Viewing pax6_4-136_1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	16.16		45th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	2.61%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	129	98.47%	Goal: >98%
	MolProbity score^	2.03		74th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	4 / 1038	0.39%	Goal: 0%
	Bad backbone angles:	1 / 1403	0.07%	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: 54.96	Clashscore: 16.16	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133
A 4		SER	50	-	-	90.8% (*p*) chi angles: 62.7	0.047Å	-	-
A 5		HIS	50	-	Favored (27.67%) General / -154.0,149.8	29.1% (*p-80*) chi angles: 70,293.6	0.031Å	OUTLIER(S) worst is CG--ND1: 4.3 σ	OUTLIER(S) worst is CB-CG-CD2: 4.405 σ
A 6		SER	50	-	Favored (38.98%) General / -74.8,153.0	43.8% (*m*) chi angles: 302.6	0.038Å	-	-
A 7		GLY	50	0.598Å O with A 14 VAL HA	Favored (27.01%) Glycine / -147.1,174.2	-	-	-	-
A 8		VAL	50	-	Favored (49.94%) Isoleucine or valine /	86.3% (*t*) chi angles: 177.3	0.074Å	-	-

				valine / -117.1,137.8				
A 9	ASN	50	0.471Å HB2 with C2019 DGU OP2	Favored (6.11%) General / -95.1,176.8	33.1% (*p30*) chi angles: 60,31.4	0.076Å	-	-
A 10	GLN	50	-	Allowed (1.26%) General / -57.2,-10.5	93.9% (*mt-30*) chi angles: 297.1,181.1,339.7	0.025Å	-	-
A 11	LEU	50	-	Favored (24.32%) General / -102.0,-5.7	9.9% (*mp*) chi angles: 275,55.4	0.046Å	-	-
A 12	GLY	50	-	Favored (84.19%) Glycine / 81.0,11.1	-	-	-	-
A 13	GLY	50	-	Favored (25.75%) Glycine / -80.4,144.5	-	-	-	-
A 14	VAL	50	0.598Å HA with A 7 GLY O	Favored (45.2%) Isoleucine or valine / -92.6,125.4	6.3% (*m*) chi angles: 309.6	0.091Å	-	-
A 15	PHE	50	-	Favored (49.31%) General / -133.5,155.6	31% (*p90*) chi angles: 67.2,281.9	0.028Å	-	-
A 16	VAL	50	-	Favored (7.86%) Isoleucine or valine / -113.9,99.1	47.9% (*t*) chi angles: 182.9	0.058Å	-	-
A 17	ASN	50	-	Allowed (0.69%) General / -51.1,112.2	47.3% (*t-20*) chi angles: 193.8,356	0.039Å	-	-
A 18	GLY	50	-	Favored (41.75%) Glycine / 105.1,-5.2	-	-	-	-
A 19	ARG	50	-	Favored (49.93%) Pre-proline / -118.7,151.4	28.5% (*mmm180*) chi angles: 300,309.2,297.7,167.2	0.036Å	-	-
A 20	PRO	50	-	Favored (90.31%) Trans-proline /	50.6% (*Cg_exo*) chi angles: 335.7	0.12Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					Trans-proline / -63.7,149.6	chi angles: 330.4			
A 21		LEU	50	-	Favored (96.5%) Pre-proline / -62.4,140.7	0.6% chi angles: 246.6,45.7	0.068Å	-	-
A 22		PRO	50	-	Favored (33.8%) Trans-proline / -52.7,146.7	86% (*Cg_exo*) chi angles: 328.8	0.062Å	-	-
A 23		ASP	50	-	Favored (66.35%) General / -57.9,-31.0	89% (*m-20*) chi angles: 289.7,334.8	0.067Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 16.16	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133
