



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 19, 2018 – 04:14 am GMT

PDB ID : 5MQ7
EMDB ID: : EMD-3544
Title : Structure of AaLS-13
Authors : Sasaki, E.; Boehringer, D.; Leibundgut, M.; Ban, N.; Hilvert, D.
Deposited on : 2016-12-20
Resolution : 5.20 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

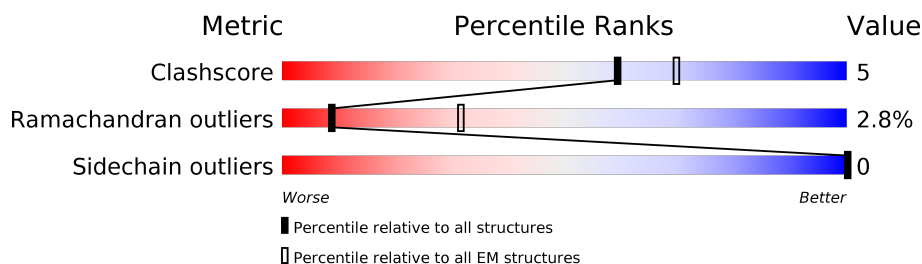
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0A	161	91% 9%
1	0B	161	88% 12%
1	0C	161	84% 14% .
1	0D	161	91% 9%
1	0E	161	86% 14% .
1	0X	161	88% 12%
1	1A	161	91% 9%
1	1B	161	88% 12%
1	1C	161	85% 14% .


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	1D	161	 89% 11%
1	1E	161	 87% 12% .
1	1X	161	 88% 12%
1	2A	161	 89% 11%
1	2B	161	 88% 12%
1	2C	161	 85% 14% .
1	2D	161	 91% 9%
1	2E	161	 85% 14% .
1	2X	161	 86% 14%
1	3A	161	 89% 11%
1	3B	161	 88% 12%
1	3C	161	 84% 14% .
1	3D	161	 91% 9%
1	3E	161	 85% 14% .
1	3X	161	 88% 12%
1	4A	161	 87% 13%
1	4B	161	 87% 12% .
1	4C	161	 85% 14% .
1	4D	161	 91% 9%
1	4E	161	 85% 14% .
1	4X	161	 88% 12%
1	5A	161	 88% 12%
1	5B	161	 87% 12% .
1	5C	161	 84% 14% .
1	5D	161	 91% 9%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	5E	161	 86% 14%
1	5X	161	 88% 12%
1	6A	161	 88% 12%
1	6B	161	 87% 12%
1	6C	161	 83% 16%
1	6D	161	 91% 9%
1	6E	161	 86% 14%
1	6X	161	 88% 12%
1	7A	161	 88% 12%
1	7B	161	 88% 12%
1	7C	161	 83% 16%
1	7D	161	 91% 9%
1	7E	161	 86% 14%
1	7X	161	 88% 12%
1	8A	161	 91% 9%
1	8B	161	 88% 12%
1	8C	161	 84% 14%
1	8D	161	 91% 9%
1	8E	161	 86% 14%
1	8X	161	 88% 12%
1	9A	161	 89% 11%
1	9B	161	 88% 12%
1	9C	161	 86% 12%
1	9D	161	 91% 9%
1	9E	161	 85% 14%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	9X	161	 88% 12%
1	AA	161	 88% 12%
1	AB	161	 87% 12% .
1	AC	161	 85% 14% .
1	AD	161	 91% 9%
1	AE	161	 84% 15% .
1	AX	161	 88% 12%
1	BA	161	 88% 12%
1	BB	161	 87% 12% .
1	BC	161	 85% 14% .
1	BD	161	 91% 9%
1	BE	161	 84% 15% .
1	BX	161	 88% 12%
1	CA	161	 87% 13%
1	CB	161	 87% 12% .
1	CC	161	 83% 16% .
1	CD	161	 91% 9%
1	CE	161	 86% 14% .
1	CX	161	 86% 14%
1	DA	161	 88% 12%
1	DB	161	 88% 12%
1	DC	161	 84% 14% .
1	DD	161	 91% 9%
1	DE	161	 85% 14% .
1	DX	161	 88% 12%

















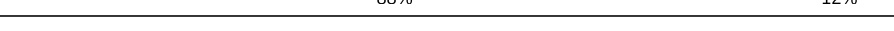

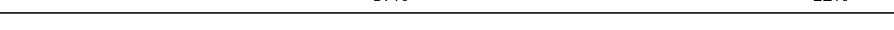
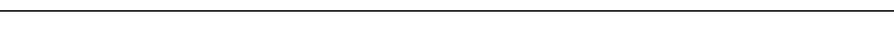
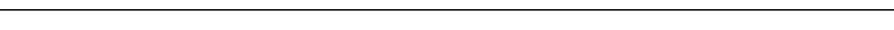
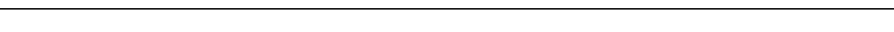
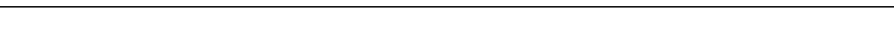
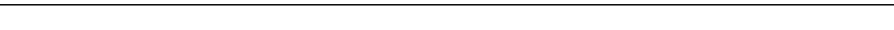

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	EA	161	 87% 13%
1	EB	161	 87% 12% .
1	EC	161	 83% 16% .
1	ED	161	 91% 9%
1	EE	161	 86% 14% .
1	EX	161	 88% 12%
1	FA	161	 88% 12%
1	FB	161	 88% 12%
1	FC	161	 84% 14% .
1	FD	161	 91% 9%
1	FE	161	 86% 14% .
1	FX	161	 88% 12%
1	GA	161	 88% 12%
1	GB	161	 87% 12% .
1	GC	161	 84% 14% .
1	GD	161	 91% 9%
1	GE	161	 85% 14% .
1	GX	161	 88% 12%
1	HA	161	 87% 13%
1	HB	161	 87% 12% .
1	HC	161	 82% 17% .
1	HD	161	 91% 9%
1	HE	161	 84% 15% .
1	HX	161	 86% 14%
1	IA	161	 89% 11%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	IB	161	 88% 12%
1	IC	161	 83% 15% .
1	ID	161	 89% 11%
1	IE	161	 86% 14% .
1	IX	161	 86% 14%
1	JA	161	 89% 11%
1	JB	161	 87% 12% .
1	JC	161	 84% 14% .
1	JD	161	 91% 9%
1	JE	161	 85% 14% .
1	JX	161	 86% 14%
1	KA	161	 87% 13%
1	KB	161	 88% 12%
1	KC	161	 84% 14% .
1	KD	161	 91% 9%
1	KE	161	 85% 14% .
1	KX	161	 88% 12%
1	LA	161	 88% 12%
1	LB	161	 87% 12% .
1	LC	161	 82% 16% .
1	LD	161	 91% 9%
1	LE	161	 86% 14% .
1	LX	161	 88% 12%
1	MA	161	 88% 12%
1	MB	161	 88% 12%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	MC	161	 83% 15% .
1	MD	161	 91% 9%
1	ME	161	 85% 14% .
1	MX	161	 88% 12%
1	NA	161	 89% 11%
1	NB	161	 88% 12%
1	NC	161	 83% 15% .
1	ND	161	 91% 9%
1	NE	161	 86% 14% .
1	NX	161	 88% 12%
1	OA	161	 89% 11%
1	OB	161	 87% 12% .
1	OC	161	 84% 14% .
1	OD	161	 91% 9%
1	OE	161	 84% 15% .
1	OX	161	 86% 14%
1	PA	161	 87% 13%
1	PB	161	 88% 12%
1	PC	161	 83% 16% .
1	PD	161	 91% 9%
1	PE	161	 84% 15% .
1	PX	161	 88% 12%
1	QA	161	 89% 11%
1	QB	161	 87% 12% .
1	QC	161	 85% 14% .















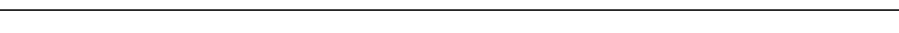




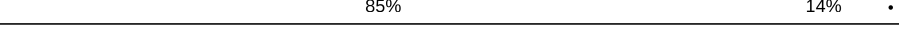





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	QD	161	 91% 9%
1	QE	161	 85% 14% .
1	QX	161	 88% 12%
1	RA	161	 89% 11%
1	RB	161	 87% 12% .
1	RC	161	 83% 15% .
1	RD	161	 91% 9%
1	RE	161	 86% 14% .
1	RX	161	 86% 14%
1	SA	161	 89% 11%
1	SB	161	 87% 12% .
1	SC	161	 84% 14% .
1	SD	161	 91% 9%
1	SE	161	 85% 14% .
1	SX	161	 88% 12%
1	TA	161	 89% 11%
1	TB	161	 88% 12%
1	TC	161	 84% 14% .
1	TD	161	 91% 9%
1	TE	161	 85% 14% .
1	TX	161	 88% 12%
1	UA	161	 88% 12%
1	UB	161	 88% 12%
1	UC	161	 82% 16% .
1	UD	161	 89% 11%








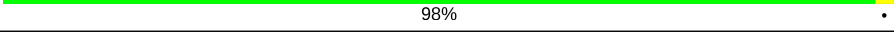
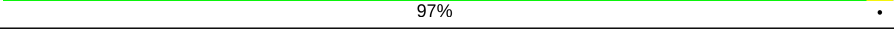
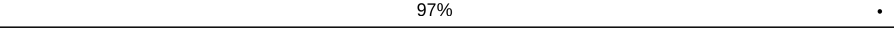
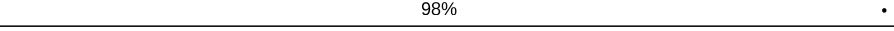
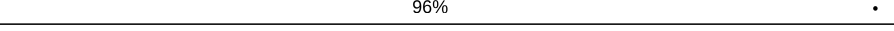
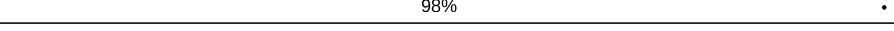
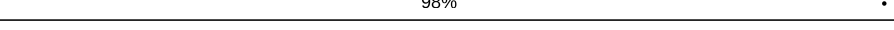
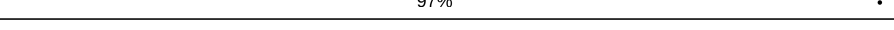
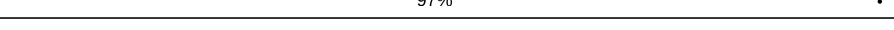
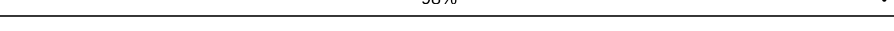
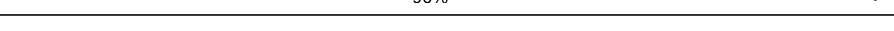
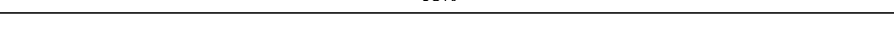
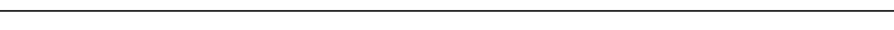
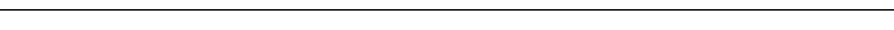
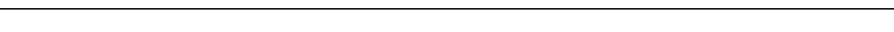
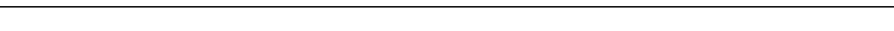
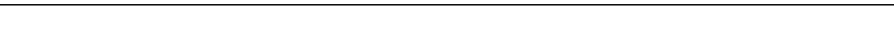

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	UE	161	 85% 14%
1	UX	161	 86% 14%
1	VA	161	 89% 11%
1	VB	161	 88% 12%
1	VC	161	 84% 15%
1	VD	161	 91% 9%
1	VE	161	 85% 14%
1	VX	161	 88% 12%
1	WA	161	 88% 12%
1	WB	161	 88% 12%
1	WC	161	 84% 14%
1	WD	161	 89% 11%
1	WE	161	 85% 14%
1	WX	161	 86% 14%
1	XA	161	 89% 11%
1	XB	161	 87% 12%
1	XC	161	 84% 15%
1	XD	161	 91% 9%
1	XE	161	 85% 14%
1	XX	161	 88% 12%
1	YA	161	 89% 11%
1	YB	161	 88% 12%
1	YC	161	 86% 13%
1	YD	161	 91% 9%
1	YE	161	 84% 15%

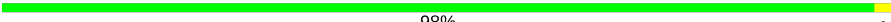
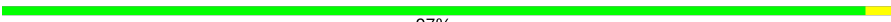













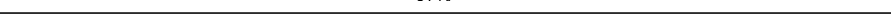
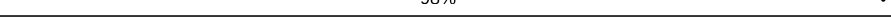
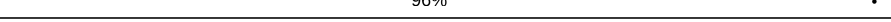
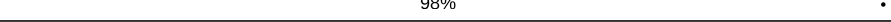
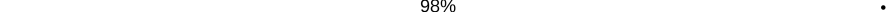
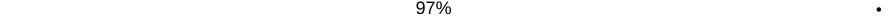
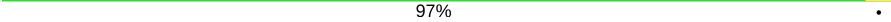
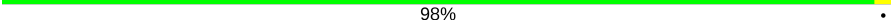
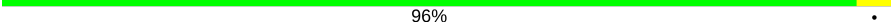
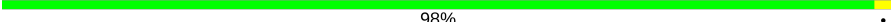
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	YX	161	 88% 12%
1	ZA	161	 86% 14%
1	ZB	161	 87% 12% .
1	ZC	161	 85% 14% .
1	ZD	161	 91% 9%
1	ZE	161	 85% 14% .
1	ZX	161	 88% 12%
1	aA	161	 98% .
1	aB	161	 97% .
1	aC	161	 97% .
1	aD	161	 98% .
1	aE	161	 96% .
1	aX	161	 98% .
1	bA	161	 98% .
1	bB	161	 97% .
1	bC	161	 97% .
1	bD	161	 98% .
1	bE	161	 96% .
1	bX	161	 98% .
1	cA	161	 98% .
1	cB	161	 97% .
1	cC	161	 97% .
1	cD	161	 98% .
1	cE	161	 96% .
1	cX	161	 98% .

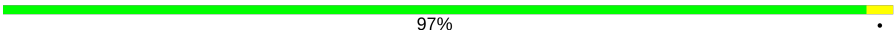

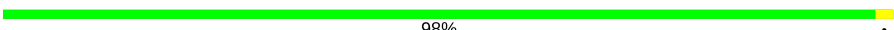
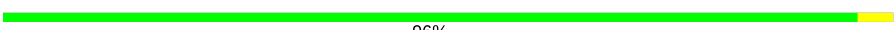











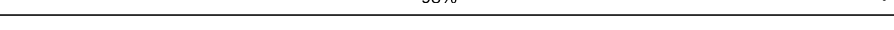
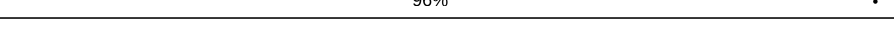
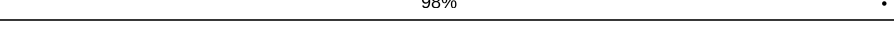
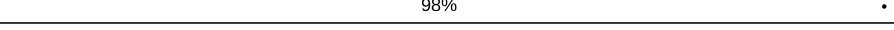
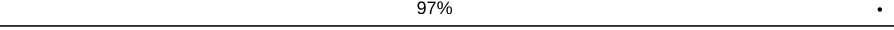
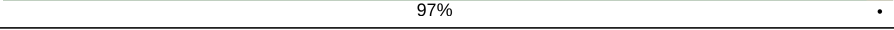
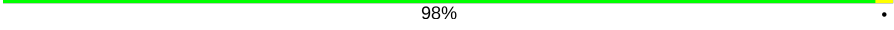
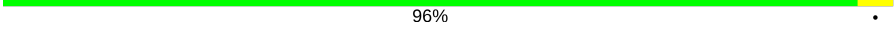
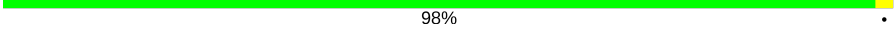
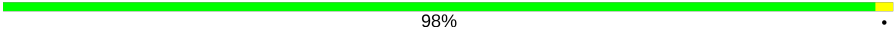
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	dA	161	 98% .
1	dB	161	 97% .
1	dC	161	 97% .
1	dD	161	 98% .
1	dE	161	 96% .
1	dX	161	 98% .
1	eA	161	 98% .
1	eB	161	 97% .
1	eC	161	 97% .
1	eD	161	 98% .
1	eE	161	 96% .
1	eX	161	 98% .
1	fA	161	 98% .
1	fB	161	 97% .
1	fC	161	 97% .
1	fD	161	 98% .
1	fE	161	 96% .
1	fX	161	 98% .
1	gA	161	 98% .
1	gB	161	 97% .
1	gC	161	 97% .
1	gD	161	 98% .
1	gE	161	 96% .
1	gX	161	 98% .
1	hA	161	 98% .

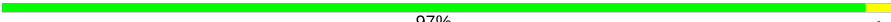
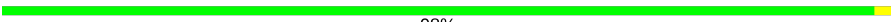
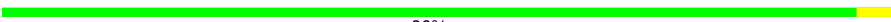












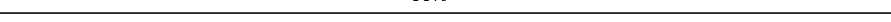
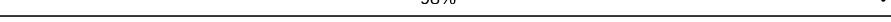
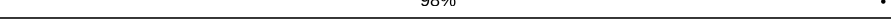
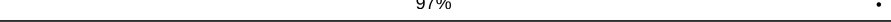
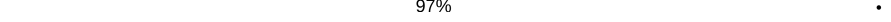
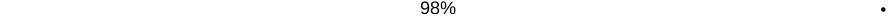
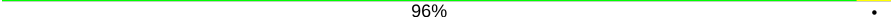
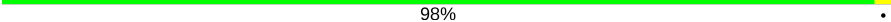
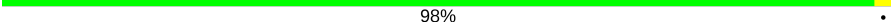
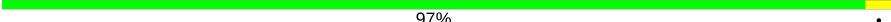
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	hB	161	 97% .
1	hC	161	 97% .
1	hD	161	 98% .
1	hE	161	 96% .
1	hX	161	 98% .
1	iA	161	 98% .
1	iB	161	 97% .
1	iC	161	 97% .
1	iD	161	 98% .
1	iE	161	 96% .
1	iX	161	 98% .
1	jA	161	 98% .
1	jB	161	 97% .
1	jC	161	 97% .
1	jD	161	 98% .
1	jE	161	 96% .
1	jX	161	 98% .
1	kA	161	 98% .
1	kB	161	 97% .
1	kC	161	 97% .
1	kD	161	 98% .
1	kE	161	 96% .
1	kX	161	 98% .
1	lA	161	 98% .
1	lB	161	 97% .

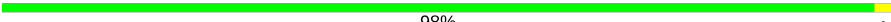
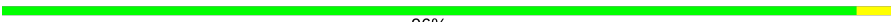
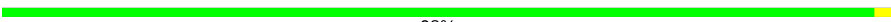












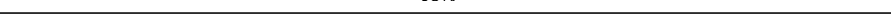
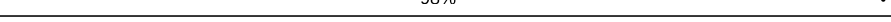
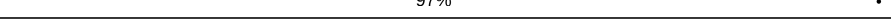
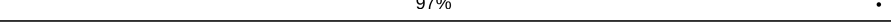
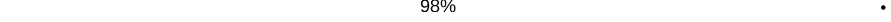
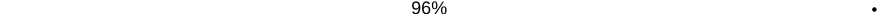
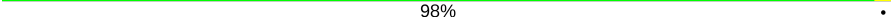
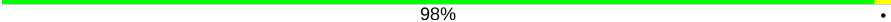
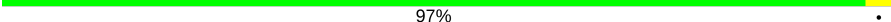
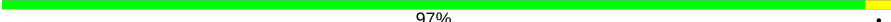
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	lC	161	 97% .
1	lD	161	 98% .
1	lE	161	 96% .
1	lX	161	 98% .
1	mA	161	 98% .
1	mB	161	 97% .
1	mC	161	 97% .
1	mD	161	 98% .
1	mE	161	 96% .
1	mX	161	 98% .
1	nA	161	 98% .
1	nB	161	 97% .
1	nC	161	 97% .
1	nD	161	 98% .
1	nE	161	 96% .
1	nX	161	 98% .
1	oA	161	 98% .
1	oB	161	 97% .
1	oC	161	 97% .
1	oD	161	 98% .
1	oE	161	 96% .
1	oX	161	 98% .
1	pA	161	 98% .
1	pB	161	 97% .
1	pC	161	 97% .

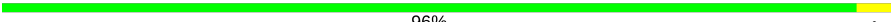
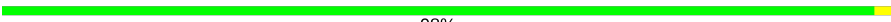
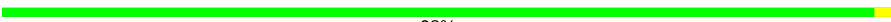












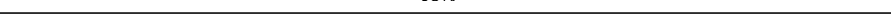
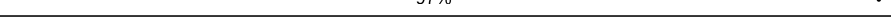
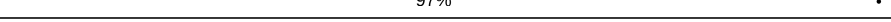
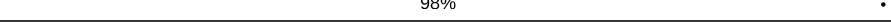
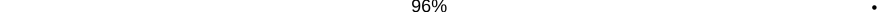
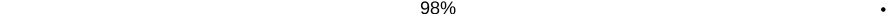
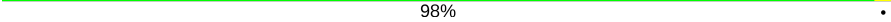
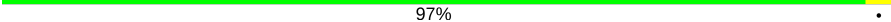
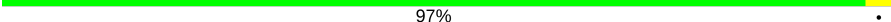
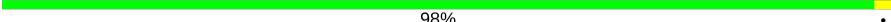
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	pD	161	 98% .
1	pE	161	 96% .
1	pX	161	 98% .
1	qA	161	 98% .
1	qB	161	 97% .
1	qC	161	 97% .
1	qD	161	 98% .
1	qE	161	 96% .
1	qX	161	 98% .
1	rA	161	 98% .
1	rB	161	 97% .
1	rC	161	 97% .
1	rD	161	 98% .
1	rE	161	 96% .
1	rX	161	 98% .
1	sA	161	 98% .
1	sB	161	 97% .
1	sC	161	 97% .
1	sD	161	 98% .
1	sE	161	 96% .
1	sX	161	 98% .
1	tA	161	 98% .
1	tB	161	 97% .
1	tC	161	 97% .
1	tD	161	 98% .

