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All-Atom Contacts	Clashscore, all atoms:	120.94	0 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	8	4.82%	Goal: <1%
	Ramachandran outliers	7	3.83%	Goal: <0.05%
	Ramachandran favored	156	85.25%	Goal: >98%
	MolProbity score [^]	3.72		5 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	1 / 1470	0.07%	Goal: 0%
	Bad backbone angles:	36 / 1968	1.83%	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	C β deviation	Bond lengths	Bond angles
		Avg: 119.21	Clashscore: 120.94	Outliers: 7 of 183	Poor rotamers: 8 of 166	Outliers: 0 of 176	Outliers: 1 of 185	Outliers: 31 of 185
769	GLU	30.45	-	-	88.9% (<i>tt0</i>) chi angles: 182.7,178.9,358	0.056Å	-	-
770	THR	44.13	0.575Å HG22 with 771 LYS N	Favored (46.28%) General / -131.1,155.8	85.9% (<i>m</i>) chi angles: 301.3	0.085Å	-	-
771	LYS	103.07	0.575Å N with 770 THR HG22	Favored (22.07%) Pre-proline / -113.9,135.8	8.1% (<i>mtpm?</i>) chi angles: 289.2,169.2,73.9,295.1	0.113Å	-	-
772	PRO	100.49	-	Favored (18.35%) Trans-proline / -81.7,164.6 Favored	61.1% (<i>Cg_exo</i>) chi angles: 334.2	0.07Å	-	-

773	ILE	124.94	0.841Å HG22 with 788 LEU O	Favored (41.15%) Isoleucine or valine / -118.0,140.5	11.1% (<i>tp</i>) chi angles: 193.2,67.5	0.1Å	-	-
774	ILE	129.38	0.514Å HD13 with 787 ARG CG	Favored (37.51%) Isoleucine or valine / -124.2,143.5	7.1% (<i>tp</i>) chi angles: 179.9,65.3	0.102Å	-	-
775	SER	80.37	-	Favored (58.24%) General / -64.6,143.0	68.6% (<i>m</i>) chi angles: 297	0.112Å	-	-
776	LYS	109.74	0.461Å HB2 with 776 LYS NZ	Favored (94.85%) General / -64.2,-43.5	3.8% (<i>ttmp?</i>) chi angles: 186.8,165.9,285.8,71.1	0.074Å	-	-
777	SER	71.11	-	Favored (35.34%) General / -122.6,155.9	70.4% (<i>m</i>) chi angles: 295.9	0.101Å	-	-
778	MET	105.33	0.621Å HA with 785 CYS SG	Favored (37.45%) General / -71.1,157.9	27.2% (<i>ptm</i>) chi angles: 63.3,175,283	0.098Å	-	-
779	ALA	48.26	0.734Å CB with 782 ASP HB2	Favored (9.91%) General / -61.9,120.0	-	0.09Å	-	-
780	LYS	133.13	-	Favored (50.72%) General / -64.8,-53.2	9.7% (<i>tmmt?</i>) chi angles: 186.9,295.1,192.1,182.5	0.06Å	-	-
781	TYR	138.49	-	Favored (79.78%) General / -68.3,-42.1	50.8% (<i>t80</i>) chi angles: 182.4,274.7	0.083Å	-	-
782	ASP	164.26	0.734Å HB2 with 779 ALA CB	Allowed (0.06%) General / -84.4,-136.9	71% (<i>m-20</i>) chi angles: 288.1,322.5	0.077Å	-	OUTLIER(S) worst is CA- CB-CG: 6.146 σ
783	PHE	328.55	-	Allowed (0.37%) General / -116.3,-140.1	83.2% (<i>m-85</i>) chi angles: 299,82.9	0.117Å	-	OUTLIER(S) worst is CA- CB-CG: 5.891 σ
784	LYS	146.91	-	Allowed (0.41%) General / 52.2,164.7	12.2% (<i>mtp</i>) chi angles: 205.0,161.7,82.4,82.2	0.105Å	-	-

				-55.2,104.7		505.9,101.7,55.4,02.2			
785	CYS	49.44	0.621Å SG with 778 MET HA	Favored (46.43%) General / -73.5,143.8	97.9% (<i>m</i>) chi angles: 294.2	0.111Å	-	-	
786	ASP	56.02	-	Favored (19.71%) General / -88.6,155.3	45.6% (<i>m-20</i>) chi angles: 289.9,299.3	0.097Å	-	OUTLIER(S) worst is CA- CB-CG: 4.315 σ	
787	ARG	101.2	0.844Å HH22 with 799 GLU HB2	Favored (36.2%) General / -136.9,133.8	86.2% (<i>mtm-85</i>) chi angles: 291.5,181.6,305,283.8	0.147Å	-	-	
788	LEU	52.64	0.841Å O with 773 ILE HG22	Favored (44.94%) General / -123.4,149.5	87.3% (<i>mt</i>) chi angles: 296.3,180.1	0.103Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 119.21	Clashscore: 120.94	Outliers: 7 of 183	Poor rotamers: 8 of 166	Outliers: 0 of 176	Outliers: 1 of 185	Outliers: 31 of 185
789	SER	85.68	0.548Å HB3 with 795 LYS NZ	Favored (47.16%) General / -138.4,156.9	47.5% (<i>t</i>) chi angles: 180	0.107Å	-	-	
790	GLU	77.7	-	Favored (52.18%) General / -112.8,136.6	58.8% (<i>mp0</i>) chi angles: 297.8,80.7,3.6	0.125Å	-	-	
791	ILE	176.33	0.986Å HG13 with 792 PRO HD2	Allowed (0.11%) Pre-proline / -145.4,-166.0	6% (<i>tp</i>) chi angles: 207.8,66.7	0.067Å	-	OUTLIER(S) worst is CA-C- N: 4.791 σ	
792	PRO	224.27	0.986Å HD2 with 791 ILE HG13	Favored (52.3%) Trans-proline / -61.1,-17.4	64.3% (<i>Cg_exo</i>) chi angles: 327.4	0.162Å	-	-	
793	GLU	233.48	0.829Å H with 791 ILE HG23	Favored (5.99%) General / -123.4,176.7	54.4% (<i>mm-40</i>) chi angles: 285.8,285.4,353.9	0.11Å	-	-	
794	GLU	94.01	-	Favored (37.27%) General / -108.2,143.3	50% (<i>mt-10</i>) chi angles: 287.6,180,291.3	0.085Å	-	-	
795	LYS	95.2	1.016Å HA with 809	Favored (45.2%) General /	7.9% (<i>mtmp?</i>) chi angles:	0.11Å	-	-	