A 24		SER	50	0.595Å O with A 28 LYS HG2	Favored (99.03%) General / -61.8,-42.5	66% (*p*) chi angles: 57	0.021Å	-	-
A 25		THR	50	-	Favored (75.62%) General / -70.1,-38.6	28.5% (*m*) chi angles: 307.6	0.022Å	-	-
A 26		ARG	50	-	Favored (92.36%) General / -64.9,-38.9	38.7% (*mtp85*) chi angles: 304,174.7,90.6,88.2	0.016Å	-	-
A 27		GLN	50	0.453Å HG2 with A 66 ILE CD1	Favored (85.83%) General / -66.6,-43.1	5.5% (*mm100*) chi angles: 264,298.7,140.7	0.042Å	-	-
A 28		LYS	50	0.595Å HG2 with A 24 SER O	Favored (90.43%) General / -59.4,-41.9	32.8% (*mmmt*) chi angles: 295.4,296.5,292.3,181.2	0.048Å	-	-
A 29		ILE	50	-	Favored (58.45%) Isoleucine or valine / -56.9,-52.2	77.9% (*mt*) chi angles: 294.1,176.5	0.079Å	-	-
A 30		VAL	50	-	Favored (83.44%) Isoleucine or valine / -66.7,-39.3	2% (*p*) chi angles: 45.5	0.198Å	-	-
A 31		GLU	50		Favored (98.15%)	89.1% (*mt-10*) chi angles:	0.038Å		

A 31	GLU	50	-	General / -63.7,-41.5	chi angles: 289.6,180.2,330.7	0.038Å	-	-
A 32	LEU	50	-	Favored (79.62%) General / -66.8,-45.0	59.1% (*mt*) chi angles: 285.5,174.7	0.03Å	-	-
A 33	ALA	50	-	Favored (87.16%) General / -59.7,-40.2	-	0.038Å	-	-
A 34	HIS	50	-	Favored (82.91%) General / -62.9,-36.3	45.6% (*t-80*) chi angles: 180.1,250.6	0.024Å	OUTLIER(S) worst is CG-- ND1: 4.39 σ	-
A 35	SER	50	-	Favored (56.27%) General / -79.9,-5.8	80.5% (*p*) chi angles: 60.2	0.104Å	-	-
A 36	GLY	50	-	Favored (11.59%) Glycine / 107.3,17.3	-	-	-	-
A 37	ALA	50	-	Favored (36.34%) General / -79.0,131.6	-	0.021Å	-	-
A 38	ARG	50	-	Favored (87.57%) Pre-proline / -66.9,156.4	83.2% (*mtm180*) chi angles: 295.4,172.1,300.8,162.1	0.055Å	-	-
A 39	PRO	50	-	Favored (65.04%) Trans-proline / -51.6,-39.9	78.9% (*Cg_exo*) chi angles: 328.5	0.052Å	-	-
A 40	CYS	50	-	Favored (87.4%) General / -65.6,-37.7	29.4% (*p*) chi angles: 62.3	0.024Å	-	-
A 41	ASP	50	-	Favored (83.29%) General / -64.1,-46.6	76.8% (*m-20*) chi angles: 294.4,322.2	0.041Å	-	-
A 42	ILE	50	-	Favored (90.68%) Isoleucine or valine / -60.6,-42.2	85.4% (*mt*) chi angles: 300.7,172.5	0.046Å	-	-
A 43	SER	50	-	Favored (90.04%) General /	29.4% (*t*) chi angles: 172.6	0.033Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 16.16	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133
A 44		ARG	50	-	Favored (61.36%) General / -66.7,-50.9	30.3% (*ttp-105*) chi angles: 188.6,185.7,68.2,262.1	0.027Å	-	-
A 45		ILE	50	-	Favored (92.83%) Isoleucine or valine / -61.1,-47.6	85.8% (*mt*) chi angles: 300.3,171.2	0.04Å	-	-
A 46		LEU	50	-	Favored (54.68%) General / -91.7,-4.8	85.1% (*mt*) chi angles: 300.1,180.3	0.05Å	-	-
