Viewing pde6b_sm_484-813H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	54.38		3rd percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	12	4.03%	Goal: <1%
	Ramachandran outliers	5	1.52%	Goal: <0.05%
	Ramachandran favored	309	94.21%	Goal: >98%
	MolProbity score^	3.06		21st percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	7	2.21%	Goal: 0
	Bad backbone bonds:	26 / 2794	0.93%	Goal: 0%
	Bad backbone angles:	52 / 3769	1.38%	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: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 484		GLU	50	0.429Å O with D 488 ILE HG22	-	85.4% (*tt0*) chi angles: 187.5,176,7	0.043Å	-	-
D 485		LEU	50	0.826Å O with D 489 LEU HD13	Favored (87.51%) General / -66.9,-39.7	64.5% (*tp*) chi angles: 179.9,62.8	0.014Å	-	-
D 486		GLY	50	-	Favored (92.81%) Glycine / -67.1,-39.5	-	-	-	-
D 487		GLU	50	-	Favored (93.73%) General / -60.2,-41.8	50.8% (*mt-10*) chi angles: 298.8,181.4,286.9	0.061Å	-	-

D 488	ILE	50	0.752Å HG21 with D 545 PHE CZ	Favored (38.06%) Isoleucine or valine / -76.1,-42.7	6.8% (*tp*) chi angles: 179.2,67.5	0.049Å	-	-
D 489	LEU	50	0.873Å HD11 with D 541 VAL HG11	Favored (71.84%) General / -63.0,-30.7	10.5% (*mp*) chi angles: 278.6,58.1	0.084Å	-	OUTLIER(S) worst is CD1-CG-CD2: 5.987 σ
D 490	LYS	50	-	Favored (25.53%) General / -84.0,-31.5	26.8% (*tptp*) chi angles: 188.7,61.4,184.2,64.6	0.047Å	-	-
D 491	GLU	50	-	Favored (50.61%) General / -60.6,144.9	43.9% (*tp10*) chi angles: 188.7,56.8,20.5	0.061Å	-	-
D 492	GLU	50	0.576Å O with D 494 PRO HD3	Favored (41.89%) General / -75.9,139.8	12% (*pt-20*) chi angles: 58.7,179.2,65.6	0.02Å	-	-
D 493	LEU	50	0.607Å HD22 with D 521 ILE HG22	Favored (10.39%) Pre-proline / -99.5,100.3	60.9% (*tp*) chi angles: 180.5,63.7	0.019Å	-	-
D 494	PRO	50	0.65Å HB2 with D 499 PHE CE1	Favored (55.32%) Trans-proline / -61.6,155.1	51.3% (*Cg_exo*) chi angles: 335.2	0.214Å	-	-
D 495	GLY	50	-	Favored (13.16%) Glycine / -59.1,162.0	-	-	-	-
D 496	PRO	99.99	-	Favored (81.04%) Trans-proline / -62.4,-32.0	78.4% (*Cg_endo*) chi angles: 29.7	0.039Å	-	-
D 497	THR	50	0.534Å HA with D 502 TYR HE1	Favored (71.22%) General / -71.0,-41.2	72.1% (*p*) chi angles: 59.8	0.038Å	-	-
D 498	THR	50	-	Favored (82.81%) General / -66.7,-36.6	15.8% (*m*) chi angles: 311.7	0.031Å	-	-
D 499	PHE	99.99	0.65Å CE1 with D 494 PRO	Favored (59.23%) General /	23.3% (*m-30*) chi angles: 297.6,323.7	0.056Å	-	OUTLIER(S) worst is CE1-CZ-CE2:

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
				HB2	-81.3,-11.8				4.504 σ
D 500		ASP	50	-	Favored (12.29%) General / 64.8,21.0	38.1% (*m-20*) chi angles: 302.1,291.5	0.06Å	-	-
D 501		ILE	50	-	Favored (12.03%) Isoleucine or valine / -77.0,-8.8	42.6% (*pt*) chi angles: 58.6,174.3	0.146Å	-	-
D 502		TYR	50	0.534Å HE1 with D 497 THR HA	Favored (43.01%) General / -83.7,-17.0	55.1% (*p90*) chi angles: 63,270.5	0.056Å	-	-
D 503		GLU	50	0.421Å HB3 with D 505 HIS CD2	Favored (44.1%) General / -72.1,132.4	35.8% (*mm-40*) chi angles: 291.9,292,8.6	0.161Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 504		PHE	50	0.487Å CZ with D 793 ILE CD1	Favored (64.17%) General / -68.2,-16.8	45.2% (*m-85*) chi angles: 283.3,292.3	0.037Å	-	-
D 505		HIS	99.99	0.421Å CD2 with D 503 GLU HB3	Favored (43.6%) General / -93.4,7.7	33.3% (*p80*) chi angles: 65.5,77.7	0.055Å	OUTLIER(S) worst is CD2--NE2: 4.226 σ	OUTLIER(S) worst is CB-CG-CD2: 4.91 σ
D 506		PHE	50	-	Favored (26.74%) General / -52.6,139.1	73.9% (*t80*) chi angles: 171.8,83	0.034Å	-	-
D 507		SER	50	-	Favored (50.63%) General / -122.2,142.3	44% (*t*) chi angles: 178.3	0.069Å	-	-
D 508		ASP	50	0.421Å OD2 with D 560 ARG HD2	Favored (19.38%) General / -100.3,-12.6	1.9% (*p-10*) chi angles: 79.3,279.8	0.025Å	-	-
D 509		LEU	99.99	-	Favored (10.49%) General / -45.3,-43.3	52.5% (*tp*) chi angles: 183.9,62.8	0.04Å	-	-
D		GLU	50	-	Favored (5.29%)	0.6%	0.155Å	-	-

510				General / -108.1,31.8	chi angles: 60.3,283.3,279.5			
D 511	CYS	50	-	Favored (44.7%) General / -110.1,140.0	70.8% (*m*) chi angles: 297.5	0.048Å	-	-
D 512	THR	50	-	Favored (31.65%) General / -73.1,160.7	70% (*p*) chi angles: 64.1	0.03Å	-	-
D 513	GLU	50	-	Favored (68.03%) General / -54.9,-38.7	51.6% (*mt-10*) chi angles: 299.8,180.6,289.4	0.071Å	-	-
D 514	LEU	50	0.553Å O with D 517 VAL HG12	Favored (89.42%) General / -64.8,-38.0	0.5% chi angles: 200,259.9	0.058Å	-	-
D 515	ASP	50	-	Favored (79.13%) General / -67.9,-35.9	96.8% (*m-20*) chi angles: 291.8,343.6	0.052Å	-	-
D 516	LEU	50	0.439Å HG with D D 563 PHE CE2	Favored (91.55%) General / -63.2,-38.5	8.7% (*mp*) chi angles: 272.5,71.8	0.054Å	-	-
D 517	VAL	50	0.927Å HG21 with D 545 PHE CE1	Favored (82.69%) Isoleucine or valine / -67.5,-39.6	10.1% (*p*) chi angles: 67.7	0.148Å	-	OUTLIER(S) worst is CA-CB-CG2: 4.291 σ
D 518	LYS	50	0.445Å O with D 493 LEU HD11	Favored (84.27%) General / -58.5,-40.9	57.3% (*mtpt*) chi angles: 291.8,182.2,62.5,178.5	0.056Å	-	-
D 519	CYS	50	-	Favored (87.02%) General / -63.1,-37.4	76.2% (*m*) chi angles: 296.4	0.046Å	-	-
D 520	GLY	50	-	Favored (88.12%) Glycine / -62.1,-47.7	-	-	-	-
D 521	ILE	50	0.607Å HG22 with D 493 LEU HD22	Favored (81.68%) Isoleucine or valine / -57.0,-48.5	60.4% (*mt*) chi angles: 296.7,181	0.108Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
D 522		GLN	50	0.946Å HE21 with D 526 GLU HG2	Favored (74.63%) General / -55.0,-44.5	71.2% (*tp60*) chi angles: 183.5,62.7,58.6	0.025Å	-	OUTLIER(S) worst is OE1-CD-NE2: 4.321 σ
D 523		MET	50	-	Favored (80.8%) General / -59.0,-39.1	38.6% (*mtm*) chi angles: 278.9,180,268.3	0.028Å	-	-
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 524		TYR	50	0.57Å CD2 with D 540 LEU HD11	Favored (65.95%) General / -72.3,-31.7	1.7% (*m-30*) chi angles: 292,33.3	0.008Å	-	-
D 525		TYR	50	0.734Å CD1 with D 530 VAL HG21	Favored (10.63%) General / -76.2,-52.1	2% (*m-30*) chi angles: 291.9,29.8	0.016Å	-	-
D 526		GLU	99.99	0.946Å HG2 with D 522 GLN HE21	Favored (69.81%) General / -65.8,-29.3	75.9% (*mm-40*) chi angles: 289.1,303.2,315.8	0.062Å	-	-
D 527		LEU	50	-	Favored (4.22%) General / -78.6,9.3	79.4% (*mt*) chi angles: 288.4,173.8	0.048Å	-	-
D 528		GLY	50	-	Favored (61.51%) Glycine / 56.9,31.8	-	-	-	-
D 529		VAL	50	0.461Å HB with D 524 TYR O	Favored (22.58%) Isoleucine or valine / -78.7,-39.1	42.6% (*t*) chi angles: 167.3	0.094Å	-	-
D 530		VAL	50	0.988Å HG22 with D 535 ILE HD11	Favored (79.95%) Isoleucine or valine / -60.4,-50.5	60.9% (*t*) chi angles: 181.6	0.02Å	-	-
D 531		ARG	50	-	Favored (48.98%) General / -65.8,-52.7	62.2% (*ttm-85*) chi angles: 182,181.9,293.9,276	0.045Å	-	-