			GLN H	-122.7,148.5	296,166.9,296.3,72.2			
796	GLU	83.5	0.631Å H with 809 GLN N	Favored (34.8%) General / -132.7,161.1	14.2% (<i>pt</i> -20) chi angles: 62.5,173,323.2	0.126Å	-	-
797	GLY	24.04	-	Favored (46.96%) Glycine / -175.7,174.6	-	-	-	-
798	ALA	40.59	-	Favored (39.64%) General / -142.3,149.6	-	0.103Å	-	-
799	GLU	131.23	0.844Å HB2 with 787 ARG HH22	Allowed (0.06%) General / -175.6,-157.9	4.1% (<i>tm</i> -20) chi angles: 206,255.3,346	0.069Å	-	-
800	ASP	227.39	0.668Å H with 799 GLU CD	Favored (7.33%) General / -72.4,174.5	89% (<i>m</i> -20) chi angles: 289.9,351.8	0.086Å	-	OUTLIER(S) worst is CA- CB-CG: 4.882 σ
801	SER	110.17	-	Favored (38.52%) General / -72.5,-5.7	75.3% (<i>m</i>) chi angles: 294.7	0.083Å	-	-
802	LYS	130.69	0.711Å HB2 with 804 ASN OD1	Favored (77.43%) General / -57.7,-39.5	34.4% (<i>mmt</i> p) chi angles: 299.5,298.4,174.4,65.3	0.091Å	-	-
803	GLY	43.89	-	Favored (48.3%) Glycine / 105.1,-11.2	-	-	-	-
804	ASN	60.2	0.711Å OD1 with 802 LYS HB2	Favored (13.26%) General / -85.1,170.1	15.3% (<i>p</i> -10) chi angles: 68.2,304.6	0.123Å	-	OUTLIER(S) worst is CA- CB-CG: 5.367 σ
805	GLY	45.91	0.455Å HA3 with 787 ARG NH2	Favored (20.98%) Glycine / 140.9,-177.3	-	-	-	-
806	ILE	123.04	0.974Å HB with 830 ILE HG13	Favored (71.41%) Isoleucine or valine / -117.2,130.9	21.1% (<i>tt</i>) chi angles: 187.5,166.6	0.079Å	-	-
			0.517Å	Favored (27.21%)	15.6% (<i>pt</i> -20)	0		

807	GLU	115.6	HG3 with 795 LYS HZ3	(27.51%) General / -139.7,131.4	chi angles: 64.7,180,291.1	0.112Å	-	-
808	GLU	128.81	0.782Å OE2 with 819 LYS HE2	Favored (4.34%) General / -149.3,110.3	12.2% (<i>pt-20</i>) chi angles: 61.1,169.8,323.6	0.1Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 119.21			Clashscore: 120.94	Outliers: 7 of 183	Poor rotamers: 8 of 166	Outliers: 0 of 176	Outliers: 1 of 185	Outliers: 31 of 185
809	GLN	68.38	1.016Å H with 795 LYS HA	Favored (88.46%) General / -66.2,-38.6	52.4% (<i>tt0</i>) chi angles: 185.8,180.1,61.5	0.097Å	-	-
810	GLU	120.45	-	Favored (12.4%) General / -144.1,172.8	23% (<i>pt-20</i>) chi angles: 61.8,175.4,0.6	0.101Å	-	-
811	VAL	53.13	0.73Å HG13 with 817 ASN HA	Favored (12.09%) Isoleucine or valine / -111.5,158.1	97.7% (<i>t</i>) chi angles: 176.2	0.108Å	-	-
812	GLU	90.96	0.568Å N with 811 VAL HG12	Favored (6.86%) General / -66.4,169.9	5.6% (<i>mm-40</i>) chi angles: 289.6,290,64	0.089Å	-	-
813	ALA	58.95	-	Favored (86.47%) General / -58.2,-42.6	-	0.108Å	-	-
814	ASN	214.41	0.69Å OD1 with 816 GLU HB2	Favored (48.68%) General / -71.6,146.1	4.6% (<i>p30</i>) chi angles: 59.1,98.7	0.072Å	-	OUTLIER(S) worst is CA- CB-CG: 4.789 σ
815	GLU	117.57	0.526Å O with 811 VAL HG11	Favored (44.89%) General / -57.9,-21.6	64.2% (<i>mt-10</i>) chi angles: 291.4,180,309.1	0.077Å	-	-
816	GLU	91.77	0.69Å HB2 with 814 ASN OD1	Favored (12.7%) General / -52.2,124.3	49.9% (<i>mt-10</i>) chi angles: 294.2,177.8,62.8	0.066Å	-	-
817	ASN	122.8	0.73Å HA with 811 VAL HG13	Favored (23.23%) General / -88.3,150.4	23.6% (<i>p-10</i>) chi angles: 60.4,325.7	0.072Å	-	OUTLIER(S) worst is CA- CB-CG: 4.403 σ