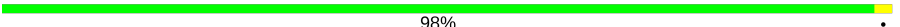
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	tE	161	 96% .
1	tX	161	 98% .
1	uA	161	 98% .
1	uB	161	 97% .
1	uC	161	 97% .
1	uD	161	 98% .
1	uE	161	 96% .
1	uX	161	 98% .
1	vA	161	 98% .
1	vB	161	 97% .
1	vC	161	 97% .
1	vD	161	 98% .
1	vE	161	 96% .
1	vX	161	 98% .
1	wA	161	 98% .
1	wB	161	 97% .
1	wC	161	 97% .
1	wD	161	 98% .
1	wE	161	 96% .
1	wX	161	 98% .
1	xA	161	 98% .
1	xB	161	 97% .
1	xC	161	 97% .
1	xD	161	 98% .
1	xE	161	 96% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	xX	161	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 286920 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 6,7-dimethyl-8-ribityllumazine synthase.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0A	161	Total	C	N	O	0	0
			797	475	161	161		
1	0B	161	Total	C	N	O	0	0
			797	475	161	161		
1	0C	161	Total	C	N	O	0	0
			797	475	161	161		
1	0D	161	Total	C	N	O	0	0
			797	475	161	161		
1	0E	161	Total	C	N	O	0	0
			797	475	161	161		
1	0X	161	Total	C	N	O	0	0
			797	475	161	161		
1	1A	161	Total	C	N	O	0	0
			797	475	161	161		
1	1B	161	Total	C	N	O	0	0
			797	475	161	161		
1	1C	161	Total	C	N	O	0	0
			797	475	161	161		
1	1D	161	Total	C	N	O	0	0
			797	475	161	161		
1	1E	161	Total	C	N	O	0	0
			797	475	161	161		
1	1X	161	Total	C	N	O	0	0
			797	475	161	161		
1	2A	161	Total	C	N	O	0	0
			797	475	161	161		
1	2B	161	Total	C	N	O	0	0
			797	475	161	161		
1	2C	161	Total	C	N	O	0	0
			797	475	161	161		
1	2D	161	Total	C	N	O	0	0
			797	475	161	161		
1	2E	161	Total	C	N	O	0	0
			797	475	161	161		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2X	161	Total	C	N	O	0	0
			797	475	161	161		
1	3A	161	Total	C	N	O	0	0
			797	475	161	161		
1	3B	161	Total	C	N	O	0	0
			797	475	161	161		
1	3C	161	Total	C	N	O	0	0
			797	475	161	161		
1	3D	161	Total	C	N	O	0	0
			797	475	161	161		
1	3E	161	Total	C	N	O	0	0
			797	475	161	161		
1	3X	161	Total	C	N	O	0	0
			797	475	161	161		
1	4A	161	Total	C	N	O	0	0
			797	475	161	161		
1	4B	161	Total	C	N	O	0	0
			797	475	161	161		
1	4C	161	Total	C	N	O	0	0
			797	475	161	161		
1	4D	161	Total	C	N	O	0	0
			797	475	161	161		
1	4E	161	Total	C	N	O	0	0
			797	475	161	161		
1	4X	161	Total	C	N	O	0	0
			797	475	161	161		
1	5A	161	Total	C	N	O	0	0
			797	475	161	161		
1	5B	161	Total	C	N	O	0	0
			797	475	161	161		
1	5C	161	Total	C	N	O	0	0
			797	475	161	161		
1	5D	161	Total	C	N	O	0	0
			797	475	161	161		
1	5E	161	Total	C	N	O	0	0
			797	475	161	161		
1	5X	161	Total	C	N	O	0	0
			797	475	161	161		
1	6A	161	Total	C	N	O	0	0
			797	475	161	161		
1	6B	161	Total	C	N	O	0	0
			797	475	161	161		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	6C	161	Total 797	C 475	N 161	O 161	0	0
1	6D	161	Total 797	C 475	N 161	O 161	0	0
1	6E	161	Total 797	C 475	N 161	O 161	0	0
1	6X	161	Total 797	C 475	N 161	O 161	0	0
1	7A	161	Total 797	C 475	N 161	O 161	0	0
1	7B	161	Total 797	C 475	N 161	O 161	0	0
1	7C	161	Total 797	C 475	N 161	O 161	0	0
1	7D	161	Total 797	C 475	N 161	O 161	0	0
1	7E	161	Total 797	C 475	N 161	O 161	0	0
1	7X	161	Total 797	C 475	N 161	O 161	0	0
1	8A	161	Total 797	C 475	N 161	O 161	0	0
1	8B	161	Total 797	C 475	N 161	O 161	0	0
1	8C	161	Total 797	C 475	N 161	O 161	0	0
1	8D	161	Total 797	C 475	N 161	O 161	0	0
1	8E	161	Total 797	C 475	N 161	O 161	0	0
1	8X	161	Total 797	C 475	N 161	O 161	0	0
1	9A	161	Total 797	C 475	N 161	O 161	0	0
1	9B	161	Total 797	C 475	N 161	O 161	0	0
1	9C	161	Total 797	C 475	N 161	O 161	0	0
1	9D	161	Total 797	C 475	N 161	O 161	0	0
1	9E	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	9X	161	Total 797	C 475	N 161	O 161	0	0
1	AA	161	Total 797	C 475	N 161	O 161	0	0
1	AB	161	Total 797	C 475	N 161	O 161	0	0
1	AC	161	Total 797	C 475	N 161	O 161	0	0
1	AD	161	Total 797	C 475	N 161	O 161	0	0
1	AE	161	Total 797	C 475	N 161	O 161	0	0
1	AX	161	Total 797	C 475	N 161	O 161	0	0
1	BA	161	Total 797	C 475	N 161	O 161	0	0
1	BB	161	Total 797	C 475	N 161	O 161	0	0
1	BC	161	Total 797	C 475	N 161	O 161	0	0
1	BD	161	Total 797	C 475	N 161	O 161	0	0
1	BE	161	Total 797	C 475	N 161	O 161	0	0
1	BX	161	Total 797	C 475	N 161	O 161	0	0
1	CA	161	Total 797	C 475	N 161	O 161	0	0
1	CB	161	Total 797	C 475	N 161	O 161	0	0
1	CC	161	Total 797	C 475	N 161	O 161	0	0
1	CD	161	Total 797	C 475	N 161	O 161	0	0
1	CE	161	Total 797	C 475	N 161	O 161	0	0
1	CX	161	Total 797	C 475	N 161	O 161	0	0
1	DA	161	Total 797	C 475	N 161	O 161	0	0
1	DB	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	DC	161	Total 797	C 475	N 161	O 161	0	0
1	DD	161	Total 797	C 475	N 161	O 161	0	0
1	DE	161	Total 797	C 475	N 161	O 161	0	0
1	DX	161	Total 797	C 475	N 161	O 161	0	0
1	EA	161	Total 797	C 475	N 161	O 161	0	0
1	EB	161	Total 797	C 475	N 161	O 161	0	0
1	EC	161	Total 797	C 475	N 161	O 161	0	0
1	ED	161	Total 797	C 475	N 161	O 161	0	0
1	EE	161	Total 797	C 475	N 161	O 161	0	0
1	EX	161	Total 797	C 475	N 161	O 161	0	0
1	FA	161	Total 797	C 475	N 161	O 161	0	0
1	FB	161	Total 797	C 475	N 161	O 161	0	0
1	FC	161	Total 797	C 475	N 161	O 161	0	0
1	FD	161	Total 797	C 475	N 161	O 161	0	0
1	FE	161	Total 797	C 475	N 161	O 161	0	0
1	FX	161	Total 797	C 475	N 161	O 161	0	0
1	GA	161	Total 797	C 475	N 161	O 161	0	0
1	GB	161	Total 797	C 475	N 161	O 161	0	0
1	GC	161	Total 797	C 475	N 161	O 161	0	0
1	GD	161	Total 797	C 475	N 161	O 161	0	0
1	GE	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	GX	161	Total 797	C 475	N 161	O 161	0	0
1	HA	161	Total 797	C 475	N 161	O 161	0	0
1	HB	161	Total 797	C 475	N 161	O 161	0	0
1	HC	161	Total 797	C 475	N 161	O 161	0	0
1	HD	161	Total 797	C 475	N 161	O 161	0	0
1	HE	161	Total 797	C 475	N 161	O 161	0	0
1	HX	161	Total 797	C 475	N 161	O 161	0	0
1	IA	161	Total 797	C 475	N 161	O 161	0	0
1	IB	161	Total 797	C 475	N 161	O 161	0	0
1	IC	161	Total 797	C 475	N 161	O 161	0	0
1	ID	161	Total 797	C 475	N 161	O 161	0	0
1	IE	161	Total 797	C 475	N 161	O 161	0	0
1	IX	161	Total 797	C 475	N 161	O 161	0	0
1	JA	161	Total 797	C 475	N 161	O 161	0	0
1	JB	161	Total 797	C 475	N 161	O 161	0	0
1	JC	161	Total 797	C 475	N 161	O 161	0	0
1	JD	161	Total 797	C 475	N 161	O 161	0	0
1	JE	161	Total 797	C 475	N 161	O 161	0	0
1	JX	161	Total 797	C 475	N 161	O 161	0	0
1	KA	161	Total 797	C 475	N 161	O 161	0	0
1	KB	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	KC	161	Total 797	C 475	N 161	O 161	0	0
1	KD	161	Total 797	C 475	N 161	O 161	0	0
1	KE	161	Total 797	C 475	N 161	O 161	0	0
1	KX	161	Total 797	C 475	N 161	O 161	0	0
1	LA	161	Total 797	C 475	N 161	O 161	0	0
1	LB	161	Total 797	C 475	N 161	O 161	0	0
1	LC	161	Total 797	C 475	N 161	O 161	0	0
1	LD	161	Total 797	C 475	N 161	O 161	0	0
1	LE	161	Total 797	C 475	N 161	O 161	0	0
1	LX	161	Total 797	C 475	N 161	O 161	0	0
1	MA	161	Total 797	C 475	N 161	O 161	0	0
1	MB	161	Total 797	C 475	N 161	O 161	0	0
1	MC	161	Total 797	C 475	N 161	O 161	0	0
1	MD	161	Total 797	C 475	N 161	O 161	0	0
1	ME	161	Total 797	C 475	N 161	O 161	0	0
1	MX	161	Total 797	C 475	N 161	O 161	0	0
1	NA	161	Total 797	C 475	N 161	O 161	0	0
1	NB	161	Total 797	C 475	N 161	O 161	0	0
1	NC	161	Total 797	C 475	N 161	O 161	0	0
1	ND	161	Total 797	C 475	N 161	O 161	0	0
1	NE	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	NX	161	Total 797	C 475	N 161	O 161	0	0
1	OA	161	Total 797	C 475	N 161	O 161	0	0
1	OB	161	Total 797	C 475	N 161	O 161	0	0
1	OC	161	Total 797	C 475	N 161	O 161	0	0
1	OD	161	Total 797	C 475	N 161	O 161	0	0
1	OE	161	Total 797	C 475	N 161	O 161	0	0
1	OX	161	Total 797	C 475	N 161	O 161	0	0
1	PA	161	Total 797	C 475	N 161	O 161	0	0
1	PB	161	Total 797	C 475	N 161	O 161	0	0
1	PC	161	Total 797	C 475	N 161	O 161	0	0
1	PD	161	Total 797	C 475	N 161	O 161	0	0
1	PE	161	Total 797	C 475	N 161	O 161	0	0
1	PX	161	Total 797	C 475	N 161	O 161	0	0
1	QA	161	Total 797	C 475	N 161	O 161	0	0
1	QB	161	Total 797	C 475	N 161	O 161	0	0
1	QC	161	Total 797	C 475	N 161	O 161	0	0
1	QD	161	Total 797	C 475	N 161	O 161	0	0
1	QE	161	Total 797	C 475	N 161	O 161	0	0
1	QX	161	Total 797	C 475	N 161	O 161	0	0
1	RA	161	Total 797	C 475	N 161	O 161	0	0
1	RB	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	RC	161	Total	C	N	O	0	0
			797	475	161	161		
1	RD	161	Total	C	N	O	0	0
			797	475	161	161		
1	RE	161	Total	C	N	O	0	0
			797	475	161	161		
1	RX	161	Total	C	N	O	0	0
			797	475	161	161		
1	SA	161	Total	C	N	O	0	0
			797	475	161	161		
1	SB	161	Total	C	N	O	0	0
			797	475	161	161		
1	SC	161	Total	C	N	O	0	0
			797	475	161	161		
1	SD	161	Total	C	N	O	0	0
			797	475	161	161		
1	SE	161	Total	C	N	O	0	0
			797	475	161	161		
1	SX	161	Total	C	N	O	0	0
			797	475	161	161		
1	TA	161	Total	C	N	O	0	0
			797	475	161	161		
1	TB	161	Total	C	N	O	0	0
			797	475	161	161		
1	TC	161	Total	C	N	O	0	0
			797	475	161	161		
1	TD	161	Total	C	N	O	0	0
			797	475	161	161		
1	TE	161	Total	C	N	O	0	0
			797	475	161	161		
1	TX	161	Total	C	N	O	0	0
			797	475	161	161		
1	UA	161	Total	C	N	O	0	0
			797	475	161	161		
1	UB	161	Total	C	N	O	0	0
			797	475	161	161		
1	UC	161	Total	C	N	O	0	0
			797	475	161	161		
1	UD	161	Total	C	N	O	0	0
			797	475	161	161		
1	UE	161	Total	C	N	O	0	0
			797	475	161	161		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	UX	161	Total 797	C 475	N 161	O 161	0	0
1	VA	161	Total 797	C 475	N 161	O 161	0	0
1	VB	161	Total 797	C 475	N 161	O 161	0	0
1	VC	161	Total 797	C 475	N 161	O 161	0	0
1	VD	161	Total 797	C 475	N 161	O 161	0	0
1	VE	161	Total 797	C 475	N 161	O 161	0	0
1	VX	161	Total 797	C 475	N 161	O 161	0	0
1	WA	161	Total 797	C 475	N 161	O 161	0	0
1	WB	161	Total 797	C 475	N 161	O 161	0	0
1	WC	161	Total 797	C 475	N 161	O 161	0	0
1	WD	161	Total 797	C 475	N 161	O 161	0	0
1	WE	161	Total 797	C 475	N 161	O 161	0	0
1	WX	161	Total 797	C 475	N 161	O 161	0	0
1	XA	161	Total 797	C 475	N 161	O 161	0	0
1	XB	161	Total 797	C 475	N 161	O 161	0	0
1	XC	161	Total 797	C 475	N 161	O 161	0	0
1	XD	161	Total 797	C 475	N 161	O 161	0	0
1	XE	161	Total 797	C 475	N 161	O 161	0	0
1	XX	161	Total 797	C 475	N 161	O 161	0	0
1	YA	161	Total 797	C 475	N 161	O 161	0	0
1	YB	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	YC	161	Total	C	N	O	0	0
			797	475	161	161		
1	YD	161	Total	C	N	O	0	0
			797	475	161	161		
1	YE	161	Total	C	N	O	0	0
			797	475	161	161		
1	YX	161	Total	C	N	O	0	0
			797	475	161	161		
1	ZA	161	Total	C	N	O	0	0
			797	475	161	161		
1	ZB	161	Total	C	N	O	0	0
			797	475	161	161		
1	ZC	161	Total	C	N	O	0	0
			797	475	161	161		
1	ZD	161	Total	C	N	O	0	0
			797	475	161	161		
1	ZE	161	Total	C	N	O	0	0
			797	475	161	161		
1	ZX	161	Total	C	N	O	0	0
			797	475	161	161		
1	aA	161	Total	C	N	O	0	0
			797	475	161	161		
1	aB	161	Total	C	N	O	0	0
			797	475	161	161		
1	aC	161	Total	C	N	O	0	0
			797	475	161	161		
1	aD	161	Total	C	N	O	0	0
			797	475	161	161		
1	aE	161	Total	C	N	O	0	0
			797	475	161	161		
1	aX	161	Total	C	N	O	0	0
			797	475	161	161		
1	bA	161	Total	C	N	O	0	0
			797	475	161	161		
1	bB	161	Total	C	N	O	0	0
			797	475	161	161		
1	bC	161	Total	C	N	O	0	0
			797	475	161	161		
1	bD	161	Total	C	N	O	0	0
			797	475	161	161		
1	bE	161	Total	C	N	O	0	0
			797	475	161	161		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	bX	161	Total 797	C 475	N 161	O 161	0	0
1	cA	161	Total 797	C 475	N 161	O 161	0	0
1	cB	161	Total 797	C 475	N 161	O 161	0	0
1	cC	161	Total 797	C 475	N 161	O 161	0	0
1	cD	161	Total 797	C 475	N 161	O 161	0	0
1	cE	161	Total 797	C 475	N 161	O 161	0	0
1	cX	161	Total 797	C 475	N 161	O 161	0	0
1	dA	161	Total 797	C 475	N 161	O 161	0	0
1	dB	161	Total 797	C 475	N 161	O 161	0	0
1	dC	161	Total 797	C 475	N 161	O 161	0	0
1	dD	161	Total 797	C 475	N 161	O 161	0	0
1	dE	161	Total 797	C 475	N 161	O 161	0	0
1	dX	161	Total 797	C 475	N 161	O 161	0	0
1	eA	161	Total 797	C 475	N 161	O 161	0	0
1	eB	161	Total 797	C 475	N 161	O 161	0	0
1	eC	161	Total 797	C 475	N 161	O 161	0	0
1	eD	161	Total 797	C 475	N 161	O 161	0	0
1	eE	161	Total 797	C 475	N 161	O 161	0	0
1	eX	161	Total 797	C 475	N 161	O 161	0	0
1	fA	161	Total 797	C 475	N 161	O 161	0	0
1	fB	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	fC	161	Total 797	C 475	N 161	O 161	0	0
1	fD	161	Total 797	C 475	N 161	O 161	0	0
1	fE	161	Total 797	C 475	N 161	O 161	0	0
1	fX	161	Total 797	C 475	N 161	O 161	0	0
1	gA	161	Total 797	C 475	N 161	O 161	0	0
1	gB	161	Total 797	C 475	N 161	O 161	0	0
1	gC	161	Total 797	C 475	N 161	O 161	0	0
1	gD	161	Total 797	C 475	N 161	O 161	0	0
1	gE	161	Total 797	C 475	N 161	O 161	0	0
1	gX	161	Total 797	C 475	N 161	O 161	0	0
1	hA	161	Total 797	C 475	N 161	O 161	0	0
1	hB	161	Total 797	C 475	N 161	O 161	0	0
1	hC	161	Total 797	C 475	N 161	O 161	0	0
1	hD	161	Total 797	C 475	N 161	O 161	0	0
1	hE	161	Total 797	C 475	N 161	O 161	0	0
1	hX	161	Total 797	C 475	N 161	O 161	0	0
1	iA	161	Total 797	C 475	N 161	O 161	0	0
1	iB	161	Total 797	C 475	N 161	O 161	0	0
1	iC	161	Total 797	C 475	N 161	O 161	0	0
1	iD	161	Total 797	C 475	N 161	O 161	0	0
1	iE	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	iX	161	Total 797	C 475	N 161	O 161	0	0
1	jA	161	Total 797	C 475	N 161	O 161	0	0
1	jB	161	Total 797	C 475	N 161	O 161	0	0
1	jC	161	Total 797	C 475	N 161	O 161	0	0
1	jD	161	Total 797	C 475	N 161	O 161	0	0
1	jE	161	Total 797	C 475	N 161	O 161	0	0
1	jX	161	Total 797	C 475	N 161	O 161	0	0
1	kA	161	Total 797	C 475	N 161	O 161	0	0
1	kB	161	Total 797	C 475	N 161	O 161	0	0
1	kC	161	Total 797	C 475	N 161	O 161	0	0
1	kD	161	Total 797	C 475	N 161	O 161	0	0
1	kE	161	Total 797	C 475	N 161	O 161	0	0
1	kX	161	Total 797	C 475	N 161	O 161	0	0
1	lA	161	Total 797	C 475	N 161	O 161	0	0
1	lB	161	Total 797	C 475	N 161	O 161	0	0
1	lC	161	Total 797	C 475	N 161	O 161	0	0
1	lD	161	Total 797	C 475	N 161	O 161	0	0
1	lE	161	Total 797	C 475	N 161	O 161	0	0
1	lX	161	Total 797	C 475	N 161	O 161	0	0
1	mA	161	Total 797	C 475	N 161	O 161	0	0
1	mB	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	mC	161	Total 797	C 475	N 161	O 161	0	0
1	mD	161	Total 797	C 475	N 161	O 161	0	0
1	mE	161	Total 797	C 475	N 161	O 161	0	0
1	mX	161	Total 797	C 475	N 161	O 161	0	0
1	nA	161	Total 797	C 475	N 161	O 161	0	0
1	nB	161	Total 797	C 475	N 161	O 161	0	0
1	nC	161	Total 797	C 475	N 161	O 161	0	0
1	nD	161	Total 797	C 475	N 161	O 161	0	0
1	nE	161	Total 797	C 475	N 161	O 161	0	0
1	nX	161	Total 797	C 475	N 161	O 161	0	0
1	oA	161	Total 797	C 475	N 161	O 161	0	0
1	oB	161	Total 797	C 475	N 161	O 161	0	0
1	oC	161	Total 797	C 475	N 161	O 161	0	0
1	oD	161	Total 797	C 475	N 161	O 161	0	0
1	oE	161	Total 797	C 475	N 161	O 161	0	0
1	oX	161	Total 797	C 475	N 161	O 161	0	0
1	pA	161	Total 797	C 475	N 161	O 161	0	0
1	pB	161	Total 797	C 475	N 161	O 161	0	0
1	pC	161	Total 797	C 475	N 161	O 161	0	0
1	pD	161	Total 797	C 475	N 161	O 161	0	0
1	pE	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	pX	161	Total 797	C 475	N 161	O 161	0	0
1	qA	161	Total 797	C 475	N 161	O 161	0	0
1	qB	161	Total 797	C 475	N 161	O 161	0	0
1	qC	161	Total 797	C 475	N 161	O 161	0	0
1	qD	161	Total 797	C 475	N 161	O 161	0	0
1	qE	161	Total 797	C 475	N 161	O 161	0	0
1	qX	161	Total 797	C 475	N 161	O 161	0	0
1	rA	161	Total 797	C 475	N 161	O 161	0	0
1	rB	161	Total 797	C 475	N 161	O 161	0	0
1	rC	161	Total 797	C 475	N 161	O 161	0	0
1	rD	161	Total 797	C 475	N 161	O 161	0	0
1	rE	161	Total 797	C 475	N 161	O 161	0	0
1	rX	161	Total 797	C 475	N 161	O 161	0	0
1	sA	161	Total 797	C 475	N 161	O 161	0	0
1	sB	161	Total 797	C 475	N 161	O 161	0	0
1	sC	161	Total 797	C 475	N 161	O 161	0	0
1	sD	161	Total 797	C 475	N 161	O 161	0	0
1	sE	161	Total 797	C 475	N 161	O 161	0	0
1	sX	161	Total 797	C 475	N 161	O 161	0	0
1	tA	161	Total 797	C 475	N 161	O 161	0	0
1	tB	161	Total 797	C 475	N 161	O 161	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	tC	161	Total	C	N	O	0	0
			797	475	161	161		
1	tD	161	Total	C	N	O	0	0
			797	475	161	161		
1	tE	161	Total	C	N	O	0	0
			797	475	161	161		
1	tX	161	Total	C	N	O	0	0
			797	475	161	161		
1	uA	161	Total	C	N	O	0	0
			797	475	161	161		
1	uB	161	Total	C	N	O	0	0
			797	475	161	161		
1	uC	161	Total	C	N	O	0	0
			797	475	161	161		
1	uD	161	Total	C	N	O	0	0
			797	475	161	161		
1	uE	161	Total	C	N	O	0	0
			797	475	161	161		
1	uX	161	Total	C	N	O	0	0
			797	475	161	161		
1	vA	161	Total	C	N	O	0	0
			797	475	161	161		
1	vB	161	Total	C	N	O	0	0
			797	475	161	161		
1	vC	161	Total	C	N	O	0	0
			797	475	161	161		
1	vD	161	Total	C	N	O	0	0
			797	475	161	161		
1	vE	161	Total	C	N	O	0	0
			797	475	161	161		
1	vX	161	Total	C	N	O	0	0
			797	475	161	161		
1	wA	161	Total	C	N	O	0	0
			797	475	161	161		
1	wB	161	Total	C	N	O	0	0
			797	475	161	161		
1	wC	161	Total	C	N	O	0	0
			797	475	161	161		
1	wD	161	Total	C	N	O	0	0
			797	475	161	161		
1	wE	161	Total	C	N	O	0	0
			797	475	161	161		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	wX	161	Total	C	N	O	0	0
			797	475	161	161		
1	xA	161	Total	C	N	O	0	0
			797	475	161	161		
1	xB	161	Total	C	N	O	0	0
			797	475	161	161		
1	xC	161	Total	C	N	O	0	0
			797	475	161	161		
1	xD	161	Total	C	N	O	0	0
			797	475	161	161		
1	xE	161	Total	C	N	O	0	0
			797	475	161	161		
1	xX	161	Total	C	N	O	0	0
			797	475	161	161		

