Viewing pax6-arg26trp_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.52		99th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	4	3.48%	Goal: <1%
	Ramachandran outliers	6	4.58%	Goal: <0.05%
	Ramachandran favored	113	86.26%	Goal: >98%
	MolProbity score^	1.94		79th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	3.28%	Goal: 0
	Bad backbone bonds:	0 / 1043	0.00%	Goal: 0%
	Bad backbone angles:	12 / 1412	0.85%	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: 1.52	Outliers: 6 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 4		SER	50	-	-	6.1% (*p*) chi angles: 44.1	0.153Å	-	-
A 5		HIS	50	-	Favored (38.76%) General / -97.5,135.8	48% (*p-80*) chi angles: 65.1,271.4	0.098Å	-	OUTLIER(S) worst is CA-CB-CG: 4.442 σ
A 6		SER	50	-	Favored (43.78%) General / -67.7,153.4	74.1% (*m*) chi angles: 295.1	0.061Å	-	-
A 7		GLY	50	-	Favored (20.72%) Glycine / -130.3,170.9	-	-	-	-
					Favored				

A 8	VAL	50	-	Favored (32.13%) Isoleucine or valine / -124.7,145.3	86% (*t*) chi angles: 177.4	0.076Å	-	-
A 9	ASN	50	0.432Å HB2 with C2019 DGU OP2	Favored (4.65%) General / -103.6,178.1	24.9% (*p30*) chi angles: 53.5,40.5	0.099Å	-	OUTLIER(S) worst is CA-CB-CG: 4.153 σ
A 10	GLN	50	-	Favored (61.63%) General / -72.6,-17.8	32.1% (*mt-30*) chi angles: 282.3,177.4,110.9	0.077Å	-	-
A 11	LEU	50	-	Favored (48.08%) General / -80.9,-18.2	4.7% (*mp*) chi angles: 302.5,93.3	0.101Å	-	-
A 12	GLY	50	-	Favored (55.2%) Glycine / 98.0,8.7	-	-	-	-
A 13	GLY	50	-	Favored (45.69%) Glycine / -89.7,-176.1	-	-	-	-
A 14	VAL	50	-	Favored (35.13%) Isoleucine or valine / -128.6,151.2	6.6% (*m*) chi angles: 286.1	0.039Å	-	-
A 15	PHE	50	-	Favored (2.89%) General / -144.6,-168.4	17.2% (*p90*) chi angles: 72.7,286.1	0.068Å	-	-
A 16	VAL	50	-	Favored (49.29%) Isoleucine or valine / -136.0,136.9	79.7% (*t*) chi angles: 174.5	0.074Å	-	-
A 17	ASN	50	-	Favored (35.64%) General / -76.6,153.0	19.2% (*t30*) chi angles: 203.3,58.8	0.03Å	-	-
A 18	GLY	50	-	Favored (41.33%) Glycine / 55.5,25.1	-	-	-	-
A 19	ARG	50	-	Favored (37.24%) Pre-proline / -150.1,157.8	26.1% (*mmm180*) chi angles: 293.4,303.3,292.7,179.4	0.04Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 20		PRO	50	-	Favored (31.13%) Trans-proline / -77.7,155.5	6.1% (*Cg_exo*) chi angles: 357.7	0.037Å	-	-
A 21		LEU	50	-	Favored (31.46%) Pre-proline / -59.5,118.5	15.2% (*tp*) chi angles: 199.4,63.5	0.029Å	-	-
A 22		PRO	50	-	Favored (20.36%) Trans-proline / -53.2,152.1	0.1% chi angles: 317.7	0.081Å	-	OUTLIER(S) worst is C-N-CA: 5.093 σ
A 23		ASP	50	-	OUTLIER (0.01%) General / -62.1,57.0	2.4% (*m-20*) chi angles: 309.7,70.5	0.124Å	-	OUTLIER(S) worst is C-N-CA: 5.235 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 24		SER	50	-	Allowed (0.29%) General / -144.0,-40.0	64.2% (*p*) chi angles: 56.8	0.05Å	-	-
A 25		THR	50	-	Favored (14.87%) General / -95.7,-28.3	1.7% (*m*) chi angles: 324	0.116Å	-	-
A 26		TRP	50	-	Favored (74.79%) General / -64.8,-32.9	7.2% (*p-90*) chi angles: 54.3,246	0.225Å	-	-
A 27		GLN	50	-	Favored (72.82%) General / -60.2,-33.8	1.4% (*tp60*) chi angles: 171.3,68.4,113.8	0.092Å	-	-
A 28		LYS	50	-	Favored (60.03%) General / -75.8,-33.6	24.3% (*mmmt*) chi angles: 313,314.8,302.3,178.9	0.145Å	-	-
A 29		ILE	50	-	Favored (99.22%) Isoleucine or valine / -62.4,-44.5	40.8% (*mt*) chi angles: 306.3,181.2	0.217Å	-	-
A 30		VAL	50	-	Favored (61.01%)	2.8% (*p*) chi angles: 80.9	0.247Å	-	-