818	VAL	143.42	1.025Å HA with 840 GLU HG3	Favored (67.38%) Isoleucine or valine / -111.3,123.6	8.7% (<i>p</i>) chi angles: 60.1	0.047Å	-	-
819	LYS	166.87	0.853Å HZ2 with 806 ILE HG12	Favored (45.97%) General / -122.8,147.9	5.4% (<i>mptp?</i>) chi angles: 263.6,61.6,181.3,52.5	0.105Å	-	-
820	VAL	112.83	0.924Å CG2 with 795 LYS HE2	Allowed (1.25%) Isoleucine or valine / -154.2,166.3	60.3% (<i>t</i>) chi angles: 180.2	0.07Å	-	-
821	HIS	274.48	1.065Å HB2 with 831 LEU HD13	OUTLIER (0%) General / 149.2,-140.7	3.9% (<i>m80</i>) chi angles: 266.9,110.6	0.149Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.554 σ
822	GLY	132.17	0.702Å C with 831 LEU HB3	Favored (24.09%) Glycine / -150.5,152.2	-	-	-	-
823	GLY	97.8	0.656Å HA3 with 832 SER N	Favored (8.56%) Glycine / 116.9,147.0	-	-	-	-
824	ARG	246.92	1.107Å HA with 837 ASP HB2	Favored (27.27%) General / -66.8,159.8	17.7% (<i>ttp-105</i>) chi angles: 180.5,189.5,76.8,273	0.097Å	-	-
825	LYS	270.35	0.656Å N with 824 ARG HG2	Favored (47.25%) General / -59.3,144.2	6.2% (<i>ttpm?</i>) chi angles: 180.5,166.4,71.5,294.7	0.101Å	-	-
826	GLU	211.5	0.458Å HG2 with 832 SER HB3	Allowed (0.49%) General / -120.7,-151.9	59.1% (<i>mm-40</i>) chi angles: 292.1,294.1,357.4	0.091Å	-	-
827	LYS	141.48	-	Favored (87.22%) General / -58.2,-42.9	14.9% (<i>mmmm</i>) chi angles: 302.2,303.6,297,296.1	0.091Å	-	-
828	THR	191.19	0.501Å HG22 with 829 GLU N	Favored (30.71%) General / -115.9,153.9	87.7% (<i>m</i>) chi angles: 301.1	0.103Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg:				Clashscore:	Outliers: 7 of	Poor rotamers: 8 of	Outliers:	Outliers: 1	Outliers: 31

		avg. clashscore: 119.21	clashes: 120.94	Outliers: 183	Outliers: 166	Outliers: 0 of 176	Outliers: 0 of 185	Outliers: 0 of 185
829	GLU 243.72		0.936Å HB2 with 842 HIS CD2	Favored (25.06%) General / -60.4,125.8	52% (<i>mp0</i>) chi angles: 283.2,77,5.2	0.103Å	-	-
830	ILE 168.54		0.974Å HG13 with 806 ILE HB	OUTLIER (0.01%) Isoleucine or valine / -169.7,-173.3	18% (<i>tt</i>) chi angles: 194.5,166	0.134Å	-	-
831	LEU 129.64		1.065Å HD13 with 821 HIS HB2	Favored (46.21%) General / -119.0,124.1	3.1% (<i>mp</i>) chi angles: 309.2,83.5	0.136Å	-	-
832	SER 75.85		0.656Å N with 823 GLY HA3	Favored (7.01%) General / -81.0,-178.7	60% (<i>p</i>) chi angles: 71.9	0.165Å	-	-
833	ASP 61.26		-	Favored (87.13%) General / -60.5,-39.3	73.1% (<i>m-20</i>) chi angles: 287.5,325.3	0.146Å	-	-
834	ASP 77.16		0.656Å CG with 836 THR HG23	Favored (66.55%) General / -66.1,-23.7	53.6% (<i>p30</i>) chi angles: 58.5,2.1	0.085Å	-	-
835	LEU 126.33		0.647Å HA with 822 GLY C	Favored (9.07%) General / 68.6,14.7	10.6% (<i>mp</i>) chi angles: 280.2,63.7	0.126Å	-	-
836	THR 136.89		0.656Å HG23 with 834 ASP CG	Favored (59.66%) General / -70.1,-48.0	62.2% (<i>p</i>) chi angles: 64.9	0.078Å	-	-
837	ASP 87.44		1.107Å HB2 with 824 ARG HA	Allowed (0.9%) General / -111.5,-164.3	66.8% (<i>m-20</i>) chi angles: 295.1,354.9	0.114Å	-	-
838	LYS 95.86		0.954Å HE3 with 851 LYS HD2	Favored (5.05%) General / -169.8,153.8	85.9% (<i>mttt</i>) chi angles: 299.6,171.9,173.7,191.9	0.207Å	-	-
839	ALA 83.64		-	Allowed (1.99%) General / -163.6,122.2	-	0.097Å	-	-
			1.025Å	Favored (0.01%)	35.8% (<i>tt0</i>)	-	-	-