There are 6840 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0A	2	GLU	GLN	conflict	UNP O66529
0A	28	GLY	ASP	conflict	UNP O66529
0A	52	CYS	ARG	conflict	UNP O66529
0A	83	GLU	ARG	conflict	UNP O66529
0A	86	GLU	THR	conflict	UNP O66529
0A	112	SER	THR	conflict	UNP O66529
0A	115	ASP	VAL	conflict	UNP O66529
0A	118	ASP	ALA	conflict	UNP O66529
0A	120	GLU	THR	conflict	UNP O66529
0A	123	GLU	GLN	conflict	UNP O66529
0A	127	CYS	ARG	conflict	UNP O66529
0A	131	GLU	LYS	conflict	UNP O66529
0A	155	LEU	-	expression tag	UNP O66529
0A	156	GLU	-	expression tag	UNP O66529
0A	157	HIS	-	expression tag	UNP O66529
0A	158	HIS	-	expression tag	UNP O66529
0A	159	HIS	-	expression tag	UNP O66529
0A	160	HIS	-	expression tag	UNP O66529
0A	161	HIS	-	expression tag	UNP O66529
0B	2	GLU	GLN	conflict	UNP O66529
0B	28	GLY	ASP	conflict	UNP O66529
0B	52	CYS	ARG	conflict	UNP O66529
0B	83	GLU	ARG	conflict	UNP O66529
0B	86	GLU	THR	conflict	UNP O66529
0B	112	SER	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
0B	115	ASP	VAL	conflict	UNP O66529
0B	118	ASP	ALA	conflict	UNP O66529
0B	120	GLU	THR	conflict	UNP O66529
0B	123	GLU	GLN	conflict	UNP O66529
0B	127	CYS	ARG	conflict	UNP O66529
0B	131	GLU	LYS	conflict	UNP O66529
0B	155	LEU	-	expression tag	UNP O66529
0B	156	GLU	-	expression tag	UNP O66529
0B	157	HIS	-	expression tag	UNP O66529
0B	158	HIS	-	expression tag	UNP O66529
0B	159	HIS	-	expression tag	UNP O66529
0B	160	HIS	-	expression tag	UNP O66529
0B	161	HIS	-	expression tag	UNP O66529
0C	2	GLU	GLN	conflict	UNP O66529
0C	28	GLY	ASP	conflict	UNP O66529
0C	52	CYS	ARG	conflict	UNP O66529
0C	83	GLU	ARG	conflict	UNP O66529
0C	86	GLU	THR	conflict	UNP O66529
0C	112	SER	THR	conflict	UNP O66529
0C	115	ASP	VAL	conflict	UNP O66529
0C	118	ASP	ALA	conflict	UNP O66529
0C	120	GLU	THR	conflict	UNP O66529
0C	123	GLU	GLN	conflict	UNP O66529
0C	127	CYS	ARG	conflict	UNP O66529
0C	131	GLU	LYS	conflict	UNP O66529
0C	155	LEU	-	expression tag	UNP O66529
0C	156	GLU	-	expression tag	UNP O66529
0C	157	HIS	-	expression tag	UNP O66529
0C	158	HIS	-	expression tag	UNP O66529
0C	159	HIS	-	expression tag	UNP O66529
0C	160	HIS	-	expression tag	UNP O66529
0C	161	HIS	-	expression tag	UNP O66529
0D	2	GLU	GLN	conflict	UNP O66529
0D	28	GLY	ASP	conflict	UNP O66529
0D	52	CYS	ARG	conflict	UNP O66529
0D	83	GLU	ARG	conflict	UNP O66529
0D	86	GLU	THR	conflict	UNP O66529
0D	112	SER	THR	conflict	UNP O66529
0D	115	ASP	VAL	conflict	UNP O66529
0D	118	ASP	ALA	conflict	UNP O66529
0D	120	GLU	THR	conflict	UNP O66529
0D	123	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
0D	127	CYS	ARG	conflict	UNP O66529
0D	131	GLU	LYS	conflict	UNP O66529
0D	155	LEU	-	expression tag	UNP O66529
0D	156	GLU	-	expression tag	UNP O66529
0D	157	HIS	-	expression tag	UNP O66529
0D	158	HIS	-	expression tag	UNP O66529
0D	159	HIS	-	expression tag	UNP O66529
0D	160	HIS	-	expression tag	UNP O66529
0D	161	HIS	-	expression tag	UNP O66529
0E	2	GLU	GLN	conflict	UNP O66529
0E	28	GLY	ASP	conflict	UNP O66529
0E	52	CYS	ARG	conflict	UNP O66529
0E	83	GLU	ARG	conflict	UNP O66529
0E	86	GLU	THR	conflict	UNP O66529
0E	112	SER	THR	conflict	UNP O66529
0E	115	ASP	VAL	conflict	UNP O66529
0E	118	ASP	ALA	conflict	UNP O66529
0E	120	GLU	THR	conflict	UNP O66529
0E	123	GLU	GLN	conflict	UNP O66529
0E	127	CYS	ARG	conflict	UNP O66529
0E	131	GLU	LYS	conflict	UNP O66529
0E	155	LEU	-	expression tag	UNP O66529
0E	156	GLU	-	expression tag	UNP O66529
0E	157	HIS	-	expression tag	UNP O66529
0E	158	HIS	-	expression tag	UNP O66529
0E	159	HIS	-	expression tag	UNP O66529
0E	160	HIS	-	expression tag	UNP O66529
0E	161	HIS	-	expression tag	UNP O66529
0X	2	GLU	GLN	conflict	UNP O66529
0X	28	GLY	ASP	conflict	UNP O66529
0X	52	CYS	ARG	conflict	UNP O66529
0X	83	GLU	ARG	conflict	UNP O66529
0X	86	GLU	THR	conflict	UNP O66529
0X	112	SER	THR	conflict	UNP O66529
0X	115	ASP	VAL	conflict	UNP O66529
0X	118	ASP	ALA	conflict	UNP O66529
0X	120	GLU	THR	conflict	UNP O66529
0X	123	GLU	GLN	conflict	UNP O66529
0X	127	CYS	ARG	conflict	UNP O66529
0X	131	GLU	LYS	conflict	UNP O66529
0X	155	LEU	-	expression tag	UNP O66529
0X	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
0X	157	HIS	-	expression tag	UNP O66529
0X	158	HIS	-	expression tag	UNP O66529
0X	159	HIS	-	expression tag	UNP O66529
0X	160	HIS	-	expression tag	UNP O66529
0X	161	HIS	-	expression tag	UNP O66529
1A	2	GLU	GLN	conflict	UNP O66529
1A	28	GLY	ASP	conflict	UNP O66529
1A	52	CYS	ARG	conflict	UNP O66529
1A	83	GLU	ARG	conflict	UNP O66529
1A	86	GLU	THR	conflict	UNP O66529
1A	112	SER	THR	conflict	UNP O66529
1A	115	ASP	VAL	conflict	UNP O66529
1A	118	ASP	ALA	conflict	UNP O66529
1A	120	GLU	THR	conflict	UNP O66529
1A	123	GLU	GLN	conflict	UNP O66529
1A	127	CYS	ARG	conflict	UNP O66529
1A	131	GLU	LYS	conflict	UNP O66529
1A	155	LEU	-	expression tag	UNP O66529
1A	156	GLU	-	expression tag	UNP O66529
1A	157	HIS	-	expression tag	UNP O66529
1A	158	HIS	-	expression tag	UNP O66529
1A	159	HIS	-	expression tag	UNP O66529
1A	160	HIS	-	expression tag	UNP O66529
1A	161	HIS	-	expression tag	UNP O66529
1B	2	GLU	GLN	conflict	UNP O66529
1B	28	GLY	ASP	conflict	UNP O66529
1B	52	CYS	ARG	conflict	UNP O66529
1B	83	GLU	ARG	conflict	UNP O66529
1B	86	GLU	THR	conflict	UNP O66529
1B	112	SER	THR	conflict	UNP O66529
1B	115	ASP	VAL	conflict	UNP O66529
1B	118	ASP	ALA	conflict	UNP O66529
1B	120	GLU	THR	conflict	UNP O66529
1B	123	GLU	GLN	conflict	UNP O66529
1B	127	CYS	ARG	conflict	UNP O66529
1B	131	GLU	LYS	conflict	UNP O66529
1B	155	LEU	-	expression tag	UNP O66529
1B	156	GLU	-	expression tag	UNP O66529
1B	157	HIS	-	expression tag	UNP O66529
1B	158	HIS	-	expression tag	UNP O66529
1B	159	HIS	-	expression tag	UNP O66529
1B	160	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1B	161	HIS	-	expression tag	UNP O66529
1C	2	GLU	GLN	conflict	UNP O66529
1C	28	GLY	ASP	conflict	UNP O66529
1C	52	CYS	ARG	conflict	UNP O66529
1C	83	GLU	ARG	conflict	UNP O66529
1C	86	GLU	THR	conflict	UNP O66529
1C	112	SER	THR	conflict	UNP O66529
1C	115	ASP	VAL	conflict	UNP O66529
1C	118	ASP	ALA	conflict	UNP O66529
1C	120	GLU	THR	conflict	UNP O66529
1C	123	GLU	GLN	conflict	UNP O66529
1C	127	CYS	ARG	conflict	UNP O66529
1C	131	GLU	LYS	conflict	UNP O66529
1C	155	LEU	-	expression tag	UNP O66529
1C	156	GLU	-	expression tag	UNP O66529
1C	157	HIS	-	expression tag	UNP O66529
1C	158	HIS	-	expression tag	UNP O66529
1C	159	HIS	-	expression tag	UNP O66529
1C	160	HIS	-	expression tag	UNP O66529
1C	161	HIS	-	expression tag	UNP O66529
1D	2	GLU	GLN	conflict	UNP O66529
1D	28	GLY	ASP	conflict	UNP O66529
1D	52	CYS	ARG	conflict	UNP O66529
1D	83	GLU	ARG	conflict	UNP O66529
1D	86	GLU	THR	conflict	UNP O66529
1D	112	SER	THR	conflict	UNP O66529
1D	115	ASP	VAL	conflict	UNP O66529
1D	118	ASP	ALA	conflict	UNP O66529
1D	120	GLU	THR	conflict	UNP O66529
1D	123	GLU	GLN	conflict	UNP O66529
1D	127	CYS	ARG	conflict	UNP O66529
1D	131	GLU	LYS	conflict	UNP O66529
1D	155	LEU	-	expression tag	UNP O66529
1D	156	GLU	-	expression tag	UNP O66529
1D	157	HIS	-	expression tag	UNP O66529
1D	158	HIS	-	expression tag	UNP O66529
1D	159	HIS	-	expression tag	UNP O66529
1D	160	HIS	-	expression tag	UNP O66529
1D	161	HIS	-	expression tag	UNP O66529
1E	2	GLU	GLN	conflict	UNP O66529
1E	28	GLY	ASP	conflict	UNP O66529
1E	52	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1E	83	GLU	ARG	conflict	UNP O66529
1E	86	GLU	THR	conflict	UNP O66529
1E	112	SER	THR	conflict	UNP O66529
1E	115	ASP	VAL	conflict	UNP O66529
1E	118	ASP	ALA	conflict	UNP O66529
1E	120	GLU	THR	conflict	UNP O66529
1E	123	GLU	GLN	conflict	UNP O66529
1E	127	CYS	ARG	conflict	UNP O66529
1E	131	GLU	LYS	conflict	UNP O66529
1E	155	LEU	-	expression tag	UNP O66529
1E	156	GLU	-	expression tag	UNP O66529
1E	157	HIS	-	expression tag	UNP O66529
1E	158	HIS	-	expression tag	UNP O66529
1E	159	HIS	-	expression tag	UNP O66529
1E	160	HIS	-	expression tag	UNP O66529
1E	161	HIS	-	expression tag	UNP O66529
1X	2	GLU	GLN	conflict	UNP O66529
1X	28	GLY	ASP	conflict	UNP O66529
1X	52	CYS	ARG	conflict	UNP O66529
1X	83	GLU	ARG	conflict	UNP O66529
1X	86	GLU	THR	conflict	UNP O66529
1X	112	SER	THR	conflict	UNP O66529
1X	115	ASP	VAL	conflict	UNP O66529
1X	118	ASP	ALA	conflict	UNP O66529
1X	120	GLU	THR	conflict	UNP O66529
1X	123	GLU	GLN	conflict	UNP O66529
1X	127	CYS	ARG	conflict	UNP O66529
1X	131	GLU	LYS	conflict	UNP O66529
1X	155	LEU	-	expression tag	UNP O66529
1X	156	GLU	-	expression tag	UNP O66529
1X	157	HIS	-	expression tag	UNP O66529
1X	158	HIS	-	expression tag	UNP O66529
1X	159	HIS	-	expression tag	UNP O66529
1X	160	HIS	-	expression tag	UNP O66529
1X	161	HIS	-	expression tag	UNP O66529
2A	2	GLU	GLN	conflict	UNP O66529
2A	28	GLY	ASP	conflict	UNP O66529
2A	52	CYS	ARG	conflict	UNP O66529
2A	83	GLU	ARG	conflict	UNP O66529
2A	86	GLU	THR	conflict	UNP O66529
2A	112	SER	THR	conflict	UNP O66529
2A	115	ASP	VAL	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
2A	118	ASP	ALA	conflict	UNP O66529
2A	120	GLU	THR	conflict	UNP O66529
2A	123	GLU	GLN	conflict	UNP O66529
2A	127	CYS	ARG	conflict	UNP O66529
2A	131	GLU	LYS	conflict	UNP O66529
2A	155	LEU	-	expression tag	UNP O66529
2A	156	GLU	-	expression tag	UNP O66529
2A	157	HIS	-	expression tag	UNP O66529
2A	158	HIS	-	expression tag	UNP O66529
2A	159	HIS	-	expression tag	UNP O66529
2A	160	HIS	-	expression tag	UNP O66529
2A	161	HIS	-	expression tag	UNP O66529
2B	2	GLU	GLN	conflict	UNP O66529
2B	28	GLY	ASP	conflict	UNP O66529
2B	52	CYS	ARG	conflict	UNP O66529
2B	83	GLU	ARG	conflict	UNP O66529
2B	86	GLU	THR	conflict	UNP O66529
2B	112	SER	THR	conflict	UNP O66529
2B	115	ASP	VAL	conflict	UNP O66529
2B	118	ASP	ALA	conflict	UNP O66529
2B	120	GLU	THR	conflict	UNP O66529
2B	123	GLU	GLN	conflict	UNP O66529
2B	127	CYS	ARG	conflict	UNP O66529
2B	131	GLU	LYS	conflict	UNP O66529
2B	155	LEU	-	expression tag	UNP O66529
2B	156	GLU	-	expression tag	UNP O66529
2B	157	HIS	-	expression tag	UNP O66529
2B	158	HIS	-	expression tag	UNP O66529
2B	159	HIS	-	expression tag	UNP O66529
2B	160	HIS	-	expression tag	UNP O66529
2B	161	HIS	-	expression tag	UNP O66529
2C	2	GLU	GLN	conflict	UNP O66529
2C	28	GLY	ASP	conflict	UNP O66529
2C	52	CYS	ARG	conflict	UNP O66529
2C	83	GLU	ARG	conflict	UNP O66529
2C	86	GLU	THR	conflict	UNP O66529
2C	112	SER	THR	conflict	UNP O66529
2C	115	ASP	VAL	conflict	UNP O66529
2C	118	ASP	ALA	conflict	UNP O66529
2C	120	GLU	THR	conflict	UNP O66529
2C	123	GLU	GLN	conflict	UNP O66529
2C	127	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
2C	131	GLU	LYS	conflict	UNP O66529
2C	155	LEU	-	expression tag	UNP O66529
2C	156	GLU	-	expression tag	UNP O66529
2C	157	HIS	-	expression tag	UNP O66529
2C	158	HIS	-	expression tag	UNP O66529
2C	159	HIS	-	expression tag	UNP O66529
2C	160	HIS	-	expression tag	UNP O66529
2C	161	HIS	-	expression tag	UNP O66529
2D	2	GLU	GLN	conflict	UNP O66529
2D	28	GLY	ASP	conflict	UNP O66529
2D	52	CYS	ARG	conflict	UNP O66529
2D	83	GLU	ARG	conflict	UNP O66529
2D	86	GLU	THR	conflict	UNP O66529
2D	112	SER	THR	conflict	UNP O66529
2D	115	ASP	VAL	conflict	UNP O66529
2D	118	ASP	ALA	conflict	UNP O66529
2D	120	GLU	THR	conflict	UNP O66529
2D	123	GLU	GLN	conflict	UNP O66529
2D	127	CYS	ARG	conflict	UNP O66529
2D	131	GLU	LYS	conflict	UNP O66529
2D	155	LEU	-	expression tag	UNP O66529
2D	156	GLU	-	expression tag	UNP O66529
2D	157	HIS	-	expression tag	UNP O66529
2D	158	HIS	-	expression tag	UNP O66529
2D	159	HIS	-	expression tag	UNP O66529
2D	160	HIS	-	expression tag	UNP O66529
2D	161	HIS	-	expression tag	UNP O66529
2E	2	GLU	GLN	conflict	UNP O66529
2E	28	GLY	ASP	conflict	UNP O66529
2E	52	CYS	ARG	conflict	UNP O66529
2E	83	GLU	ARG	conflict	UNP O66529
2E	86	GLU	THR	conflict	UNP O66529
2E	112	SER	THR	conflict	UNP O66529
2E	115	ASP	VAL	conflict	UNP O66529
2E	118	ASP	ALA	conflict	UNP O66529
2E	120	GLU	THR	conflict	UNP O66529
2E	123	GLU	GLN	conflict	UNP O66529
2E	127	CYS	ARG	conflict	UNP O66529
2E	131	GLU	LYS	conflict	UNP O66529
2E	155	LEU	-	expression tag	UNP O66529
2E	156	GLU	-	expression tag	UNP O66529
2E	157	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
2E	158	HIS	-	expression tag	UNP O66529
2E	159	HIS	-	expression tag	UNP O66529
2E	160	HIS	-	expression tag	UNP O66529
2E	161	HIS	-	expression tag	UNP O66529
2X	2	GLU	GLN	conflict	UNP O66529
2X	28	GLY	ASP	conflict	UNP O66529
2X	52	CYS	ARG	conflict	UNP O66529
2X	83	GLU	ARG	conflict	UNP O66529
2X	86	GLU	THR	conflict	UNP O66529
2X	112	SER	THR	conflict	UNP O66529
2X	115	ASP	VAL	conflict	UNP O66529
2X	118	ASP	ALA	conflict	UNP O66529
2X	120	GLU	THR	conflict	UNP O66529
2X	123	GLU	GLN	conflict	UNP O66529
2X	127	CYS	ARG	conflict	UNP O66529
2X	131	GLU	LYS	conflict	UNP O66529
2X	155	LEU	-	expression tag	UNP O66529
2X	156	GLU	-	expression tag	UNP O66529
2X	157	HIS	-	expression tag	UNP O66529
2X	158	HIS	-	expression tag	UNP O66529
2X	159	HIS	-	expression tag	UNP O66529
2X	160	HIS	-	expression tag	UNP O66529
2X	161	HIS	-	expression tag	UNP O66529
3A	2	GLU	GLN	conflict	UNP O66529
3A	28	GLY	ASP	conflict	UNP O66529
3A	52	CYS	ARG	conflict	UNP O66529
3A	83	GLU	ARG	conflict	UNP O66529
3A	86	GLU	THR	conflict	UNP O66529
3A	112	SER	THR	conflict	UNP O66529
3A	115	ASP	VAL	conflict	UNP O66529
3A	118	ASP	ALA	conflict	UNP O66529
3A	120	GLU	THR	conflict	UNP O66529
3A	123	GLU	GLN	conflict	UNP O66529
3A	127	CYS	ARG	conflict	UNP O66529
3A	131	GLU	LYS	conflict	UNP O66529
3A	155	LEU	-	expression tag	UNP O66529
3A	156	GLU	-	expression tag	UNP O66529
3A	157	HIS	-	expression tag	UNP O66529
3A	158	HIS	-	expression tag	UNP O66529
3A	159	HIS	-	expression tag	UNP O66529
3A	160	HIS	-	expression tag	UNP O66529
3A	161	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
3B	2	GLU	GLN	conflict	UNP O66529
3B	28	GLY	ASP	conflict	UNP O66529
3B	52	CYS	ARG	conflict	UNP O66529
3B	83	GLU	ARG	conflict	UNP O66529
3B	86	GLU	THR	conflict	UNP O66529
3B	112	SER	THR	conflict	UNP O66529
3B	115	ASP	VAL	conflict	UNP O66529
3B	118	ASP	ALA	conflict	UNP O66529
3B	120	GLU	THR	conflict	UNP O66529
3B	123	GLU	GLN	conflict	UNP O66529
3B	127	CYS	ARG	conflict	UNP O66529
3B	131	GLU	LYS	conflict	UNP O66529
3B	155	LEU	-	expression tag	UNP O66529
3B	156	GLU	-	expression tag	UNP O66529
3B	157	HIS	-	expression tag	UNP O66529
3B	158	HIS	-	expression tag	UNP O66529
3B	159	HIS	-	expression tag	UNP O66529
3B	160	HIS	-	expression tag	UNP O66529
3B	161	HIS	-	expression tag	UNP O66529
3C	2	GLU	GLN	conflict	UNP O66529
3C	28	GLY	ASP	conflict	UNP O66529
3C	52	CYS	ARG	conflict	UNP O66529
3C	83	GLU	ARG	conflict	UNP O66529
3C	86	GLU	THR	conflict	UNP O66529
3C	112	SER	THR	conflict	UNP O66529
3C	115	ASP	VAL	conflict	UNP O66529
3C	118	ASP	ALA	conflict	UNP O66529
3C	120	GLU	THR	conflict	UNP O66529
3C	123	GLU	GLN	conflict	UNP O66529
3C	127	CYS	ARG	conflict	UNP O66529
3C	131	GLU	LYS	conflict	UNP O66529
3C	155	LEU	-	expression tag	UNP O66529
3C	156	GLU	-	expression tag	UNP O66529
3C	157	HIS	-	expression tag	UNP O66529
3C	158	HIS	-	expression tag	UNP O66529
3C	159	HIS	-	expression tag	UNP O66529
3C	160	HIS	-	expression tag	UNP O66529
3C	161	HIS	-	expression tag	UNP O66529
3D	2	GLU	GLN	conflict	UNP O66529
3D	28	GLY	ASP	conflict	UNP O66529
3D	52	CYS	ARG	conflict	UNP O66529
3D	83	GLU	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
3D	86	GLU	THR	conflict	UNP O66529
3D	112	SER	THR	conflict	UNP O66529
3D	115	ASP	VAL	conflict	UNP O66529
3D	118	ASP	ALA	conflict	UNP O66529
3D	120	GLU	THR	conflict	UNP O66529
3D	123	GLU	GLN	conflict	UNP O66529
3D	127	CYS	ARG	conflict	UNP O66529
3D	131	GLU	LYS	conflict	UNP O66529
3D	155	LEU	-	expression tag	UNP O66529
3D	156	GLU	-	expression tag	UNP O66529
3D	157	HIS	-	expression tag	UNP O66529
3D	158	HIS	-	expression tag	UNP O66529
3D	159	HIS	-	expression tag	UNP O66529
3D	160	HIS	-	expression tag	UNP O66529
3D	161	HIS	-	expression tag	UNP O66529
3E	2	GLU	GLN	conflict	UNP O66529
3E	28	GLY	ASP	conflict	UNP O66529
3E	52	CYS	ARG	conflict	UNP O66529
3E	83	GLU	ARG	conflict	UNP O66529
3E	86	GLU	THR	conflict	UNP O66529
3E	112	SER	THR	conflict	UNP O66529
3E	115	ASP	VAL	conflict	UNP O66529
3E	118	ASP	ALA	conflict	UNP O66529
3E	120	GLU	THR	conflict	UNP O66529
3E	123	GLU	GLN	conflict	UNP O66529
3E	127	CYS	ARG	conflict	UNP O66529
3E	131	GLU	LYS	conflict	UNP O66529
3E	155	LEU	-	expression tag	UNP O66529
3E	156	GLU	-	expression tag	UNP O66529
3E	157	HIS	-	expression tag	UNP O66529
3E	158	HIS	-	expression tag	UNP O66529
3E	159	HIS	-	expression tag	UNP O66529
3E	160	HIS	-	expression tag	UNP O66529
3E	161	HIS	-	expression tag	UNP O66529
3X	2	GLU	GLN	conflict	UNP O66529
3X	28	GLY	ASP	conflict	UNP O66529
3X	52	CYS	ARG	conflict	UNP O66529
3X	83	GLU	ARG	conflict	UNP O66529
3X	86	GLU	THR	conflict	UNP O66529
3X	112	SER	THR	conflict	UNP O66529
3X	115	ASP	VAL	conflict	UNP O66529
3X	118	ASP	ALA	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
3X	120	GLU	THR	conflict	UNP O66529
3X	123	GLU	GLN	conflict	UNP O66529
3X	127	CYS	ARG	conflict	UNP O66529
3X	131	GLU	LYS	conflict	UNP O66529
3X	155	LEU	-	expression tag	UNP O66529
3X	156	GLU	-	expression tag	UNP O66529
3X	157	HIS	-	expression tag	UNP O66529
3X	158	HIS	-	expression tag	UNP O66529
3X	159	HIS	-	expression tag	UNP O66529
3X	160	HIS	-	expression tag	UNP O66529
3X	161	HIS	-	expression tag	UNP O66529
4A	2	GLU	GLN	conflict	UNP O66529
4A	28	GLY	ASP	conflict	UNP O66529
4A	52	CYS	ARG	conflict	UNP O66529
4A	83	GLU	ARG	conflict	UNP O66529
4A	86	GLU	THR	conflict	UNP O66529
4A	112	SER	THR	conflict	UNP O66529
4A	115	ASP	VAL	conflict	UNP O66529
4A	118	ASP	ALA	conflict	UNP O66529
4A	120	GLU	THR	conflict	UNP O66529
4A	123	GLU	GLN	conflict	UNP O66529
4A	127	CYS	ARG	conflict	UNP O66529
4A	131	GLU	LYS	conflict	UNP O66529
4A	155	LEU	-	expression tag	UNP O66529
4A	156	GLU	-	expression tag	UNP O66529
4A	157	HIS	-	expression tag	UNP O66529
4A	158	HIS	-	expression tag	UNP O66529
4A	159	HIS	-	expression tag	UNP O66529
4A	160	HIS	-	expression tag	UNP O66529
4A	161	HIS	-	expression tag	UNP O66529
4B	2	GLU	GLN	conflict	UNP O66529
4B	28	GLY	ASP	conflict	UNP O66529
4B	52	CYS	ARG	conflict	UNP O66529
4B	83	GLU	ARG	conflict	UNP O66529
4B	86	GLU	THR	conflict	UNP O66529
4B	112	SER	THR	conflict	UNP O66529
4B	115	ASP	VAL	conflict	UNP O66529
4B	118	ASP	ALA	conflict	UNP O66529
4B	120	GLU	THR	conflict	UNP O66529
4B	123	GLU	GLN	conflict	UNP O66529
4B	127	CYS	ARG	conflict	UNP O66529
4B	131	GLU	LYS	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
4B	155	LEU	-	expression tag	UNP O66529
4B	156	GLU	-	expression tag	UNP O66529
4B	157	HIS	-	expression tag	UNP O66529
4B	158	HIS	-	expression tag	UNP O66529
4B	159	HIS	-	expression tag	UNP O66529
4B	160	HIS	-	expression tag	UNP O66529
4B	161	HIS	-	expression tag	UNP O66529
4C	2	GLU	GLN	conflict	UNP O66529
4C	28	GLY	ASP	conflict	UNP O66529
4C	52	CYS	ARG	conflict	UNP O66529
4C	83	GLU	ARG	conflict	UNP O66529
4C	86	GLU	THR	conflict	UNP O66529
4C	112	SER	THR	conflict	UNP O66529
4C	115	ASP	VAL	conflict	UNP O66529
4C	118	ASP	ALA	conflict	UNP O66529
4C	120	GLU	THR	conflict	UNP O66529
4C	123	GLU	GLN	conflict	UNP O66529
4C	127	CYS	ARG	conflict	UNP O66529
4C	131	GLU	LYS	conflict	UNP O66529
4C	155	LEU	-	expression tag	UNP O66529
4C	156	GLU	-	expression tag	UNP O66529
4C	157	HIS	-	expression tag	UNP O66529
4C	158	HIS	-	expression tag	UNP O66529
4C	159	HIS	-	expression tag	UNP O66529
4C	160	HIS	-	expression tag	UNP O66529
4C	161	HIS	-	expression tag	UNP O66529
4D	2	GLU	GLN	conflict	UNP O66529
4D	28	GLY	ASP	conflict	UNP O66529
4D	52	CYS	ARG	conflict	UNP O66529
4D	83	GLU	ARG	conflict	UNP O66529
4D	86	GLU	THR	conflict	UNP O66529
4D	112	SER	THR	conflict	UNP O66529
4D	115	ASP	VAL	conflict	UNP O66529
4D	118	ASP	ALA	conflict	UNP O66529
4D	120	GLU	THR	conflict	UNP O66529
4D	123	GLU	GLN	conflict	UNP O66529
4D	127	CYS	ARG	conflict	UNP O66529
4D	131	GLU	LYS	conflict	UNP O66529
4D	155	LEU	-	expression tag	UNP O66529
4D	156	GLU	-	expression tag	UNP O66529
4D	157	HIS	-	expression tag	UNP O66529
4D	158	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
4D	159	HIS	-	expression tag	UNP O66529
4D	160	HIS	-	expression tag	UNP O66529