D 532	LYS	50	0.805A HE2 with D 584 ASP CG	(67.76%) General / -64.7,-25.0	29.3% (*mtpp*) chi angles: 293.3,185.1,64,79	0.028Å	-	-
D 533	PHE	50	0.521Å HA with D 647 ASN HD22	Favored (8.56%) General / -124.3,22.5	65.4% (*m-85*) chi angles: 302.4,292.5	0.087Å	-	-
D 534	GLN	50	0.482Å HB2 with D 647 ASN CG	Favored (22.22%) General / 50.1,40.6	3.1% (*mp0*) chi angles: 270.8,54.7,78.9	0.039Å	-	-
D 535	ILE	50	0.988Å HD11 with D 530 VAL HG22	Favored (88.42%) Pre-proline / -75.7,123.5	25% (*pt*) chi angles: 68.9,165.5	0.126Å	-	-
D 536	PRO	50	0.74Å HG2 with D 539 VAL HB	Favored (39.52%) Trans-proline / -70.9,141.0	43.9% (*Cg_endo*) chi angles: 24.4	0.039Å	-	-
D 537	GLN	50	-	Favored (95.1%) General / -60.3,-44.7	53.3% (*tt0*) chi angles: 183.3,182.2,57	0.02Å	-	-
D 538	GLU	50	0.519Å HG3 with D 489 LEU HD21	Favored (75.83%) General / -60.4,-35.4	0.1% chi angles: 250.4,74.9,342.6	0.1Å	-	-
D 539	VAL	50	0.74Å HB with D 536 PRO HG2	Favored (46.06%) Isoleucine or valine / -74.9,-43.4	69.2% (*t*) chi angles: 171.7	0.101Å	-	-
D 540	LEU	50	0.57Å HD11 with D 524 TYR CD2	Favored (97.38%) General / -60.9,-42.1	55% (*tp*) chi angles: 176.1,58.4	0.007Å	-	-
D 541	VAL	50	0.873Å HG11 with D 489 LEU HD11	Favored (88.89%) Isoleucine or valine / -65.5,-46.8	7.7% (*p*) chi angles: 59.2	0.148Å	-	-
D 542	ARG	50	0.596Å HG2 with D 642 LEU HD21	Favored (74.77%) General / -61.1,-34.4	30.7% (*ttm105*) chi angles: 194.9,182.2,287.4,98.5	0.08Å	-	-
D 543	PHE	50	0.693Å HA with D 642 LEU HD22	Favored (63.83%) General /	87.6% (*t80*) chi angles: 179,82.4	0.028Å	-	-

HD22   General /
-66.3,-50.4

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 544		LEU	50	0.576Å O with D 547 ILE HG12	Favored (62.67%) General / -55.1,-33.3	96.5% (*mt*) chi angles: 294.4,173.9	0.035Å	-	-
D 545		PHE	50	0.927Å CE1 with D 517 VAL HG21	Favored (29.01%) General / -82.2,-34.1	2% (*m-30*) chi angles: 290.6,32.2	0.006Å	-	-
D 546		SER	50	-	Favored (91.2%) General / -64.6,-38.5	74.7% (*m*) chi angles: 294.9	0.036Å	-	-
D 547		ILE	50	0.576Å HG12 with D 544 LEU O	Favored (80.09%) Isoleucine or valine / -65.8,-49.0	28.7% (*pt*) chi angles: 66.8,178	0.073Å	-	-
D 548		SER	50	0.508Å N with D 547 ILE HG13	Favored (79.08%) General / -59.3,-37.9	48% (*t*) chi angles: 179.8	0.046Å	-	-
D 549		LYS	50	-	Favored (60.89%) General / -74.8,-28.9	33.1% (*ttpt*) chi angles: 187.3,184.3,61.7,192.8	0.075Å	-	-
D 550		GLY	50	0.487Å C with D 599 ILE HD11	Favored (72.37%) Glycine / -64.3,-28.0	-	-	-	-
D 551		TYR	50	-	Favored (37.38%) General / -75.8,151.9	65.9% (*m-85*) chi angles: 284.9,273.2	0.025Å	-	-
D 552		ARG	99.99	0.667Å NH1 with D 602 ARG HG3	Favored (8.65%) General / -118.1,170.7	17.5% (*ptp180*) chi angles: 64.5,175.8,68.4,183	0.044Å	-	-
D 553		ARG	99.99	0.489Å HG3 with D 553 ARG O	Favored (9.63%) General / -97.0,97.9	29% (*ptt-85*) chi angles: 60.9,171.9,183.8,279.7	0.036Å	-	-

Allowed

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
D 554		ILE	99.99	0.708Å HG13 with D 555 THR H	Allowed (0.89%) Isoleucine or valine / -115.8,-69.9	10.3% (*pt*) chi angles: 53.8,186.2	0.184Å	-	-
D 555		THR	50	0.708Å H with D 554 ILE HG13	OUTLIER (0.03%) General / -165.5,-43.0	40.7% (*p*) chi angles: 54	0.105Å	-	OUTLIER(S) worst is CA-CB-CG2: 4.145 σ
D 556		TYR	50	-	Allowed (1.8%) General / -122.8,-55.6	75.5% (*t80*) chi angles: 173.4,72.1	0.069Å	-	-
D 557		HIS	50	0.452Å HB2 with D 554 ILE HD11	Allowed (0.39%) General / -71.5,63.0	60.3% (*m80*) chi angles: 289.4,100.7	0.05Å	OUTLIER(S) worst is CG--ND1: 4.791 σ	-
D 558		ASN	50	-	Allowed (1.41%) General / -120.5,-167.1	22.8% (*p30*) chi angles: 55.6,58.1	0.066Å	-	-
D 559		TRP	50	-	Favored (72.71%) General / -55.2,-42.0	39.1% (*t-105*) chi angles: 163.9,252.7	0.037Å	-	-
D 560		ARG	50	0.421Å HD2 with D 508 ASP OD2	Favored (82.64%) General / -57.4,-42.6	11.9% (*mmt85*) chi angles: 297.2,300.8,176,117.9	0.064Å	-	-
D 561		HIS	50	-	Favored (85.32%) General / -61.2,-47.6	69.8% (*t60*) chi angles: 170.4,68.2	0.017Å	OUTLIER(S) worst is CG--ND1: 4.628 σ	OUTLIER(S) worst is CB-CG-CD2: 4.202 σ
D 562		GLY	50	0.588Å O with D 565 VAL HG12	Favored (92.04%) Glycine / -60.1,-37.0	-	-	-	-
D 563		PHE	50	0.439Å CE2 with D 516 LEU HG	Favored (57.15%) General / -70.2,-48.4	44.6% (*t80*) chi angles: 172.2,62.6	0.074Å	-	-
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 564		ASN	50	-	Favored (83.15%) General /	69% (*m-20*) chi angles: 284.6,307.1	0.043Å	-	-