				Isoleucine or valine / -70.0,-34.7				
A 31	GLU	50	-	Favored (94.51%) General / -60.4,-41.7	28.9% (*mt-10*) chi angles: 275.1,176.8,47.6	0.09Å	-	-
A 32	LEU	50	-	Favored (2.32%) General / -87.5,-59.2	28.4% (*mt*) chi angles: 307,188.5	0.143Å	-	-
A 33	ALA	50	-	Favored (99.81%) General / -62.8,-42.6	-	0.103Å	-	-
A 34	HIS	50	-	Favored (37.4%) General / -72.5,-5.5	2.2% (*t-80*) chi angles: 212.2,313.8	0.077Å	-	-
A 35	SER	50	-	Favored (20.56%) General / -101.3,-10.2	58.4% (*m*) chi angles: 290.9	0.063Å	-	-
A 36	GLY	50	-	Allowed (0.57%) Glycine / 132.3,28.8	-	-	-	-
A 37	ALA	50	-	Favored (47.09%) General / -124.5,149.2	-	0.051Å	-	-
A 38	ARG	50	-	Favored (19.23%) Pre-proline / -82.5,169.1	72.7% (*mtm180*) chi angles: 299.2,180,300,155	0.07Å	-	-
A 39	PRO	50	-	Favored (12.87%) Trans-proline / -53.7,-50.7	3.3% (*Cg_exo*) chi angles: 321.8	0.045Å	-	-
A 40	CYS	50	-	Favored (72.54%) General / -65.8,-31.5	1.1% (*p*) chi angles: 88.3	0.214Å	-	-
A 41	ASP	50	-	Favored (89.16%) General / -66.4,-39.8	32.4% (*m-20*) chi angles: 308.3,321.9	0.169Å	-	-
A 42	ILE	50	-	Favored (10.78%)	6% (*pt*)	0.229Å		

| A 42 | | ILE | 50 | - | Isoleucine or valine / -81.3,-29.4 | chi angles: 65.6,149.3 | 0.329Å | - | - |
| A 43 | | SER | 50 | - | Favored (92.44%) General / -64.5,-43.9 | 79.1% (*p*) chi angles: 59.5 | 0.102Å | - | - |