4D	161	HIS	-	expression tag	UNP O66529
4E	2	GLU	GLN	conflict	UNP O66529
4E	28	GLY	ASP	conflict	UNP O66529
4E	52	CYS	ARG	conflict	UNP O66529
4E	83	GLU	ARG	conflict	UNP O66529
4E	86	GLU	THR	conflict	UNP O66529
4E	112	SER	THR	conflict	UNP O66529
4E	115	ASP	VAL	conflict	UNP O66529
4E	118	ASP	ALA	conflict	UNP O66529
4E	120	GLU	THR	conflict	UNP O66529
4E	123	GLU	GLN	conflict	UNP O66529
4E	127	CYS	ARG	conflict	UNP O66529
4E	131	GLU	LYS	conflict	UNP O66529
4E	155	LEU	-	expression tag	UNP O66529
4E	156	GLU	-	expression tag	UNP O66529
4E	157	HIS	-	expression tag	UNP O66529
4E	158	HIS	-	expression tag	UNP O66529
4E	159	HIS	-	expression tag	UNP O66529
4E	160	HIS	-	expression tag	UNP O66529
4E	161	HIS	-	expression tag	UNP O66529
4X	2	GLU	GLN	conflict	UNP O66529
4X	28	GLY	ASP	conflict	UNP O66529
4X	52	CYS	ARG	conflict	UNP O66529
4X	83	GLU	ARG	conflict	UNP O66529
4X	86	GLU	THR	conflict	UNP O66529
4X	112	SER	THR	conflict	UNP O66529
4X	115	ASP	VAL	conflict	UNP O66529
4X	118	ASP	ALA	conflict	UNP O66529
4X	120	GLU	THR	conflict	UNP O66529
4X	123	GLU	GLN	conflict	UNP O66529
4X	127	CYS	ARG	conflict	UNP O66529
4X	131	GLU	LYS	conflict	UNP O66529
4X	155	LEU	-	expression tag	UNP O66529
4X	156	GLU	-	expression tag	UNP O66529
4X	157	HIS	-	expression tag	UNP O66529
4X	158	HIS	-	expression tag	UNP O66529
4X	159	HIS	-	expression tag	UNP O66529
4X	160	HIS	-	expression tag	UNP O66529
4X	161	HIS	-	expression tag	UNP O66529
5A	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
5A	28	GLY	ASP	conflict	UNP O66529
5A	52	CYS	ARG	conflict	UNP O66529
5A	83	GLU	ARG	conflict	UNP O66529
5A	86	GLU	THR	conflict	UNP O66529
5A	112	SER	THR	conflict	UNP O66529
5A	115	ASP	VAL	conflict	UNP O66529
5A	118	ASP	ALA	conflict	UNP O66529
5A	120	GLU	THR	conflict	UNP O66529
5A	123	GLU	GLN	conflict	UNP O66529
5A	127	CYS	ARG	conflict	UNP O66529
5A	131	GLU	LYS	conflict	UNP O66529
5A	155	LEU	-	expression tag	UNP O66529
5A	156	GLU	-	expression tag	UNP O66529
5A	157	HIS	-	expression tag	UNP O66529
5A	158	HIS	-	expression tag	UNP O66529
5A	159	HIS	-	expression tag	UNP O66529
5A	160	HIS	-	expression tag	UNP O66529
5A	161	HIS	-	expression tag	UNP O66529
5B	2	GLU	GLN	conflict	UNP O66529
5B	28	GLY	ASP	conflict	UNP O66529
5B	52	CYS	ARG	conflict	UNP O66529
5B	83	GLU	ARG	conflict	UNP O66529
5B	86	GLU	THR	conflict	UNP O66529
5B	112	SER	THR	conflict	UNP O66529
5B	115	ASP	VAL	conflict	UNP O66529
5B	118	ASP	ALA	conflict	UNP O66529
5B	120	GLU	THR	conflict	UNP O66529
5B	123	GLU	GLN	conflict	UNP O66529
5B	127	CYS	ARG	conflict	UNP O66529
5B	131	GLU	LYS	conflict	UNP O66529
5B	155	LEU	-	expression tag	UNP O66529
5B	156	GLU	-	expression tag	UNP O66529
5B	157	HIS	-	expression tag	UNP O66529
5B	158	HIS	-	expression tag	UNP O66529
5B	159	HIS	-	expression tag	UNP O66529
5B	160	HIS	-	expression tag	UNP O66529
5B	161	HIS	-	expression tag	UNP O66529
5C	2	GLU	GLN	conflict	UNP O66529
5C	28	GLY	ASP	conflict	UNP O66529
5C	52	CYS	ARG	conflict	UNP O66529
5C	83	GLU	ARG	conflict	UNP O66529
5C	86	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
5C	112	SER	THR	conflict	UNP O66529
5C	115	ASP	VAL	conflict	UNP O66529
5C	118	ASP	ALA	conflict	UNP O66529
5C	120	GLU	THR	conflict	UNP O66529
5C	123	GLU	GLN	conflict	UNP O66529
5C	127	CYS	ARG	conflict	UNP O66529
5C	131	GLU	LYS	conflict	UNP O66529
5C	155	LEU	-	expression tag	UNP O66529
5C	156	GLU	-	expression tag	UNP O66529
5C	157	HIS	-	expression tag	UNP O66529
5C	158	HIS	-	expression tag	UNP O66529
5C	159	HIS	-	expression tag	UNP O66529
5C	160	HIS	-	expression tag	UNP O66529
5C	161	HIS	-	expression tag	UNP O66529
5D	2	GLU	GLN	conflict	UNP O66529
5D	28	GLY	ASP	conflict	UNP O66529
5D	52	CYS	ARG	conflict	UNP O66529
5D	83	GLU	ARG	conflict	UNP O66529
5D	86	GLU	THR	conflict	UNP O66529
5D	112	SER	THR	conflict	UNP O66529
5D	115	ASP	VAL	conflict	UNP O66529
5D	118	ASP	ALA	conflict	UNP O66529
5D	120	GLU	THR	conflict	UNP O66529
5D	123	GLU	GLN	conflict	UNP O66529
5D	127	CYS	ARG	conflict	UNP O66529
5D	131	GLU	LYS	conflict	UNP O66529
5D	155	LEU	-	expression tag	UNP O66529
5D	156	GLU	-	expression tag	UNP O66529
5D	157	HIS	-	expression tag	UNP O66529
5D	158	HIS	-	expression tag	UNP O66529
5D	159	HIS	-	expression tag	UNP O66529
5D	160	HIS	-	expression tag	UNP O66529
5D	161	HIS	-	expression tag	UNP O66529
5E	2	GLU	GLN	conflict	UNP O66529
5E	28	GLY	ASP	conflict	UNP O66529
5E	52	CYS	ARG	conflict	UNP O66529
5E	83	GLU	ARG	conflict	UNP O66529
5E	86	GLU	THR	conflict	UNP O66529
5E	112	SER	THR	conflict	UNP O66529
5E	115	ASP	VAL	conflict	UNP O66529
5E	118	ASP	ALA	conflict	UNP O66529
5E	120	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
5E	123	GLU	GLN	conflict	UNP O66529
5E	127	CYS	ARG	conflict	UNP O66529
5E	131	GLU	LYS	conflict	UNP O66529
5E	155	LEU	-	expression tag	UNP O66529
5E	156	GLU	-	expression tag	UNP O66529
5E	157	HIS	-	expression tag	UNP O66529
5E	158	HIS	-	expression tag	UNP O66529
5E	159	HIS	-	expression tag	UNP O66529
5E	160	HIS	-	expression tag	UNP O66529
5E	161	HIS	-	expression tag	UNP O66529
5X	2	GLU	GLN	conflict	UNP O66529
5X	28	GLY	ASP	conflict	UNP O66529
5X	52	CYS	ARG	conflict	UNP O66529
5X	83	GLU	ARG	conflict	UNP O66529
5X	86	GLU	THR	conflict	UNP O66529
5X	112	SER	THR	conflict	UNP O66529
5X	115	ASP	VAL	conflict	UNP O66529
5X	118	ASP	ALA	conflict	UNP O66529
5X	120	GLU	THR	conflict	UNP O66529
5X	123	GLU	GLN	conflict	UNP O66529
5X	127	CYS	ARG	conflict	UNP O66529
5X	131	GLU	LYS	conflict	UNP O66529
5X	155	LEU	-	expression tag	UNP O66529
5X	156	GLU	-	expression tag	UNP O66529
5X	157	HIS	-	expression tag	UNP O66529
5X	158	HIS	-	expression tag	UNP O66529
5X	159	HIS	-	expression tag	UNP O66529
5X	160	HIS	-	expression tag	UNP O66529
5X	161	HIS	-	expression tag	UNP O66529
6A	2	GLU	GLN	conflict	UNP O66529
6A	28	GLY	ASP	conflict	UNP O66529
6A	52	CYS	ARG	conflict	UNP O66529
6A	83	GLU	ARG	conflict	UNP O66529
6A	86	GLU	THR	conflict	UNP O66529
6A	112	SER	THR	conflict	UNP O66529
6A	115	ASP	VAL	conflict	UNP O66529
6A	118	ASP	ALA	conflict	UNP O66529
6A	120	GLU	THR	conflict	UNP O66529
6A	123	GLU	GLN	conflict	UNP O66529
6A	127	CYS	ARG	conflict	UNP O66529
6A	131	GLU	LYS	conflict	UNP O66529
6A	155	LEU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
6A	156	GLU	-	expression tag	UNP O66529
6A	157	HIS	-	expression tag	UNP O66529
6A	158	HIS	-	expression tag	UNP O66529
6A	159	HIS	-	expression tag	UNP O66529
6A	160	HIS	-	expression tag	UNP O66529
6A	161	HIS	-	expression tag	UNP O66529
6B	2	GLU	GLN	conflict	UNP O66529
6B	28	GLY	ASP	conflict	UNP O66529
6B	52	CYS	ARG	conflict	UNP O66529
6B	83	GLU	ARG	conflict	UNP O66529
6B	86	GLU	THR	conflict	UNP O66529
6B	112	SER	THR	conflict	UNP O66529
6B	115	ASP	VAL	conflict	UNP O66529
6B	118	ASP	ALA	conflict	UNP O66529
6B	120	GLU	THR	conflict	UNP O66529
6B	123	GLU	GLN	conflict	UNP O66529
6B	127	CYS	ARG	conflict	UNP O66529
6B	131	GLU	LYS	conflict	UNP O66529
6B	155	LEU	-	expression tag	UNP O66529
6B	156	GLU	-	expression tag	UNP O66529
6B	157	HIS	-	expression tag	UNP O66529
6B	158	HIS	-	expression tag	UNP O66529
6B	159	HIS	-	expression tag	UNP O66529
6B	160	HIS	-	expression tag	UNP O66529
6B	161	HIS	-	expression tag	UNP O66529
6C	2	GLU	GLN	conflict	UNP O66529
6C	28	GLY	ASP	conflict	UNP O66529
6C	52	CYS	ARG	conflict	UNP O66529
6C	83	GLU	ARG	conflict	UNP O66529
6C	86	GLU	THR	conflict	UNP O66529
6C	112	SER	THR	conflict	UNP O66529
6C	115	ASP	VAL	conflict	UNP O66529
6C	118	ASP	ALA	conflict	UNP O66529
6C	120	GLU	THR	conflict	UNP O66529
6C	123	GLU	GLN	conflict	UNP O66529
6C	127	CYS	ARG	conflict	UNP O66529
6C	131	GLU	LYS	conflict	UNP O66529
6C	155	LEU	-	expression tag	UNP O66529
6C	156	GLU	-	expression tag	UNP O66529
6C	157	HIS	-	expression tag	UNP O66529
6C	158	HIS	-	expression tag	UNP O66529
6C	159	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
6C	160	HIS	-	expression tag	UNP O66529
6C	161	HIS	-	expression tag	UNP O66529
6D	2	GLU	GLN	conflict	UNP O66529
6D	28	GLY	ASP	conflict	UNP O66529
6D	52	CYS	ARG	conflict	UNP O66529
6D	83	GLU	ARG	conflict	UNP O66529
6D	86	GLU	THR	conflict	UNP O66529
6D	112	SER	THR	conflict	UNP O66529
6D	115	ASP	VAL	conflict	UNP O66529
6D	118	ASP	ALA	conflict	UNP O66529
6D	120	GLU	THR	conflict	UNP O66529
6D	123	GLU	GLN	conflict	UNP O66529
6D	127	CYS	ARG	conflict	UNP O66529
6D	131	GLU	LYS	conflict	UNP O66529
6D	155	LEU	-	expression tag	UNP O66529
6D	156	GLU	-	expression tag	UNP O66529
6D	157	HIS	-	expression tag	UNP O66529
6D	158	HIS	-	expression tag	UNP O66529
6D	159	HIS	-	expression tag	UNP O66529
6D	160	HIS	-	expression tag	UNP O66529
6D	161	HIS	-	expression tag	UNP O66529
6E	2	GLU	GLN	conflict	UNP O66529
6E	28	GLY	ASP	conflict	UNP O66529
6E	52	CYS	ARG	conflict	UNP O66529
6E	83	GLU	ARG	conflict	UNP O66529
6E	86	GLU	THR	conflict	UNP O66529
6E	112	SER	THR	conflict	UNP O66529
6E	115	ASP	VAL	conflict	UNP O66529
6E	118	ASP	ALA	conflict	UNP O66529
6E	120	GLU	THR	conflict	UNP O66529
6E	123	GLU	GLN	conflict	UNP O66529
6E	127	CYS	ARG	conflict	UNP O66529
6E	131	GLU	LYS	conflict	UNP O66529
6E	155	LEU	-	expression tag	UNP O66529
6E	156	GLU	-	expression tag	UNP O66529
6E	157	HIS	-	expression tag	UNP O66529
6E	158	HIS	-	expression tag	UNP O66529
6E	159	HIS	-	expression tag	UNP O66529
6E	160	HIS	-	expression tag	UNP O66529
6E	161	HIS	-	expression tag	UNP O66529
6X	2	GLU	GLN	conflict	UNP O66529
6X	28	GLY	ASP	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
6X	52	CYS	ARG	conflict	UNP O66529
6X	83	GLU	ARG	conflict	UNP O66529
6X	86	GLU	THR	conflict	UNP O66529
6X	112	SER	THR	conflict	UNP O66529
6X	115	ASP	VAL	conflict	UNP O66529
6X	118	ASP	ALA	conflict	UNP O66529
6X	120	GLU	THR	conflict	UNP O66529
6X	123	GLU	GLN	conflict	UNP O66529
6X	127	CYS	ARG	conflict	UNP O66529
6X	131	GLU	LYS	conflict	UNP O66529
6X	155	LEU	-	expression tag	UNP O66529
6X	156	GLU	-	expression tag	UNP O66529
6X	157	HIS	-	expression tag	UNP O66529
6X	158	HIS	-	expression tag	UNP O66529
6X	159	HIS	-	expression tag	UNP O66529
6X	160	HIS	-	expression tag	UNP O66529
6X	161	HIS	-	expression tag	UNP O66529
7A	2	GLU	GLN	conflict	UNP O66529
7A	28	GLY	ASP	conflict	UNP O66529
7A	52	CYS	ARG	conflict	UNP O66529
7A	83	GLU	ARG	conflict	UNP O66529
7A	86	GLU	THR	conflict	UNP O66529
7A	112	SER	THR	conflict	UNP O66529
7A	115	ASP	VAL	conflict	UNP O66529
7A	118	ASP	ALA	conflict	UNP O66529
7A	120	GLU	THR	conflict	UNP O66529
7A	123	GLU	GLN	conflict	UNP O66529
7A	127	CYS	ARG	conflict	UNP O66529
7A	131	GLU	LYS	conflict	UNP O66529
7A	155	LEU	-	expression tag	UNP O66529
7A	156	GLU	-	expression tag	UNP O66529
7A	157	HIS	-	expression tag	UNP O66529
7A	158	HIS	-	expression tag	UNP O66529
7A	159	HIS	-	expression tag	UNP O66529
7A	160	HIS	-	expression tag	UNP O66529
7A	161	HIS	-	expression tag	UNP O66529
7B	2	GLU	GLN	conflict	UNP O66529
7B	28	GLY	ASP	conflict	UNP O66529
7B	52	CYS	ARG	conflict	UNP O66529
7B	83	GLU	ARG	conflict	UNP O66529
7B	86	GLU	THR	conflict	UNP O66529
7B	112	SER	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
7B	115	ASP	VAL	conflict	UNP O66529
7B	118	ASP	ALA	conflict	UNP O66529
7B	120	GLU	THR	conflict	UNP O66529
7B	123	GLU	GLN	conflict	UNP O66529
7B	127	CYS	ARG	conflict	UNP O66529
7B	131	GLU	LYS	conflict	UNP O66529
7B	155	LEU	-	expression tag	UNP O66529
7B	156	GLU	-	expression tag	UNP O66529
7B	157	HIS	-	expression tag	UNP O66529
7B	158	HIS	-	expression tag	UNP O66529
7B	159	HIS	-	expression tag	UNP O66529
7B	160	HIS	-	expression tag	UNP O66529
7B	161	HIS	-	expression tag	UNP O66529
7C	2	GLU	GLN	conflict	UNP O66529
7C	28	GLY	ASP	conflict	UNP O66529
7C	52	CYS	ARG	conflict	UNP O66529
7C	83	GLU	ARG	conflict	UNP O66529
7C	86	GLU	THR	conflict	UNP O66529
7C	112	SER	THR	conflict	UNP O66529
7C	115	ASP	VAL	conflict	UNP O66529
7C	118	ASP	ALA	conflict	UNP O66529
7C	120	GLU	THR	conflict	UNP O66529
7C	123	GLU	GLN	conflict	UNP O66529
7C	127	CYS	ARG	conflict	UNP O66529
7C	131	GLU	LYS	conflict	UNP O66529
7C	155	LEU	-	expression tag	UNP O66529
7C	156	GLU	-	expression tag	UNP O66529
7C	157	HIS	-	expression tag	UNP O66529
7C	158	HIS	-	expression tag	UNP O66529
7C	159	HIS	-	expression tag	UNP O66529
7C	160	HIS	-	expression tag	UNP O66529
7C	161	HIS	-	expression tag	UNP O66529
7D	2	GLU	GLN	conflict	UNP O66529
7D	28	GLY	ASP	conflict	UNP O66529
7D	52	CYS	ARG	conflict	UNP O66529
7D	83	GLU	ARG	conflict	UNP O66529
7D	86	GLU	THR	conflict	UNP O66529
7D	112	SER	THR	conflict	UNP O66529
7D	115	ASP	VAL	conflict	UNP O66529
7D	118	ASP	ALA	conflict	UNP O66529
7D	120	GLU	THR	conflict	UNP O66529
7D	123	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
7D	127	CYS	ARG	conflict	UNP O66529
7D	131	GLU	LYS	conflict	UNP O66529
7D	155	LEU	-	expression tag	UNP O66529
7D	156	GLU	-	expression tag	UNP O66529
7D	157	HIS	-	expression tag	UNP O66529
7D	158	HIS	-	expression tag	UNP O66529
7D	159	HIS	-	expression tag	UNP O66529
7D	160	HIS	-	expression tag	UNP O66529
7D	161	HIS	-	expression tag	UNP O66529
7E	2	GLU	GLN	conflict	UNP O66529
7E	28	GLY	ASP	conflict	UNP O66529
7E	52	CYS	ARG	conflict	UNP O66529
7E	83	GLU	ARG	conflict	UNP O66529
7E	86	GLU	THR	conflict	UNP O66529
7E	112	SER	THR	conflict	UNP O66529
7E	115	ASP	VAL	conflict	UNP O66529
7E	118	ASP	ALA	conflict	UNP O66529
7E	120	GLU	THR	conflict	UNP O66529
7E	123	GLU	GLN	conflict	UNP O66529
7E	127	CYS	ARG	conflict	UNP O66529
7E	131	GLU	LYS	conflict	UNP O66529
7E	155	LEU	-	expression tag	UNP O66529
7E	156	GLU	-	expression tag	UNP O66529
7E	157	HIS	-	expression tag	UNP O66529
7E	158	HIS	-	expression tag	UNP O66529
7E	159	HIS	-	expression tag	UNP O66529
7E	160	HIS	-	expression tag	UNP O66529
7E	161	HIS	-	expression tag	UNP O66529
7X	2	GLU	GLN	conflict	UNP O66529
7X	28	GLY	ASP	conflict	UNP O66529
7X	52	CYS	ARG	conflict	UNP O66529
7X	83	GLU	ARG	conflict	UNP O66529
7X	86	GLU	THR	conflict	UNP O66529
7X	112	SER	THR	conflict	UNP O66529
7X	115	ASP	VAL	conflict	UNP O66529
7X	118	ASP	ALA	conflict	UNP O66529
7X	120	GLU	THR	conflict	UNP O66529
7X	123	GLU	GLN	conflict	UNP O66529
7X	127	CYS	ARG	conflict	UNP O66529
7X	131	GLU	LYS	conflict	UNP O66529
7X	155	LEU	-	expression tag	UNP O66529
7X	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
7X	157	HIS	-	expression tag	UNP O66529
7X	158	HIS	-	expression tag	UNP O66529
7X	159	HIS	-	expression tag	UNP O66529
7X	160	HIS	-	expression tag	UNP O66529
7X	161	HIS	-	expression tag	UNP O66529
8A	2	GLU	GLN	conflict	UNP O66529
8A	28	GLY	ASP	conflict	UNP O66529
8A	52	CYS	ARG	conflict	UNP O66529
8A	83	GLU	ARG	conflict	UNP O66529
8A	86	GLU	THR	conflict	UNP O66529
8A	112	SER	THR	conflict	UNP O66529
8A	115	ASP	VAL	conflict	UNP O66529
8A	118	ASP	ALA	conflict	UNP O66529
8A	120	GLU	THR	conflict	UNP O66529
8A	123	GLU	GLN	conflict	UNP O66529
8A	127	CYS	ARG	conflict	UNP O66529
8A	131	GLU	LYS	conflict	UNP O66529
8A	155	LEU	-	expression tag	UNP O66529
8A	156	GLU	-	expression tag	UNP O66529
8A	157	HIS	-	expression tag	UNP O66529
8A	158	HIS	-	expression tag	UNP O66529
8A	159	HIS	-	expression tag	UNP O66529
8A	160	HIS	-	expression tag	UNP O66529
8A	161	HIS	-	expression tag	UNP O66529
8B	2	GLU	GLN	conflict	UNP O66529
8B	28	GLY	ASP	conflict	UNP O66529
8B	52	CYS	ARG	conflict	UNP O66529
8B	83	GLU	ARG	conflict	UNP O66529
8B	86	GLU	THR	conflict	UNP O66529
8B	112	SER	THR	conflict	UNP O66529
8B	115	ASP	VAL	conflict	UNP O66529
8B	118	ASP	ALA	conflict	UNP O66529
8B	120	GLU	THR	conflict	UNP O66529
8B	123	GLU	GLN	conflict	UNP O66529
8B	127	CYS	ARG	conflict	UNP O66529
8B	131	GLU	LYS	conflict	UNP O66529
8B	155	LEU	-	expression tag	UNP O66529
8B	156	GLU	-	expression tag	UNP O66529
8B	157	HIS	-	expression tag	UNP O66529
8B	158	HIS	-	expression tag	UNP O66529
8B	159	HIS	-	expression tag	UNP O66529
8B	160	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
8B	161	HIS	-	expression tag	UNP O66529
8C	2	GLU	GLN	conflict	UNP O66529
8C	28	GLY	ASP	conflict	UNP O66529
8C	52	CYS	ARG	conflict	UNP O66529
8C	83	GLU	ARG	conflict	UNP O66529
8C	86	GLU	THR	conflict	UNP O66529
8C	112	SER	THR	conflict	UNP O66529
8C	115	ASP	VAL	conflict	UNP O66529
8C	118	ASP	ALA	conflict	UNP O66529
8C	120	GLU	THR	conflict	UNP O66529
8C	123	GLU	GLN	conflict	UNP O66529
8C	127	CYS	ARG	conflict	UNP O66529
8C	131	GLU	LYS	conflict	UNP O66529
8C	155	LEU	-	expression tag	UNP O66529
8C	156	GLU	-	expression tag	UNP O66529
8C	157	HIS	-	expression tag	UNP O66529
8C	158	HIS	-	expression tag	UNP O66529
8C	159	HIS	-	expression tag	UNP O66529
8C	160	HIS	-	expression tag	UNP O66529
8C	161	HIS	-	expression tag	UNP O66529
8D	2	GLU	GLN	conflict	UNP O66529
8D	28	GLY	ASP	conflict	UNP O66529
8D	52	CYS	ARG	conflict	UNP O66529
8D	83	GLU	ARG	conflict	UNP O66529
8D	86	GLU	THR	conflict	UNP O66529
8D	112	SER	THR	conflict	UNP O66529
8D	115	ASP	VAL	conflict	UNP O66529
8D	118	ASP	ALA	conflict	UNP O66529
8D	120	GLU	THR	conflict	UNP O66529
8D	123	GLU	GLN	conflict	UNP O66529
8D	127	CYS	ARG	conflict	UNP O66529
8D	131	GLU	LYS	conflict	UNP O66529
8D	155	LEU	-	expression tag	UNP O66529
8D	156	GLU	-	expression tag	UNP O66529
8D	157	HIS	-	expression tag	UNP O66529
8D	158	HIS	-	expression tag	UNP O66529
8D	159	HIS	-	expression tag	UNP O66529
8D	160	HIS	-	expression tag	UNP O66529
8D	161	HIS	-	expression tag	UNP O66529
8E	2	GLU	GLN	conflict	UNP O66529
8E	28	GLY	ASP	conflict	UNP O66529
8E	52	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
8E	83	GLU	ARG	conflict	UNP O66529
8E	86	GLU	THR	conflict	UNP O66529
8E	112	SER	THR	conflict	UNP O66529
8E	115	ASP	VAL	conflict	UNP O66529
8E	118	ASP	ALA	conflict	UNP O66529
8E	120	GLU	THR	conflict	UNP O66529
8E	123	GLU	GLN	conflict	UNP O66529
8E	127	CYS	ARG	conflict	UNP O66529
8E	131	GLU	LYS	conflict	UNP O66529
8E	155	LEU	-	expression tag	UNP O66529
8E	156	GLU	-	expression tag	UNP O66529
8E	157	HIS	-	expression tag	UNP O66529
8E	158	HIS	-	expression tag	UNP O66529
8E	159	HIS	-	expression tag	UNP O66529
8E	160	HIS	-	expression tag	UNP O66529
8E	161	HIS	-	expression tag	UNP O66529
8X	2	GLU	GLN	conflict	UNP O66529
8X	28	GLY	ASP	conflict	UNP O66529
8X	52	CYS	ARG	conflict	UNP O66529
8X	83	GLU	ARG	conflict	UNP O66529
8X	86	GLU	THR	conflict	UNP O66529
8X	112	SER	THR	conflict	UNP O66529
8X	115	ASP	VAL	conflict	UNP O66529
8X	118	ASP	ALA	conflict	UNP O66529
8X	120	GLU	THR	conflict	UNP O66529
8X	123	GLU	GLN	conflict	UNP O66529
8X	127	CYS	ARG	conflict	UNP O66529
8X	131	GLU	LYS	conflict	UNP O66529
8X	155	LEU	-	expression tag	UNP O66529
8X	156	GLU	-	expression tag	UNP O66529
8X	157	HIS	-	expression tag	UNP O66529
8X	158	HIS	-	expression tag	UNP O66529
8X	159	HIS	-	expression tag	UNP O66529
8X	160	HIS	-	expression tag	UNP O66529
8X	161	HIS	-	expression tag	UNP O66529
9A	2	GLU	GLN	conflict	UNP O66529
9A	28	GLY	ASP	conflict	UNP O66529
9A	52	CYS	ARG	conflict	UNP O66529
9A	83	GLU	ARG	conflict	UNP O66529
9A	86	GLU	THR	conflict	UNP O66529
9A	112	SER	THR	conflict	UNP O66529
9A	115	ASP	VAL	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
9A	118	ASP	ALA	conflict	UNP O66529
9A	120	GLU	THR	conflict	UNP O66529
9A	123	GLU	GLN	conflict	UNP O66529
9A	127	CYS	ARG	conflict	UNP O66529
9A	131	GLU	LYS	conflict	UNP O66529
9A	155	LEU	-	expression tag	UNP O66529
9A	156	GLU	-	expression tag	UNP O66529
9A	157	HIS	-	expression tag	UNP O66529
9A	158	HIS	-	expression tag	UNP O66529
9A	159	HIS	-	expression tag	UNP O66529
9A	160	HIS	-	expression tag	UNP O66529
9A	161	HIS	-	expression tag	UNP O66529
9B	2	GLU	GLN	conflict	UNP O66529
9B	28	GLY	ASP	conflict	UNP O66529
9B	52	CYS	ARG	conflict	UNP O66529
9B	83	GLU	ARG	conflict	UNP O66529
9B	86	GLU	THR	conflict	UNP O66529
9B	112	SER	THR	conflict	UNP O66529
9B	115	ASP	VAL	conflict	UNP O66529
9B	118	ASP	ALA	conflict	UNP O66529
9B	120	GLU	THR	conflict	UNP O66529
9B	123	GLU	GLN	conflict	UNP O66529
9B	127	CYS	ARG	conflict	UNP O66529
9B	131	GLU	LYS	conflict	UNP O66529
9B	155	LEU	-	expression tag	UNP O66529
9B	156	GLU	-	expression tag	UNP O66529
9B	157	HIS	-	expression tag	UNP O66529
9B	158	HIS	-	expression tag	UNP O66529
9B	159	HIS	-	expression tag	UNP O66529
9B	160	HIS	-	expression tag	UNP O66529
9B	161	HIS	-	expression tag	UNP O66529
9C	2	GLU	GLN	conflict	UNP O66529
9C	28	GLY	ASP	conflict	UNP O66529