840	GLU 143.01	HG3 with 818 VAL HA	(8.04%) General / -81.1,-51.8	chi angles: 179.9,192.1,46.8	0.13Å	-	-	
841	ASP 173.67	0.713Å OD1 with 843 GLU HB2	Favored (75.47%) General / -66.1,-47.0	7% (<i>t70</i>) chi angles: 200.3,295	0.109Å	-	OUTLIER(S) worst is CA-CB-CG: 6.403 σ	
842	HIS 142.1	0.936Å CD2 with 829 GLU HB2	Favored (14.88%) General / 62.9,25.1	25.8% (<i>m80</i>) chi angles: 295.7,61.6	0.123Å	-	OUTLIER(S) worst is CD2-NE2-CE1: 4.357 σ	
843	GLU 211.91	0.713Å HB2 with 841 ASP OD1	Allowed (0.13%) General / -171.6,-158.5	51.9% (<i>mt-10</i>) chi angles: 292.2,178.9,60.9	0.173Å	-	-	
844	PHE 195.61	0.401Å C with 844 PHE CD2	Favored (50.58%) General / -62.6,147.0	49.4% (<i>p90</i>) chi angles: 67,273.5	0.133Å	-	OUTLIER(S) worst is CA-CB-CG: 5.66 σ	
845	SER 123.16	0.672Å HB3 with 859 ILE HD12	Favored (53.51%) General / -107.2,127.4	47.4% (<i>t</i>) chi angles: 180.1	0.09Å	-	-	
846	LYS 113.15	-	Favored (9.64%) General / -74.5,-53.4	83.2% (<i>tttt</i>) chi angles: 183.7,167,179.8,176.4	0.091Å	-	-	
847	THR 77.96	0.436Å O with 848 GLU HB3	Favored (30.65%) General / -157.5,155.6	69.1% (<i>p</i>) chi angles: 62	0.092Å	-	OUTLIER(S) worst is C-N-CA: 4.462 σ	
848	GLU 134.74	0.789Å OE2 with 850 LEU HD11	Favored (2.24%) General / -177.0,170.6	23.3% (<i>pt-20</i>) chi angles: 59.1,180.1,356.6	0.091Å	-	-	
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 119.21	Clashscore: 120.94	Outliers: 7 of 183	Poor rotamers: 8 of 166	Outliers: 0 of 176	Outliers: 1 of 185	Outliers: 31 of 185	
849	GLU 152.81	0.814Å HG2 with 855 VAL O	Favored (7.42%) General / -120.5,100.9	0.1% chi angles: 182.5,264.1,82.1	0.088Å	-	-	
850	LEU 146.78	0.789Å HD11 with 848 GLU OE2	Favored (28.47%) General / -81.0,151.5	5.7% (<i>mp</i>) chi angles: 293.3,64.9	0.111Å	-	OUTLIER(S) worst is C-N-CA: 5.286 σ	
		0.054Å	Favored	10.10% (<i>tttt</i>)				

851	LYS	160.24	0.554Å HD2 with 838 LYS HE3	(46.45%) General / -129.7,132.0	19.1% (<i>tttt</i>) chi angles: 179.9,167.2,265.4,195.9	0.121Å	-	-
852	LEU	112.79	0.564Å O with 851 LYS HG2	Allowed (0.33%) General / -116.8,-115.9	5% (<i>mp</i>) chi angles: 295.3,64.8	0.187Å	-	OUTLIER(S) worst is N-CA- C: 5.229 σ
853	GLU	139.77	0.548Å O with 854 ASP HB2	Favored (84.76%) General / -63.6,-46.7	23.5% (<i>mm-40</i>) chi angles: 292.6,291.6,278.2	0.108Å	-	-
854	ASP	276.61	0.548Å HB2 with 853 GLU O	OUTLIER (0.02%) General / 169.2,135.5	9.7% (<i>t70</i>) chi angles: 193.1,296.9	0.087Å	-	OUTLIER(S) worst is CA- CB-CG: 4.991 σ
855	VAL	127.6	0.814Å O with 849 GLU HG2	Favored (9.72%) Isoleucine or valine / -151.4,153.6	12.9% (<i>p</i>) chi angles: 65.4	0.075Å	-	-
856	ASP	54.72	0.502Å N with 855 VAL HG22	Favored (52.55%) General / -124.1,140.9	81% (<i>m-20</i>) chi angles: 292.1,326.7	0.107Å	-	OUTLIER(S) worst is CA- CB-CG: 5.123 σ
857	GLU	60.13	-	Favored (40.57%) General / -142.6,150.6	99.6% (<i>mt-10</i>) chi angles: 291.5,176,350.6	0.1Å	-	-
858	GLU	83.86	-	Favored (54.23%) General / -122.0,139.0	41.3% (<i>tt0</i>) chi angles: 180,179.1,304.5	0.117Å	-	-
859	ILE	47.64	0.754Å HG22 with 860 ASN O	Favored (32.16%) Isoleucine or valine / -127.5,148.6	96.3% (<i>mt</i>) chi angles: 294.9,167.8	0.094Å	-	-
860	ASN	73.34	0.754Å O with 859 ILE HG22	Favored (7.11%) General / -85.5,179.6	27.7% (<i>p30</i>) chi angles: 56.1,40.5	0.066Å	-	-
861	ALA	56.72	-	Favored (76.38%) General / -61.5,-35.0	-	0.086Å	-	-
862	GLU	70.05	0.568Å HB2 with 860 ASN O	Favored (60.33%) General /	60.1% (<i>mt-10</i>) chi angles: 294.7,176.5,306.0	0.093Å	-	OUTLIER(S) worst is C-N- CA: 4.45 σ