A 47		GLN	50	-	Favored (30.56%) General / 55.3,42.1	31.8% (*mt-30*) chi angles: 301.9,173.9,117.2	0.045Å	-	-
A 48		VAL	50	-	Favored (26.39%) Isoleucine or valine / -110.3,141.2	75.9% (*t*) chi angles: 179.3	0.076Å	-	-
A 49		SER	50	-	Favored (46.75%) General / -56.8,140.8	93.8% (*p*) chi angles: 66.1	0.016Å	-	-
A 50		ASN	50	-	Favored (70.71%) General / -55.6,-39.3	15.9% (*m-80*) chi angles: 269.7,285.3	0.046Å	-	-
A 51		GLY	50	-	Favored (94.42%) Glycine / -59.9,-38.6	-	-	-	-
A 52		CYS	50	-	Favored (65.51%) General / -71.9,-43.3	48.2% (*t*) chi angles: 182.6	0.009Å	-	-
A 53		VAL	50	-	Favored (88.74%) Isoleucine or valine / -58.4,-44.5	98.7% (*t*) chi angles: 178.4	0.029Å	-	-
A 54		SER	50	-	Favored (85.5%) General /	43.2% (*t*) chi angles: 178.1	0.03Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					General / -59.7,-47.5	chi angles: 178.1			
A 55		LYS	50	0.453Å NZ with C2017 DGU OP2	Favored (80.11%) General / -68.4,-41.7	3% (*tmmt?*) chi angles: 195.6,248.9,291.9,169.9	0.067Å	-	-
A 56		ILE	50	-	Favored (79.62%) Isoleucine or valine / -67.1,-48.2	79% (*mt*) chi angles: 297.2,177.2	0.116Å	-	-
A 57		LEU	50	0.409Å HA with A 57 LEU HD23	Favored (98.08%) General / -61.6,-43.9	14.1% (*mt*) chi angles: 276.4,184.3	0.072Å	-	-
A 58		GLY	50	-	Favored (94.22%) Glycine / -58.7,-45.8	-	-	-	-
A 59		ARG	50	0.661Å HA with A 62 GLU HG2	Favored (74.13%) General / -70.2,-35.7	40.7% (*ttm180*) chi angles: 189.3,182.5,294,163.2	0.069Å	-	-
A 60		TYR	50	-	Favored (98.04%) General / -63.5,-40.8	51.7% (*t80*) chi angles: 173.9,63.7	0.012Å	-	-
A 61		TYR	50	-	Favored (64.24%) General / -70.9,-28.1	18.1% (*m-30*) chi angles: 291.9,323.3	0.09Å	-	-
A 62		GLU	50	0.766Å HG3 with A 63 THR HG23	Favored (22.39%) General / -85.0,-33.9	12.3% (*pt-20*) chi angles: 64.3,178.6,62.1	0.112Å	-	-
A 63		THR	50	0.766Å HG23 with A 62 GLU HG3	Favored (7.86%) General / -122.3,-14.5	33.7% (*p*) chi angles: 68.8	0.055Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 16.16	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133
A 64		GLY	50	-	Favored (65.61%) Glycine / 64.8,19.8	-	-	-	-
A 65		SER	50	-	Favored (48.15%)	46.3% (*t*)	0.043Å	-	-

A 65	SER	50		General / -113.5,140.4	chi angles: 180.5	0.049Å	
A 66	ILE	50	0.453Å CD1 with A 27 GLN HG2	Favored (5.49%) Isoleucine or valine / -101.5,-20.6	6.2% (*pt*) chi angles: 77.5,162	0.05Å	-	-
A 67	ARG	50	-	Favored (97.65%) Pre-proline / -63.3,140.1	25.5% (*mmm-85*) chi angles: 294.7,316.4,312,295.3	0.06Å	-	-
A 68	PRO	50	-	Favored (81.17%) Trans-proline / -67.3,151.0	91.8% (*Cg_endo*) chi angles: 30.9	0.044Å	-	-
A 69	ARG	50	-	Favored (31.49%) General / -75.5,159.3	26% (*mtt85*) chi angles: 300.1,205.1,203.5,115.9	0.035Å	-	-