564

				General / -58.7,-40.2	chi angles: 264.0,307.1			
D 565	VAL	50	0.588Å HG12 with D 562 GLY O	Favored (90.21%) Isoleucine or valine / -59.8,-42.8	11.7% (*p*) chi angles: 66.4	0.091Å	-	-
D 566	ALA	50	-	Favored (78.72%) General / -67.7,-35.4	-	0.061Å	-	-
D 567	GLN	50	-	Favored (75.05%) General / -69.4,-34.9	19% (*tm0?*) chi angles: 182.1,279.4,321.8	0.068Å	-	-
D 568	THR	50	0.602Å HG21 with D 720 SER OG	Favored (67.94%) General / -72.6,-35.3	72.4% (*p*) chi angles: 63.4	0.034Å	-	-
D 569	MET	50	-	Favored (99.19%) General / -62.4,-42.1	63.4% (*tpp*) chi angles: 181.2,66.2,74	0.072Å	-	-
D 570	PHE	50	-	Favored (86.37%) General / -67.2,-39.1	89.7% (*t80*) chi angles: 178.4,81.4	0.021Å	-	-
D 571	THR	50	-	Favored (66.61%) General / -73.1,-35.8	30.6% (*p*) chi angles: 51.3	0.06Å	-	-
D 572	LEU	99.99	0.86Å HD21 with D 796 MET SD	Favored (77.59%) General / -65.9,-34.2	72.8% (*mt*) chi angles: 289.3,177.9	0.101Å	-	-
D 573	LEU	50	-	Favored (55.95%) General / -74.7,-43.3	88.2% (*mt*) chi angles: 291.3,175.9	0.019Å	-	-
D 574	MET	50	0.635Å HE3 with D 579 LYS HD3	Allowed (0.21%) General / -83.2,-78.8	35.3% (*mmp*) chi angles: 294.6,297.3,94.4	0.072Å	-	-
D 575	THR	50	0.53Å HG21 with D 502 TYR O	Favored (85.67%) General / -63.3,-37.0	69.1% (*p*) chi angles: 59.7	0.012Å	-	-
D			0.498Å	Favored (88.59%)				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
D 576		GLY	50	0.498Å O with D 790 HIS CD2	(88.59%) Glycine / -79.1,-4.0	-	-	-	-
D 577		LYS	50	0.816Å HB2 with D 790 HIS CE1	Favored (6.4%) General / 48.1,36.3	52.5% (*mttp*) chi angles: 301.9,195.8,175.2,59.6	0.156Å	-	-
D 578		LEU	99.99	0.808Å HD11 with D 786 PHE CZ	Favored (40.54%) General / -79.8,-27.1	78.2% (*mt*) chi angles: 291.9,179.4	0.091Å	-	OUTLIER(S) worst is CB-CG-CD1: 4.832 σ
D 579		LYS	50	0.635Å HD3 with D 574 MET HE3	Allowed (0.13%) General / -34.0,-67.7	35% (*ttpt*) chi angles: 182.6,183.9,56.2,186.7	0.036Å	-	-
D 580		SER	50	-	Allowed (0.09%) General / -74.6,23.6	94% (*p*) chi angles: 63.3	0.06Å	-	-
D 581		TYR	99.99	-	Favored (15.01%) General / -109.2,-9.8	98.1% (*m-85*) chi angles: 295.7,273.6	0.022Å	-	-
D 582		TYR	99.99	-	Favored (39.34%) General / -123.6,154.4	98.8% (*m-85*) chi angles: 296.9,273.3	0.06Å	-	-
D 583		THR	50	-	Favored (26.76%) General / -76.3,163.7	62% (*p*) chi angles: 64.9	0.025Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 584		ASP	50	0.805Å CG with D 532 LYS HE2	Favored (72.88%) General / -64.4,-31.6	30.6% (*m-20*) chi angles: 294.7,286.6	0.022Å	-	OUTLIER(S) worst is CA-CB-CG: 4.212 σ
D 585		LEU	50	-	Favored (96.85%) General / -62.4,-40.5	0.6% chi angles: 275.5,327.6	0.114Å	-	-
D 586		GLU	50	0.512Å O with D 590 MET HG3	Favored (73.93%) General / -70.5,-39.9	83.3% (*mt-10*) chi angles: 295.8,173.7,325.5	0.018Å	-	-
D					Favored				

D 587	ALA	50	-	Favored (90.64%) General / -66.0,-41.6	-	0.038Å	-	-
D 588	PHE	99.99	0.496Å CE2 with D 645 TYR CE1	Favored (98.96%) General / -61.4,-42.6	84.1% (*t80*) chi angles: 181.4,81.8	0.046Å	-	-
D 589	ALA	50	-	Favored (86.77%) General / -66.7,-42.2	-	0.033Å	-	-
D 590	MET	99.99	0.512Å HG3 with D 586 GLU O	Favored (93.89%) General / -65.4,-40.7	98.6% (*mtp*) chi angles: 293.5,179.7,72.6	0.025Å	-	-
D 591	VAL	50	-	Favored (78.64%) Isoleucine or valine / -68.6,-47.1	14.2% (*p*) chi angles: 63.2	0.089Å	-	-
D 592	THR	50	0.982Å HB with D 660 MET HE1	Favored (98.12%) General / -63.7,-42.0	38.7% (*m*) chi angles: 305.9	0.021Å	-	-
D 593	ALA	50	0.478Å HA with D 660 MET SD	Favored (91.83%) General / -59.5,-42.2	-	0.083Å	-	-
D 594	GLY	50	-	Favored (93.67%) Glycine / -59.5,-46.6	-	-	-	-
D 595	LEU	50	-	Favored (61.52%) General / -71.9,-23.9	80.8% (*mt*) chi angles: 290.6,167.6	0.02Å	-	-
D 596	CYS	50	-	Favored (16.78%) General / -105.3,-10.8	80.6% (*m*) chi angles: 299.7	0.049Å	-	-
D 597	HIS	50	0.514Å CE1 with D 565 VAL HG11	Favored (67.96%) General / -63.9,-25.0	21.7% (*p-80*) chi angles: 81,271.9	0.116Å	OUTLIER(S) worst is CG--ND1: 5.036 σ	OUTLIER(S) worst is CB-CG-CD2: 4.577 σ
D 598	ASP	50	-	Favored (10.83%) General / -119.2,24.3	24.9% (*m-20*) chi angles: 275.3,329.8	0.042Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
D 599		ILE	50	1.029Å HG12 with D 632 PHE CD1	Favored (12.83%) Isoleucine or valine / -59.4,144.2	6.7% (*tp*) chi angles: 192.9,77.1	0.119Å	-	OUTLIER(S) worst is CA-CB-CG1: 6.235 σ
D 600		ASP	50	0.672Å N with D 599 ILE HG13	Favored (9.9%) General / 56.0,26.5	22.5% (*t70*) chi angles: 195.5,46.6	0.039Å	-	-
D 601		HIS	50	-	Favored (52.2%) General / -61.4,145.2	55.3% (*t-80*) chi angles: 197.4,280.9	0.141Å	OUTLIER(S) worst is CG--ND1: 4.364 σ	OUTLIER(S) worst is CB-CG-CD2: 4.447 σ
D 602		ARG	50	0.667Å HG3 with D 552 ARG NH1	Favored (23.82%) General / -108.8,15.2	1.7% (*mpt_?*) chi angles: 294.2,79.7,193.8,286.1	0.046Å	-	-
D 603		GLY	50	0.591Å CA with D 554 ILE HD12	Favored (93.33%) Glycine / 66.7,38.6	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 604		THR	50	0.572Å O with D 625 LEU HD21	Favored (23.58%) General / -153.1,144.9	71.5% (*p*) chi angles: 61.9	0.012Å	-	-
D 605		ASN	50	-	Allowed (0.15%) General / -52.0,166.6	6.5% (*m120*) chi angles: 284.2,165.1	0.07Å	-	-
D 606		ASN	50	0.463Å OD1 with D 625 LEU HD13	Favored (78.11%) General / -69.3,-38.4	86.7% (*m-20*) chi angles: 287.5,323.6	0.07Å	-	-
D 607		LEU	50	0.518Å HG with D 611 LYS HE2	Favored (73.28%) General / -60.0,-50.5	56% (*tp*) chi angles: 183.1,63	0.01Å	-	-
D 608		TYR	50	-	Favored (97.63%) General / -63.8,-42.4	81% (*t80*) chi angles: 172.8,80.4	0.022Å	-	-
D 609		GLN	50	0.867Å NE2 with D 616 LEU HB2	Favored (99.65%) General /	65.8% (*tt0*) chi angles: 181.5,176.4,24.2	0.077Å	-	-