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 44		ARG	50	-	Favored (61.18%) General / -73.6,-17.4	33.4% (*ttp-105*) chi angles: 197.8,179.6,66.6,250	0.059Å	-	-
A 45		ILE	50	-	Favored (9.04%) Isoleucine or valine / -111.1,-16.6	18.8% (*mt*) chi angles: 304.8,188.1	0.264Å	-	-
A 46		LEU	50	-	Favored (20.43%) General / -98.6,-13.3	75.6% (*mt*) chi angles: 298.8,170.1	0.125Å	-	-
A 47		GLN	50	-	Allowed (0.71%) General / 71.3,42.3	35.5% (*mt-30*) chi angles: 305.5,181.1,252	0.155Å	-	-
A 48		VAL	50	-	Favored (24.57%) Isoleucine or valine / -121.0,154.2	55% (*t*) chi angles: 169.8	0.129Å	-	-
A 49		SER	50	-	Favored (20.52%) General / -64.9,160.4	82.5% (*p*) chi angles: 69.4	0.047Å	-	-
A 50		ASN	50	-	Favored (85.52%) General / -66.9,-42.5	21.9% (*m-20*) chi angles: 316.1,306	0.104Å	-	-
A 51		GLY	50	0.413Å HA3 with C2019 DGU O6	Favored (57.66%) Glycine / -74.8,-31.9	-	-	-	-
A 52		CYS	50	-	Favored (97.98%) General / -63.0,-43.7	41.8% (*t*) chi angles: 175.8	0.044Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 53		VAL	50	-	Allowed (1.28%) Isoleucine or valine / -46.1,-56.1	2.3% (*t*) chi angles: 151.1	0.166Å	-	-
A 54		SER	50	-	Favored (49.08%) General / -86.2,-12.7	69.6% (*m*) chi angles: 297.2	0.198Å	-	-
A 55		LYS	50	-	Favored (61.55%) General / -73.0,-14.9	47.8% (*mtmt*) chi angles: 283.9,187.2,283.4,197.1	0.189Å	-	-
A 56		ILE	50	-	Favored (13.64%) Isoleucine or valine / -93.6,-47.3	3.3% (*mp*) chi angles: 287.7,82.3	0.17Å	-	-
A 57		LEU	50	-	Favored (99.2%) General / -62.5,-41.9	86.7% (*mt*) chi angles: 298.7,180.5	0.2Å	-	-
A 58		GLY	50	-	Favored (91.63%) Glycine / -60.7,-36.4	-	-	-	-
A 59		ARG	50	-	Favored (57.9%) General / -75.3,-25.3	71.7% (*mtm180*) chi angles: 292.6,182.7,277,185.5	0.152Å	-	-
A 60		TYR	50	-	Favored (81.87%) General / -68.0,-37.8	80.9% (*t80*) chi angles: 180.4,71	0.132Å	-	-
A 61		TYR	50	-	Favored (66.8%) General / -57.5,-32.3	19% (*m-30*) chi angles: 299.9,340.4	0.143Å	-	-
A 62		GLU	50	-	Allowed (0.18%) General / -94.9,-93.8	15.3% (*tm-20*) chi angles: 186.4,275.6,324.6	0.2Å	-	-
A 63		THR	50	-	Favored (82.04%) General / -58.8,-39.8	1.3% (*p*) chi angles: 35.6	0.132Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles

Avg: Clashscore: Outliers: 6 of   Poor rotamers: 4 of   Outliers: Outliers: Outliers: 11