		ASN OD1	-60.5,-20.6	294.7,176.5,506.9		CA: 4.45 Å		
863	ASN 143.42	0.646Å HA with 859 ILE CG2	Allowed (0.79%) General / 81.9,10.2	25.5% (<i>p30</i>) chi angles: 76.7,10.2	0.179Å	-	-	
864	VAL 49.2	0.604Å O with 859 ILE HG23	Favored (4.71%) Isoleucine or valine / -79.4,155.1	93.9% (<i>t</i>) chi angles: 175.7	0.068Å	-	-	
865	GLU 120.67	0.55Å HG2 with 865 GLU O	Favored (23.44%) General / -88.9,112.6	0.4% chi angles: 60.8,286.8,276.6	0.083Å	-	-	
866	SER 96.54	0.506Å O with 881 TYR HD2	Favored (10.84%) General / -72.6,-53.8	47.1% (<i>t</i>) chi angles: 180.2	0.077Å	-	-	
867	LYS 85.7	0.956Å HG2 with 880 GLY HA2	Favored (46.64%) General / -140.0,152.9	60.7% (<i>mtpt</i>) chi angles: 290.4,175.7,72.3,177.4	0.096Å	-	-	
868	LYS 128.34	0.781Å O with 879 THR HG22	Favored (38.04%) General / -143.5,161.6	0% chi angles: 62,75.4,179.7,180.8	0.083Å	-	-	
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 119.21	Clashscore: 120.94	Outliers: 7 of 183	Poor rotamers: 8 of 166	Outliers: 0 of 176	Outliers: 1 of 185	Outliers: 31 of 185
869	LYS 178.12	0.616Å HB2 with 877 VAL O	Favored (4.87%) General / -162.3,132.9	0% chi angles: 71.8,78.3,74.2,179.8	0.069Å	-	-	
870	THR 117.49	0.514Å HG22 with 871 VAL N	OUTLIER (0%) General / 126.2,147.5	98% (<i>m</i>) chi angles: 299.1	0.124Å	-	-	
871	VAL 106.02	0.816Å HG12 with 875 GLU O	Favored (2.67%) Isoleucine or valine / -151.7,163.1	8% (<i>p</i>) chi angles: 68.9	0.089Å	-	-	
872	GLY 38.34	0.628Å N with 871 VAL HG22	Favored (93.27%) Glycine / -65.6,-37.1	-	-	-	-	
873	ASP 112.24	0.505Å OD1 with	Allowed (0.41%)	11.9% (<i>p30</i>)	0.072Å	-	-	

			8 / 1 VAL HG11	General / -82.3,33.5 Favored (7.51%) General / 57.7,21.6	chi angles: 60.6,39.6 88.6% (<i>m</i> -20) chi angles: 290.6,351.5	0.076Å	-	OUTLIER(S) worst is CA- CB-CG: 4.388 σ
874	ASP	75.39	-					
875	GLU	117.93	0.816Å O with 871 VAL HG12	Favored (37.26%) General / -92.3,126.2	39.3% (<i>tt0</i>) chi angles: 184.1,179.9,300.1	0.118Å	-	-
876	SER	104.43	0.539Å O with 877 VAL HB	Favored (45.74%) General / -141.5,156.5	89.9% (<i>p</i>) chi angles: 67.3	0.131Å	-	-
877	VAL	157.28	0.616Å O with 869 LYS HB2	OUTLIER (0%) Pre-proline / 151.2,169.1	11.1% (<i>p</i>) chi angles: 67	0.153Å	-	-
878	PRO	133.53	0.574Å N with 877 VAL HG22	Favored (7.52%) Trans-proline / -86.6,143.9	11.2% (<i>Cg_endo</i>) chi angles: 14.4	0.202Å	-	-
879	THR	134.33	0.781Å HG22 with 868 LYS O	Favored (39.44%) General / -119.8,151.0	14.7% (<i>t</i>) chi angles: 189.1	0.111Å	-	-
880	GLY	40.52	0.956Å HA2 with 867 LYS HG2	Favored (16.14%) Glycine / -131.7,144.5	-	-	-	-
881	TYR	68.15	0.506Å HD2 with 866 SER O	Favored (50.62%) General / -122.1,142.2	91.5% (<i>m</i> -85) chi angles: 301.4,276.3	0.088Å	-	OUTLIER(S) worst is CA- CB-CG: 4.417 σ
882	HIS	145.98	0.542Å CD2 with 884 LYS H	Allowed (0.36%) General / -90.7,-154.8	27.3% (<i>p</i> -80) chi angles: 70.2,263.6	0.165Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.516 σ
883	SER	51.11	0.427Å N with 882 HIS CD2	Favored (92.3%) General / -59.2,-44.3	65.5% (<i>m</i>) chi angles: 298.6	0.092Å	-	-
884	LYS	194.56	0.542Å H with 882 HIS CD2	Allowed (1.11%) General / -100.3,42.4	20.3% (<i>ptmt</i>) chi angles: 66.4,170,297.9,176	0.088Å	-	-
885	THR	182.51	-	Favored (3.93%) General /	69.8% (<i>p</i>) chi angles: 64.2	0.059Å	-	-