A 70	ALA	50	-	Favored (18.35%) General / -63.9,123.2	-	0.026Å	-	-
A 71	ILE	50	0.428Å O with B1017 DGU C5'	Favored (3.5%) Isoleucine or valine / -92.1,151.8	72.5% (*mt*) chi angles: 303.2,171.2	0.056Å	-	-
A 72	GLY	50	0.795Å HA3 with B1016 DTY O2	Favored (46.73%) Glycine / 61.7,-136.7	-	-	-	-
A 73	GLY	50	-	Favored (41.3%) Glycine / 61.4,-152.5	-	-	-	-
A 74	SER	50	-	Favored (7.89%) General / -170.0,159.9	74.2% (*p*) chi angles: 58.1	0.049Å	-	-
A 75	LYS	50	-	Favored (46.41%) Pre-proline / -89.2,151.3	7.4% (*mmpt?*) chi angles: 291.6,263.8,73.7,182	0.036Å	-	-
A 76	PRO	50	-	Favored (50.96%) Trans-proline / -53.4,132.9	94.4% (*Cg_exo*) chi angles: 329.2	0.069Å	-	-
A 77	ARG	50	0.489Å NH2 with B1019 DGU C1'	Favored (4.79%) General / -107.0,-42.8	27.1% (*mtm180*) chi angles: 279,149.2,280.5,158.5	0.027Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-107.0,-42.0				
A 78		VAL	50	-	Favored (3.71%) Isoleucine or valine / -113.2,-41.2	33.2% (*m*) chi angles: 299.9	0.076Å	-	-
A 79		ALA	50	-	Favored (2.43%) General / -87.6,52.2	-	0.076Å	-	-
A 80		THR	50	-	Favored (65.26%) Pre-proline / -64.5,158.7	30.5% (*p*) chi angles: 69.9	0.031Å	-	-
A 81		PRO	50	-	Favored (24.58%) Trans-proline / -50.8,-47.6	83.1% (*Cg_exo*) chi angles: 328.7	0.055Å	-	-
A 82		GLU	50	-	Favored (98.71%) General / -61.3,-42.5	86.1% (*tt0*) chi angles: 184.3,182.4,354.9	0.011Å	-	-
A 83		VAL	50	-	Favored (98.76%) Isoleucine or valine / -61.9,-44.4	96.9% (*t*) chi angles: 176.1	0.039Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 16.16	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133
A 84		VAL	50	-	Favored (96.18%) Isoleucine or valine / -62.1,-42.7	85.5% (*t*) chi angles: 177.6	0.066Å	-	-
A 85		SER	50	-	Favored (98.34%) General / -61.1,-42.3	66.5% (*m*) chi angles: 296.6	0.056Å	-	-
A 86		LYS	50	-	Favored (95.52%) General / -64.8,-41.7	62.6% (*mmtt*) chi angles: 279.5,295.7,174.7,181.2	0.059Å	-	-
A 87		ILE	50	-	Favored (93.87%) Isoleucine or valine / -62.0,-47.3	76.8% (*mt*) chi angles: 294.7,177	0.064Å	-	-
				0.55Å	Favored				

A 88	ALA	50	O.55Å O with A 92 ARG HG3	(84.73%) General / -61.6,-37.7	-	0.037Å	-	-
A 89	GLN	50	0.599Å O with A 93 GLU HG2	Favored (96.91%) General / -64.2,-41.8	2.9% (*tt0*) chi angles: 204.9,202.6,274.6	0.03Å	-	-
A 90	TYR	50	0.475Å HE2 with A 106 LEU HD22	Favored (65.07%) General / -69.3,-47.2	17.8% (*m-30*) chi angles: 300.9,339.9	0.036Å	-	-
A 91	LYS	50	0.419Å HG3 with A 127 LEU CD2	Favored (79.07%) General / -61.4,-36.0	7.3% (*mmtt*) chi angles: 248.4,275.3,180.6,165.6	0.022Å	-	-
A 92	ARG	50	0.55Å HG3 with A 88 ALA O	Favored (76.72%) General / -61.4,-49.5	74.3% (*mtp85*) chi angles: 289.5,175.7,70.7,81.5	0.032Å	-	-