		Avg. 54.96	Clashscore. 1.52	Outliers. 6 of 131	Poor rotamers. 4 of 115	Outliers. 4 of 122	Outliers. 0 of 133	Outliers. 11 of 133
A 64	GLY	50	-	Favored (36.07%) Glycine / 103.9,9.9	-	-	-	-
A 65	SER	50	-	Favored (23.06%) General / -65.0,124.8	19.4% (*t*) chi angles: 188.8	0.105Å	-	-
A 66	ILE	50	-	Favored (9.21%) Isoleucine or valine / -101.7,-5.3	3.1% (*mt*) chi angles: 301,122.2	0.176Å	-	-
A 67	ARG	50	-	Favored (63.64%) Pre-proline / -81.2,148.5	2.3% (*mmm180*) chi angles: 259.7,298.8,310.4,186.3	0.121Å	-	-
A 68	PRO	50	-	Favored (4.9%) Trans-proline / -85.9,177.1	36.6% (*Cg_endo*) chi angles: 36.8	0.05Å	-	-
A 69	ARG	50	-	OUTLIER (0.03%) General / -68.6,-159.9	83.3% (*mtm180*) chi angles: 295,180.6,281,176.4	0.124Å	-	-
A 70	ALA	50	-	Favored (54.48%) General / -120.6,131.2	-	0.098Å	-	-
A 71	ILE	50	-	Favored (4.83%) Isoleucine or valine / -79.2,152.4	33% (*mt*) chi angles: 292,153.7	0.119Å	-	-
A 72	GLY	50	0.465Å HA2 with C2013 DAD H2	Favored (43.76%) Glycine / 81.1,170.7	-	-	-	-
A 73	GLY	50	-	Favored (3.15%) Glycine / 97.0,114.5	-	-	-	-
A 74	SER	50	-	Allowed (0.12%) General / -81.8,-154.6	14.9% (*p*) chi angles: 81.9	0.231Å	-	-
		50		Favored (29.6%)	29.6% (*mmtm*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 75		LYS	50	-	(39.6%) Pre-proline / -141.2,163.8	chi angles: 307.9,298.9,161.8,307	0.042A	-	-
A 76		PRO	50	-	Allowed (0.12%) Trans-proline / -55.6,104.2	0.1% chi angles: 318.3	0.063Å	-	-
A 77		ARG	50	-	Favored (18.52%) General / -88.9,-30.9	84.1% (*mtm180*) chi angles: 283.6,174.3,283.5,176.4	0.181Å	-	-
A 78		VAL	50	-	Allowed (1.03%) Isoleucine or valine / -125.7,-31.8	8.3% (*m*) chi angles: 309	0.18Å	-	-
A 79		ALA	50	-	Allowed (0.87%) General / -78.7,49.2	-	0.04Å	-	-
A 80		THR	50	-	Favored (3.37%) Pre-proline / -55.5,160.9	64.8% (*p*) chi angles: 62.9	0.071Å	-	-
A 81		PRO	50	-	Favored (29.2%) Trans-proline / -47.5,-39.6	0.1% chi angles: 318.1	0.092Å	-	-
A 82		GLU	50	-	Favored (41.88%) General / -79.6,-32.5	44.4% (*tt0*) chi angles: 185.3,155.3,354.3	0.236Å	-	-
A 83		VAL	50	-	Favored (85.47%) Isoleucine or valine / -59.0,-42.2	21.9% (*t*) chi angles: 163.1	0.109Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 84		VAL	50	-	Favored (96.07%) Isoleucine or valine / -60.6,-46.2	80.9% (*t*) chi angles: 174.6	0.071Å	-	-
A 85		SER	50	-	Favored (77.17%) General /	55.4% (*m*) chi angles: 299.7	0.081Å	-	-