886	GLU	127.08	0.439Å HB3 with 882 HIS CE1	Favored (30.43%) General / -85.1,141.2	4% (<i>tp10</i>) chi angles: 207,85.3,53.7	0.084Å	-	-
887	GLY	48.14	0.442Å O with 902 LYS HD2	Favored (5.77%) Glycine / -72.7,116.6	-	-	-	-
888	ALA	73.32	1.082Å HA with 902 LYS HD2	Favored (41.88%) General / -73.7,-47.1	-	0.077Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 119.21			Clashscore: 120.94	Outliers: 7 of 183	Poor rotamers: 8 of 166	Outliers: 0 of 176	Outliers: 1 of 185	Outliers: 31 of 185
889	GLU	99.22	0.603Å O with 890 ARG HG3	Favored (28.17%) General / -152.4,167.6	36.3% (<i>mt-10</i>) chi angles: 304.6,179,86.9	0.143Å	-	-
890	ARG	216.01	0.645Å H with 900 ILE CG2	Favored (12.03%) General / -163.8,174.1	74.4% (<i>mtm180</i>) chi angles: 293.9,170.1,292.1,152.3	0.083Å	OUTLIER(S) worst is C--N: 5.117 σ	OUTLIER(S) worst is C-N- CA: 5.302 σ
891	THR	123.15	0.582Å HG22 with 892 ASN N	Favored (47.17%) General / -139.6,155.9	96.5% (<i>m</i>) chi angles: 299.5	0.083Å	-	-
892	ASN	85.67	0.582Å N with 891 THR HG22	Favored (8.61%) General / -121.9,171.8	96.3% (<i>m-20</i>) chi angles: 292.1,333.9	0.1Å	-	OUTLIER(S) worst is C-N- CA: 4.979 σ
893	ASP	93.97	-	Favored (64.88%) General / -68.1,-23.4	48.8% (<i>t0</i>) chi angles: 191.3,9.1	0.097Å	-	-
894	ASP	149.83	0.587Å OD2 with 896 SER HB3	Favored (29.63%) General / -56.8,-21.5	10.1% (<i>t0</i>) chi angles: 171.5,38.8	0.131Å	-	OUTLIER(S) worst is CA- CB-CG: 4.711 σ
895	SER	225.64	0.49Å HB3 with 894 ASP O	Favored (2.58%) General / 78.6,2.1	47.6% (<i>t</i>) chi angles: 180	0.074Å	-	-
896	SER	158.96	0.587Å HB3 with 894 ASP OD2	Favored (28.99%) General / -80.0,153.3	99.6% (<i>p</i>) chi angles: 64.5	0.109Å	-	-