D 609					-61.9,-42.9		
D 610	MET	50	-	Favored (69.38%) General / -57.8,-51.5	62.3% (*ttp*) chi angles: 181,184.1,66.9	0.063Å	-	-
D 611	LYS	50	0.518Å HE2 with D 607 LEU HG	Favored (68.29%) General / -63.6,-25.6	54.7% (*mtmt*) chi angles: 293.4,181,297.2,178.7	0.033Å	-	-
D 612	SER	50	-	Favored (56.02%) General / -94.1,2.4	35.3% (*p*) chi angles: 53.1	0.013Å	-	-
D 613	GLN	50	-	Favored (22.87%) General / 54.6,35.1	75.1% (*mt-30*) chi angles: 298.1,181.4,55.2	0.019Å	-	-
D 614	ASN	99.99	-	Favored (95.86%) Pre-proline / -62.4,143.4	90.8% (*m-20*) chi angles: 294.5,340.3	0.025Å	-	-
D 615	PRO	50	-	Favored (17.53%) Trans-proline / -49.1,-30.1	40.5% (*Cg_exo*) chi angles: 325.9	0.058Å	-	-
D 616	LEU	50	0.867Å HB2 with D 609 GLN NE2	Favored (66.86%) General / -65.4,-22.9	2.8% (*mm?*) chi angles: 296.1,311.7	0.157Å	-	-
D 617	ALA	50	-	Favored (79.25%) General / -58.8,-38.8	-	0.012Å	-	-
D 618	LYS	50	-	Favored (58.96%) General / -85.6,-3.7	30.9% (*mtpp*) chi angles: 296,183.4,65.9,64.6	0.008Å	-	-
D 619	LEU	50	-	Favored (25.95%) General / -82.6,-36.6	2.3% (*mp*) chi angles: 252.2,55.4	0.029Å	-	-
D 620	HIS	50	0.898Å HB3 with D 627 ARG HD2	Favored (49.07%) General / -130.5,153.2	79.4% (*m-70*) chi angles: 285.6,294.4	0.206Å	OUTLIER(S) worst is CD2-- NE2: 4.41 σ	OUTLIER(S) worst is CB- CG-CD2: 6.825 σ
D 621	GLY	50	-	Allowed (0.2%)	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
~~624~~		~~GLY~~	~~50~~		(0.2%) Glycine / -60.1,-77.0				
D 622	SER	50		-	Favored (7.86%) General / -125.2,174.8	78.5% (*p*) chi angles: 59.2	0.059Å	-	-
D 623	SER	50		-	Favored (2.97%) General / 50.0,61.8	37.7% (*m*) chi angles: 303.4	0.054Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 624	ILE	50		-	Favored (5.71%) Isoleucine or valine / -56.7,-58.4	89% (*mt*) chi angles: 299.4,170.5	0.085Å	-	-
D 625	LEU	50		0.6Å HD12 with D 609 GLN OE1	Favored (82.53%) General / -56.9,-44.6	9.3% (*mp*) chi angles: 276.1,71.6	0.071Å	-	-
D 626	GLU	50		0.513Å HG2 with D 668 ASP HB2	Favored (80.1%) General / -64.5,-35.2	26.8% (*mp0*) chi angles: 290.1,66.8,33.8	0.071Å	-	-
D 627	ARG	50		0.898Å HD2 with D 620 HIS HB3	Favored (72.6%) General / -71.0,-36.6	95% (*mtt-85*) chi angles: 291.3,186,180.8,270.3	0.045Å	-	-
D 628	HIS	50		-	Favored (92.87%) General / -65.4,-40.1	86.1% (*t60*) chi angles: 182.2,66.4	0.01Å	OUTLIER(S) worst is CG--ND1: 4.511 σ	-
D 629	HIS	50		-	Favored (91.11%) General / -58.9,-43.2	20.9% (*m-70*) chi angles: 295,325.4	0.05Å	OUTLIER(S) worst is CG--ND1: 4.852 σ	-
D 630	LEU	50		0.41Å HD13 with D 661 ASP HA	Favored (80.14%) General / -68.6,-37.9	33.2% (*tp*) chi angles: 182.9,71.1	0.045Å	-	-
D 631	GLU	50		0.448Å HG3 with D 627 ARG O	Favored (90.42%) General / -64.0,-38.3	51.9% (*mt-10*) chi angles: 296.6,182.6,290.9	0.045Å	-	-
				1.029Å	Favored				

D 632	PHE	99.99	1.029Å CD1 with D 599 ILE HG12	Favored (77.53%) General / -69.5,-38.3	53.6% (*t80*) chi angles: 178.9,273.3	0.032Å	-	-
D 633	GLY	50	-	Favored (62.33%) Glycine / -62.7,-50.6	-	-	-	-
D 634	LYS	50	-	Favored (75.5%) General / -59.0,-36.8	28.9% (*tptp*) chi angles: 184.1,64,180.7,65	0.047Å	-	-
D 635	PHE	50	0.666Å O with D 639 GLU HG3	Favored (75.45%) General / -67.5,-33.6	69.2% (*t80*) chi angles: 186.6,80.3	0.037Å	-	-
D 636	LEU	50	0.565Å HD13 with D 632 PHE O	Favored (22.66%) General / -80.9,-41.6	11.2% (*mp*) chi angles: 275,62	0.02Å	-	-
D 637	LEU	50	0.492Å HD23 with D 543 PHE CE1	Favored (36.03%) General / -57.2,-21.7	85.1% (*mt*) chi angles: 289.4,173.3	0.034Å	-	-
D 638	SER	50	-	Favored (13.96%) General / -112.6,-6.2	70.3% (*m*) chi angles: 297.7	0.05Å	-	-
D 639	GLU	99.99	0.666Å HG3 with D 635 PHE O	Favored (44.61%) General / -74.2,139.7	51.1% (*mt-10*) chi angles: 294.8,180.7,61.3	0.009Å	-	-
D 640	GLU	50	-	Favored (56.48%) General / -59.4,140.1	55% (*mm-40*) chi angles: 289.2,294.9,356.8	0.138Å	-	OUTLIER(S) worst is O-C-N: 4.799 σ
D 641	THR	50	0.504Å HB with D 542 ARG NH1	Allowed (1.24%) General / 82.7,1.1	19.2% (*p*) chi angles: 73.6	0.102Å	-	-
D 642	LEU	99.99	0.693Å HD22 with D 543 PHE HA	Favored (7.92%) General / -125.8,12.9	89.1% (*mt*) chi angles: 299.9,179	0.096Å	-	-
D 643	ASN	50	-	Favored (8.06%) General / -87.0,81.5	58% (*m-80*) chi angles: 293.6,275.2	0.046Å	-	-