9C	52	CYS	ARG	conflict	UNP O66529
9C	83	GLU	ARG	conflict	UNP O66529
9C	86	GLU	THR	conflict	UNP O66529
9C	112	SER	THR	conflict	UNP O66529
9C	115	ASP	VAL	conflict	UNP O66529
9C	118	ASP	ALA	conflict	UNP O66529
9C	120	GLU	THR	conflict	UNP O66529
9C	123	GLU	GLN	conflict	UNP O66529
9C	127	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
9C	131	GLU	LYS	conflict	UNP O66529
9C	155	LEU	-	expression tag	UNP O66529
9C	156	GLU	-	expression tag	UNP O66529
9C	157	HIS	-	expression tag	UNP O66529
9C	158	HIS	-	expression tag	UNP O66529
9C	159	HIS	-	expression tag	UNP O66529
9C	160	HIS	-	expression tag	UNP O66529
9C	161	HIS	-	expression tag	UNP O66529
9D	2	GLU	GLN	conflict	UNP O66529
9D	28	GLY	ASP	conflict	UNP O66529
9D	52	CYS	ARG	conflict	UNP O66529
9D	83	GLU	ARG	conflict	UNP O66529
9D	86	GLU	THR	conflict	UNP O66529
9D	112	SER	THR	conflict	UNP O66529
9D	115	ASP	VAL	conflict	UNP O66529
9D	118	ASP	ALA	conflict	UNP O66529
9D	120	GLU	THR	conflict	UNP O66529
9D	123	GLU	GLN	conflict	UNP O66529
9D	127	CYS	ARG	conflict	UNP O66529
9D	131	GLU	LYS	conflict	UNP O66529
9D	155	LEU	-	expression tag	UNP O66529
9D	156	GLU	-	expression tag	UNP O66529
9D	157	HIS	-	expression tag	UNP O66529
9D	158	HIS	-	expression tag	UNP O66529
9D	159	HIS	-	expression tag	UNP O66529
9D	160	HIS	-	expression tag	UNP O66529
9D	161	HIS	-	expression tag	UNP O66529
9E	2	GLU	GLN	conflict	UNP O66529
9E	28	GLY	ASP	conflict	UNP O66529
9E	52	CYS	ARG	conflict	UNP O66529
9E	83	GLU	ARG	conflict	UNP O66529
9E	86	GLU	THR	conflict	UNP O66529
9E	112	SER	THR	conflict	UNP O66529
9E	115	ASP	VAL	conflict	UNP O66529
9E	118	ASP	ALA	conflict	UNP O66529
9E	120	GLU	THR	conflict	UNP O66529
9E	123	GLU	GLN	conflict	UNP O66529
9E	127	CYS	ARG	conflict	UNP O66529
9E	131	GLU	LYS	conflict	UNP O66529
9E	155	LEU	-	expression tag	UNP O66529
9E	156	GLU	-	expression tag	UNP O66529
9E	157	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
9E	158	HIS	-	expression tag	UNP O66529
9E	159	HIS	-	expression tag	UNP O66529
9E	160	HIS	-	expression tag	UNP O66529
9E	161	HIS	-	expression tag	UNP O66529
9X	2	GLU	GLN	conflict	UNP O66529
9X	28	GLY	ASP	conflict	UNP O66529
9X	52	CYS	ARG	conflict	UNP O66529
9X	83	GLU	ARG	conflict	UNP O66529
9X	86	GLU	THR	conflict	UNP O66529
9X	112	SER	THR	conflict	UNP O66529
9X	115	ASP	VAL	conflict	UNP O66529
9X	118	ASP	ALA	conflict	UNP O66529
9X	120	GLU	THR	conflict	UNP O66529
9X	123	GLU	GLN	conflict	UNP O66529
9X	127	CYS	ARG	conflict	UNP O66529
9X	131	GLU	LYS	conflict	UNP O66529
9X	155	LEU	-	expression tag	UNP O66529
9X	156	GLU	-	expression tag	UNP O66529
9X	157	HIS	-	expression tag	UNP O66529
9X	158	HIS	-	expression tag	UNP O66529
9X	159	HIS	-	expression tag	UNP O66529
9X	160	HIS	-	expression tag	UNP O66529
9X	161	HIS	-	expression tag	UNP O66529
AA	2	GLU	GLN	conflict	UNP O66529
AA	28	GLY	ASP	conflict	UNP O66529
AA	52	CYS	ARG	conflict	UNP O66529
AA	83	GLU	ARG	conflict	UNP O66529
AA	86	GLU	THR	conflict	UNP O66529
AA	112	SER	THR	conflict	UNP O66529
AA	115	ASP	VAL	conflict	UNP O66529
AA	118	ASP	ALA	conflict	UNP O66529
AA	120	GLU	THR	conflict	UNP O66529
AA	123	GLU	GLN	conflict	UNP O66529
AA	127	CYS	ARG	conflict	UNP O66529
AA	131	GLU	LYS	conflict	UNP O66529
AA	155	LEU	-	expression tag	UNP O66529
AA	156	GLU	-	expression tag	UNP O66529
AA	157	HIS	-	expression tag	UNP O66529
AA	158	HIS	-	expression tag	UNP O66529
AA	159	HIS	-	expression tag	UNP O66529
AA	160	HIS	-	expression tag	UNP O66529
AA	161	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AB	2	GLU	GLN	conflict	UNP O66529
AB	28	GLY	ASP	conflict	UNP O66529
AB	52	CYS	ARG	conflict	UNP O66529
AB	83	GLU	ARG	conflict	UNP O66529
AB	86	GLU	THR	conflict	UNP O66529
AB	112	SER	THR	conflict	UNP O66529
AB	115	ASP	VAL	conflict	UNP O66529
AB	118	ASP	ALA	conflict	UNP O66529
AB	120	GLU	THR	conflict	UNP O66529
AB	123	GLU	GLN	conflict	UNP O66529
AB	127	CYS	ARG	conflict	UNP O66529
AB	131	GLU	LYS	conflict	UNP O66529
AB	155	LEU	-	expression tag	UNP O66529
AB	156	GLU	-	expression tag	UNP O66529
AB	157	HIS	-	expression tag	UNP O66529
AB	158	HIS	-	expression tag	UNP O66529
AB	159	HIS	-	expression tag	UNP O66529
AB	160	HIS	-	expression tag	UNP O66529
AB	161	HIS	-	expression tag	UNP O66529
AC	2	GLU	GLN	conflict	UNP O66529
AC	28	GLY	ASP	conflict	UNP O66529
AC	52	CYS	ARG	conflict	UNP O66529
AC	83	GLU	ARG	conflict	UNP O66529
AC	86	GLU	THR	conflict	UNP O66529
AC	112	SER	THR	conflict	UNP O66529
AC	115	ASP	VAL	conflict	UNP O66529
AC	118	ASP	ALA	conflict	UNP O66529
AC	120	GLU	THR	conflict	UNP O66529
AC	123	GLU	GLN	conflict	UNP O66529
AC	127	CYS	ARG	conflict	UNP O66529
AC	131	GLU	LYS	conflict	UNP O66529
AC	155	LEU	-	expression tag	UNP O66529
AC	156	GLU	-	expression tag	UNP O66529
AC	157	HIS	-	expression tag	UNP O66529
AC	158	HIS	-	expression tag	UNP O66529
AC	159	HIS	-	expression tag	UNP O66529
AC	160	HIS	-	expression tag	UNP O66529
AC	161	HIS	-	expression tag	UNP O66529
AD	2	GLU	GLN	conflict	UNP O66529
AD	28	GLY	ASP	conflict	UNP O66529
AD	52	CYS	ARG	conflict	UNP O66529
AD	83	GLU	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AD	86	GLU	THR	conflict	UNP O66529
AD	112	SER	THR	conflict	UNP O66529
AD	115	ASP	VAL	conflict	UNP O66529
AD	118	ASP	ALA	conflict	UNP O66529
AD	120	GLU	THR	conflict	UNP O66529
AD	123	GLU	GLN	conflict	UNP O66529
AD	127	CYS	ARG	conflict	UNP O66529
AD	131	GLU	LYS	conflict	UNP O66529
AD	155	LEU	-	expression tag	UNP O66529
AD	156	GLU	-	expression tag	UNP O66529
AD	157	HIS	-	expression tag	UNP O66529
AD	158	HIS	-	expression tag	UNP O66529
AD	159	HIS	-	expression tag	UNP O66529
AD	160	HIS	-	expression tag	UNP O66529
AD	161	HIS	-	expression tag	UNP O66529
AE	2	GLU	GLN	conflict	UNP O66529
AE	28	GLY	ASP	conflict	UNP O66529
AE	52	CYS	ARG	conflict	UNP O66529
AE	83	GLU	ARG	conflict	UNP O66529
AE	86	GLU	THR	conflict	UNP O66529
AE	112	SER	THR	conflict	UNP O66529
AE	115	ASP	VAL	conflict	UNP O66529
AE	118	ASP	ALA	conflict	UNP O66529
AE	120	GLU	THR	conflict	UNP O66529
AE	123	GLU	GLN	conflict	UNP O66529
AE	127	CYS	ARG	conflict	UNP O66529
AE	131	GLU	LYS	conflict	UNP O66529
AE	155	LEU	-	expression tag	UNP O66529
AE	156	GLU	-	expression tag	UNP O66529
AE	157	HIS	-	expression tag	UNP O66529
AE	158	HIS	-	expression tag	UNP O66529
AE	159	HIS	-	expression tag	UNP O66529
AE	160	HIS	-	expression tag	UNP O66529
AE	161	HIS	-	expression tag	UNP O66529
AX	2	GLU	GLN	conflict	UNP O66529
AX	28	GLY	ASP	conflict	UNP O66529
AX	52	CYS	ARG	conflict	UNP O66529
AX	83	GLU	ARG	conflict	UNP O66529
AX	86	GLU	THR	conflict	UNP O66529
AX	112	SER	THR	conflict	UNP O66529
AX	115	ASP	VAL	conflict	UNP O66529
AX	118	ASP	ALA	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AX	120	GLU	THR	conflict	UNP O66529
AX	123	GLU	GLN	conflict	UNP O66529
AX	127	CYS	ARG	conflict	UNP O66529
AX	131	GLU	LYS	conflict	UNP O66529
AX	155	LEU	-	expression tag	UNP O66529
AX	156	GLU	-	expression tag	UNP O66529
AX	157	HIS	-	expression tag	UNP O66529
AX	158	HIS	-	expression tag	UNP O66529
AX	159	HIS	-	expression tag	UNP O66529
AX	160	HIS	-	expression tag	UNP O66529
AX	161	HIS	-	expression tag	UNP O66529
BA	2	GLU	GLN	conflict	UNP O66529
BA	28	GLY	ASP	conflict	UNP O66529
BA	52	CYS	ARG	conflict	UNP O66529
BA	83	GLU	ARG	conflict	UNP O66529
BA	86	GLU	THR	conflict	UNP O66529
BA	112	SER	THR	conflict	UNP O66529
BA	115	ASP	VAL	conflict	UNP O66529
BA	118	ASP	ALA	conflict	UNP O66529
BA	120	GLU	THR	conflict	UNP O66529
BA	123	GLU	GLN	conflict	UNP O66529
BA	127	CYS	ARG	conflict	UNP O66529
BA	131	GLU	LYS	conflict	UNP O66529
BA	155	LEU	-	expression tag	UNP O66529
BA	156	GLU	-	expression tag	UNP O66529
BA	157	HIS	-	expression tag	UNP O66529
BA	158	HIS	-	expression tag	UNP O66529
BA	159	HIS	-	expression tag	UNP O66529
BA	160	HIS	-	expression tag	UNP O66529
BA	161	HIS	-	expression tag	UNP O66529
BB	2	GLU	GLN	conflict	UNP O66529
BB	28	GLY	ASP	conflict	UNP O66529
BB	52	CYS	ARG	conflict	UNP O66529
BB	83	GLU	ARG	conflict	UNP O66529
BB	86	GLU	THR	conflict	UNP O66529
BB	112	SER	THR	conflict	UNP O66529
BB	115	ASP	VAL	conflict	UNP O66529
BB	118	ASP	ALA	conflict	UNP O66529
BB	120	GLU	THR	conflict	UNP O66529
BB	123	GLU	GLN	conflict	UNP O66529
BB	127	CYS	ARG	conflict	UNP O66529
BB	131	GLU	LYS	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BB	155	LEU	-	expression tag	UNP O66529
BB	156	GLU	-	expression tag	UNP O66529
BB	157	HIS	-	expression tag	UNP O66529
BB	158	HIS	-	expression tag	UNP O66529
BB	159	HIS	-	expression tag	UNP O66529
BB	160	HIS	-	expression tag	UNP O66529
BB	161	HIS	-	expression tag	UNP O66529
BC	2	GLU	GLN	conflict	UNP O66529
BC	28	GLY	ASP	conflict	UNP O66529
BC	52	CYS	ARG	conflict	UNP O66529
BC	83	GLU	ARG	conflict	UNP O66529
BC	86	GLU	THR	conflict	UNP O66529
BC	112	SER	THR	conflict	UNP O66529
BC	115	ASP	VAL	conflict	UNP O66529
BC	118	ASP	ALA	conflict	UNP O66529
BC	120	GLU	THR	conflict	UNP O66529
BC	123	GLU	GLN	conflict	UNP O66529
BC	127	CYS	ARG	conflict	UNP O66529
BC	131	GLU	LYS	conflict	UNP O66529
BC	155	LEU	-	expression tag	UNP O66529
BC	156	GLU	-	expression tag	UNP O66529
BC	157	HIS	-	expression tag	UNP O66529
BC	158	HIS	-	expression tag	UNP O66529
BC	159	HIS	-	expression tag	UNP O66529
BC	160	HIS	-	expression tag	UNP O66529
BC	161	HIS	-	expression tag	UNP O66529
BD	2	GLU	GLN	conflict	UNP O66529
BD	28	GLY	ASP	conflict	UNP O66529
BD	52	CYS	ARG	conflict	UNP O66529
BD	83	GLU	ARG	conflict	UNP O66529
BD	86	GLU	THR	conflict	UNP O66529
BD	112	SER	THR	conflict	UNP O66529
BD	115	ASP	VAL	conflict	UNP O66529
BD	118	ASP	ALA	conflict	UNP O66529
BD	120	GLU	THR	conflict	UNP O66529
BD	123	GLU	GLN	conflict	UNP O66529
BD	127	CYS	ARG	conflict	UNP O66529
BD	131	GLU	LYS	conflict	UNP O66529
BD	155	LEU	-	expression tag	UNP O66529
BD	156	GLU	-	expression tag	UNP O66529
BD	157	HIS	-	expression tag	UNP O66529
BD	158	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BD	159	HIS	-	expression tag	UNP O66529
BD	160	HIS	-	expression tag	UNP O66529
BD	161	HIS	-	expression tag	UNP O66529
BE	2	GLU	GLN	conflict	UNP O66529
BE	28	GLY	ASP	conflict	UNP O66529
BE	52	CYS	ARG	conflict	UNP O66529
BE	83	GLU	ARG	conflict	UNP O66529
BE	86	GLU	THR	conflict	UNP O66529
BE	112	SER	THR	conflict	UNP O66529
BE	115	ASP	VAL	conflict	UNP O66529
BE	118	ASP	ALA	conflict	UNP O66529
BE	120	GLU	THR	conflict	UNP O66529
BE	123	GLU	GLN	conflict	UNP O66529
BE	127	CYS	ARG	conflict	UNP O66529
BE	131	GLU	LYS	conflict	UNP O66529
BE	155	LEU	-	expression tag	UNP O66529
BE	156	GLU	-	expression tag	UNP O66529
BE	157	HIS	-	expression tag	UNP O66529
BE	158	HIS	-	expression tag	UNP O66529
BE	159	HIS	-	expression tag	UNP O66529
BE	160	HIS	-	expression tag	UNP O66529
BE	161	HIS	-	expression tag	UNP O66529
BX	2	GLU	GLN	conflict	UNP O66529
BX	28	GLY	ASP	conflict	UNP O66529
BX	52	CYS	ARG	conflict	UNP O66529
BX	83	GLU	ARG	conflict	UNP O66529
BX	86	GLU	THR	conflict	UNP O66529
BX	112	SER	THR	conflict	UNP O66529
BX	115	ASP	VAL	conflict	UNP O66529
BX	118	ASP	ALA	conflict	UNP O66529
BX	120	GLU	THR	conflict	UNP O66529
BX	123	GLU	GLN	conflict	UNP O66529
BX	127	CYS	ARG	conflict	UNP O66529
BX	131	GLU	LYS	conflict	UNP O66529
BX	155	LEU	-	expression tag	UNP O66529
BX	156	GLU	-	expression tag	UNP O66529
BX	157	HIS	-	expression tag	UNP O66529
BX	158	HIS	-	expression tag	UNP O66529
BX	159	HIS	-	expression tag	UNP O66529
BX	160	HIS	-	expression tag	UNP O66529
BX	161	HIS	-	expression tag	UNP O66529
CA	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CA	28	GLY	ASP	conflict	UNP O66529
CA	52	CYS	ARG	conflict	UNP O66529
CA	83	GLU	ARG	conflict	UNP O66529
CA	86	GLU	THR	conflict	UNP O66529
CA	112	SER	THR	conflict	UNP O66529
CA	115	ASP	VAL	conflict	UNP O66529
CA	118	ASP	ALA	conflict	UNP O66529
CA	120	GLU	THR	conflict	UNP O66529
CA	123	GLU	GLN	conflict	UNP O66529
CA	127	CYS	ARG	conflict	UNP O66529
CA	131	GLU	LYS	conflict	UNP O66529
CA	155	LEU	-	expression tag	UNP O66529
CA	156	GLU	-	expression tag	UNP O66529
CA	157	HIS	-	expression tag	UNP O66529
CA	158	HIS	-	expression tag	UNP O66529
CA	159	HIS	-	expression tag	UNP O66529
CA	160	HIS	-	expression tag	UNP O66529
CA	161	HIS	-	expression tag	UNP O66529
CB	2	GLU	GLN	conflict	UNP O66529
CB	28	GLY	ASP	conflict	UNP O66529
CB	52	CYS	ARG	conflict	UNP O66529
CB	83	GLU	ARG	conflict	UNP O66529
CB	86	GLU	THR	conflict	UNP O66529
CB	112	SER	THR	conflict	UNP O66529
CB	115	ASP	VAL	conflict	UNP O66529
CB	118	ASP	ALA	conflict	UNP O66529
CB	120	GLU	THR	conflict	UNP O66529
CB	123	GLU	GLN	conflict	UNP O66529
CB	127	CYS	ARG	conflict	UNP O66529
CB	131	GLU	LYS	conflict	UNP O66529
CB	155	LEU	-	expression tag	UNP O66529
CB	156	GLU	-	expression tag	UNP O66529
CB	157	HIS	-	expression tag	UNP O66529
CB	158	HIS	-	expression tag	UNP O66529
CB	159	HIS	-	expression tag	UNP O66529
CB	160	HIS	-	expression tag	UNP O66529
CB	161	HIS	-	expression tag	UNP O66529
CC	2	GLU	GLN	conflict	UNP O66529
CC	28	GLY	ASP	conflict	UNP O66529
CC	52	CYS	ARG	conflict	UNP O66529
CC	83	GLU	ARG	conflict	UNP O66529
CC	86	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CC	112	SER	THR	conflict	UNP O66529
CC	115	ASP	VAL	conflict	UNP O66529
CC	118	ASP	ALA	conflict	UNP O66529
CC	120	GLU	THR	conflict	UNP O66529
CC	123	GLU	GLN	conflict	UNP O66529
CC	127	CYS	ARG	conflict	UNP O66529
CC	131	GLU	LYS	conflict	UNP O66529
CC	155	LEU	-	expression tag	UNP O66529
CC	156	GLU	-	expression tag	UNP O66529
CC	157	HIS	-	expression tag	UNP O66529
CC	158	HIS	-	expression tag	UNP O66529
CC	159	HIS	-	expression tag	UNP O66529
CC	160	HIS	-	expression tag	UNP O66529
CC	161	HIS	-	expression tag	UNP O66529
CD	2	GLU	GLN	conflict	UNP O66529
CD	28	GLY	ASP	conflict	UNP O66529
CD	52	CYS	ARG	conflict	UNP O66529
CD	83	GLU	ARG	conflict	UNP O66529
CD	86	GLU	THR	conflict	UNP O66529
CD	112	SER	THR	conflict	UNP O66529
CD	115	ASP	VAL	conflict	UNP O66529
CD	118	ASP	ALA	conflict	UNP O66529
CD	120	GLU	THR	conflict	UNP O66529
CD	123	GLU	GLN	conflict	UNP O66529
CD	127	CYS	ARG	conflict	UNP O66529
CD	131	GLU	LYS	conflict	UNP O66529
CD	155	LEU	-	expression tag	UNP O66529
CD	156	GLU	-	expression tag	UNP O66529
CD	157	HIS	-	expression tag	UNP O66529
CD	158	HIS	-	expression tag	UNP O66529
CD	159	HIS	-	expression tag	UNP O66529
CD	160	HIS	-	expression tag	UNP O66529
CD	161	HIS	-	expression tag	UNP O66529
CE	2	GLU	GLN	conflict	UNP O66529
CE	28	GLY	ASP	conflict	UNP O66529
CE	52	CYS	ARG	conflict	UNP O66529
CE	83	GLU	ARG	conflict	UNP O66529
CE	86	GLU	THR	conflict	UNP O66529
CE	112	SER	THR	conflict	UNP O66529
CE	115	ASP	VAL	conflict	UNP O66529
CE	118	ASP	ALA	conflict	UNP O66529
CE	120	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CE	123	GLU	GLN	conflict	UNP O66529
CE	127	CYS	ARG	conflict	UNP O66529
CE	131	GLU	LYS	conflict	UNP O66529
CE	155	LEU	-	expression tag	UNP O66529
CE	156	GLU	-	expression tag	UNP O66529
CE	157	HIS	-	expression tag	UNP O66529
CE	158	HIS	-	expression tag	UNP O66529
CE	159	HIS	-	expression tag	UNP O66529
CE	160	HIS	-	expression tag	UNP O66529
CE	161	HIS	-	expression tag	UNP O66529
CX	2	GLU	GLN	conflict	UNP O66529
CX	28	GLY	ASP	conflict	UNP O66529
CX	52	CYS	ARG	conflict	UNP O66529
CX	83	GLU	ARG	conflict	UNP O66529
CX	86	GLU	THR	conflict	UNP O66529
CX	112	SER	THR	conflict	UNP O66529
CX	115	ASP	VAL	conflict	UNP O66529
CX	118	ASP	ALA	conflict	UNP O66529
CX	120	GLU	THR	conflict	UNP O66529
CX	123	GLU	GLN	conflict	UNP O66529
CX	127	CYS	ARG	conflict	UNP O66529
CX	131	GLU	LYS	conflict	UNP O66529
CX	155	LEU	-	expression tag	UNP O66529
CX	156	GLU	-	expression tag	UNP O66529
CX	157	HIS	-	expression tag	UNP O66529
CX	158	HIS	-	expression tag	UNP O66529
CX	159	HIS	-	expression tag	UNP O66529
CX	160	HIS	-	expression tag	UNP O66529
CX	161	HIS	-	expression tag	UNP O66529
DA	2	GLU	GLN	conflict	UNP O66529
DA	28	GLY	ASP	conflict	UNP O66529
DA	52	CYS	ARG	conflict	UNP O66529
DA	83	GLU	ARG	conflict	UNP O66529
DA	86	GLU	THR	conflict	UNP O66529
DA	112	SER	THR	conflict	UNP O66529
DA	115	ASP	VAL	conflict	UNP O66529
DA	118	ASP	ALA	conflict	UNP O66529
DA	120	GLU	THR	conflict	UNP O66529
DA	123	GLU	GLN	conflict	UNP O66529
DA	127	CYS	ARG	conflict	UNP O66529
DA	131	GLU	LYS	conflict	UNP O66529
DA	155	LEU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DA	156	GLU	-	expression tag	UNP O66529
DA	157	HIS	-	expression tag	UNP O66529
DA	158	HIS	-	expression tag	UNP O66529
DA	159	HIS	-	expression tag	UNP O66529
DA	160	HIS	-	expression tag	UNP O66529
DA	161	HIS	-	expression tag	UNP O66529
DB	2	GLU	GLN	conflict	UNP O66529
DB	28	GLY	ASP	conflict	UNP O66529
DB	52	CYS	ARG	conflict	UNP O66529
DB	83	GLU	ARG	conflict	UNP O66529
DB	86	GLU	THR	conflict	UNP O66529
DB	112	SER	THR	conflict	UNP O66529
DB	115	ASP	VAL	conflict	UNP O66529
DB	118	ASP	ALA	conflict	UNP O66529
DB	120	GLU	THR	conflict	UNP O66529
DB	123	GLU	GLN	conflict	UNP O66529
DB	127	CYS	ARG	conflict	UNP O66529
DB	131	GLU	LYS	conflict	UNP O66529
DB	155	LEU	-	expression tag	UNP O66529
DB	156	GLU	-	expression tag	UNP O66529
DB	157	HIS	-	expression tag	UNP O66529
DB	158	HIS	-	expression tag	UNP O66529
DB	159	HIS	-	expression tag	UNP O66529
DB	160	HIS	-	expression tag	UNP O66529
DB	161	HIS	-	expression tag	UNP O66529
DC	2	GLU	GLN	conflict	UNP O66529
DC	28	GLY	ASP	conflict	UNP O66529
DC	52	CYS	ARG	conflict	UNP O66529
DC	83	GLU	ARG	conflict	UNP O66529
DC	86	GLU	THR	conflict	UNP O66529
DC	112	SER	THR	conflict	UNP O66529
DC	115	ASP	VAL	conflict	UNP O66529
DC	118	ASP	ALA	conflict	UNP O66529
DC	120	GLU	THR	conflict	UNP O66529
DC	123	GLU	GLN	conflict	UNP O66529
DC	127	CYS	ARG	conflict	UNP O66529
DC	131	GLU	LYS	conflict	UNP O66529
DC	155	LEU	-	expression tag	UNP O66529
DC	156	GLU	-	expression tag	UNP O66529
DC	157	HIS	-	expression tag	UNP O66529
DC	158	HIS	-	expression tag	UNP O66529
DC	159	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DC	160	HIS	-	expression tag	UNP O66529
DC	161	HIS	-	expression tag	UNP O66529
DD	2	GLU	GLN	conflict	UNP O66529
DD	28	GLY	ASP	conflict	UNP O66529
DD	52	CYS	ARG	conflict	UNP O66529
DD	83	GLU	ARG	conflict	UNP O66529
DD	86	GLU	THR	conflict	UNP O66529
DD	112	SER	THR	conflict	UNP O66529
DD	115	ASP	VAL	conflict	UNP O66529
DD	118	ASP	ALA	conflict	UNP O66529
DD	120	GLU	THR	conflict	UNP O66529
DD	123	GLU	GLN	conflict	UNP O66529
DD	127	CYS	ARG	conflict	UNP O66529
DD	131	GLU	LYS	conflict	UNP O66529
DD	155	LEU	-	expression tag	UNP O66529
DD	156	GLU	-	expression tag	UNP O66529
DD	157	HIS	-	expression tag	UNP O66529
DD	158	HIS	-	expression tag	UNP O66529
DD	159	HIS	-	expression tag	UNP O66529
DD	160	HIS	-	expression tag	UNP O66529
DD	161	HIS	-	expression tag	UNP O66529
DE	2	GLU	GLN	conflict	UNP O66529
DE	28	GLY	ASP	conflict	UNP O66529
DE	52	CYS	ARG	conflict	UNP O66529
DE	83	GLU	ARG	conflict	UNP O66529
DE	86	GLU	THR	conflict	UNP O66529
DE	112	SER	THR	conflict	UNP O66529
DE	115	ASP	VAL	conflict	UNP O66529
DE	118	ASP	ALA	conflict	UNP O66529
DE	120	GLU	THR	conflict	UNP O66529
DE	123	GLU	GLN	conflict	UNP O66529
DE	127	CYS	ARG	conflict	UNP O66529
DE	131	GLU	LYS	conflict	UNP O66529
DE	155	LEU	-	expression tag	UNP O66529
DE	156	GLU	-	expression tag	UNP O66529
DE	157	HIS	-	expression tag	UNP O66529
DE	158	HIS	-	expression tag	UNP O66529
DE	159	HIS	-	expression tag	UNP O66529
DE	160	HIS	-	expression tag	UNP O66529
DE	161	HIS	-	expression tag	UNP O66529
DX	2	GLU	GLN	conflict	UNP O66529
DX	28	GLY	ASP	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DX	52	CYS	ARG	conflict	UNP O66529
DX	83	GLU	ARG	conflict	UNP O66529
DX	86	GLU	THR	conflict	UNP O66529
DX	112	SER	THR	conflict	UNP O66529
DX	115	ASP	VAL	conflict	UNP O66529
DX	118	ASP	ALA	conflict	UNP O66529
DX	120	GLU	THR	conflict	UNP O66529
DX	123	GLU	GLN	conflict	UNP O66529
DX	127	CYS	ARG	conflict	UNP O66529
DX	131	GLU	LYS	conflict	UNP O66529
DX	155	LEU	-	expression tag	UNP O66529
DX	156	GLU	-	expression tag	UNP O66529
DX	157	HIS	-	expression tag	UNP O66529
DX	158	HIS	-	expression tag	UNP O66529
DX	159	HIS	-	expression tag	UNP O66529
DX	160	HIS	-	expression tag	UNP O66529
DX	161	HIS	-	expression tag	UNP O66529
EA	2	GLU	GLN	conflict	UNP O66529
EA	28	GLY	ASP	conflict	UNP O66529
EA	52	CYS	ARG	conflict	UNP O66529