A 93	GLU	50	0.599Å HG2 with A 89 GLN O	Favored (55.26%) General / -80.8,-15.8	3.8% (*pt-20*) chi angles: 37,194.2,62.3	0.202Å	-	-
A 94	CYS	50	-	Favored (3.83%) Pre-proline / -153.6,87.2	52.6% (*t*) chi angles: 181.3	0.071Å	-	-
A 95	PRO	50	-	Favored (98.57%) Trans-proline / -58.7,-33.9	80.5% (*Cg_exo*) chi angles: 330.6	0.065Å	-	-
A 96	SER	50	-	Favored (32.22%) General / -71.8,-5.2	78.5% (*p*) chi angles: 59.2	0.028Å	-	-
A 97	ILE	50	-	Favored (15.4%) Isoleucine or valine / -63.1,143.6	16.3% (*tt*) chi angles: 196.5,169.1	0.105Å	-	-
A 98	PHE	50	-	Favored (19.93%) General / -86.5,156.9	82.7% (*m-85*) chi angles: 293,285.2	0.022Å	-	-
A 99	ALA	50	-	Favored (88.05%) General / -58.2,-43.9	-	0.031Å	-	-
A 100	TRP	50	-	Favored (79.03%)	48.4% (*p-90*)	0.036Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 100		TRP	50		General / -64.6,-34.8	chi angles: 71.9,271	0.058Å		
A 101		GLU	50	-	Favored (89.75%) General / -65.8,-38.7	52.5% (*mt-10*) chi angles: 294.2,190.7,306.5	0.046Å	-	-
A 102		ILE	50	-	Favored (98.34%) Isoleucine or valine / -63.5,-43.3	71.2% (*mt*) chi angles: 293.4,177.8	0.059Å	-	-
A 103		ARG	50	-	Favored (69.06%) General / -58.6,-51.6	24.5% (*ttt180*) chi angles: 198,177.1,194,238.5	0.051Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 16.16	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133
A 104		ASP	50	-	Favored (72.45%) General / -57.5,-37.2	74.6% (*m-20*) chi angles: 297.8,346	0.029Å	-	-
A 105		ARG	50	0.421Å HB3 with A 90 TYR CE2	Favored (24.07%) General / -60.4,-56.2	0.1% chi angles: 257.2,262,215.5,172.5	0.053Å	-	-
A 106		LEU	50	0.475Å HD22 with A 90 TYR HE2	Favored (47.35%) General / -51.1,-37.7	3.1% (*mm?*) chi angles: 276.5,310.6	0.085Å	-	-
A 107		LEU	50	-	Favored (3.22%) General / -71.2,-58.8	18.2% (*mt*) chi angles: 275.6,168.3	0.064Å	-	-
A 108		SER	50	-	Favored (90.54%) General / -60.7,-39.9	91.6% (*p*) chi angles: 62.8	0.03Å	-	-
A 109		GLU	50	-	Favored (61.03%) General / -73.5,-19.1	66% (*mt-10*) chi angles: 299.9,197.2,344.4	0.055Å	-	-
A 110		GLY	50	-	Favored (46.17%) Glycine / 81.3,28.0	-	-	-	-
A 111		VAL	50		Favored (45.74%)	22.6% (*t*)	0.04Å		

A 111	VAL	50	-	Isoleucine or valine / -70.9,-31.6	chi angles: 187.4	0.04Å	-	-
A 112	CYS	50	-	Favored (52.39%) General / -132.3,149.3	92.8% (*m*) chi angles: 295	0.085Å	-	-
A 113	THR	50	-	Favored (11.69%) General / -95.1,166.9	30.3% (*p*) chi angles: 70.1	0.043Å	-	-
A 114	ASN	50	-	Favored (2.66%) General / -59.4,-9.8	74.2% (*m-20*) chi angles: 286.1,310.9	0.039Å	-	-
A 115	ASP	50	-	Favored (16.67%) General / -90.9,-30.9	31.6% (*m-20*) chi angles: 301.7,287.9	0.033Å	-	-
A 116	ASN	50	-	Favored (11.84%) General / -120.7,15.2	38.4% (*p30*) chi angles: 62.5,28	0.09Å	-	-