High   Clash >   **Cβ   Bond   Bond**

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 644		ILE	50	0.665Å HG13 with D 645 TYR CD1	Favored (16.58%) Isoleucine or valine / -72.1,-13.3	44.5% (*pt*) chi angles: 58.4,170.6	0.159Å	-	-
D 645		TYR	99.99	0.665Å CD1 with D 644 ILE HG13	Favored (41.05%) General / -101.2,10.3	1.7% (*m-85*) chi angles: 291.4,35.1	0.066Å	-	-
D 646		GLN	50	-	Favored (63.21%) General / -70.1,-20.9	19.1% (*pt20*) chi angles: 62.8,180.4,58.9	0.105Å	-	-
D 647		ASN	50	0.521Å HD22 with D 533 PHE HA	Favored (61.48%) General / -73.0,-17.0	51.8% (*t30*) chi angles: 183.7,57.9	0.029Å	-	-
D 648		LEU	50	-	Favored (37.21%) General / -75.8,153.1	9.7% (*mp*) chi angles: 283.3,62.9	0.012Å	-	-
D 649		ASN	50	-	Favored (32.18%) General / -75.1,159.0	53.1% (*t30*) chi angles: 184,52.5	0.045Å	-	-
D 650		ARG	50	0.42Å O with D 654 GLU HG3	Favored (33.17%) General / -51.0,-35.2	61.9% (*ttm-85*) chi angles: 182.4,181.7,292.7,275.5	0.043Å	-	-
D 651		ARG	50	-	Favored (62.06%) General / -69.7,-47.8	56.7% (*mmm-85*) chi angles: 294.2,296.5,293.7,278.1	0.012Å	-	-
D 652		GLN	50	0.559Å O with D 656 VAL HG13	Favored (82.8%) General / -66.3,-36.4	74.9% (*mt-30*) chi angles: 296.8,182.1,55.8	0.031Å	-	-
D 653		HIS	50	0.53Å O with D 656 VAL HG22	Favored (98.44%) General / -63.5,-42.9	80.3% (*t60*) chi angles: 185.6,61.7	0.006Å	OUTLIER(S) worst is CG-- ND1: 4.306 σ	-
D 654		GLU	50	0.42Å HG3 with D	Favored (86.21%) General /	54.3% (*mt-10*) chi angles:	0.02Å	-	-

			650 ARG O	-67.2,-39.4	296.4,181.6,296			

D 655	HIS	50	-	Favored (95.73%) General / -64.6,-40.6	21.1% (*t-160*) chi angles: 181,202.9	0.05Å	OUTLIER(S) worst is CG--ND1: 4.514 σ	-
D 656	VAL	50	0.559Å HG13 with D 652 GLN O	Favored (82.92%) Isoleucine or valine / -65.6,-48.4	33.9% (*m*) chi angles: 299.3	0.122Å	-	-
D 657	ILE	50	-	Favored (74.98%) Isoleucine or valine / -61.1,-36.8	47.7% (*pt*) chi angles: 63.6,172.2	0.037Å	-	-
D 658	HIS	50	0.434Å O with D 662 ILE HG23	Favored (95.13%) General / -63.7,-43.9	21.8% (*t-160*) chi angles: 181.5,201.9	0.035Å	OUTLIER(S) worst is CG--ND1: 4.557 σ	-
D 659	LEU	50	-	Favored (80.78%) General / -67.2,-36.0	93.4% (*mt*) chi angles: 293.6,176.7	0.021Å	-	-
D 660	MET	50	0.982Å HE1 with D 592 THR HB	Favored (85.8%) General / -66.6,-43.1	44.4% (*tpp*) chi angles: 180.2,63.3,58.1	0.095Å	-	-
D 661	ASP	50	0.41Å HA with D 630 LEU HD13	Favored (88.62%) General / -63.4,-46.0	51.8% (*t0*) chi angles: 184.9,336.7	0.035Å	-	-
D 662	ILE	50	0.494Å HA with D 665 ILE HG12	Favored (78.52%) Isoleucine or valine / -66.0,-36.9	36.1% (*pt*) chi angles: 66.9,170.8	0.073Å	-	-
D 663	ALA	50	-	Favored (78.41%) General / -67.8,-35.3	-	0.032Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 664		ILE	50	-	Favored (25.62%) Isoleucine or	51.1% (*mt*) chi angles: 294.7,182.6	0.076Å	-	-

D 665	ILE	50	0.494Å HG12 with D 662 ILE HA	Favored (39.94%) Isoleucine or valine / -61.1,-26.7	37.7% (*pt*) chi angles: 65.5,174.7	0.051Å	-	-
D 666	ALA	50	-	Favored (68.4%) General / -66.3,-28.0	-	0.045Å	-	-
D 667	THR	50	-	Favored (2.15%) General / -77.1,10.8	61.9% (*p*) chi angles: 62.3	0.052Å	-	-
D 668	ASP	50	0.513Å HB2 with D 626 GLU HG2	Favored (20%) General / -90.2,108.8	43.9% (*t0*) chi angles: 180.3,18.5	0.012Å	-	-
D 669	LEU	50	0.563Å HG with D 673 PHE CE1	Favored (12.55%) General / -49.7,-32.0	3.3% (*tp*) chi angles: 227,56.7	0.044Å	-	-
D 670	ALA	50	-	Favored (96.64%) General / -60.4,-43.5	-	0.022Å	-	-
D 671	LEU	50	-	Favored (77.7%) General / -68.6,-35.7	13% (*mt*) chi angles: 298.6,198.3	0.082Å	-	-
D 672	TYR	50	0.638Å CZ with D 676 ARG HD3	Favored (79.08%) General / -60.8,-49.0	28.2% (*t80*) chi angles: 163.5,67.8	0.037Å	-	-
D 673	PHE	50	0.563Å CE1 with D 669 LEU HG	Favored (87.37%) General / -62.7,-37.7	2% (*m-30*) chi angles: 292.1,29.7	0.049Å	-	-
D 674	LYS	50	0.732Å HE2 with D 701 LEU HD13	Favored (74.57%) General / -63.2,-33.0	80.9% (*tttt*) chi angles: 175.5,187.9,170.7,184.3	0.035Å	-	-
D 675	LYS	99.99	0.725Å CG with D 701 LEU HD11	Favored (10.2%) General / -106.8,-28.3	54.4% (*mtmt*) chi angles: 292.5,183.3,279.5,184.9	0.082Å	-	-
			0.638Å	OUTLIER	10.8% (*mtm180*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
D 676		ARG	50	0.638Å HD3 with D 672 TYR CZ	(0.03%) General / -20.9,-62.7	10.8% (*mtm180*) chi angles: 286.6,216.5,288.2,210.7	0.142Å	-	-
D 677		ALA	50	0.879Å HA with D 680 GLN HE21	Favored (59.79%) General / -52.1,-39.4	-	0.061Å	-	-
D 678		MET	50	0.756Å O with D 682 ILE HG23	Favored (74.97%) General / -70.3,-38.1	62.1% (*ttp*) chi angles: 187.4,179.4,66.8	0.082Å	-	-
D 679		PHE	50	0.778Å O with D 682 ILE HG12	Favored (77.39%) General / -65.9,-46.7	24.2% (*t80*) chi angles: 185.7,51	0.097Å	-	-
D 680		GLN	99.99	0.879Å HE21 with D 677 ALA HA	Favored (82.93%) General / -66.0,-36.3	16.8% (*pt20*) chi angles: 72.5,173.9,289.1	0.201Å	-	OUTLIER(S) worst is N-CA-CB: 4.705 σ
D 681		LYS	50	0.695Å O with D 685 GLU HG2	Favored (86.28%) General / -66.4,-37.9	32.1% (*mmmt*) chi angles: 290.8,296.7,294.2,182.3	0.028Å	-	-
D 682		ILE	50	0.778Å HG12 with D 679 PHE O	Favored (80.6%) Isoleucine or valine / -60.8,-50.4	18.2% (*pt*) chi angles: 72.1,177.2	0.165Å	OUTLIER(S) worst is C--O: 4.215 σ	-
D 683		VAL	50	0.697Å HG11 with D 785 GLU OE1	Favored (95.94%) Isoleucine or valine / -63.7,-46.0	7.8% (*p*) chi angles: 70	0.21Å	-	OUTLIER(S) worst is N-CA-CB: 4.745 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 684		ASP	50	-	Favored (67.88%) General / -58.4,-31.7	43% (*t0*) chi angles: 186.6,328.5	0.03Å	-	-
D 685		GLU	99.99	0.695Å HG2 with D 681 LYS O	Favored (7.08%) General / -113.8,-29.5	12.5% (*pt-20*) chi angles: 64.4,180.8,58.7	0.081Å	OUTLIER(S) worst is C--N: 6.701 σ	OUTLIER(S) worst is C-N-CA: 5.877 σ
D		SER	99.99	0.621Å O with D 683 VAL ...	Favored (7.54%)	19% (*t*)	0.056Å	-	-