EA	83	GLU	ARG	conflict	UNP O66529
EA	86	GLU	THR	conflict	UNP O66529
EA	112	SER	THR	conflict	UNP O66529
EA	115	ASP	VAL	conflict	UNP O66529
EA	118	ASP	ALA	conflict	UNP O66529
EA	120	GLU	THR	conflict	UNP O66529
EA	123	GLU	GLN	conflict	UNP O66529
EA	127	CYS	ARG	conflict	UNP O66529
EA	131	GLU	LYS	conflict	UNP O66529
EA	155	LEU	-	expression tag	UNP O66529
EA	156	GLU	-	expression tag	UNP O66529
EA	157	HIS	-	expression tag	UNP O66529
EA	158	HIS	-	expression tag	UNP O66529
EA	159	HIS	-	expression tag	UNP O66529
EA	160	HIS	-	expression tag	UNP O66529
EA	161	HIS	-	expression tag	UNP O66529
EB	2	GLU	GLN	conflict	UNP O66529
EB	28	GLY	ASP	conflict	UNP O66529
EB	52	CYS	ARG	conflict	UNP O66529
EB	83	GLU	ARG	conflict	UNP O66529
EB	86	GLU	THR	conflict	UNP O66529
EB	112	SER	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
EB	115	ASP	VAL	conflict	UNP O66529
EB	118	ASP	ALA	conflict	UNP O66529
EB	120	GLU	THR	conflict	UNP O66529
EB	123	GLU	GLN	conflict	UNP O66529
EB	127	CYS	ARG	conflict	UNP O66529
EB	131	GLU	LYS	conflict	UNP O66529
EB	155	LEU	-	expression tag	UNP O66529
EB	156	GLU	-	expression tag	UNP O66529
EB	157	HIS	-	expression tag	UNP O66529
EB	158	HIS	-	expression tag	UNP O66529
EB	159	HIS	-	expression tag	UNP O66529
EB	160	HIS	-	expression tag	UNP O66529
EB	161	HIS	-	expression tag	UNP O66529
EC	2	GLU	GLN	conflict	UNP O66529
EC	28	GLY	ASP	conflict	UNP O66529
EC	52	CYS	ARG	conflict	UNP O66529
EC	83	GLU	ARG	conflict	UNP O66529
EC	86	GLU	THR	conflict	UNP O66529
EC	112	SER	THR	conflict	UNP O66529
EC	115	ASP	VAL	conflict	UNP O66529
EC	118	ASP	ALA	conflict	UNP O66529
EC	120	GLU	THR	conflict	UNP O66529
EC	123	GLU	GLN	conflict	UNP O66529
EC	127	CYS	ARG	conflict	UNP O66529
EC	131	GLU	LYS	conflict	UNP O66529
EC	155	LEU	-	expression tag	UNP O66529
EC	156	GLU	-	expression tag	UNP O66529
EC	157	HIS	-	expression tag	UNP O66529
EC	158	HIS	-	expression tag	UNP O66529
EC	159	HIS	-	expression tag	UNP O66529
EC	160	HIS	-	expression tag	UNP O66529
EC	161	HIS	-	expression tag	UNP O66529
ED	2	GLU	GLN	conflict	UNP O66529
ED	28	GLY	ASP	conflict	UNP O66529
ED	52	CYS	ARG	conflict	UNP O66529
ED	83	GLU	ARG	conflict	UNP O66529
ED	86	GLU	THR	conflict	UNP O66529
ED	112	SER	THR	conflict	UNP O66529
ED	115	ASP	VAL	conflict	UNP O66529
ED	118	ASP	ALA	conflict	UNP O66529
ED	120	GLU	THR	conflict	UNP O66529
ED	123	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ED	127	CYS	ARG	conflict	UNP O66529
ED	131	GLU	LYS	conflict	UNP O66529
ED	155	LEU	-	expression tag	UNP O66529
ED	156	GLU	-	expression tag	UNP O66529
ED	157	HIS	-	expression tag	UNP O66529
ED	158	HIS	-	expression tag	UNP O66529
ED	159	HIS	-	expression tag	UNP O66529
ED	160	HIS	-	expression tag	UNP O66529
ED	161	HIS	-	expression tag	UNP O66529
EE	2	GLU	GLN	conflict	UNP O66529
EE	28	GLY	ASP	conflict	UNP O66529
EE	52	CYS	ARG	conflict	UNP O66529
EE	83	GLU	ARG	conflict	UNP O66529
EE	86	GLU	THR	conflict	UNP O66529
EE	112	SER	THR	conflict	UNP O66529
EE	115	ASP	VAL	conflict	UNP O66529
EE	118	ASP	ALA	conflict	UNP O66529
EE	120	GLU	THR	conflict	UNP O66529
EE	123	GLU	GLN	conflict	UNP O66529
EE	127	CYS	ARG	conflict	UNP O66529
EE	131	GLU	LYS	conflict	UNP O66529
EE	155	LEU	-	expression tag	UNP O66529
EE	156	GLU	-	expression tag	UNP O66529
EE	157	HIS	-	expression tag	UNP O66529
EE	158	HIS	-	expression tag	UNP O66529
EE	159	HIS	-	expression tag	UNP O66529
EE	160	HIS	-	expression tag	UNP O66529
EE	161	HIS	-	expression tag	UNP O66529
EX	2	GLU	GLN	conflict	UNP O66529
EX	28	GLY	ASP	conflict	UNP O66529
EX	52	CYS	ARG	conflict	UNP O66529
EX	83	GLU	ARG	conflict	UNP O66529
EX	86	GLU	THR	conflict	UNP O66529
EX	112	SER	THR	conflict	UNP O66529
EX	115	ASP	VAL	conflict	UNP O66529
EX	118	ASP	ALA	conflict	UNP O66529
EX	120	GLU	THR	conflict	UNP O66529
EX	123	GLU	GLN	conflict	UNP O66529
EX	127	CYS	ARG	conflict	UNP O66529
EX	131	GLU	LYS	conflict	UNP O66529
EX	155	LEU	-	expression tag	UNP O66529
EX	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
EX	157	HIS	-	expression tag	UNP O66529
EX	158	HIS	-	expression tag	UNP O66529
EX	159	HIS	-	expression tag	UNP O66529
EX	160	HIS	-	expression tag	UNP O66529
EX	161	HIS	-	expression tag	UNP O66529
FA	2	GLU	GLN	conflict	UNP O66529
FA	28	GLY	ASP	conflict	UNP O66529
FA	52	CYS	ARG	conflict	UNP O66529
FA	83	GLU	ARG	conflict	UNP O66529
FA	86	GLU	THR	conflict	UNP O66529
FA	112	SER	THR	conflict	UNP O66529
FA	115	ASP	VAL	conflict	UNP O66529
FA	118	ASP	ALA	conflict	UNP O66529
FA	120	GLU	THR	conflict	UNP O66529
FA	123	GLU	GLN	conflict	UNP O66529
FA	127	CYS	ARG	conflict	UNP O66529
FA	131	GLU	LYS	conflict	UNP O66529
FA	155	LEU	-	expression tag	UNP O66529
FA	156	GLU	-	expression tag	UNP O66529
FA	157	HIS	-	expression tag	UNP O66529
FA	158	HIS	-	expression tag	UNP O66529
FA	159	HIS	-	expression tag	UNP O66529
FA	160	HIS	-	expression tag	UNP O66529
FA	161	HIS	-	expression tag	UNP O66529
FB	2	GLU	GLN	conflict	UNP O66529
FB	28	GLY	ASP	conflict	UNP O66529
FB	52	CYS	ARG	conflict	UNP O66529
FB	83	GLU	ARG	conflict	UNP O66529
FB	86	GLU	THR	conflict	UNP O66529
FB	112	SER	THR	conflict	UNP O66529
FB	115	ASP	VAL	conflict	UNP O66529
FB	118	ASP	ALA	conflict	UNP O66529
FB	120	GLU	THR	conflict	UNP O66529
FB	123	GLU	GLN	conflict	UNP O66529
FB	127	CYS	ARG	conflict	UNP O66529
FB	131	GLU	LYS	conflict	UNP O66529
FB	155	LEU	-	expression tag	UNP O66529
FB	156	GLU	-	expression tag	UNP O66529
FB	157	HIS	-	expression tag	UNP O66529
FB	158	HIS	-	expression tag	UNP O66529
FB	159	HIS	-	expression tag	UNP O66529
FB	160	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FB	161	HIS	-	expression tag	UNP O66529
FC	2	GLU	GLN	conflict	UNP O66529
FC	28	GLY	ASP	conflict	UNP O66529
FC	52	CYS	ARG	conflict	UNP O66529
FC	83	GLU	ARG	conflict	UNP O66529
FC	86	GLU	THR	conflict	UNP O66529
FC	112	SER	THR	conflict	UNP O66529
FC	115	ASP	VAL	conflict	UNP O66529
FC	118	ASP	ALA	conflict	UNP O66529
FC	120	GLU	THR	conflict	UNP O66529
FC	123	GLU	GLN	conflict	UNP O66529
FC	127	CYS	ARG	conflict	UNP O66529
FC	131	GLU	LYS	conflict	UNP O66529
FC	155	LEU	-	expression tag	UNP O66529
FC	156	GLU	-	expression tag	UNP O66529
FC	157	HIS	-	expression tag	UNP O66529
FC	158	HIS	-	expression tag	UNP O66529
FC	159	HIS	-	expression tag	UNP O66529
FC	160	HIS	-	expression tag	UNP O66529
FC	161	HIS	-	expression tag	UNP O66529
FD	2	GLU	GLN	conflict	UNP O66529
FD	28	GLY	ASP	conflict	UNP O66529
FD	52	CYS	ARG	conflict	UNP O66529
FD	83	GLU	ARG	conflict	UNP O66529
FD	86	GLU	THR	conflict	UNP O66529
FD	112	SER	THR	conflict	UNP O66529
FD	115	ASP	VAL	conflict	UNP O66529
FD	118	ASP	ALA	conflict	UNP O66529
FD	120	GLU	THR	conflict	UNP O66529
FD	123	GLU	GLN	conflict	UNP O66529
FD	127	CYS	ARG	conflict	UNP O66529
FD	131	GLU	LYS	conflict	UNP O66529
FD	155	LEU	-	expression tag	UNP O66529
FD	156	GLU	-	expression tag	UNP O66529
FD	157	HIS	-	expression tag	UNP O66529
FD	158	HIS	-	expression tag	UNP O66529
FD	159	HIS	-	expression tag	UNP O66529
FD	160	HIS	-	expression tag	UNP O66529
FD	161	HIS	-	expression tag	UNP O66529
FE	2	GLU	GLN	conflict	UNP O66529
FE	28	GLY	ASP	conflict	UNP O66529
FE	52	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FE	83	GLU	ARG	conflict	UNP O66529
FE	86	GLU	THR	conflict	UNP O66529
FE	112	SER	THR	conflict	UNP O66529
FE	115	ASP	VAL	conflict	UNP O66529
FE	118	ASP	ALA	conflict	UNP O66529
FE	120	GLU	THR	conflict	UNP O66529
FE	123	GLU	GLN	conflict	UNP O66529
FE	127	CYS	ARG	conflict	UNP O66529
FE	131	GLU	LYS	conflict	UNP O66529
FE	155	LEU	-	expression tag	UNP O66529
FE	156	GLU	-	expression tag	UNP O66529
FE	157	HIS	-	expression tag	UNP O66529
FE	158	HIS	-	expression tag	UNP O66529
FE	159	HIS	-	expression tag	UNP O66529
FE	160	HIS	-	expression tag	UNP O66529
FE	161	HIS	-	expression tag	UNP O66529
FX	2	GLU	GLN	conflict	UNP O66529
FX	28	GLY	ASP	conflict	UNP O66529
FX	52	CYS	ARG	conflict	UNP O66529
FX	83	GLU	ARG	conflict	UNP O66529
FX	86	GLU	THR	conflict	UNP O66529
FX	112	SER	THR	conflict	UNP O66529
FX	115	ASP	VAL	conflict	UNP O66529
FX	118	ASP	ALA	conflict	UNP O66529
FX	120	GLU	THR	conflict	UNP O66529
FX	123	GLU	GLN	conflict	UNP O66529
FX	127	CYS	ARG	conflict	UNP O66529
FX	131	GLU	LYS	conflict	UNP O66529
FX	155	LEU	-	expression tag	UNP O66529
FX	156	GLU	-	expression tag	UNP O66529
FX	157	HIS	-	expression tag	UNP O66529
FX	158	HIS	-	expression tag	UNP O66529
FX	159	HIS	-	expression tag	UNP O66529
FX	160	HIS	-	expression tag	UNP O66529
FX	161	HIS	-	expression tag	UNP O66529
GA	2	GLU	GLN	conflict	UNP O66529
GA	28	GLY	ASP	conflict	UNP O66529
GA	52	CYS	ARG	conflict	UNP O66529
GA	83	GLU	ARG	conflict	UNP O66529
GA	86	GLU	THR	conflict	UNP O66529
GA	112	SER	THR	conflict	UNP O66529
GA	115	ASP	VAL	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GA	118	ASP	ALA	conflict	UNP O66529
GA	120	GLU	THR	conflict	UNP O66529
GA	123	GLU	GLN	conflict	UNP O66529
GA	127	CYS	ARG	conflict	UNP O66529
GA	131	GLU	LYS	conflict	UNP O66529
GA	155	LEU	-	expression tag	UNP O66529
GA	156	GLU	-	expression tag	UNP O66529
GA	157	HIS	-	expression tag	UNP O66529
GA	158	HIS	-	expression tag	UNP O66529
GA	159	HIS	-	expression tag	UNP O66529
GA	160	HIS	-	expression tag	UNP O66529
GA	161	HIS	-	expression tag	UNP O66529
GB	2	GLU	GLN	conflict	UNP O66529
GB	28	GLY	ASP	conflict	UNP O66529
GB	52	CYS	ARG	conflict	UNP O66529
GB	83	GLU	ARG	conflict	UNP O66529
GB	86	GLU	THR	conflict	UNP O66529
GB	112	SER	THR	conflict	UNP O66529
GB	115	ASP	VAL	conflict	UNP O66529
GB	118	ASP	ALA	conflict	UNP O66529
GB	120	GLU	THR	conflict	UNP O66529
GB	123	GLU	GLN	conflict	UNP O66529
GB	127	CYS	ARG	conflict	UNP O66529
GB	131	GLU	LYS	conflict	UNP O66529
GB	155	LEU	-	expression tag	UNP O66529
GB	156	GLU	-	expression tag	UNP O66529
GB	157	HIS	-	expression tag	UNP O66529
GB	158	HIS	-	expression tag	UNP O66529
GB	159	HIS	-	expression tag	UNP O66529
GB	160	HIS	-	expression tag	UNP O66529
GB	161	HIS	-	expression tag	UNP O66529
GC	2	GLU	GLN	conflict	UNP O66529
GC	28	GLY	ASP	conflict	UNP O66529
GC	52	CYS	ARG	conflict	UNP O66529
GC	83	GLU	ARG	conflict	UNP O66529
GC	86	GLU	THR	conflict	UNP O66529
GC	112	SER	THR	conflict	UNP O66529
GC	115	ASP	VAL	conflict	UNP O66529
GC	118	ASP	ALA	conflict	UNP O66529
GC	120	GLU	THR	conflict	UNP O66529
GC	123	GLU	GLN	conflict	UNP O66529
GC	127	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GC	131	GLU	LYS	conflict	UNP O66529
GC	155	LEU	-	expression tag	UNP O66529
GC	156	GLU	-	expression tag	UNP O66529
GC	157	HIS	-	expression tag	UNP O66529
GC	158	HIS	-	expression tag	UNP O66529
GC	159	HIS	-	expression tag	UNP O66529
GC	160	HIS	-	expression tag	UNP O66529
GC	161	HIS	-	expression tag	UNP O66529
GD	2	GLU	GLN	conflict	UNP O66529
GD	28	GLY	ASP	conflict	UNP O66529
GD	52	CYS	ARG	conflict	UNP O66529
GD	83	GLU	ARG	conflict	UNP O66529
GD	86	GLU	THR	conflict	UNP O66529
GD	112	SER	THR	conflict	UNP O66529
GD	115	ASP	VAL	conflict	UNP O66529
GD	118	ASP	ALA	conflict	UNP O66529
GD	120	GLU	THR	conflict	UNP O66529
GD	123	GLU	GLN	conflict	UNP O66529
GD	127	CYS	ARG	conflict	UNP O66529
GD	131	GLU	LYS	conflict	UNP O66529
GD	155	LEU	-	expression tag	UNP O66529
GD	156	GLU	-	expression tag	UNP O66529
GD	157	HIS	-	expression tag	UNP O66529
GD	158	HIS	-	expression tag	UNP O66529
GD	159	HIS	-	expression tag	UNP O66529
GD	160	HIS	-	expression tag	UNP O66529
GD	161	HIS	-	expression tag	UNP O66529
GE	2	GLU	GLN	conflict	UNP O66529
GE	28	GLY	ASP	conflict	UNP O66529
GE	52	CYS	ARG	conflict	UNP O66529
GE	83	GLU	ARG	conflict	UNP O66529
GE	86	GLU	THR	conflict	UNP O66529
GE	112	SER	THR	conflict	UNP O66529
GE	115	ASP	VAL	conflict	UNP O66529
GE	118	ASP	ALA	conflict	UNP O66529
GE	120	GLU	THR	conflict	UNP O66529
GE	123	GLU	GLN	conflict	UNP O66529
GE	127	CYS	ARG	conflict	UNP O66529
GE	131	GLU	LYS	conflict	UNP O66529
GE	155	LEU	-	expression tag	UNP O66529
GE	156	GLU	-	expression tag	UNP O66529
GE	157	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
GE	158	HIS	-	expression tag	UNP O66529
GE	159	HIS	-	expression tag	UNP O66529
GE	160	HIS	-	expression tag	UNP O66529
GE	161	HIS	-	expression tag	UNP O66529
GX	2	GLU	GLN	conflict	UNP O66529
GX	28	GLY	ASP	conflict	UNP O66529
GX	52	CYS	ARG	conflict	UNP O66529
GX	83	GLU	ARG	conflict	UNP O66529
GX	86	GLU	THR	conflict	UNP O66529
GX	112	SER	THR	conflict	UNP O66529
GX	115	ASP	VAL	conflict	UNP O66529
GX	118	ASP	ALA	conflict	UNP O66529
GX	120	GLU	THR	conflict	UNP O66529
GX	123	GLU	GLN	conflict	UNP O66529
GX	127	CYS	ARG	conflict	UNP O66529
GX	131	GLU	LYS	conflict	UNP O66529
GX	155	LEU	-	expression tag	UNP O66529
GX	156	GLU	-	expression tag	UNP O66529
GX	157	HIS	-	expression tag	UNP O66529
GX	158	HIS	-	expression tag	UNP O66529
GX	159	HIS	-	expression tag	UNP O66529
GX	160	HIS	-	expression tag	UNP O66529
GX	161	HIS	-	expression tag	UNP O66529
HA	2	GLU	GLN	conflict	UNP O66529
HA	28	GLY	ASP	conflict	UNP O66529
HA	52	CYS	ARG	conflict	UNP O66529
HA	83	GLU	ARG	conflict	UNP O66529
HA	86	GLU	THR	conflict	UNP O66529
HA	112	SER	THR	conflict	UNP O66529
HA	115	ASP	VAL	conflict	UNP O66529
HA	118	ASP	ALA	conflict	UNP O66529
HA	120	GLU	THR	conflict	UNP O66529
HA	123	GLU	GLN	conflict	UNP O66529
HA	127	CYS	ARG	conflict	UNP O66529
HA	131	GLU	LYS	conflict	UNP O66529
HA	155	LEU	-	expression tag	UNP O66529
HA	156	GLU	-	expression tag	UNP O66529
HA	157	HIS	-	expression tag	UNP O66529
HA	158	HIS	-	expression tag	UNP O66529
HA	159	HIS	-	expression tag	UNP O66529
HA	160	HIS	-	expression tag	UNP O66529
HA	161	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
HB	2	GLU	GLN	conflict	UNP O66529
HB	28	GLY	ASP	conflict	UNP O66529
HB	52	CYS	ARG	conflict	UNP O66529
HB	83	GLU	ARG	conflict	UNP O66529
HB	86	GLU	THR	conflict	UNP O66529
HB	112	SER	THR	conflict	UNP O66529
HB	115	ASP	VAL	conflict	UNP O66529
HB	118	ASP	ALA	conflict	UNP O66529
HB	120	GLU	THR	conflict	UNP O66529
HB	123	GLU	GLN	conflict	UNP O66529
HB	127	CYS	ARG	conflict	UNP O66529
HB	131	GLU	LYS	conflict	UNP O66529
HB	155	LEU	-	expression tag	UNP O66529
HB	156	GLU	-	expression tag	UNP O66529
HB	157	HIS	-	expression tag	UNP O66529
HB	158	HIS	-	expression tag	UNP O66529
HB	159	HIS	-	expression tag	UNP O66529
HB	160	HIS	-	expression tag	UNP O66529
HB	161	HIS	-	expression tag	UNP O66529
HC	2	GLU	GLN	conflict	UNP O66529
HC	28	GLY	ASP	conflict	UNP O66529
HC	52	CYS	ARG	conflict	UNP O66529
HC	83	GLU	ARG	conflict	UNP O66529
HC	86	GLU	THR	conflict	UNP O66529
HC	112	SER	THR	conflict	UNP O66529
HC	115	ASP	VAL	conflict	UNP O66529
HC	118	ASP	ALA	conflict	UNP O66529
HC	120	GLU	THR	conflict	UNP O66529
HC	123	GLU	GLN	conflict	UNP O66529
HC	127	CYS	ARG	conflict	UNP O66529
HC	131	GLU	LYS	conflict	UNP O66529
HC	155	LEU	-	expression tag	UNP O66529
HC	156	GLU	-	expression tag	UNP O66529
HC	157	HIS	-	expression tag	UNP O66529
HC	158	HIS	-	expression tag	UNP O66529
HC	159	HIS	-	expression tag	UNP O66529
HC	160	HIS	-	expression tag	UNP O66529
HC	161	HIS	-	expression tag	UNP O66529
HD	2	GLU	GLN	conflict	UNP O66529
HD	28	GLY	ASP	conflict	UNP O66529
HD	52	CYS	ARG	conflict	UNP O66529
HD	83	GLU	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
HD	86	GLU	THR	conflict	UNP O66529
HD	112	SER	THR	conflict	UNP O66529
HD	115	ASP	VAL	conflict	UNP O66529
HD	118	ASP	ALA	conflict	UNP O66529
HD	120	GLU	THR	conflict	UNP O66529
HD	123	GLU	GLN	conflict	UNP O66529
HD	127	CYS	ARG	conflict	UNP O66529
HD	131	GLU	LYS	conflict	UNP O66529
HD	155	LEU	-	expression tag	UNP O66529
HD	156	GLU	-	expression tag	UNP O66529
HD	157	HIS	-	expression tag	UNP O66529
HD	158	HIS	-	expression tag	UNP O66529
HD	159	HIS	-	expression tag	UNP O66529
HD	160	HIS	-	expression tag	UNP O66529
HD	161	HIS	-	expression tag	UNP O66529
HE	2	GLU	GLN	conflict	UNP O66529
HE	28	GLY	ASP	conflict	UNP O66529
HE	52	CYS	ARG	conflict	UNP O66529
HE	83	GLU	ARG	conflict	UNP O66529
HE	86	GLU	THR	conflict	UNP O66529
HE	112	SER	THR	conflict	UNP O66529
HE	115	ASP	VAL	conflict	UNP O66529
HE	118	ASP	ALA	conflict	UNP O66529
HE	120	GLU	THR	conflict	UNP O66529
HE	123	GLU	GLN	conflict	UNP O66529
HE	127	CYS	ARG	conflict	UNP O66529
HE	131	GLU	LYS	conflict	UNP O66529
HE	155	LEU	-	expression tag	UNP O66529
HE	156	GLU	-	expression tag	UNP O66529
HE	157	HIS	-	expression tag	UNP O66529
HE	158	HIS	-	expression tag	UNP O66529
HE	159	HIS	-	expression tag	UNP O66529
HE	160	HIS	-	expression tag	UNP O66529
HE	161	HIS	-	expression tag	UNP O66529
HX	2	GLU	GLN	conflict	UNP O66529
HX	28	GLY	ASP	conflict	UNP O66529
HX	52	CYS	ARG	conflict	UNP O66529
HX	83	GLU	ARG	conflict	UNP O66529
HX	86	GLU	THR	conflict	UNP O66529
HX	112	SER	THR	conflict	UNP O66529
HX	115	ASP	VAL	conflict	UNP O66529
HX	118	ASP	ALA	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
HX	120	GLU	THR	conflict	UNP O66529
HX	123	GLU	GLN	conflict	UNP O66529
HX	127	CYS	ARG	conflict	UNP O66529
HX	131	GLU	LYS	conflict	UNP O66529
HX	155	LEU	-	expression tag	UNP O66529
HX	156	GLU	-	expression tag	UNP O66529
HX	157	HIS	-	expression tag	UNP O66529
HX	158	HIS	-	expression tag	UNP O66529
HX	159	HIS	-	expression tag	UNP O66529
HX	160	HIS	-	expression tag	UNP O66529
HX	161	HIS	-	expression tag	UNP O66529
IA	2	GLU	GLN	conflict	UNP O66529
IA	28	GLY	ASP	conflict	UNP O66529
IA	52	CYS	ARG	conflict	UNP O66529
IA	83	GLU	ARG	conflict	UNP O66529
IA	86	GLU	THR	conflict	UNP O66529
IA	112	SER	THR	conflict	UNP O66529
IA	115	ASP	VAL	conflict	UNP O66529
IA	118	ASP	ALA	conflict	UNP O66529
IA	120	GLU	THR	conflict	UNP O66529
IA	123	GLU	GLN	conflict	UNP O66529
IA	127	CYS	ARG	conflict	UNP O66529
IA	131	GLU	LYS	conflict	UNP O66529
IA	155	LEU	-	expression tag	UNP O66529
IA	156	GLU	-	expression tag	UNP O66529
IA	157	HIS	-	expression tag	UNP O66529
IA	158	HIS	-	expression tag	UNP O66529
IA	159	HIS	-	expression tag	UNP O66529
IA	160	HIS	-	expression tag	UNP O66529
IA	161	HIS	-	expression tag	UNP O66529
IB	2	GLU	GLN	conflict	UNP O66529
IB	28	GLY	ASP	conflict	UNP O66529
IB	52	CYS	ARG	conflict	UNP O66529
IB	83	GLU	ARG	conflict	UNP O66529
IB	86	GLU	THR	conflict	UNP O66529
IB	112	SER	THR	conflict	UNP O66529
IB	115	ASP	VAL	conflict	UNP O66529
IB	118	ASP	ALA	conflict	UNP O66529
IB	120	GLU	THR	conflict	UNP O66529
IB	123	GLU	GLN	conflict	UNP O66529
IB	127	CYS	ARG	conflict	UNP O66529
IB	131	GLU	LYS	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
IB	155	LEU	-	expression tag	UNP O66529
IB	156	GLU	-	expression tag	UNP O66529
IB	157	HIS	-	expression tag	UNP O66529
IB	158	HIS	-	expression tag	UNP O66529
IB	159	HIS	-	expression tag	UNP O66529
IB	160	HIS	-	expression tag	UNP O66529
IB	161	HIS	-	expression tag	UNP O66529
IC	2	GLU	GLN	conflict	UNP O66529
IC	28	GLY	ASP	conflict	UNP O66529
IC	52	CYS	ARG	conflict	UNP O66529
IC	83	GLU	ARG	conflict	UNP O66529
IC	86	GLU	THR	conflict	UNP O66529
IC	112	SER	THR	conflict	UNP O66529
IC	115	ASP	VAL	conflict	UNP O66529
IC	118	ASP	ALA	conflict	UNP O66529
IC	120	GLU	THR	conflict	UNP O66529
IC	123	GLU	GLN	conflict	UNP O66529
IC	127	CYS	ARG	conflict	UNP O66529
IC	131	GLU	LYS	conflict	UNP O66529
IC	155	LEU	-	expression tag	UNP O66529
IC	156	GLU	-	expression tag	UNP O66529
IC	157	HIS	-	expression tag	UNP O66529
IC	158	HIS	-	expression tag	UNP O66529
IC	159	HIS	-	expression tag	UNP O66529
IC	160	HIS	-	expression tag	UNP O66529
IC	161	HIS	-	expression tag	UNP O66529
ID	2	GLU	GLN	conflict	UNP O66529
ID	28	GLY	ASP	conflict	UNP O66529
ID	52	CYS	ARG	conflict	UNP O66529
ID	83	GLU	ARG	conflict	UNP O66529
ID	86	GLU	THR	conflict	UNP O66529
ID	112	SER	THR	conflict	UNP O66529
ID	115	ASP	VAL	conflict	UNP O66529
ID	118	ASP	ALA	conflict	UNP O66529
ID	120	GLU	THR	conflict	UNP O66529
ID	123	GLU	GLN	conflict	UNP O66529
ID	127	CYS	ARG	conflict	UNP O66529
ID	131	GLU	LYS	conflict	UNP O66529
ID	155	LEU	-	expression tag	UNP O66529
ID	156	GLU	-	expression tag	UNP O66529
ID	157	HIS	-	expression tag	UNP O66529
ID	158	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ID	159	HIS	-	expression tag	UNP O66529
ID	160	HIS	-	expression tag	UNP O66529
ID	161	HIS	-	expression tag	UNP O66529
IE	2	GLU	GLN	conflict	UNP O66529
IE	28	GLY	ASP	conflict	UNP O66529
IE	52	CYS	ARG	conflict	UNP O66529
IE	83	GLU	ARG	conflict	UNP O66529
IE	86	GLU	THR	conflict	UNP O66529