897	ALA	85.46	0.526Å O with 898 GLU HG3	Favored (46.64%) General / -135.2,143.8	-	0.1Å	-	-
898	GLU	103.48	0.997Å HG2 with 913 ILE HD13	Favored (5.89%) General / -164.0,-178.9	45.3% (<i>mp0</i>) chi angles: 302.4,86.1,11.9	0.157Å	-	-
899	THR	137.32	0.496Å O with 911 ARG HA	Favored (43.63%) General / -118.1,122.7	73.9% (<i>p</i>) chi angles: 61.8	0.097Å	-	-
900	ILE	169.45	0.987Å HG12 with 908 LEU HD13	Favored (70.09%) Isoleucine or valine / -112.8,127.3	0% chi angles: 184.4,291.1	0.066Å	-	-
901	GLU	81.63	0.738Å O with 908 LEU HD12	Favored (53.03%) General / -109.2,133.4	37.8% (<i>tp10</i>) chi angles: 180,72.1,359.7	0.117Å	-	-
902	LYS	165.45	1.082Å HD2 with 888 ALA HA	Favored (36.2%) General / -107.3,143.0	0% chi angles: 95.7,299.3,179.9,180.1	0.126Å	-	-
903	LYS	88.99	0.684Å HG2 with 904 GLU H	Favored (5.34%) General / -87.0,-175.4	78.7% (<i>tttt</i>) chi angles: 192.5,165.5,180.2,179.9	0.069Å	-	-
904	GLU	86.38	0.684Å H with 903 LYS HG2	Favored (81.15%) General / -56.6,-44.7	99.7% (<i>mt-10</i>) chi angles: 291.6,180,353.7	0.108Å	-	-
905	LYS	262.48	-	Favored (38.33%) General / -77.0,144.9	18.5% (<i>mtp</i>) chi angles: 292.5,162.2,42.4,74.3	0.149Å	-	-
906	ALA	109.67	-	Favored (38.72%) General / -56.9,-22.6	-	0.077Å	-	-
907	ASN	65.57	-	Favored (4.82%) General / -57.4,159.4	88.3% (<i>m-20</i>) chi angles: 293.1,318	0.081Å	-	OUTLIER(S) worst is CA- CB-CG: 4.701 σ
908	LEU	85.65	1.136Å HD21 with 911 ARG HB2	Favored (19.74%) General / -84.4,111.8	27.4% (<i>tp</i>) chi angles: 167.5,60.3	0.089Å	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 119.21	Clashscore: 120.94	Outliers: 7 of 183	Poor rotamers: 8 of 166	Outliers: 0 of 176	Outliers: 1 of 185	Outliers: 31 of 185
909	GLU	100.08	0.488Å HG2 with 910 GLU HG3	Favored (35.52%) General / -74.0,-47.7	86.3% (<i>tt0</i>) chi angles: 180.2,180,10.2	0.084Å	-	-
910	GLU	80.96	0.699Å O with 908 LEU HD11	Favored (23.13%) General / -147.4,137.6	21.6% (<i>mt-10</i>) chi angles: 292.4,157.6,278.1	0.115Å	-	-
911	ARG	125.72	1.136Å HB2 with 908 LEU HD21	Favored (26.07%) General / -139.2,165.9	52.2% (<i>ttp180</i>) chi angles: 180.3,168.7,55.7,191.9	0.082Å	-	OUTLIER(S) worst is C-N- CA: 4.036 σ
912	ALA	93.01	0.597Å HA with 914 CYS O	Allowed (1.25%) General / -126.1,71.3	-	0.105Å	-	-
913	ILE	202.9	0.997Å HD13 with 898 GLU HG2	Favored (18.99%) Isoleucine or valine / -75.9,-52.0	37.2% (<i>mm</i>) chi angles: 302.2,293.9	0.246Å	-	OUTLIER(S) worst is C-N- CA: 5.43 σ
914	CYS	166.49	0.597Å O with 912 ALA HA	Allowed (1.28%) General / -117.0,-167.3	52.7% (<i>t</i>) chi angles: 180.1	0.159Å	-	OUTLIER(S) worst is N-CA- C: 4.892 σ
915	GLU	165.41	0.789Å HG3 with 919 ASN OD1	Favored (63.5%) General / -68.8,-15.4	30.2% (<i>mm-40</i>) chi angles: 287.2,282.3,292.7	0.095Å	-	-
916	TYR	287.77	0.432Å HB2 with 911 ARG O	Favored (7.05%) General / 65.1,36.9	36.3% (<i>t80</i>) chi angles: 195.2,77.7	0.08Å	-	OUTLIER(S) worst is C-N- CA: 6.528 σ
917	ASN	184.53	0.742Å O with 915 GLU HB2	OUTLIER (0.01%) General / 170.5,107.4	0.2% chi angles: 184.4,155	0.184Å	-	OUTLIER(S) worst is C-N- CA: 5.386 σ
918	GLU	106.74	0.846Å CG with 933 LEU HD22	Favored (26.89%) General / -74.2,124.7	84.1% (<i>mt-10</i>) chi angles: 288.8,180.6,15.4	0.116Å	-	-
919	ASN	119.63	0.789Å OD1 with 915 GLU	Favored (35.68%) Pre-proline /	35.2% (<i>p-10</i>) chi angles: 58.4,342.7	0.074Å	-	-

920	PRO	159.98	0.732Å HG2 with 923 TYR CE1	HG3 -112.6,96.2 Favored (19.26%) Trans-proline / -81.4,164.2	77.7% (<i>Cg_exo</i>) chi angles: 333.4	0.045Å	-	-
921	LYS	152.75	-	Favored (26.87%) General / -74.3,124.7	12.2% (<i>tppt?</i>) chi angles: 181.9,60.5,44.4,183.1	0.08Å	-	-
922	GLY	31.11	-	Favored (4.15%) Glycine / 106.0,-36.8	-	-	-	-
923	TYR	59.13	0.732Å CE1 with 920 PRO HG2	Favored (41.4%) General / -147.1,161.2	51.7% (<i>p90</i>) chi angles: 60.6,86.8	0.076Å	-	-
924	MET	91.94	0.453Å HA with 920 PRO HD2	Favored (44.2%) General / -138.8,148.7	25.6% (<i>ptp</i>) chi angles: 62.1,180.5,71.8	0.064Å	-	-
925	LEU	76.91	0.839Å HB2 with 933 LEU HD23	Favored (42.44%) General / -116.8,147.0	82.9% (<i>mt</i>) chi angles: 301.7,180	0.075Å	-	-
926	ASP	109.66	-	Favored (8.5%) General / -129.1,175.7	77.1% (<i>m-20</i>) chi angles: 292.1,322.4	0.141Å	-	-
927	ASP	136.98	0.51Å HB3 with 930 SER O	OUTLIER (0.01%) General / 170.6,103.4	30.2% (<i>t0</i>) chi angles: 197,340.6	0.047Å	-	-
928	ALA	56.6	-	Favored (59.52%) General / -66.5,-51.2	-	0.077Å	-	-
<div> <div>#</div> <div>Alt Res High B</div> <div>Clash > 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> </div> <div> <div>Avg: 119.21</div> <div>Clashscore: 120.94</div> <div>Outliers: 7 of 183</div> <div>Poor rotamers: 8 of 166</div> <div>Outliers: 0 of 176</div> <div>Outliers: 1 of 185</div> <div>Outliers: 31 of 185</div> </div>								
929	ASP	53.89	-	Favored (54.58%) General / -68.3,-50.3	83.9% (<i>m-20</i>) chi angles: 291.8,352.9	0.097Å	-	-
930	SER	98.55	0.51Å O with 927 ASP HB3	Favored (29.13%) General / -127.4,161.2	47.8% (<i>t</i>) chi angles: 179.9	0.135Å	-	-