686		VAL HA		General / -155.4,-178.8	chi angles: 188.9			
D 687	LYS	99.99	-	Favored (50.88%) General / -134.4,150.8	22.5% (*pttp*) chi angles: 61.5,180.3,183.1,63.9	0.048Å	-	-
D 688	ASN	99.99	0.807Å HB2 with D 705 ARG HB3	Favored (41.02%) General / -72.7,153.8	39.5% (*p30*) chi angles: 63.7,26.7	0.054Å	-	-
D 689	TYR	99.99	1.084Å HD2 with D 690 GLN HB2	Allowed (0.35%) General / -115.2,-111.9	6.6% (*p90*) chi angles: 48.5,284.8	0.472Å	-	OUTLIER(S) worst is C-N-CA: 13.454 σ
D 690	GLN	50	1.084Å HB2 with D 689 TYR HD2	OUTLIER (0.02%) General / 101.5,-26.4	5.3% (*mt-30*) chi angles: 330.5,162.8,326	0.535Å	-	OUTLIER(S) worst is CA-CB-CG: 12.614 σ
D 691	ASP	50	-	Favored (33.94%) General / -88.8,124.2	28.9% (*t0*) chi angles: 174.8,20.7	0.105Å	-	-
D 692	LYS	50	0.694Å HG2 with D 693 LYS H	OUTLIER (0%) General / -53.8,-130.9	75.2% (*tttt*) chi angles: 186.6,195,173.4,169.6	0.055Å	-	-
D 693	LYS	99.99	0.937Å CB with D 707 GLU HB2	Favored (23.38%) General / -157.6,150.7	0% chi angles: 58.7,188.4,227,21.4	0.408Å	-	OUTLIER(S) worst is CG-CD-CE: 6.936 σ
D 694	SER	99.99	-	Favored (51.17%) General / -127.4,143.7	77.9% (*p*) chi angles: 58.9	0.04Å	-	-
D 695	TRP	99.99	0.939Å CZ3 with D 702 GLU HB3	Favored (54.25%) General / -109.9,132.3	96.2% (*m95*) chi angles: 296.4,97.2	0.069Å	OUTLIER(S) worst is NE1--CE2: 4.908 σ	-
D 696	VAL	99.99	-	Favored (31.85%) Isoleucine or valine / -110.6,110.3	97.7% (*t*) chi angles: 178.4	0.046Å	-	-
D 697	GLU	99.99	-	Favored (66.36%) General / -58.0,-30.7	85.4% (*mt-10*) chi angles: 300.7,183.9,333.8	0.044Å	-	-
D	TYR	99.99	-	Favored (68.63%)	96.6% (*m-85*)	0.034Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
698					General / -70.2,-44.5	chi angles: 292.7,276.4			
D 699		LEU	99.99	-	Favored (25.2%) General / -93.3,-16.0	85.4% (*mt*) chi angles: 293.1,178.8	0.062Å	-	-
D 700		SER	99.99	-	Favored (14.32%) General / 61.7,39.4	93.8% (*p*) chi angles: 66.9	0.057Å	-	-
D 701		LEU	99.99	0.732Å HD13 with D 674 LYS HE2	Favored (34.72%) General / -120.5,154.9	37.3% (*tp*) chi angles: 186.3,58.2	0.076Å	-	-
D 702		GLU	99.99	0.939Å HB3 with D 695 TRP CZ3	Favored (56.71%) General / -114.4,130.8	14.1% (*pt-20*) chi angles: 71.2,179.4,289.4	0.286Å	-	OUTLIER(S) worst is CA-CB-CG: 5.579 σ
D 703		THR	99.99	0.698Å HG23 with D 678 MET SD	Favored (55.01%) General / -119.7,135.0	20.2% (*m*) chi angles: 290	0.201Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 704		THR	99.99	0.926Å OG1 with D 705 ARG HA	OUTLIER (0%) General / -49.3,-168.2	0.5% chi angles: 220.4	0.383Å	-	OUTLIER(S) worst is CA-CB-CG2: 9.91 σ
D 705		ARG	99.99	0.926Å HA with D 704 THR OG1	Favored (14.72%) General / -92.2,-33.4	84.4% (*mtt-85*) chi angles: 309.7,176.7,184.7,276.9	0.563Å	-	OUTLIER(S) worst is N-CA-C: 5.124 σ
D 706		LYS	50	0.606Å O with D 709 VAL HG12	Favored (36.39%) General / -75.5,-45.7	4.5% (*tppp?*) chi angles: 178.2,63.4,65.4,53.4	0.098Å	-	-
D 707		GLU	50	0.937Å HB2 with D 693 LYS CB	Favored (77.75%) General / -58.2,-49.3	7.2% (*tt0*) chi angles: 207.7,150.9,330.9	0.475Å	-	OUTLIER(S) worst is C-CA-CB: 8.714 σ
D 708		ILE	99.99	0.919Å HB with D 704 THR CB	Favored (81.57%) Isoleucine or valine / -57.2,-48.8	1.5% (*tt*) chi angles: 223.9,175.1	0.217Å	-	OUTLIER(S) worst is N-CA-CB: 5.432 σ

D 709	VAL	50	0.606Å HG12 with D 706 LYS O	Favored (78.44%) Isoleucine or valine / -62.7,-37.2	12.5% (*p*) chi angles: 65.7	0.092Å	-	-
D 710	MET	99.99	-	Favored (97.42%) General / -63.7,-43.1	87.9% (*mtp*) chi angles: 295.7,185.1,66.1	0.038Å	-	-
D 711	ALA	50	-	Favored (97.65%) General / -60.9,-42.3	-	0.017Å	-	-
D 712	MET	50	-	Favored (80.85%) General / -68.4,-38.0	39% (*mmp*) chi angles: 295.6,298.2,108.5	0.013Å	-	-
D 713	MET	50	0.649Å HE1 with D 572 LEU HB3	Favored (89.96%) General / -61.5,-46.5	14.5% (*tpt*) chi angles: 182.6,62.3,175.2	0.064Å	-	OUTLIER(S) worst is CG-SD-CE: 5.491 σ
D 714	MET	50	-	Favored (85.34%) General / -57.7,-45.7	83.5% (*mmm*) chi angles: 287.7,298.8,303.9	0.039Å	-	-
D 715	THR	50	-	Favored (83.21%) General / -66.3,-36.5	99.2% (*m*) chi angles: 298.7	0.037Å	-	-
D 716	ALA	50	-	Favored (93.93%) General / -61.5,-40.2	-	0.031Å	-	-
D 717	CYS	50	0.621Å SG with D 572 LEU HD12	Favored (49.89%) General / -77.7,-37.3	73.6% (*m*) chi angles: 298.3	0.064Å	-	-
D 718	ASP	50	-	Favored (69.16%) General / -66.1,-28.9	43.5% (*t0*) chi angles: 191.1,22.4	0.046Å	-	-
D 719	LEU	50	0.434Å O with D 722 ILE HG22	Favored (35.79%) General / -104.3,7.8	83.9% (*mt*) chi angles: 301.7,179.5	0.105Å	-	-
D 720	SER	50	0.602Å OG with D 568 THR HG21	Favored (64.95%) General / -62.8,-30.4	78.2% (*p*) chi angles: 59	0.037Å	-	-

HG21							-62.8,-20.4

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
D 721		ALA	50	-	Favored (38.43%) General / -55.0,-26.7	-	0.043Å	-	-
D 722		ILE	50	0.434Å HG22 with D 719 LEU O	Favored (3.24%) Isoleucine or valine / -69.7,-3.7	8.7% (*tp*) chi angles: 201.6,65.3	0.095Å	-	-
D 723		THR	50	0.56Å O with D 799 ARG HB3	Favored (11.2%) General / -120.4,10.4	17.7% (*p*) chi angles: 74.5	0.055Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 724		LYS	50	0.715Å HB3 with D 728 VAL HG21	Favored (34.21%) Pre-proline / -89.7,163.1	72.6% (*mmtt*) chi angles: 290.9,300.6,187.8,182.4	0.214Å	-	OUTLIER(S) worst is N-CA-CB: 4.564 σ
D 725		PRO	50	0.565Å O with D 728 VAL HG22	Favored (2.64%) Trans-proline / -48.8,155.2	40.9% (*Cg_exo*) chi angles: 326	0.011Å	-	-
D 726		TRP	50	-	Favored (97.64%) General / -61.2,-44.2	63.3% (*t-105*) chi angles: 174.5,243.7	0.114Å	-	-
D 727		GLU	50	0.414Å O with D 731 LYS HG3	Favored (62.26%) General / -51.6,-43.1	49% (*mm-40*) chi angles: 288.5,293.2,359.8	0.03Å	-	-
D 728		VAL	50	0.715Å HG21 with D 724 LYS HB3	Favored (52.93%) Isoleucine or valine / -70.1,-49.8	11.4% (*m*) chi angles: 307.6	0.133Å	-	OUTLIER(S) worst is CG1-CB-CG2: 4.743 σ
D 729		GLN	50	0.578Å HA with D 732 VAL HG22	Favored (82.64%) General / -56.9,-45.2	1.6% (*tp-100*) chi angles: 156.8,54,203.3	0.049Å	-	-
D 730		SER	50	-	Favored (92.68%) General / -63.8,-38.9	31.4% (*t*) chi angles: 184.6	0.034Å	-	-