IE	112	SER	THR	conflict	UNP O66529
IE	115	ASP	VAL	conflict	UNP O66529
IE	118	ASP	ALA	conflict	UNP O66529
IE	120	GLU	THR	conflict	UNP O66529
IE	123	GLU	GLN	conflict	UNP O66529
IE	127	CYS	ARG	conflict	UNP O66529
IE	131	GLU	LYS	conflict	UNP O66529
IE	155	LEU	-	expression tag	UNP O66529
IE	156	GLU	-	expression tag	UNP O66529
IE	157	HIS	-	expression tag	UNP O66529
IE	158	HIS	-	expression tag	UNP O66529
IE	159	HIS	-	expression tag	UNP O66529
IE	160	HIS	-	expression tag	UNP O66529
IE	161	HIS	-	expression tag	UNP O66529
IX	2	GLU	GLN	conflict	UNP O66529
IX	28	GLY	ASP	conflict	UNP O66529
IX	52	CYS	ARG	conflict	UNP O66529
IX	83	GLU	ARG	conflict	UNP O66529
IX	86	GLU	THR	conflict	UNP O66529
IX	112	SER	THR	conflict	UNP O66529
IX	115	ASP	VAL	conflict	UNP O66529
IX	118	ASP	ALA	conflict	UNP O66529
IX	120	GLU	THR	conflict	UNP O66529
IX	123	GLU	GLN	conflict	UNP O66529
IX	127	CYS	ARG	conflict	UNP O66529
IX	131	GLU	LYS	conflict	UNP O66529
IX	155	LEU	-	expression tag	UNP O66529
IX	156	GLU	-	expression tag	UNP O66529
IX	157	HIS	-	expression tag	UNP O66529
IX	158	HIS	-	expression tag	UNP O66529
IX	159	HIS	-	expression tag	UNP O66529
IX	160	HIS	-	expression tag	UNP O66529
IX	161	HIS	-	expression tag	UNP O66529
JA	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JA	28	GLY	ASP	conflict	UNP O66529
JA	52	CYS	ARG	conflict	UNP O66529
JA	83	GLU	ARG	conflict	UNP O66529
JA	86	GLU	THR	conflict	UNP O66529
JA	112	SER	THR	conflict	UNP O66529
JA	115	ASP	VAL	conflict	UNP O66529
JA	118	ASP	ALA	conflict	UNP O66529
JA	120	GLU	THR	conflict	UNP O66529
JA	123	GLU	GLN	conflict	UNP O66529
JA	127	CYS	ARG	conflict	UNP O66529
JA	131	GLU	LYS	conflict	UNP O66529
JA	155	LEU	-	expression tag	UNP O66529
JA	156	GLU	-	expression tag	UNP O66529
JA	157	HIS	-	expression tag	UNP O66529
JA	158	HIS	-	expression tag	UNP O66529
JA	159	HIS	-	expression tag	UNP O66529
JA	160	HIS	-	expression tag	UNP O66529
JA	161	HIS	-	expression tag	UNP O66529
JB	2	GLU	GLN	conflict	UNP O66529
JB	28	GLY	ASP	conflict	UNP O66529
JB	52	CYS	ARG	conflict	UNP O66529
JB	83	GLU	ARG	conflict	UNP O66529
JB	86	GLU	THR	conflict	UNP O66529
JB	112	SER	THR	conflict	UNP O66529
JB	115	ASP	VAL	conflict	UNP O66529
JB	118	ASP	ALA	conflict	UNP O66529
JB	120	GLU	THR	conflict	UNP O66529
JB	123	GLU	GLN	conflict	UNP O66529
JB	127	CYS	ARG	conflict	UNP O66529
JB	131	GLU	LYS	conflict	UNP O66529
JB	155	LEU	-	expression tag	UNP O66529
JB	156	GLU	-	expression tag	UNP O66529
JB	157	HIS	-	expression tag	UNP O66529
JB	158	HIS	-	expression tag	UNP O66529
JB	159	HIS	-	expression tag	UNP O66529
JB	160	HIS	-	expression tag	UNP O66529
JB	161	HIS	-	expression tag	UNP O66529
JC	2	GLU	GLN	conflict	UNP O66529
JC	28	GLY	ASP	conflict	UNP O66529
JC	52	CYS	ARG	conflict	UNP O66529
JC	83	GLU	ARG	conflict	UNP O66529
JC	86	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JC	112	SER	THR	conflict	UNP O66529
JC	115	ASP	VAL	conflict	UNP O66529
JC	118	ASP	ALA	conflict	UNP O66529
JC	120	GLU	THR	conflict	UNP O66529
JC	123	GLU	GLN	conflict	UNP O66529
JC	127	CYS	ARG	conflict	UNP O66529
JC	131	GLU	LYS	conflict	UNP O66529
JC	155	LEU	-	expression tag	UNP O66529
JC	156	GLU	-	expression tag	UNP O66529
JC	157	HIS	-	expression tag	UNP O66529
JC	158	HIS	-	expression tag	UNP O66529
JC	159	HIS	-	expression tag	UNP O66529
JC	160	HIS	-	expression tag	UNP O66529
JC	161	HIS	-	expression tag	UNP O66529
JD	2	GLU	GLN	conflict	UNP O66529
JD	28	GLY	ASP	conflict	UNP O66529
JD	52	CYS	ARG	conflict	UNP O66529
JD	83	GLU	ARG	conflict	UNP O66529
JD	86	GLU	THR	conflict	UNP O66529
JD	112	SER	THR	conflict	UNP O66529
JD	115	ASP	VAL	conflict	UNP O66529
JD	118	ASP	ALA	conflict	UNP O66529
JD	120	GLU	THR	conflict	UNP O66529
JD	123	GLU	GLN	conflict	UNP O66529
JD	127	CYS	ARG	conflict	UNP O66529
JD	131	GLU	LYS	conflict	UNP O66529
JD	155	LEU	-	expression tag	UNP O66529
JD	156	GLU	-	expression tag	UNP O66529
JD	157	HIS	-	expression tag	UNP O66529
JD	158	HIS	-	expression tag	UNP O66529
JD	159	HIS	-	expression tag	UNP O66529
JD	160	HIS	-	expression tag	UNP O66529
JD	161	HIS	-	expression tag	UNP O66529
JE	2	GLU	GLN	conflict	UNP O66529
JE	28	GLY	ASP	conflict	UNP O66529
JE	52	CYS	ARG	conflict	UNP O66529
JE	83	GLU	ARG	conflict	UNP O66529
JE	86	GLU	THR	conflict	UNP O66529
JE	112	SER	THR	conflict	UNP O66529
JE	115	ASP	VAL	conflict	UNP O66529
JE	118	ASP	ALA	conflict	UNP O66529
JE	120	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JE	123	GLU	GLN	conflict	UNP O66529
JE	127	CYS	ARG	conflict	UNP O66529
JE	131	GLU	LYS	conflict	UNP O66529
JE	155	LEU	-	expression tag	UNP O66529
JE	156	GLU	-	expression tag	UNP O66529
JE	157	HIS	-	expression tag	UNP O66529
JE	158	HIS	-	expression tag	UNP O66529
JE	159	HIS	-	expression tag	UNP O66529
JE	160	HIS	-	expression tag	UNP O66529
JE	161	HIS	-	expression tag	UNP O66529
JX	2	GLU	GLN	conflict	UNP O66529
JX	28	GLY	ASP	conflict	UNP O66529
JX	52	CYS	ARG	conflict	UNP O66529
JX	83	GLU	ARG	conflict	UNP O66529
JX	86	GLU	THR	conflict	UNP O66529
JX	112	SER	THR	conflict	UNP O66529
JX	115	ASP	VAL	conflict	UNP O66529
JX	118	ASP	ALA	conflict	UNP O66529
JX	120	GLU	THR	conflict	UNP O66529
JX	123	GLU	GLN	conflict	UNP O66529
JX	127	CYS	ARG	conflict	UNP O66529
JX	131	GLU	LYS	conflict	UNP O66529
JX	155	LEU	-	expression tag	UNP O66529
JX	156	GLU	-	expression tag	UNP O66529
JX	157	HIS	-	expression tag	UNP O66529
JX	158	HIS	-	expression tag	UNP O66529
JX	159	HIS	-	expression tag	UNP O66529
JX	160	HIS	-	expression tag	UNP O66529
JX	161	HIS	-	expression tag	UNP O66529
KA	2	GLU	GLN	conflict	UNP O66529
KA	28	GLY	ASP	conflict	UNP O66529
KA	52	CYS	ARG	conflict	UNP O66529
KA	83	GLU	ARG	conflict	UNP O66529
KA	86	GLU	THR	conflict	UNP O66529
KA	112	SER	THR	conflict	UNP O66529
KA	115	ASP	VAL	conflict	UNP O66529
KA	118	ASP	ALA	conflict	UNP O66529
KA	120	GLU	THR	conflict	UNP O66529
KA	123	GLU	GLN	conflict	UNP O66529
KA	127	CYS	ARG	conflict	UNP O66529
KA	131	GLU	LYS	conflict	UNP O66529
KA	155	LEU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
KA	156	GLU	-	expression tag	UNP O66529
KA	157	HIS	-	expression tag	UNP O66529
KA	158	HIS	-	expression tag	UNP O66529
KA	159	HIS	-	expression tag	UNP O66529
KA	160	HIS	-	expression tag	UNP O66529
KA	161	HIS	-	expression tag	UNP O66529
KB	2	GLU	GLN	conflict	UNP O66529
KB	28	GLY	ASP	conflict	UNP O66529
KB	52	CYS	ARG	conflict	UNP O66529
KB	83	GLU	ARG	conflict	UNP O66529
KB	86	GLU	THR	conflict	UNP O66529
KB	112	SER	THR	conflict	UNP O66529
KB	115	ASP	VAL	conflict	UNP O66529
KB	118	ASP	ALA	conflict	UNP O66529
KB	120	GLU	THR	conflict	UNP O66529
KB	123	GLU	GLN	conflict	UNP O66529
KB	127	CYS	ARG	conflict	UNP O66529
KB	131	GLU	LYS	conflict	UNP O66529
KB	155	LEU	-	expression tag	UNP O66529
KB	156	GLU	-	expression tag	UNP O66529
KB	157	HIS	-	expression tag	UNP O66529
KB	158	HIS	-	expression tag	UNP O66529
KB	159	HIS	-	expression tag	UNP O66529
KB	160	HIS	-	expression tag	UNP O66529
KB	161	HIS	-	expression tag	UNP O66529
KC	2	GLU	GLN	conflict	UNP O66529
KC	28	GLY	ASP	conflict	UNP O66529
KC	52	CYS	ARG	conflict	UNP O66529
KC	83	GLU	ARG	conflict	UNP O66529
KC	86	GLU	THR	conflict	UNP O66529
KC	112	SER	THR	conflict	UNP O66529
KC	115	ASP	VAL	conflict	UNP O66529
KC	118	ASP	ALA	conflict	UNP O66529
KC	120	GLU	THR	conflict	UNP O66529
KC	123	GLU	GLN	conflict	UNP O66529
KC	127	CYS	ARG	conflict	UNP O66529
KC	131	GLU	LYS	conflict	UNP O66529
KC	155	LEU	-	expression tag	UNP O66529
KC	156	GLU	-	expression tag	UNP O66529
KC	157	HIS	-	expression tag	UNP O66529
KC	158	HIS	-	expression tag	UNP O66529
KC	159	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
KC	160	HIS	-	expression tag	UNP O66529
KC	161	HIS	-	expression tag	UNP O66529
KD	2	GLU	GLN	conflict	UNP O66529
KD	28	GLY	ASP	conflict	UNP O66529
KD	52	CYS	ARG	conflict	UNP O66529
KD	83	GLU	ARG	conflict	UNP O66529
KD	86	GLU	THR	conflict	UNP O66529
KD	112	SER	THR	conflict	UNP O66529
KD	115	ASP	VAL	conflict	UNP O66529
KD	118	ASP	ALA	conflict	UNP O66529
KD	120	GLU	THR	conflict	UNP O66529
KD	123	GLU	GLN	conflict	UNP O66529
KD	127	CYS	ARG	conflict	UNP O66529
KD	131	GLU	LYS	conflict	UNP O66529
KD	155	LEU	-	expression tag	UNP O66529
KD	156	GLU	-	expression tag	UNP O66529
KD	157	HIS	-	expression tag	UNP O66529
KD	158	HIS	-	expression tag	UNP O66529
KD	159	HIS	-	expression tag	UNP O66529
KD	160	HIS	-	expression tag	UNP O66529
KD	161	HIS	-	expression tag	UNP O66529
KE	2	GLU	GLN	conflict	UNP O66529
KE	28	GLY	ASP	conflict	UNP O66529
KE	52	CYS	ARG	conflict	UNP O66529
KE	83	GLU	ARG	conflict	UNP O66529
KE	86	GLU	THR	conflict	UNP O66529
KE	112	SER	THR	conflict	UNP O66529
KE	115	ASP	VAL	conflict	UNP O66529
KE	118	ASP	ALA	conflict	UNP O66529
KE	120	GLU	THR	conflict	UNP O66529
KE	123	GLU	GLN	conflict	UNP O66529
KE	127	CYS	ARG	conflict	UNP O66529
KE	131	GLU	LYS	conflict	UNP O66529
KE	155	LEU	-	expression tag	UNP O66529
KE	156	GLU	-	expression tag	UNP O66529
KE	157	HIS	-	expression tag	UNP O66529
KE	158	HIS	-	expression tag	UNP O66529
KE	159	HIS	-	expression tag	UNP O66529
KE	160	HIS	-	expression tag	UNP O66529
KE	161	HIS	-	expression tag	UNP O66529
KX	2	GLU	GLN	conflict	UNP O66529
KX	28	GLY	ASP	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
KX	52	CYS	ARG	conflict	UNP O66529
KX	83	GLU	ARG	conflict	UNP O66529
KX	86	GLU	THR	conflict	UNP O66529
KX	112	SER	THR	conflict	UNP O66529
KX	115	ASP	VAL	conflict	UNP O66529
KX	118	ASP	ALA	conflict	UNP O66529
KX	120	GLU	THR	conflict	UNP O66529
KX	123	GLU	GLN	conflict	UNP O66529
KX	127	CYS	ARG	conflict	UNP O66529
KX	131	GLU	LYS	conflict	UNP O66529
KX	155	LEU	-	expression tag	UNP O66529
KX	156	GLU	-	expression tag	UNP O66529
KX	157	HIS	-	expression tag	UNP O66529
KX	158	HIS	-	expression tag	UNP O66529
KX	159	HIS	-	expression tag	UNP O66529
KX	160	HIS	-	expression tag	UNP O66529
KX	161	HIS	-	expression tag	UNP O66529
LA	2	GLU	GLN	conflict	UNP O66529
LA	28	GLY	ASP	conflict	UNP O66529
LA	52	CYS	ARG	conflict	UNP O66529
LA	83	GLU	ARG	conflict	UNP O66529
LA	86	GLU	THR	conflict	UNP O66529
LA	112	SER	THR	conflict	UNP O66529
LA	115	ASP	VAL	conflict	UNP O66529
LA	118	ASP	ALA	conflict	UNP O66529
LA	120	GLU	THR	conflict	UNP O66529
LA	123	GLU	GLN	conflict	UNP O66529
LA	127	CYS	ARG	conflict	UNP O66529
LA	131	GLU	LYS	conflict	UNP O66529
LA	155	LEU	-	expression tag	UNP O66529
LA	156	GLU	-	expression tag	UNP O66529
LA	157	HIS	-	expression tag	UNP O66529
LA	158	HIS	-	expression tag	UNP O66529
LA	159	HIS	-	expression tag	UNP O66529
LA	160	HIS	-	expression tag	UNP O66529
LA	161	HIS	-	expression tag	UNP O66529
LB	2	GLU	GLN	conflict	UNP O66529
LB	28	GLY	ASP	conflict	UNP O66529
LB	52	CYS	ARG	conflict	UNP O66529
LB	83	GLU	ARG	conflict	UNP O66529
LB	86	GLU	THR	conflict	UNP O66529
LB	112	SER	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LB	115	ASP	VAL	conflict	UNP O66529
LB	118	ASP	ALA	conflict	UNP O66529
LB	120	GLU	THR	conflict	UNP O66529
LB	123	GLU	GLN	conflict	UNP O66529
LB	127	CYS	ARG	conflict	UNP O66529
LB	131	GLU	LYS	conflict	UNP O66529
LB	155	LEU	-	expression tag	UNP O66529
LB	156	GLU	-	expression tag	UNP O66529
LB	157	HIS	-	expression tag	UNP O66529
LB	158	HIS	-	expression tag	UNP O66529
LB	159	HIS	-	expression tag	UNP O66529
LB	160	HIS	-	expression tag	UNP O66529
LB	161	HIS	-	expression tag	UNP O66529
LC	2	GLU	GLN	conflict	UNP O66529
LC	28	GLY	ASP	conflict	UNP O66529
LC	52	CYS	ARG	conflict	UNP O66529
LC	83	GLU	ARG	conflict	UNP O66529
LC	86	GLU	THR	conflict	UNP O66529
LC	112	SER	THR	conflict	UNP O66529
LC	115	ASP	VAL	conflict	UNP O66529
LC	118	ASP	ALA	conflict	UNP O66529
LC	120	GLU	THR	conflict	UNP O66529
LC	123	GLU	GLN	conflict	UNP O66529
LC	127	CYS	ARG	conflict	UNP O66529
LC	131	GLU	LYS	conflict	UNP O66529
LC	155	LEU	-	expression tag	UNP O66529
LC	156	GLU	-	expression tag	UNP O66529
LC	157	HIS	-	expression tag	UNP O66529
LC	158	HIS	-	expression tag	UNP O66529
LC	159	HIS	-	expression tag	UNP O66529
LC	160	HIS	-	expression tag	UNP O66529
LC	161	HIS	-	expression tag	UNP O66529
LD	2	GLU	GLN	conflict	UNP O66529
LD	28	GLY	ASP	conflict	UNP O66529
LD	52	CYS	ARG	conflict	UNP O66529
LD	83	GLU	ARG	conflict	UNP O66529
LD	86	GLU	THR	conflict	UNP O66529
LD	112	SER	THR	conflict	UNP O66529
LD	115	ASP	VAL	conflict	UNP O66529
LD	118	ASP	ALA	conflict	UNP O66529
LD	120	GLU	THR	conflict	UNP O66529
LD	123	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LD	127	CYS	ARG	conflict	UNP O66529
LD	131	GLU	LYS	conflict	UNP O66529
LD	155	LEU	-	expression tag	UNP O66529
LD	156	GLU	-	expression tag	UNP O66529
LD	157	HIS	-	expression tag	UNP O66529
LD	158	HIS	-	expression tag	UNP O66529
LD	159	HIS	-	expression tag	UNP O66529
LD	160	HIS	-	expression tag	UNP O66529
LD	161	HIS	-	expression tag	UNP O66529
LE	2	GLU	GLN	conflict	UNP O66529
LE	28	GLY	ASP	conflict	UNP O66529
LE	52	CYS	ARG	conflict	UNP O66529
LE	83	GLU	ARG	conflict	UNP O66529
LE	86	GLU	THR	conflict	UNP O66529
LE	112	SER	THR	conflict	UNP O66529
LE	115	ASP	VAL	conflict	UNP O66529
LE	118	ASP	ALA	conflict	UNP O66529
LE	120	GLU	THR	conflict	UNP O66529
LE	123	GLU	GLN	conflict	UNP O66529
LE	127	CYS	ARG	conflict	UNP O66529
LE	131	GLU	LYS	conflict	UNP O66529
LE	155	LEU	-	expression tag	UNP O66529
LE	156	GLU	-	expression tag	UNP O66529
LE	157	HIS	-	expression tag	UNP O66529
LE	158	HIS	-	expression tag	UNP O66529
LE	159	HIS	-	expression tag	UNP O66529
LE	160	HIS	-	expression tag	UNP O66529
LE	161	HIS	-	expression tag	UNP O66529
LX	2	GLU	GLN	conflict	UNP O66529
LX	28	GLY	ASP	conflict	UNP O66529
LX	52	CYS	ARG	conflict	UNP O66529
LX	83	GLU	ARG	conflict	UNP O66529
LX	86	GLU	THR	conflict	UNP O66529
LX	112	SER	THR	conflict	UNP O66529
LX	115	ASP	VAL	conflict	UNP O66529
LX	118	ASP	ALA	conflict	UNP O66529
LX	120	GLU	THR	conflict	UNP O66529
LX	123	GLU	GLN	conflict	UNP O66529
LX	127	CYS	ARG	conflict	UNP O66529
LX	131	GLU	LYS	conflict	UNP O66529
LX	155	LEU	-	expression tag	UNP O66529
LX	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LX	157	HIS	-	expression tag	UNP O66529
LX	158	HIS	-	expression tag	UNP O66529
LX	159	HIS	-	expression tag	UNP O66529
LX	160	HIS	-	expression tag	UNP O66529
LX	161	HIS	-	expression tag	UNP O66529
MA	2	GLU	GLN	conflict	UNP O66529
MA	28	GLY	ASP	conflict	UNP O66529
MA	52	CYS	ARG	conflict	UNP O66529
MA	83	GLU	ARG	conflict	UNP O66529
MA	86	GLU	THR	conflict	UNP O66529
MA	112	SER	THR	conflict	UNP O66529
MA	115	ASP	VAL	conflict	UNP O66529
MA	118	ASP	ALA	conflict	UNP O66529
MA	120	GLU	THR	conflict	UNP O66529
MA	123	GLU	GLN	conflict	UNP O66529
MA	127	CYS	ARG	conflict	UNP O66529
MA	131	GLU	LYS	conflict	UNP O66529
MA	155	LEU	-	expression tag	UNP O66529
MA	156	GLU	-	expression tag	UNP O66529
MA	157	HIS	-	expression tag	UNP O66529
MA	158	HIS	-	expression tag	UNP O66529
MA	159	HIS	-	expression tag	UNP O66529
MA	160	HIS	-	expression tag	UNP O66529
MA	161	HIS	-	expression tag	UNP O66529
MB	2	GLU	GLN	conflict	UNP O66529
MB	28	GLY	ASP	conflict	UNP O66529
MB	52	CYS	ARG	conflict	UNP O66529
MB	83	GLU	ARG	conflict	UNP O66529
MB	86	GLU	THR	conflict	UNP O66529
MB	112	SER	THR	conflict	UNP O66529
MB	115	ASP	VAL	conflict	UNP O66529
MB	118	ASP	ALA	conflict	UNP O66529
MB	120	GLU	THR	conflict	UNP O66529
MB	123	GLU	GLN	conflict	UNP O66529
MB	127	CYS	ARG	conflict	UNP O66529
MB	131	GLU	LYS	conflict	UNP O66529
MB	155	LEU	-	expression tag	UNP O66529
MB	156	GLU	-	expression tag	UNP O66529
MB	157	HIS	-	expression tag	UNP O66529
MB	158	HIS	-	expression tag	UNP O66529
MB	159	HIS	-	expression tag	UNP O66529
MB	160	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
MB	161	HIS	-	expression tag	UNP O66529
MC	2	GLU	GLN	conflict	UNP O66529
MC	28	GLY	ASP	conflict	UNP O66529
MC	52	CYS	ARG	conflict	UNP O66529
MC	83	GLU	ARG	conflict	UNP O66529
MC	86	GLU	THR	conflict	UNP O66529
MC	112	SER	THR	conflict	UNP O66529
MC	115	ASP	VAL	conflict	UNP O66529
MC	118	ASP	ALA	conflict	UNP O66529
MC	120	GLU	THR	conflict	UNP O66529
MC	123	GLU	GLN	conflict	UNP O66529
MC	127	CYS	ARG	conflict	UNP O66529
MC	131	GLU	LYS	conflict	UNP O66529
MC	155	LEU	-	expression tag	UNP O66529
MC	156	GLU	-	expression tag	UNP O66529
MC	157	HIS	-	expression tag	UNP O66529
MC	158	HIS	-	expression tag	UNP O66529
MC	159	HIS	-	expression tag	UNP O66529
MC	160	HIS	-	expression tag	UNP O66529
MC	161	HIS	-	expression tag	UNP O66529
MD	2	GLU	GLN	conflict	UNP O66529
MD	28	GLY	ASP	conflict	UNP O66529
MD	52	CYS	ARG	conflict	UNP O66529
MD	83	GLU	ARG	conflict	UNP O66529
MD	86	GLU	THR	conflict	UNP O66529
MD	112	SER	THR	conflict	UNP O66529
MD	115	ASP	VAL	conflict	UNP O66529
MD	118	ASP	ALA	conflict	UNP O66529
MD	120	GLU	THR	conflict	UNP O66529
MD	123	GLU	GLN	conflict	UNP O66529
MD	127	CYS	ARG	conflict	UNP O66529
MD	131	GLU	LYS	conflict	UNP O66529
MD	155	LEU	-	expression tag	UNP O66529
MD	156	GLU	-	expression tag	UNP O66529
MD	157	HIS	-	expression tag	UNP O66529
MD	158	HIS	-	expression tag	UNP O66529
MD	159	HIS	-	expression tag	UNP O66529
MD	160	HIS	-	expression tag	UNP O66529
MD	161	HIS	-	expression tag	UNP O66529
ME	2	GLU	GLN	conflict	UNP O66529
ME	28	GLY	ASP	conflict	UNP O66529
ME	52	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ME	83	GLU	ARG	conflict	UNP O66529
ME	86	GLU	THR	conflict	UNP O66529
ME	112	SER	THR	conflict	UNP O66529
ME	115	ASP	VAL	conflict	UNP O66529
ME	118	ASP	ALA	conflict	UNP O66529
ME	120	GLU	THR	conflict	UNP O66529
ME	123	GLU	GLN	conflict	UNP O66529
ME	127	CYS	ARG	conflict	UNP O66529
ME	131	GLU	LYS	conflict	UNP O66529
ME	155	LEU	-	expression tag	UNP O66529
ME	156	GLU	-	expression tag	UNP O66529
ME	157	HIS	-	expression tag	UNP O66529
ME	158	HIS	-	expression tag	UNP O66529
ME	159	HIS	-	expression tag	UNP O66529
ME	160	HIS	-	expression tag	UNP O66529
ME	161	HIS	-	expression tag	UNP O66529
MX	2	GLU	GLN	conflict	UNP O66529
MX	28	GLY	ASP	conflict	UNP O66529
MX	52	CYS	ARG	conflict	UNP O66529
MX	83	GLU	ARG	conflict	UNP O66529
MX	86	GLU	THR	conflict	UNP O66529
MX	112	SER	THR	conflict	UNP O66529
MX	115	ASP	VAL	conflict	UNP O66529
MX	118	ASP	ALA	conflict	UNP O66529
MX	120	GLU	THR	conflict	UNP O66529
MX	123	GLU	GLN	conflict	UNP O66529
MX	127	CYS	ARG	conflict	UNP O66529
MX	131	GLU	LYS	conflict	UNP O66529
MX	155	LEU	-	expression tag	UNP O66529
MX	156	GLU	-	expression tag	UNP O66529
MX	157	HIS	-	expression tag	UNP O66529
MX	158	HIS	-	expression tag	UNP O66529
MX	159	HIS	-	expression tag	UNP O66529
MX	160	HIS	-	expression tag	UNP O66529
MX	161	HIS	-	expression tag	UNP O66529
NA	2	GLU	GLN	conflict	UNP O66529
NA	28	GLY	ASP	conflict	UNP O66529
NA	52	CYS	ARG	conflict	UNP O66529
NA	83	GLU	ARG	conflict	UNP O66529
NA	86	GLU	THR	conflict	UNP O66529
NA	112	SER	THR	conflict	UNP O66529
NA	115	ASP	VAL	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
NA	118	ASP	ALA	conflict	UNP O66529
NA	120	GLU	THR	conflict	UNP O66529
NA	123	GLU	GLN	conflict	UNP O66529
NA	127	CYS	ARG	conflict	UNP O66529
NA	131	GLU	LYS	conflict	UNP O66529
NA	155	LEU	-	expression tag	UNP O66529
NA	156	GLU	-	expression tag	UNP O66529
NA	157	HIS	-	expression tag	UNP O66529
NA	158	HIS	-	expression tag	UNP O66529
NA	159	HIS	-	expression tag	UNP O66529
NA	160	HIS	-	expression tag	UNP O66529
NA	161	HIS	-	expression tag	UNP O66529
NB	2	GLU	GLN	conflict	UNP O66529
NB	28	GLY	ASP	conflict	UNP O66529
NB	52	CYS	ARG	conflict	UNP O66529
NB	83	GLU	ARG	conflict	UNP O66529
NB	86	GLU	THR	conflict	UNP O66529
NB	112	SER	THR	conflict	UNP O66529
NB	115	ASP	VAL	conflict	UNP O66529
NB	118	ASP	ALA	conflict	UNP O66529
NB	120	GLU	THR	conflict	UNP O66529
NB	123	GLU	GLN	conflict	UNP O66529
NB	127	CYS	ARG	conflict	UNP O66529
NB	131	GLU	LYS	conflict	UNP O66529
NB	155	LEU	-	expression tag	UNP O66529
NB	156	GLU	-	expression tag	UNP O66529
NB	157	HIS	-	expression tag	UNP O66529
NB	158	HIS	-	expression tag	UNP O66529
NB	159	HIS	-	expression tag	UNP O66529
NB	160	HIS	-	expression tag	UNP O66529
NB	161	HIS	-	expression tag	UNP O66529
NC	2	GLU	GLN	conflict	UNP O66529
NC	28	GLY	ASP	conflict	UNP O66529
NC	52	CYS	ARG	conflict	UNP O66529
NC	83	GLU	ARG	conflict	UNP O66529
NC	86	GLU	THR	conflict	UNP O66529
NC	112	SER	THR	conflict	UNP O66529
NC	115	ASP	VAL	conflict	UNP O66529