931	SER 122.54	0.783Å OG with 947 MET HB3	-127.4,161.2 Favored (21.29%) General / -110.5,110.5	83.1% (<i>p</i>) chi angles: 60.8	0.07Å	-	-
932	SER 131.42	0.599Å HA with 945 LYS O	Favored (13.58%) General / -130.1,112.6	47.2% (<i>t</i>) chi angles: 180.2	0.118Å	-	-
933	LEU 130.59	0.846Å HD22 with 918 GLU CG	Favored (53.91%) General / -114.7,135.7	4.8% (<i>mp</i>) chi angles: 298.9,75	0.068Å	-	-
934	GLU 53.23	-	Favored (51.32%) General / -109.1,134.7	97.5% (<i>mt-10</i>) chi angles: 292.9,179.9,0.7	0.108Å	-	-
935	ILE 105.37	0.702Å O with 943 PRO HD2	Favored (44.16%) Isoleucine or valine / -119.5,140.2	20.5% (<i>tt</i>) chi angles: 191.8,167.9	0.091Å	-	-
936	LEU 150.09	0.596Å N with 936 LEU HD12	Favored (79.24%) General / -66.4,-45.7	4.7% (<i>mp</i>) chi angles: 295.9,64.1	0.081Å	-	-
937	GLU 100.38	0.503Å HB3 with 936 LEU O	Allowed (0.23%) General / 74.3,160.6	33.7% (<i>tt0</i>) chi angles: 180,174.4,286.8	0.093Å	-	-
938	ASN 147.81	0.453Å N with 937 GLU HG2	Favored (97.49%) General / -61.6,-44.2	20.1% (<i>p-10</i>) chi angles: 62.2,310.9	0.069Å	-	-
939	SER 131.16	-	Favored (22.81%) General / -85.9,152.6	95.2% (<i>p</i>) chi angles: 63.6	0.099Å	-	-
940	GLU 199.01	-	Allowed (1.63%) General / -73.5,88.3	88% (<i>tt0</i>) chi angles: 182.3,180.1,5.6	0.099Å	-	-
941	THR 141.08	1.013Å HG23 with 943 PRO HD3	Favored (41.95%) General / -144.3,153.4	15.2% (<i>t</i>) chi angles: 188	0.128Å	-	-
942	THR 59.17	-	Favored (53.22%) Pro-proline /	82.3% (<i>p</i>) chi angles: 60.7	0.061Å	-	-

943	PRO	95.5	1.013Å HD3 with 941 THR HG23	Favored (20.59%) Trans-proline / -80.9,156.5	75.4% (Cg_exo) chi angles: 333.1	0.086Å	-	-	
944	SER	41.59	-	Favored (34.56%) General / -140.5,138.4	75% (m) chi angles: 294.8	0.095Å	-	-	
945	LYS	87.11	0.599Å O with 932 SER HA	Favored (34.32%) General / -107.8,117.5	34.7% (ttmt) chi angles: 179.8,167.6,284.5,179.8	0.138Å	-	-	
946	ASP	50.78	-	Favored (53.06%) General / -111.3,124.8	78.1% (m-20) chi angles: 290.1,326.5	0.111Å	-	OUTLIER(S) worst is CA- CB-CG: 4.183 σ	
947	MET	134.99	0.783Å HB3 with 931 SER OG	Favored (42.27%) General / -139.8,148.5	27.6% (ttt) chi angles: 180,180.1,180.6	0.114Å	-	-	
948	LYS	77.65	0.683Å HB2 with 950 THR HG22	Favored (3.44%) General / -127.9,-175.3	53.5% (mttp) chi angles: 289.5,168.3,172.7,67.8	0.086Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 119.21	Clashscore: 120.94	Outliers: 7 of 183	Poor rotamers: 8 of 166	Outliers: 0 of 176	Outliers: 1 of 185	Outliers: 31 of 185
949	LYS	103.24	-	Favored (82.48%) General / -59.7,-38.7	23.8% (tptm) chi angles: 173.9,68.6,180.1,299.1	0.115Å	-	-	
950	THR	115.54	0.992Å HG23 with 952 LYS H	Favored (67.05%) General / -65.7,-24.5	10.2% (t) chi angles: 184.1	0.069Å	-	-	
951	LYS	114.73	0.651Å HG3 with 947 MET CE	Allowed (1.94%) General / 72.9,29.0	27.7% (ttpt) chi angles: 188.7,168.6,94.6,175.9	0.098Å	-	-	
952	LYS	88.96	0.992Å H with 950 THR HG23	Favored (36.44%) General / -101.1,139.7	7.7% (tmтт?) chi angles: 193.6,296.4,179.1,170.4	0.08Å	-	-	
953	ILE	125.53	0.824Å N with 952	-	0% chi angles: 190.1,291.4	0.039Å	-	-	

LYS HD3

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