				General / -59.9,-36.6	chi angles: 299.7			
A 86	LYS	50	-	Favored (60.75%) General / -73.0,-44.7	69.7% (*mmtt*) chi angles: 284.8,292.6,176.8,186.7	0.086Å	-	-
A 87	ILE	50	-	Favored (63.62%) Isoleucine or valine / -67.6,-33.7	10.5% (*mt*) chi angles: 298.3,144.2	0.249Å	-	-
A 88	ALA	50	-	Favored (81.24%) General / -57.7,-47.9	-	0.073Å	-	-
A 89	GLN	50	-	Favored (72.84%) General / -55.0,-48.7	28.9% (*tt0*) chi angles: 188.7,197.3,312.2	0.061Å	-	-
A 90	TYR	50	-	Favored (53.03%) General / -71.7,-47.6	4% (*m-30*) chi angles: 315.9,324.5	0.117Å	-	-
A 91	LYS	50	0.413Å NZ with C2004 DTY OP1	Favored (60.75%) General / -74.8,-15.4	65.4% (*mmtt*) chi angles: 290.7,281.3,181.4,170.4	0.103Å	-	-
A 92	ARG	50	-	Favored (13.51%) General / -109.7,-18.3	36.7% (*mtp180*) chi angles: 303.7,158.7,76.1,165.3	0.165Å	-	-
A 93	GLU	50	-	Favored (13.57%) General / -92.3,-35.7	9% (*pt-20*) chi angles: 88.2,182.6,345.9	0.143Å	-	-
A 94	CYS	50	-	Favored (25.31%) Pre-proline / -139.4,79.4	38% (*t*) chi angles: 187.9	0.048Å	-	-
A 95	PRO	50	-	Favored (7.79%) Trans-proline / -46.2,-30.5	11% (*Cg_exo*) chi angles: 323	0.108Å	-	-
A 96	SER	50	-	Favored (9.55%) General / -85.6,78.9	88.5% (*p*) chi angles: 65.4	0.058Å	-	-
A 97	ILE	50		Favored (20.58%)	19.3% (*mt*)	0.081Å		

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 97		ILE	50	-	Isoleucine or valine / -145.5,137.8	chi angles: 286.6,185.2	0.081Å	-	-
A 98		PHE	50	-	Favored (9.36%) General / -92.1,171.0	49.6% (m-85) chi angles: 307.1,293.4	0.049Å	-	-
A 99		ALA	50	-	Favored (87.56%) General / -60.3,-39.6	-	0.09Å	-	-
A 100		TRP	50	-	Favored (76.06%) General / -69.5,-35.9	63.5% (p-90) chi angles: 53.9,271.7	0.177Å	-	-
A 101		GLU	50	-	Favored (81.82%) General / -61.2,-37.1	47.5% (mt-10) chi angles: 292.1,188.2,280.5	0.104Å	-	-
A 102		ILE	50	-	Favored (39.16%) Isoleucine or valine / -71.2,-30.2	54.4% (mt) chi angles: 303,180.9	0.318Å	-	-
A 103		ARG	50	-	Favored (90.14%) General / -60.9,-39.7	32.3% (ttt180) chi angles: 202,169.1,185.4,151.9	0.145Å	-	-

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			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 104		ASP	50	-	Favored (53.73%) General / -80.7,-16.5	26% (m-20) chi angles: 283.8,13.1	0.152Å	-	-
A 105		ARG	50	-	Favored (98.25%) General / -61.1,-42.3	9.4% (mmt180) chi angles: 274.1,281.5,206.5,138.6	0.109Å	-	-
A 106		LEU	50	-	Favored (81.61%) General / -61.3,-37.0	4% (mm?) chi angles: 281.9,305.1	0.101Å	-	-
A 107		LEU	50	-	Favored (45.21%) General / -78.6,-25.5	71.9% (mt) chi angles: 302.6,173.3	0.078Å	-	-