Favored

D 731	LYS	99.99	0.414Å HG3 with D 727 GLU O	Favored (83.88%) General / -65.9,-44.9	99.2% (*mttt*) chi angles: 293.6,179.9,179.7,181.2	0.033Å	-	-
D 732	VAL	50	0.578Å HG22 with D 729 GLN HA	Favored (75.74%) Isoleucine or valine / -65.7,-35.7	25.9% (*m*) chi angles: 301.9	0.098Å	-	-
D 733	ALA	50	-	Favored (87.92%) General / -63.2,-37.6	-	0.029Å	-	-
D 734	LEU	50	-	Favored (83.6%) General / -65.8,-36.5	87.1% (*mt*) chi angles: 291.5,176.7	0.03Å	-	-
D 735	LEU	50	-	Favored (96.09%) General / -62.5,-44.6	82.7% (*mt*) chi angles: 295.8,181	0.053Å	-	-
D 736	VAL	50	-	Favored (91.73%) Isoleucine or valine / -65.5,-41.8	93.1% (*t*) chi angles: 175.6	0.044Å	-	-
D 737	ALA	50	-	Favored (83.6%) General / -67.4,-37.8	-	0.04Å	-	-
D 738	ALA	50	-	Favored (98%) General / -62.1,-41.2	-	0.049Å	-	-
D 739	GLU	50	0.48Å HB2 with D 555 THR OG1	Favored (84.57%) General / -67.2,-42.3	16.3% (*tt0*) chi angles: 198.9,159.6,308.2	0.061Å	-	-
D 740	PHE	50	-	Favored (98.56%) General / -63.5,-41.2	19.2% (*m-30*) chi angles: 292.2,349.3	0.059Å	-	-
D 741	TRP	50	-	Favored (70.91%) General / -66.1,-30.4	26.5% (*m0*) chi angles: 291.4,326.3	0.03Å	-	-
D 742	GLU	50	-	Favored (63.7%) General / -73.3,-41.4	69% (*tt0*) chi angles: 183.6,176,23.4	0.026Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
D 743		GLN	50	-	Favored (70.59%) General / -60.8,-31.2	49.7% (*tt0*) chi angles: 181.6,174.9,316.4	0.013Å	-	-
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 744		GLY	50	-	Favored (95.33%) Glycine / -58.9,-45.2	-	-	-	-
D 745		ASP	50	-	Favored (48.92%) General / -60.8,-54.1	80.7% (*m-20*) chi angles: 292.5,325.8	0.028Å	-	-
D 746		LEU	50	-	Favored (20.3%) General / -48.6,-38.3	0% chi angles: 261.9,8.2	0.02Å	-	-
D 747		GLU	50	-	Favored (61.27%) General / -72.2,-23.8	7.2% (*mt-10*) chi angles: 288.7,217.9,23.9	0.148Å	-	-
D 748		ARG	50	-	Favored (10.52%) General / -85.0,-47.1	64.4% (*mtm-85*) chi angles: 281.7,196.6,306.4,294.2	0.152Å	-	-
D 749		THR	50	-	Favored (83.96%) General / -64.3,-46.4	7.2% (*m*) chi angles: 285.8	0.168Å	-	-
D 750		VAL	50	-	Favored (2.72%) Isoleucine or valine / -108.3,-34.6	1.8% (*m*) chi angles: 320.7	0.155Å	-	-
D 751		LEU	50	-	Favored (18.3%) General / -90.4,-29.0	20.7% (*mt*) chi angles: 291.1,191.8	0.125Å	-	-
D 752		ASP	50	-	Favored (17.22%) General / 62.5,30.9	49.5% (*m-20*) chi angles: 297.7,294.9	0.056Å	-	-

Favored

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
D 753		GLN	50	-	Favored (24.4%) General / -101.9,149.2	71.3% (*mt-30*) chi angles: 290.2,189.2,29.6	0.085Å	-	-
D 754		GLN	50	-	Favored (94.38%) Pre-proline / -64.8,129.5	0% chi angles: 228.4,257.1,33.7	0.079Å	-	-
D 755		PRO	50	-	Favored (28.49%) Trans-proline / -73.5,139.4	93.6% (*Cg_endo*) chi angles: 30.8	0.034Å	-	-
D 756		ILE	50	-	Favored (6.11%) Pre-proline / -52.0,151.9	30.1% (*pt*) chi angles: 66,178	0.075Å	-	-
D 757		PRO	50	-	Favored (62.32%) Trans-proline / -51.7,-36.7	75.5% (*Cg_exo*) chi angles: 328.2	0.07Å	-	-
D 758		MET	50	0.408Å HG2 with D 758 MET O	Favored (58.14%) General / -62.2,-17.3	26.2% (*ttm*) chi angles: 190.6,198.2,310.3	0.047Å	-	-
D 759		MET	50	-	Favored (9.39%) General / -122.9,9.4	61.3% (*mtt*) chi angles: 300.4,185,186.8	0.061Å	-	-
D 760		ASP	50	-	Favored (46.8%) General / -100.5,125.6	40.7% (*t0*) chi angles: 184.4,328.6	0.087Å	-	-
D 761		ARG	50	-	Favored (83.58%) General / -67.9,-39.5	8.8% (*mtp85*) chi angles: 329.7,192.8,68.4,116.8	0.075Å	-	-
D 762		ASN	50	-	Favored (68.8%) General / -63.4,-26.6	40.5% (*m-80*) chi angles: 307.5,287.1	0.04Å	-	-
D 763		LYS	50	-	Favored (2.85%) General / -99.6,32.4	0.1% chi angles: 276,96,197.2,300	0.056Å	-	-
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330

		56.93	54.38	328	298	7 of 317	of 330	of 330
D 764	ALA	50	-	Favored (69.47%) General / -62.6,-27.8	-	0.029Å	-	-
D 765	ALA	50	-	Favored (63.51%) General / -67.0,-15.1	-	0.015Å	-	-
D 766	GLU	50	-	Favored (55.69%) General / -94.5,2.1	67.9% (*mt-10*) chi angles: 296.8,179.8,26.7	0.042Å	-	-
D 767	LEU	50	0.406Å HA with D 767 LEU HD12	Favored (78.45%) Pre-proline / -64.3,-46.1	0.2% chi angles: 242.7,30.3	0.071Å	-	-
D 768	PRO	50	-	Allowed (1.02%) Trans-proline / -51.5,-59.8	17.8% (*Cg_exo*) chi angles: 323.9	0.045Å	-	-
D 769	LYS	50	-	Favored (63.41%) General / -62.1,-19.9	19.7% (*ptmt*) chi angles: 55.2,192.1,286.1,181.2	0.203Å	-	-
D 770	LEU	50	-	Favored (68.57%) General / -71.9,-40.7	0.9% chi angles: 252.1,45.5	0.059Å	-	-
D 771	GLN	50	-	Favored (91.17%) General / -65.7,-39.4	10.2% (*mm100*) chi angles: 275.3,296.7,88.9	0.045Å	-	-
D 772	VAL	50	-	Favored (55.5%) Isoleucine or valine / -60.0,-52.9	97.9% (*t*) chi angles: 176.3	0.034Å	-	-
D 773	GLY	50	-	Favored (73.95%) Glycine / -56.0,-38.2	-	-	-	-
D 774	PHE	50	-	Favored (72.95%) General / -61.4,-50.4	30.1% (*t80*) chi angles: 174.5,54.5	0.023Å	-	-
D	ILE	50		Favored (80.94%)	78.6% (*mt*)	0.082Å		