A 117	ILE	50	0.415Å HD12 with A 118 PRO HD2	Favored (90.77%) Pre-proline / -65.6,126.0	10.9% (*tp*) chi angles: 190.3,65.7	0.114Å	-	-
A 118	PRO	50	0.415Å HD2 with A 117 ILE HD12	Favored (92.64%) Trans-proline / -63.5,148.3	78.2% (*Cg_exo*) chi angles: 333.5	0.082Å	-	-
A 119	SER	50	-	Favored (31.78%) General / -64.9,156.2	83.8% (*p*) chi angles: 68.8	0.047Å	-	-
A 120	VAL	50	-	Favored (58.86%) Isoleucine or valine / -56.5,-39.0	47.6% (*t*) chi angles: 168.2	0.054Å	-	-
A 121	SER	50	-	Favored (78.03%) General / -57.1,-48.7	44.8% (*t*) chi angles: 178.6	0.038Å	-	-
A 122	SER	50	0.422Å O with A 126 VAL HG23	Favored (87.5%) General / -64.9,-37.4	70.5% (*m*) chi angles: 297.4	0.037Å	-	-
A 123	ILE	50	-	Favored (80.31%) Isoleucine or	70.7% (*mt*) chi angles: 293,177.8	0.077Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 16.16	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133
A 124		ASN	50	-	Favored (71.76%) General / -67.2,-31.4	74.9% (*m-20*) chi angles: 284.9,314.6	0.052Å	-	-
A 125		ARG	50	-	Favored (88.49%) General / -66.5,-41.6	64.7% (*ttp85*) chi angles: 176.3,172.1,55.2,82.5	0.047Å	-	-
A 126		VAL	50	0.422Å HG23 with A 122 SER O	Favored (95.95%) Isoleucine or valine / -60.9,-46.7	70.3% (*t*) chi angles: 171.8	0.034Å	-	-
A 127		LEU	50	0.419Å CD2 with A 91 LYS HG3	Favored (83.95%) General / -60.0,-38.9	54.3% (*mt*) chi angles: 285.1,175.8	0.053Å	-	-
A 128		ARG	50	-	Favored (66.51%) General / -72.9,-39.1	92.7% (*mtm-85*) chi angles: 292.3,196.2,306.2,277.2	0.065Å	-	-
A 129		ASN	50	0.559Å O with A 133 GLU HB2	Favored (83.79%) General / -60.2,-38.6	97.1% (*m-20*) chi angles: 292.6,340.1	0.047Å	-	-
A 130		LEU	50	-	Favored (83.17%) General / -68.0,-39.3	85.4% (*mt*) chi angles: 289.7,171.1	0.017Å	-	-
A 131		ALA	50	-	Favored (72.28%) General / -61.9,-50.4	-	0.021Å	-	-
A 132		SER	50	-	Favored (63.6%) General / -73.6,-31.5	99.4% (*p*) chi angles: 64.4	0.015Å	-	-
A 133		GLU	50	0.559Å HB2 with A 129 ASN O	Favored (75.67%) General / -57.8,-38.5	24.8% (*tt0*) chi angles: 200.5,178.2,69.1	0.071Å	-	-
A 134		LYS	50	-	Favored (52.5%) General /	37.1% (*pttt*) chi angles: 69,155.6,175.1,166.8	0.17Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 135		GLN	50	-	-93.8,5.2 Favored (21.83%) General / -86.9,-29.8	84.3% (*mt-30*) chi angles: 286.4,187.5,321.5	0.085Å	-	-
A 136		GLN	99.99	-	-	0% chi angles: 241.1,75.2,308	0.07Å	-	-
B1001		DAD	100.5	0.696Å H2'1 with B1002 DAD OP2	-	-	-	-	-
B1002		DAD	102.72	0.761Å H2'1 with B1003 DGU C5'	-	-	-	-	-
B1003		DGU	95.24	0.761Å C5' with B1002 DAD H2'1	-	-	-	-	-
B1004		DCY	83.06	-	-	-	-	-	-
B1005		DAD	74.41	0.584Å N1 with C2024 DTY N3	-	-	-	-	-