A 108	SER	50	-	Favored (12.15%) General / -98.3,-31.2	80.7% (*p*) chi angles: 60.3	0.166Å	-	-
A 109	GLU	50	-	Favored (52.75%) General / -77.3,-26.8	21.4% (*mt-10*) chi angles: 284.2,205.4,26.1	0.116Å	-	-
A 110	GLY	50	-	Favored (8.36%) Glycine / 89.9,34.4	-	-	-	-
A 111	VAL	50	-	Favored (17.99%) Isoleucine or valine / -83.3,-42.8	98.7% (*t*) chi angles: 176.6	0.082Å	-	-
A 112	CYS	50	-	Favored (11.05%) General / -98.5,167.1	77.7% (*m*) chi angles: 299.1	0.025Å	-	-
A 113	THR	50	0.407Å HB with A 115 ASP OD1	Allowed (0.16%) General / -98.6,-112.4	53.5% (*m*) chi angles: 304.7	0.244Å	-	OUTLIER(S) worst is C-CA-CB: 4.361 σ
A 114	ASN	50	-	Allowed (1.46%) General / -142.7,31.2	8.7% (*m120*) chi angles: 291.8,164	0.045Å	-	OUTLIER(S) worst is CA-CB-CG: 9.235 σ
A 115	ASP	50	0.407Å OD1 with A 113 THR HB	OUTLIER (0.04%) General / -165.4,18.3	1.4% (*p30*) chi angles: 36.8,16.5	0.053Å	-	OUTLIER(S) worst is CA-CB-CG: 4.847 σ
A 116	ASN	50	-	OUTLIER (0.02%) General / -170.5,34.8	20.6% (*p30*) chi angles: 48.9,17.8	0.032Å	-	-
A 117	ILE	50	-	Favored (59.18%) Pre-proline / -95.5,122.5	7.7% (*tp*) chi angles: 184.9,71.7	0.074Å	-	-
A 118	PRO	50	-	Favored (94.92%) Trans-proline / -60.5,147.2	43.1% (*Cg_exo*) chi angles: 326.1	0.097Å	-	-
A 119	SER	50	-	Favored (5.15%) General /	51% (*m*) chi angles: 301.5	0.155Å	-	-

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					-95.7,179.4				
A 120		VAL	50	-	Favored (20.17%) Isoleucine or valine / -73.3,-52.8	48.5% (*t*) chi angles: 182.7	0.122Å	-	-
A 121		SER	50	-	Favored (93.53%) General / -64.3,-39.3	8.7% (*t*) chi angles: 193.6	0.088Å	-	-
A 122		SER	50	-	Favored (97.54%) General / -61.2,-41.9	70% (*m*) chi angles: 297.3	0.076Å	-	-
A 123		ILE	50	-	Favored (82.49%) Isoleucine or valine / -64.2,-38.4	29.9% (*mt*) chi angles: 298.5,186.5	0.253Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
A 124		ASN	50	-	Favored (62.34%) General / -73.9,-30.0	8.2% (*m-20*) chi angles: 287.5,23.2	0.133Å	-	-
A 125		ARG	50	-	Favored (94.68%) General / -59.9,-42.8	41.6% (*ttp85*) chi angles: 182.5,162.9,52.3,65.1	0.092Å	-	-
A 126		VAL	50	-	Favored (98.03%) Isoleucine or valine / -63.9,-44.1	97.5% (*t*) chi angles: 176.2	0.078Å	-	-
A 127		LEU	50	-	Favored (73.6%) General / -57.5,-37.8	96.1% (*mt*) chi angles: 298.4,177.9	0.159Å	-	-
A 128		ARG	50	-	Favored (58.87%) General / -75.1,-25.9	84.8% (*mtm-85*) chi angles: 297.1,196.5,295.2,289.2	0.222Å	-	-
A 129		ASN	50	-	Favored (83.82%) General / -66.6,-36.9	92.4% (*m-20*) chi angles: 293.9,332.1	0.107Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					00.0, 00.9				
A 130		LEU	50	-	Favored (61.06%) General / -73.2,-19.5	35.6% (*mt*) chi angles: 299.4,163.5	0.109Å	-	-
A 131		ALA	50	-	Favored (68.1%) General / -62.5,-25.5	-	0.113Å	-	-
A 132		SER	50	-	OUTLIER (0.01%) General / -75.5,-123.6	14.3% (*p*) chi angles: 82.1	0.236Å	-	OUTLIER(S) worst is C-CA-CB: 4.209 σ
A 133		GLU	50	-	Allowed (1.99%) General / 53.7,-122.4	0.6% chi angles: 195.2,230.1,259.6	0.246Å	-	OUTLIER(S) worst is C-N-CA: 8.534 σ
A 134		LYS	50	-	OUTLIER (0%) General / -26.2,11.8	2.7% (*pttm*) chi angles: 63.8,227.3,175.4,285.5	0.052Å	-	OUTLIER(S) worst is N-CA-C: 4.953 σ
A 135		GLN	50	-	Favored (12.42%) General / -117.7,6.6	24.7% (*mt-30*) chi angles: 289.5,161.2,112.4	0.078Å	-	-
A 136		GLN	99.99	-	-	5.1% (*tp-100*) chi angles: 177,47.3,205.4	0.079Å	-	OUTLIER(S) worst is CB-CG-CD: 4.174 σ
B1001		DAD	100.5	-	-	-	-	-	-
B1002		DAD	102.72	-	-	-	-	-	-
B1003		DGU	95.24	-	-	-	-	-	-
B1004		DCY	83.06	-	-	-	-	-	-
B1005		DAD	74.41	-	-	-	-	-	-
B1006		DTY	64.72	-	-	-	-	-	-
B1007		DTY	55.15	-	-	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
B1008		DTY	63.52	-	-	-	-	-	-
B1009		DTY	50.43	-	-	-	-	-	-
B1010		DCY	60.49	-	-	-	-	-	-
B1011		DAD	62.65	-	-	-	-	-	-
B1012		DCY	60.46	-	-	-	-	-	-
B1013		DGU	62.87						

