	47.2% (*m*) chi angles: 293.7	0.087Å	-	-
A 802		PHE	50	1.183Å CE2 with A 652 LYS HA	Favored (85.42%) General / -66.7,-43.0	1.9% (*m-30*) chi angles: 292.2,30.2	0.03Å	-	OUTLIER(S) worst is CE1-CZ-CE2: 4.011 σ
A 803		ASP	50	-	Favored (86.99%) General / -61.8,-38.1	86.1% (*m-20*) chi angles: 295.6,338.5	0.04Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 65.20	Clashscore: 208.45	Outliers: 10 of 225	Poor rotamers: 1 of 196	Outliers: 12 of 214	Outliers: 33 of 227	Outliers: 33 of 227
A 804		LEU	50	0.907Å HB3 with A 783 LEU HD21	Favored (62.68%) General / -74.5,-32.9	97.1% (*mt*) chi angles: 294.5,172.9	0.05Å	-	-
A				1.127Å	Favored	21.3% (m-30)			

A 805	PHE	99.99	CE1 with A 783 LEU HD13	(34.9%) General / -81.2,-28.2	21.3% (*m-30*) chi angles: 295.1,328.5	0.031Å	-	-
A 806	LYS	50	0.748Å CG with A 810 LYS HE3	Favored (88.39%) General / -59.7,-40.6	40.4% (*ttmt*) chi angles: 181.5,176.6,295.8,179.1	0.014Å	-	-
A 807	ASN	50	-	Favored (89.26%) General / -62.5,-38.2	33% (*m120*) chi angles: 293,117.8	0.013Å	-	-
A 808	ILE	50	0.894Å HG22 with A 805 PHE O	Favored (83.21%) Isoleucine or valine / -67.8,-46.0	7.5% (*tp*) chi angles: 181.3,60.7	0.042Å	-	-
A 809	ASN	50	0.574Å HD21 with A 644 SER C	Favored (77.12%) General / -69.2,-36.2	32.2% (*m120*) chi angles: 292.1,117.2	0.024Å	-	-
A 810	LYS	99.99	0.748Å HE3 with A 806 LYS CG	-	96.8% (*mttt*) chi angles: 292.4,185.3,172.9,182.4	0.007Å	-	-

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