B1006		DTY	64.72	0.561Å N3 with C2023 DAD N1	-	-	-	-	-
B1007		DTY	55.15	-	-	-	-	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 16.16	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133
B1008		DTY	63.52	-	-	-	-	-	-
B1009		DTY	50.43	0.478Å N3 with C2020 DAD N1	-	-	-	-	-
B1010		DCY	60.49	0.412Å O2 with C2019 DGU N2	-	-	-	-	-
B1011		DAD	62.65	0.889Å H2'1 with B1012 DCY C5'	-	-	-	-	-
B1012		DCY	60.46	0.889Å C5' with B1011 DAD H2'1	-	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
B1013		DGU	62.87	-	-	-	-	-	-
B1014		DCY	66.18	-	-	-	-	-	-
B1015		DAD	53.92	0.533Å N1 with C2014 DTY N3	-	-	-	-	-
B1016		DTY	60.67	0.795Å O2 with A 72 GLY HA3	-	-	-	-	-
B1017		DGU	53.38	0.428Å C5' with A 71 ILE O	-	-	-	-	-
B1018		DAD	45.88	0.424Å N1 with C2011 DTY N3	-	-	-	-	-
B1019		DGU	45.01	0.489Å C1' with A 77 ARG NH2	-	-	-	-	-
B1020		DTY	47.07	-	-	-	-	-	-
B1021		DGU	57.3	0.445Å N2 with C2008 DCY O2	-	-	-	-	-
B1022		DCY	69.79	0.542Å N3 with C2007 DGU N1	-	-	-	-	-
B1023		DAD	85.8	-	-	-	-	-	-
B1024		DCY	89.37	0.475Å C2' with B1025 DAD OP2	-	-	-	-	-
B1025		DAD	84.51	0.475Å OP2 with B1024 DCY C2'	-	-	-	-	-
B1026		DGU	87.98	0.468Å N1 with C2003 DCY N3	-	-	-	-	-
C2001		DTY	75.67	0.813Å C2' with C2002 DTY C5'	-	-	-	-	-
			Avg: 54.96	Clashscore: 16.16 0.869Å	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133

C2002	DTY	77.07	C2' with C2003 DCY C5'	-	-	-	-	-
C2003	DCY	78.78	0.869Å C5' with C2002 DTY C2'	-	-	-	-	-
C2004	DTY	48.81	-	-	-	-	-	-
C2005	DGU	57.01	-	-	-	-	-	-
C2006	DTY	69.23	-	-	-	-	-	-
C2007	DGU	76.12	0.542Å N1 with B1022 DCY N3	-	-	-	-	-
C2008	DCY	80.78	0.445Å O2 with B1021 DGU N2	-	-	-	-	-
C2009	DAD	74.88	-	-	-	-	-	-
C2010	DCY	75.39	0.538Å C2' with C2011 DTY C5'	-	-	-	-	-
C2011	DTY	73.29	0.538Å C5' with C2010 DCY C2'	-	-	-	-	-
C2012	DCY	61.25	0.416Å C2' with C2013 DAD N7	-	-	-	-	-
C2013	DAD	63.28	0.664Å N6 with B1016 DTY O4	-	-	-	-	-
C2014	DTY	61.51	0.533Å N3 with B1015 DAD N1	-	-	-	-	-
C2015	DGU	43.87	-	-	-	-	-	-
C2016	DCY	43.32	-	-	-	-	-	-
C2017	DGU	43.75	0.453Å OP2 with A 55 LYS NZ	-	-	-	-	-
C2018	DTY	44.55	-	-	-	-	-	-
C2019	DGU	51.15	0.471Å OP2 with A 9 ASN HB2	-	-	-	-	-
C2020	DAD	67.99	0.478Å N1 with B1009 DTY	-	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
				B1009 DTY N3					
C2021		DAD	76.69	-	-	-	-	-	-
			Avg: 54.96	Clashscore: 16.16	Outliers: 0 of 131	Poor rotamers: 3 of 115	Outliers: 0 of 122	Outliers: 2 of 133	Outliers: 1 of 133
C2022		DAD	70.65	-	-	-	-	-	-
C2023		DAD	68.53	1.139Å H2'1 with C2024 DTY C5'	-	-	-	-	-
C2024		DTY	68.92	1.139Å C5' with C2023 DAD H2'1	-	-	-	-	-
C2025		DGU	68.54	-	-	-	-	-	-
C2026		DCY	62.68	-	-	-	-	-	-

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