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
775	ILE 50	-	(80.94%) Isoleucine or valine / -61.8,-50.2	chi angles: 293.8,176.3	0.082Å	-	-
D 776	ASP 50	-	Favored (84.04%) General / -62.1,-47.6	87.5% (*m-20*) chi angles: 292.1,332.5	0.036Å	-	-
D 777	PHE 50	-	Favored (59.71%) General / -76.0,-32.9	42.4% (*t80*) chi angles: 180.9,57.9	0.076Å	-	-
D 778	VAL 50	-	Favored (4.72%) Isoleucine or valine / -114.5,-54.0	61.6% (*t*) chi angles: 181.4	0.038Å	-	-
D 779	CYS 50	0.745Å O with D 782 VAL HG12	Allowed (0.98%) General / -79.0,-65.6	98.6% (*m*) chi angles: 294.6	0.088Å	-	-
D 780	THR 50	0.485Å O with D 784 LYS HG3	Favored (27.62%) General / -47.7,-44.4	0.2% chi angles: 143.2	0.179Å	-	-
D 781	PHE 99.99	0.813Å HZ with D 680 GLN HB2	Favored (74.8%) General / -61.9,-33.7	75.6% (*t80*) chi angles: 184.4,81.7	0.021Å	-	-
D 782	VAL 50	0.745Å HG12 with D 779 CYS O	Favored (58.64%) Isoleucine or valine / -71.7,-47.1	9.2% (*p*) chi angles: 71	0.131Å	-	-
D 783	TYR 50	-	Favored (70.01%) General / -69.4,-31.6	55.3% (*m-85*) chi angles: 291.7,297.6	0.06Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 784	LYS 50	0.544Å HG3 with D 797 PHE CE1	Favored (78.87%) General / -58.0,-39.8	30.2% (*mtpp*) chi angles: 288.7,180,70.4,65.8	0.168Å	-	-
D 785	GLU 50	0.697Å OE1 with D	Favored (63.52%) General /	27.3% (*mm-40*) chi angles:	0.029Å	-	-

785			CE1 with D 683 VAL HG11	General / -71.9,-44.6	chi angles: 293.2,302.9,5			
D 786	PHE	50	0.808Å CZ with D 578 LEU HD11	Favored (73.85%) General / -63.0,-32.5	69.2% (*t80*) chi angles: 186.5,80.9	0.076Å	-	OUTLIER(S) worst is CA-CB-CG: 4.085 σ
D 787	SER	50	0.533Å HA with D 793 ILE CG2	Favored (76.04%) General / -64.2,-33.5	23% (*t*) chi angles: 187	0.033Å	-	-
D 788	ARG	50	0.605Å HE with D 683 VAL HG22	Favored (73.62%) General / -68.8,-33.3	71.5% (*mtp85*) chi angles: 292.5,185.5,57.1,95.9	0.006Å	-	-
D 789	PHE	50	0.64Å CZ with D 679 PHE CE1	Favored (63.06%) General / -74.6,-36.7	1.8% (*m-30*) chi angles: 292,31.9	0.038Å	-	-
D 790	HIS	50	0.816Å CE1 with D 577 LYS HB2	Favored (4.56%) General / -148.8,110.6	79.9% (*t60*) chi angles: 188,68.9	0.088Å	OUTLIER(S) worst is CG--CD2: 4.797 σ	OUTLIER(S) worst is CA-CB-CG: 9.424 σ
D 791	GLU	50	-	Favored (44%) General / -51.7,-35.7	58.5% (*tt0*) chi angles: 181.8,183.5,32.7	0.108Å	-	-
D 792	GLU	50	0.703Å HB2 with D 790 HIS NE2	Favored (7.87%) General / -76.6,5.2	26.5% (*mt-10*) chi angles: 310,166.5,51.5	0.194Å	-	-
D 793	ILE	50	0.792Å HG22 with D 790 HIS O	Favored (9.17%) Isoleucine or valine / -95.0,3.4	8.5% (*tp*) chi angles: 190,55.9	0.059Å	-	-
D 794	LEU	50	0.407Å C with D 793 ILE O	Allowed (1.83%) Pre-proline / -42.8,-37.1	40.6% (*tp*) chi angles: 186.6,61.9	0.033Å	-	-
D 795	PRO	50	0.518Å O with D 799 ARG HG2	Favored (51.64%) Trans-proline / -50.5,-37.3	61.8% (*Cg_exo*) chi angles: 327.3	0.074Å	-	-
D 796	MET	99.99	0.86Å SD with D 572 LEU HD21	Favored (85.87%) General / -66.3,-43.5	74.8% (*mtp*) chi angles: 288.3,180.1,88.3	0.041Å	-	-
D 797	PHE	50	0.544Å CE1 with D	Favored (78.86%) General /	87.9% (*t80*) chi angles: 182.1,76.9	0.022Å	-	-

7 97				784 LYS HG3	General / -69.2,-38.9	chi angles: 182.7,-0.9		
D 798		ASP	50	-	Favored (85.86%) General / -62.7,-46.9	38.3% (*t0*) chi angles: 188.6,28.1	0.052Å	-	-
D 799		ARG	99.99	0.56Å HB3 with D 723 THR O	Favored (86.39%) General / -66.1,-37.7	37.5% (*mmt180*) chi angles: 289.3,297.7,179.2,183.1	0.223Å	-	OUTLIER(S) worst is N-CA-CB: 4.199 σ
D 800		LEU	50	0.656Å HD11 with D 779 CYS HB3	Favored (96.31%) General / -61.0,-45.1	8.7% (*tt*) chi angles: 179.9,156.2	0.053Å	-	-
D 801		GLN	50	0.406Å CD with D 797 PHE CE2	Favored (92.77%) General / -65.2,-39.4	84.9% (*mt-30*) chi angles: 292.2,182.9,296.4	0.043Å	-	-
D 802		ASN	50	-	Favored (97.75%) General / -62.9,-40.5	32% (*m120*) chi angles: 292.3,119.5	0.022Å	-	-
D 803		ASN	50	-	Favored (65.35%) General / -69.0,-27.1	81.9% (*m-20*) chi angles: 284.9,324.2	0.065Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.93	Clashscore: 54.38	Outliers: 5 of 328	Poor rotamers: 12 of 298	Outliers: 7 of 317	Outliers: 15 of 330	Outliers: 31 of 330
D 804		ARG	50	-	Favored (71.97%) General / -67.7,-46.5	54.9% (*ttt-85*) chi angles: 187.8,187.8,180.7,292.9	0.032Å	-	-
D 805		LYS	50	-	Favored (85.54%) General / -60.5,-38.8	31% (*mtpp*) chi angles: 293.8,182.7,64.8,65	0.054Å	-	-
D 806		GLU	50	-	Favored (63.61%) General / -64.6,-51.3	58.7% (*mm-40*) chi angles: 290.8,294.4,356.6	0.017Å	-	-
D 807		TRP	50	-	Favored (89.88%) General / -65.3,-38.3	48.9% (*m95*) chi angles: 286.2,121.1	0.044Å	-	-
					Favored	28.5% (*tptp*)			

D 808	LYS	50	-	(79.6%) General / -62.6,-35.4	28.5 % (tptp) chi angles: 184.7,62.6,180.5,66.1	0.011Å	-	-
D 809	ALA	50	-	Favored (90.4%) General / -65.5,-38.6	-	0.03Å	-	-
D 810	LEU	50	-	Favored (66.17%) General / -72.0,-31.5	45.2% (mt) chi angles: 283.6,175.3	0.039Å	-	-
D 811	ALA	50	-	Favored (63.81%) General / -61.0,-21.8	-	0.015Å	-	-
D 812	ASP	50	-	Favored (18.47%) General / -112.8,18.1	59.8% (m-20) chi angles: 296.2,300.6	0.029Å	-	-
D 813	GLU	99.99	-	-	9.7% (tm-20) chi angles: 181.2,288.8,319.8	0.147Å	-	-
z 1	ZN	42.97	-	-	-	-	-	-

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