#	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	-	-	-	-	-	-
B1016		DTY	60.67	-	-	-	-	-	-
B1017		DGU	53.38	-	-	-	-	-	-
B1018		DAD	45.88	-	-	-	-	-	-
B1019		DGU	45.01	-	-	-	-	-	-
B1020		DTY	47.07	-	-	-	-	-	-
B1021		DGU	57.3	-	-	-	-	-	-
B1022		DCY	69.79	-	-	-	-	-	-
B1023		DAD	85.8	-	-	-	-	-	-
B1024		DCY	89.37	-	-	-	-	-	-
B1025		DAD	84.51	-	-	-	-	-	-
B1026		DGU	87.98	-	-	-	-	-	-
C2001		DTY	75.67	-	-	-	-	-	-
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
C2002		DTY	77.07	-	-	-	-	-	-
C2003		DCY	78.78	-	-	-	-	-	-
C2004		DTY	48.81	0.413Å OP1 with A 91 LYS NZ	-	-	-	-	-
C2005		DGU	57.01	-	-	-	-	-	-
C2006		DTY	69.23	-	-	-	-	-	-
C2007		DGU	76.12	-	-	-	-	-	-
C2008		DCY	80.78	-	-	-	-	-	-
C2009		DAD	74.88	-	-	-	-	-	-
C2010		DCY	75.39	-	-	-	-	-	-
C2011		DTY	73.29	-	-	-	-	-	-
C2012		DCY	61.25	-	-	-	-	-	-
C2013		DAD	63.28	0.465Å H2 with A 72 GLY HA2	-	-	-	-	-
C2014		DTY	61.51	-	-	-	-	-	-
C2015		DGU	43.87	-	-	-	-	-	-
C2016		DCY	43.32	-	-	-	-	-	-
C2017		DGU	43.75	-	-	-	-	-	-
C2018		DTY	44.55	-	-	-	-	-	-
				0.432Å					

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
C2019		DGU	51.15	OP2 with A 9 ASN HB2	-	-	-	-	-
C2020		DAD	67.99	-	-	-	-	-	-
C2021		DAD	76.69	-	-	-	-	-	-
			Avg: 54.96	Clashscore: 1.52	Outliers: 6 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122	Outliers: 0 of 133	Outliers: 11 of 133
C2022		DAD	70.65	-	-	-	-	-	-
C2023		DAD	68.53	-	-	-	-	-	-
C2024		DTY	68.92	-	-	-	-	-	-
C2025		DGU	68.54	-	-	-	-	-	-
C2026		DCY	62.68	-	-	-	-	-	-

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