NC	118	ASP	ALA	conflict	UNP O66529
NC	120	GLU	THR	conflict	UNP O66529
NC	123	GLU	GLN	conflict	UNP O66529
NC	127	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
NC	131	GLU	LYS	conflict	UNP O66529
NC	155	LEU	-	expression tag	UNP O66529
NC	156	GLU	-	expression tag	UNP O66529
NC	157	HIS	-	expression tag	UNP O66529
NC	158	HIS	-	expression tag	UNP O66529
NC	159	HIS	-	expression tag	UNP O66529
NC	160	HIS	-	expression tag	UNP O66529
NC	161	HIS	-	expression tag	UNP O66529
ND	2	GLU	GLN	conflict	UNP O66529
ND	28	GLY	ASP	conflict	UNP O66529
ND	52	CYS	ARG	conflict	UNP O66529
ND	83	GLU	ARG	conflict	UNP O66529
ND	86	GLU	THR	conflict	UNP O66529
ND	112	SER	THR	conflict	UNP O66529
ND	115	ASP	VAL	conflict	UNP O66529
ND	118	ASP	ALA	conflict	UNP O66529
ND	120	GLU	THR	conflict	UNP O66529
ND	123	GLU	GLN	conflict	UNP O66529
ND	127	CYS	ARG	conflict	UNP O66529
ND	131	GLU	LYS	conflict	UNP O66529
ND	155	LEU	-	expression tag	UNP O66529
ND	156	GLU	-	expression tag	UNP O66529
ND	157	HIS	-	expression tag	UNP O66529
ND	158	HIS	-	expression tag	UNP O66529
ND	159	HIS	-	expression tag	UNP O66529
ND	160	HIS	-	expression tag	UNP O66529
ND	161	HIS	-	expression tag	UNP O66529
NE	2	GLU	GLN	conflict	UNP O66529
NE	28	GLY	ASP	conflict	UNP O66529
NE	52	CYS	ARG	conflict	UNP O66529
NE	83	GLU	ARG	conflict	UNP O66529
NE	86	GLU	THR	conflict	UNP O66529
NE	112	SER	THR	conflict	UNP O66529
NE	115	ASP	VAL	conflict	UNP O66529
NE	118	ASP	ALA	conflict	UNP O66529
NE	120	GLU	THR	conflict	UNP O66529
NE	123	GLU	GLN	conflict	UNP O66529
NE	127	CYS	ARG	conflict	UNP O66529
NE	131	GLU	LYS	conflict	UNP O66529
NE	155	LEU	-	expression tag	UNP O66529
NE	156	GLU	-	expression tag	UNP O66529
NE	157	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
NE	158	HIS	-	expression tag	UNP O66529
NE	159	HIS	-	expression tag	UNP O66529
NE	160	HIS	-	expression tag	UNP O66529
NE	161	HIS	-	expression tag	UNP O66529
NX	2	GLU	GLN	conflict	UNP O66529
NX	28	GLY	ASP	conflict	UNP O66529
NX	52	CYS	ARG	conflict	UNP O66529
NX	83	GLU	ARG	conflict	UNP O66529
NX	86	GLU	THR	conflict	UNP O66529
NX	112	SER	THR	conflict	UNP O66529
NX	115	ASP	VAL	conflict	UNP O66529
NX	118	ASP	ALA	conflict	UNP O66529
NX	120	GLU	THR	conflict	UNP O66529
NX	123	GLU	GLN	conflict	UNP O66529
NX	127	CYS	ARG	conflict	UNP O66529
NX	131	GLU	LYS	conflict	UNP O66529
NX	155	LEU	-	expression tag	UNP O66529
NX	156	GLU	-	expression tag	UNP O66529
NX	157	HIS	-	expression tag	UNP O66529
NX	158	HIS	-	expression tag	UNP O66529
NX	159	HIS	-	expression tag	UNP O66529
NX	160	HIS	-	expression tag	UNP O66529
NX	161	HIS	-	expression tag	UNP O66529
OA	2	GLU	GLN	conflict	UNP O66529
OA	28	GLY	ASP	conflict	UNP O66529
OA	52	CYS	ARG	conflict	UNP O66529
OA	83	GLU	ARG	conflict	UNP O66529
OA	86	GLU	THR	conflict	UNP O66529
OA	112	SER	THR	conflict	UNP O66529
OA	115	ASP	VAL	conflict	UNP O66529
OA	118	ASP	ALA	conflict	UNP O66529
OA	120	GLU	THR	conflict	UNP O66529
OA	123	GLU	GLN	conflict	UNP O66529
OA	127	CYS	ARG	conflict	UNP O66529
OA	131	GLU	LYS	conflict	UNP O66529
OA	155	LEU	-	expression tag	UNP O66529
OA	156	GLU	-	expression tag	UNP O66529
OA	157	HIS	-	expression tag	UNP O66529
OA	158	HIS	-	expression tag	UNP O66529
OA	159	HIS	-	expression tag	UNP O66529
OA	160	HIS	-	expression tag	UNP O66529
OA	161	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
OB	2	GLU	GLN	conflict	UNP O66529
OB	28	GLY	ASP	conflict	UNP O66529
OB	52	CYS	ARG	conflict	UNP O66529
OB	83	GLU	ARG	conflict	UNP O66529
OB	86	GLU	THR	conflict	UNP O66529
OB	112	SER	THR	conflict	UNP O66529
OB	115	ASP	VAL	conflict	UNP O66529
OB	118	ASP	ALA	conflict	UNP O66529
OB	120	GLU	THR	conflict	UNP O66529
OB	123	GLU	GLN	conflict	UNP O66529
OB	127	CYS	ARG	conflict	UNP O66529
OB	131	GLU	LYS	conflict	UNP O66529
OB	155	LEU	-	expression tag	UNP O66529
OB	156	GLU	-	expression tag	UNP O66529
OB	157	HIS	-	expression tag	UNP O66529
OB	158	HIS	-	expression tag	UNP O66529
OB	159	HIS	-	expression tag	UNP O66529
OB	160	HIS	-	expression tag	UNP O66529
OB	161	HIS	-	expression tag	UNP O66529
OC	2	GLU	GLN	conflict	UNP O66529
OC	28	GLY	ASP	conflict	UNP O66529
OC	52	CYS	ARG	conflict	UNP O66529
OC	83	GLU	ARG	conflict	UNP O66529
OC	86	GLU	THR	conflict	UNP O66529
OC	112	SER	THR	conflict	UNP O66529
OC	115	ASP	VAL	conflict	UNP O66529
OC	118	ASP	ALA	conflict	UNP O66529
OC	120	GLU	THR	conflict	UNP O66529
OC	123	GLU	GLN	conflict	UNP O66529
OC	127	CYS	ARG	conflict	UNP O66529
OC	131	GLU	LYS	conflict	UNP O66529
OC	155	LEU	-	expression tag	UNP O66529
OC	156	GLU	-	expression tag	UNP O66529
OC	157	HIS	-	expression tag	UNP O66529
OC	158	HIS	-	expression tag	UNP O66529
OC	159	HIS	-	expression tag	UNP O66529
OC	160	HIS	-	expression tag	UNP O66529
OC	161	HIS	-	expression tag	UNP O66529
OD	2	GLU	GLN	conflict	UNP O66529
OD	28	GLY	ASP	conflict	UNP O66529
OD	52	CYS	ARG	conflict	UNP O66529
OD	83	GLU	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
OD	86	GLU	THR	conflict	UNP O66529
OD	112	SER	THR	conflict	UNP O66529
OD	115	ASP	VAL	conflict	UNP O66529
OD	118	ASP	ALA	conflict	UNP O66529
OD	120	GLU	THR	conflict	UNP O66529
OD	123	GLU	GLN	conflict	UNP O66529
OD	127	CYS	ARG	conflict	UNP O66529
OD	131	GLU	LYS	conflict	UNP O66529
OD	155	LEU	-	expression tag	UNP O66529
OD	156	GLU	-	expression tag	UNP O66529
OD	157	HIS	-	expression tag	UNP O66529
OD	158	HIS	-	expression tag	UNP O66529
OD	159	HIS	-	expression tag	UNP O66529
OD	160	HIS	-	expression tag	UNP O66529
OD	161	HIS	-	expression tag	UNP O66529
OE	2	GLU	GLN	conflict	UNP O66529
OE	28	GLY	ASP	conflict	UNP O66529
OE	52	CYS	ARG	conflict	UNP O66529
OE	83	GLU	ARG	conflict	UNP O66529
OE	86	GLU	THR	conflict	UNP O66529
OE	112	SER	THR	conflict	UNP O66529
OE	115	ASP	VAL	conflict	UNP O66529
OE	118	ASP	ALA	conflict	UNP O66529
OE	120	GLU	THR	conflict	UNP O66529
OE	123	GLU	GLN	conflict	UNP O66529
OE	127	CYS	ARG	conflict	UNP O66529
OE	131	GLU	LYS	conflict	UNP O66529
OE	155	LEU	-	expression tag	UNP O66529
OE	156	GLU	-	expression tag	UNP O66529
OE	157	HIS	-	expression tag	UNP O66529
OE	158	HIS	-	expression tag	UNP O66529
OE	159	HIS	-	expression tag	UNP O66529
OE	160	HIS	-	expression tag	UNP O66529
OE	161	HIS	-	expression tag	UNP O66529
OX	2	GLU	GLN	conflict	UNP O66529
OX	28	GLY	ASP	conflict	UNP O66529
OX	52	CYS	ARG	conflict	UNP O66529
OX	83	GLU	ARG	conflict	UNP O66529
OX	86	GLU	THR	conflict	UNP O66529
OX	112	SER	THR	conflict	UNP O66529
OX	115	ASP	VAL	conflict	UNP O66529
OX	118	ASP	ALA	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
OX	120	GLU	THR	conflict	UNP O66529
OX	123	GLU	GLN	conflict	UNP O66529
OX	127	CYS	ARG	conflict	UNP O66529
OX	131	GLU	LYS	conflict	UNP O66529
OX	155	LEU	-	expression tag	UNP O66529
OX	156	GLU	-	expression tag	UNP O66529
OX	157	HIS	-	expression tag	UNP O66529
OX	158	HIS	-	expression tag	UNP O66529
OX	159	HIS	-	expression tag	UNP O66529
OX	160	HIS	-	expression tag	UNP O66529
OX	161	HIS	-	expression tag	UNP O66529
PA	2	GLU	GLN	conflict	UNP O66529
PA	28	GLY	ASP	conflict	UNP O66529
PA	52	CYS	ARG	conflict	UNP O66529
PA	83	GLU	ARG	conflict	UNP O66529
PA	86	GLU	THR	conflict	UNP O66529
PA	112	SER	THR	conflict	UNP O66529
PA	115	ASP	VAL	conflict	UNP O66529
PA	118	ASP	ALA	conflict	UNP O66529
PA	120	GLU	THR	conflict	UNP O66529
PA	123	GLU	GLN	conflict	UNP O66529
PA	127	CYS	ARG	conflict	UNP O66529
PA	131	GLU	LYS	conflict	UNP O66529
PA	155	LEU	-	expression tag	UNP O66529
PA	156	GLU	-	expression tag	UNP O66529
PA	157	HIS	-	expression tag	UNP O66529
PA	158	HIS	-	expression tag	UNP O66529
PA	159	HIS	-	expression tag	UNP O66529
PA	160	HIS	-	expression tag	UNP O66529
PA	161	HIS	-	expression tag	UNP O66529
PB	2	GLU	GLN	conflict	UNP O66529
PB	28	GLY	ASP	conflict	UNP O66529
PB	52	CYS	ARG	conflict	UNP O66529
PB	83	GLU	ARG	conflict	UNP O66529
PB	86	GLU	THR	conflict	UNP O66529
PB	112	SER	THR	conflict	UNP O66529
PB	115	ASP	VAL	conflict	UNP O66529
PB	118	ASP	ALA	conflict	UNP O66529
PB	120	GLU	THR	conflict	UNP O66529
PB	123	GLU	GLN	conflict	UNP O66529
PB	127	CYS	ARG	conflict	UNP O66529
PB	131	GLU	LYS	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
PB	155	LEU	-	expression tag	UNP O66529
PB	156	GLU	-	expression tag	UNP O66529
PB	157	HIS	-	expression tag	UNP O66529
PB	158	HIS	-	expression tag	UNP O66529
PB	159	HIS	-	expression tag	UNP O66529
PB	160	HIS	-	expression tag	UNP O66529
PB	161	HIS	-	expression tag	UNP O66529
PC	2	GLU	GLN	conflict	UNP O66529
PC	28	GLY	ASP	conflict	UNP O66529
PC	52	CYS	ARG	conflict	UNP O66529
PC	83	GLU	ARG	conflict	UNP O66529
PC	86	GLU	THR	conflict	UNP O66529
PC	112	SER	THR	conflict	UNP O66529
PC	115	ASP	VAL	conflict	UNP O66529
PC	118	ASP	ALA	conflict	UNP O66529
PC	120	GLU	THR	conflict	UNP O66529
PC	123	GLU	GLN	conflict	UNP O66529
PC	127	CYS	ARG	conflict	UNP O66529
PC	131	GLU	LYS	conflict	UNP O66529
PC	155	LEU	-	expression tag	UNP O66529
PC	156	GLU	-	expression tag	UNP O66529
PC	157	HIS	-	expression tag	UNP O66529
PC	158	HIS	-	expression tag	UNP O66529
PC	159	HIS	-	expression tag	UNP O66529
PC	160	HIS	-	expression tag	UNP O66529
PC	161	HIS	-	expression tag	UNP O66529
PD	2	GLU	GLN	conflict	UNP O66529
PD	28	GLY	ASP	conflict	UNP O66529
PD	52	CYS	ARG	conflict	UNP O66529
PD	83	GLU	ARG	conflict	UNP O66529
PD	86	GLU	THR	conflict	UNP O66529
PD	112	SER	THR	conflict	UNP O66529
PD	115	ASP	VAL	conflict	UNP O66529
PD	118	ASP	ALA	conflict	UNP O66529
PD	120	GLU	THR	conflict	UNP O66529
PD	123	GLU	GLN	conflict	UNP O66529
PD	127	CYS	ARG	conflict	UNP O66529
PD	131	GLU	LYS	conflict	UNP O66529
PD	155	LEU	-	expression tag	UNP O66529
PD	156	GLU	-	expression tag	UNP O66529
PD	157	HIS	-	expression tag	UNP O66529
PD	158	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
PD	159	HIS	-	expression tag	UNP O66529
PD	160	HIS	-	expression tag	UNP O66529
PD	161	HIS	-	expression tag	UNP O66529
PE	2	GLU	GLN	conflict	UNP O66529
PE	28	GLY	ASP	conflict	UNP O66529
PE	52	CYS	ARG	conflict	UNP O66529
PE	83	GLU	ARG	conflict	UNP O66529
PE	86	GLU	THR	conflict	UNP O66529
PE	112	SER	THR	conflict	UNP O66529
PE	115	ASP	VAL	conflict	UNP O66529
PE	118	ASP	ALA	conflict	UNP O66529
PE	120	GLU	THR	conflict	UNP O66529
PE	123	GLU	GLN	conflict	UNP O66529
PE	127	CYS	ARG	conflict	UNP O66529
PE	131	GLU	LYS	conflict	UNP O66529
PE	155	LEU	-	expression tag	UNP O66529
PE	156	GLU	-	expression tag	UNP O66529
PE	157	HIS	-	expression tag	UNP O66529
PE	158	HIS	-	expression tag	UNP O66529
PE	159	HIS	-	expression tag	UNP O66529
PE	160	HIS	-	expression tag	UNP O66529
PE	161	HIS	-	expression tag	UNP O66529
PX	2	GLU	GLN	conflict	UNP O66529
PX	28	GLY	ASP	conflict	UNP O66529
PX	52	CYS	ARG	conflict	UNP O66529
PX	83	GLU	ARG	conflict	UNP O66529
PX	86	GLU	THR	conflict	UNP O66529
PX	112	SER	THR	conflict	UNP O66529
PX	115	ASP	VAL	conflict	UNP O66529
PX	118	ASP	ALA	conflict	UNP O66529
PX	120	GLU	THR	conflict	UNP O66529
PX	123	GLU	GLN	conflict	UNP O66529
PX	127	CYS	ARG	conflict	UNP O66529
PX	131	GLU	LYS	conflict	UNP O66529
PX	155	LEU	-	expression tag	UNP O66529
PX	156	GLU	-	expression tag	UNP O66529
PX	157	HIS	-	expression tag	UNP O66529
PX	158	HIS	-	expression tag	UNP O66529
PX	159	HIS	-	expression tag	UNP O66529
PX	160	HIS	-	expression tag	UNP O66529
PX	161	HIS	-	expression tag	UNP O66529
QA	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
QA	28	GLY	ASP	conflict	UNP O66529
QA	52	CYS	ARG	conflict	UNP O66529
QA	83	GLU	ARG	conflict	UNP O66529
QA	86	GLU	THR	conflict	UNP O66529
QA	112	SER	THR	conflict	UNP O66529
QA	115	ASP	VAL	conflict	UNP O66529
QA	118	ASP	ALA	conflict	UNP O66529
QA	120	GLU	THR	conflict	UNP O66529
QA	123	GLU	GLN	conflict	UNP O66529
QA	127	CYS	ARG	conflict	UNP O66529
QA	131	GLU	LYS	conflict	UNP O66529
QA	155	LEU	-	expression tag	UNP O66529
QA	156	GLU	-	expression tag	UNP O66529
QA	157	HIS	-	expression tag	UNP O66529
QA	158	HIS	-	expression tag	UNP O66529
QA	159	HIS	-	expression tag	UNP O66529
QA	160	HIS	-	expression tag	UNP O66529
QA	161	HIS	-	expression tag	UNP O66529
QB	2	GLU	GLN	conflict	UNP O66529
QB	28	GLY	ASP	conflict	UNP O66529
QB	52	CYS	ARG	conflict	UNP O66529
QB	83	GLU	ARG	conflict	UNP O66529
QB	86	GLU	THR	conflict	UNP O66529
QB	112	SER	THR	conflict	UNP O66529
QB	115	ASP	VAL	conflict	UNP O66529
QB	118	ASP	ALA	conflict	UNP O66529
QB	120	GLU	THR	conflict	UNP O66529
QB	123	GLU	GLN	conflict	UNP O66529
QB	127	CYS	ARG	conflict	UNP O66529
QB	131	GLU	LYS	conflict	UNP O66529
QB	155	LEU	-	expression tag	UNP O66529
QB	156	GLU	-	expression tag	UNP O66529
QB	157	HIS	-	expression tag	UNP O66529
QB	158	HIS	-	expression tag	UNP O66529
QB	159	HIS	-	expression tag	UNP O66529
QB	160	HIS	-	expression tag	UNP O66529
QB	161	HIS	-	expression tag	UNP O66529
QC	2	GLU	GLN	conflict	UNP O66529
QC	28	GLY	ASP	conflict	UNP O66529
QC	52	CYS	ARG	conflict	UNP O66529
QC	83	GLU	ARG	conflict	UNP O66529
QC	86	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
QC	112	SER	THR	conflict	UNP O66529
QC	115	ASP	VAL	conflict	UNP O66529
QC	118	ASP	ALA	conflict	UNP O66529
QC	120	GLU	THR	conflict	UNP O66529
QC	123	GLU	GLN	conflict	UNP O66529
QC	127	CYS	ARG	conflict	UNP O66529
QC	131	GLU	LYS	conflict	UNP O66529
QC	155	LEU	-	expression tag	UNP O66529
QC	156	GLU	-	expression tag	UNP O66529
QC	157	HIS	-	expression tag	UNP O66529
QC	158	HIS	-	expression tag	UNP O66529
QC	159	HIS	-	expression tag	UNP O66529
QC	160	HIS	-	expression tag	UNP O66529
QC	161	HIS	-	expression tag	UNP O66529
QD	2	GLU	GLN	conflict	UNP O66529
QD	28	GLY	ASP	conflict	UNP O66529
QD	52	CYS	ARG	conflict	UNP O66529
QD	83	GLU	ARG	conflict	UNP O66529
QD	86	GLU	THR	conflict	UNP O66529
QD	112	SER	THR	conflict	UNP O66529
QD	115	ASP	VAL	conflict	UNP O66529
QD	118	ASP	ALA	conflict	UNP O66529
QD	120	GLU	THR	conflict	UNP O66529
QD	123	GLU	GLN	conflict	UNP O66529
QD	127	CYS	ARG	conflict	UNP O66529
QD	131	GLU	LYS	conflict	UNP O66529
QD	155	LEU	-	expression tag	UNP O66529
QD	156	GLU	-	expression tag	UNP O66529
QD	157	HIS	-	expression tag	UNP O66529
QD	158	HIS	-	expression tag	UNP O66529
QD	159	HIS	-	expression tag	UNP O66529
QD	160	HIS	-	expression tag	UNP O66529
QD	161	HIS	-	expression tag	UNP O66529
QE	2	GLU	GLN	conflict	UNP O66529
QE	28	GLY	ASP	conflict	UNP O66529
QE	52	CYS	ARG	conflict	UNP O66529
QE	83	GLU	ARG	conflict	UNP O66529
QE	86	GLU	THR	conflict	UNP O66529
QE	112	SER	THR	conflict	UNP O66529
QE	115	ASP	VAL	conflict	UNP O66529
QE	118	ASP	ALA	conflict	UNP O66529
QE	120	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
QE	123	GLU	GLN	conflict	UNP O66529
QE	127	CYS	ARG	conflict	UNP O66529
QE	131	GLU	LYS	conflict	UNP O66529
QE	155	LEU	-	expression tag	UNP O66529
QE	156	GLU	-	expression tag	UNP O66529
QE	157	HIS	-	expression tag	UNP O66529
QE	158	HIS	-	expression tag	UNP O66529
QE	159	HIS	-	expression tag	UNP O66529
QE	160	HIS	-	expression tag	UNP O66529
QE	161	HIS	-	expression tag	UNP O66529
QX	2	GLU	GLN	conflict	UNP O66529
QX	28	GLY	ASP	conflict	UNP O66529
QX	52	CYS	ARG	conflict	UNP O66529
QX	83	GLU	ARG	conflict	UNP O66529
QX	86	GLU	THR	conflict	UNP O66529
QX	112	SER	THR	conflict	UNP O66529
QX	115	ASP	VAL	conflict	UNP O66529
QX	118	ASP	ALA	conflict	UNP O66529
QX	120	GLU	THR	conflict	UNP O66529
QX	123	GLU	GLN	conflict	UNP O66529
QX	127	CYS	ARG	conflict	UNP O66529
QX	131	GLU	LYS	conflict	UNP O66529
QX	155	LEU	-	expression tag	UNP O66529
QX	156	GLU	-	expression tag	UNP O66529
QX	157	HIS	-	expression tag	UNP O66529
QX	158	HIS	-	expression tag	UNP O66529
QX	159	HIS	-	expression tag	UNP O66529
QX	160	HIS	-	expression tag	UNP O66529
QX	161	HIS	-	expression tag	UNP O66529
RA	2	GLU	GLN	conflict	UNP O66529
RA	28	GLY	ASP	conflict	UNP O66529
RA	52	CYS	ARG	conflict	UNP O66529
RA	83	GLU	ARG	conflict	UNP O66529
RA	86	GLU	THR	conflict	UNP O66529
RA	112	SER	THR	conflict	UNP O66529
RA	115	ASP	VAL	conflict	UNP O66529
RA	118	ASP	ALA	conflict	UNP O66529
RA	120	GLU	THR	conflict	UNP O66529
RA	123	GLU	GLN	conflict	UNP O66529
RA	127	CYS	ARG	conflict	UNP O66529
RA	131	GLU	LYS	conflict	UNP O66529
RA	155	LEU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
RA	156	GLU	-	expression tag	UNP O66529
RA	157	HIS	-	expression tag	UNP O66529
RA	158	HIS	-	expression tag	UNP O66529
RA	159	HIS	-	expression tag	UNP O66529
RA	160	HIS	-	expression tag	UNP O66529
RA	161	HIS	-	expression tag	UNP O66529
RB	2	GLU	GLN	conflict	UNP O66529
RB	28	GLY	ASP	conflict	UNP O66529
RB	52	CYS	ARG	conflict	UNP O66529
RB	83	GLU	ARG	conflict	UNP O66529
RB	86	GLU	THR	conflict	UNP O66529
RB	112	SER	THR	conflict	UNP O66529
RB	115	ASP	VAL	conflict	UNP O66529
RB	118	ASP	ALA	conflict	UNP O66529
RB	120	GLU	THR	conflict	UNP O66529
RB	123	GLU	GLN	conflict	UNP O66529
RB	127	CYS	ARG	conflict	UNP O66529
RB	131	GLU	LYS	conflict	UNP O66529
RB	155	LEU	-	expression tag	UNP O66529
RB	156	GLU	-	expression tag	UNP O66529
RB	157	HIS	-	expression tag	UNP O66529
RB	158	HIS	-	expression tag	UNP O66529
RB	159	HIS	-	expression tag	UNP O66529
RB	160	HIS	-	expression tag	UNP O66529
RB	161	HIS	-	expression tag	UNP O66529
RC	2	GLU	GLN	conflict	UNP O66529
RC	28	GLY	ASP	conflict	UNP O66529
RC	52	CYS	ARG	conflict	UNP O66529
RC	83	GLU	ARG	conflict	UNP O66529
RC	86	GLU	THR	conflict	UNP O66529
RC	112	SER	THR	conflict	UNP O66529
RC	115	ASP	VAL	conflict	UNP O66529
RC	118	ASP	ALA	conflict	UNP O66529
RC	120	GLU	THR	conflict	UNP O66529
RC	123	GLU	GLN	conflict	UNP O66529
RC	127	CYS	ARG	conflict	UNP O66529
RC	131	GLU	LYS	conflict	UNP O66529
RC	155	LEU	-	expression tag	UNP O66529
RC	156	GLU	-	expression tag	UNP O66529
RC	157	HIS	-	expression tag	UNP O66529
RC	158	HIS	-	expression tag	UNP O66529
RC	159	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
RC	160	HIS	-	expression tag	UNP O66529
RC	161	HIS	-	expression tag	UNP O66529
RD	2	GLU	GLN	conflict	UNP O66529
RD	28	GLY	ASP	conflict	UNP O66529
RD	52	CYS	ARG	conflict	UNP O66529
RD	83	GLU	ARG	conflict	UNP O66529
RD	86	GLU	THR	conflict	UNP O66529
RD	112	SER	THR	conflict	UNP O66529
RD	115	ASP	VAL	conflict	UNP O66529
RD	118	ASP	ALA	conflict	UNP O66529
RD	120	GLU	THR	conflict	UNP O66529
RD	123	GLU	GLN	conflict	UNP O66529
RD	127	CYS	ARG	conflict	UNP O66529
RD	131	GLU	LYS	conflict	UNP O66529
RD	155	LEU	-	expression tag	UNP O66529
RD	156	GLU	-	expression tag	UNP O66529
RD	157	HIS	-	expression tag	UNP O66529
RD	158	HIS	-	expression tag	UNP O66529
RD	159	HIS	-	expression tag	UNP O66529
RD	160	HIS	-	expression tag	UNP O66529
RD	161	HIS	-	expression tag	UNP O66529
RE	2	GLU	GLN	conflict	UNP O66529
RE	28	GLY	ASP	conflict	UNP O66529
RE	52	CYS	ARG	conflict	UNP O66529
RE	83	GLU	ARG	conflict	UNP O66529
RE	86	GLU	THR	conflict	UNP O66529
RE	112	SER	THR	conflict	UNP O66529
RE	115	ASP	VAL	conflict	UNP O66529
RE	118	ASP	ALA	conflict	UNP O66529
RE	120	GLU	THR	conflict	UNP O66529
RE	123	GLU	GLN	conflict	UNP O66529
RE	127	CYS	ARG	conflict	UNP O66529
RE	131	GLU	LYS	conflict	UNP O66529
RE	155	LEU	-	expression tag	UNP O66529
RE	156	GLU	-	expression tag	UNP O66529
RE	157	HIS	-	expression tag	UNP O66529
RE	158	HIS	-	expression tag	UNP O66529
RE	159	HIS	-	expression tag	UNP O66529
RE	160	HIS	-	expression tag	UNP O66529
RE	161	HIS	-	expression tag	UNP O66529
RX	2	GLU	GLN	conflict	UNP O66529
RX	28	GLY	ASP	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
RX	52	CYS	ARG	conflict	UNP O66529
RX	83	GLU	ARG	conflict	UNP O66529
RX	86	GLU	THR	conflict	UNP O66529
RX	112	SER	THR	conflict	UNP O66529
RX	115	ASP	VAL	conflict	UNP O66529
RX	118	ASP	ALA	conflict	UNP O66529
RX	120	GLU	THR	conflict	UNP O66529
RX	123	GLU	GLN	conflict	UNP O66529
RX	127	CYS	ARG	conflict	UNP O66529
RX	131	GLU	LYS	conflict	UNP O66529
RX	155	LEU	-	expression tag	UNP O66529
RX	156	GLU	-	expression tag	UNP O66529
RX	157	HIS	-	expression tag	UNP O66529
RX	158	HIS	-	expression tag	UNP O66529
RX	159	HIS	-	expression tag	UNP O66529
RX	160	HIS	-	expression tag	UNP O66529
RX	161	HIS	-	expression tag	UNP O66529
SA	2	GLU	GLN	conflict	UNP O66529
SA	28	GLY	ASP	conflict	UNP O66529
SA	52	CYS	ARG	conflict	UNP O66529
SA	83	GLU	ARG	conflict	UNP O66529
SA	86	GLU	THR	conflict	UNP O66529
SA	112	SER	THR	conflict	UNP O66529
SA	115	ASP	VAL	conflict	UNP O66529
SA	118	ASP	ALA	conflict	UNP O66529
SA	120	GLU	THR	conflict	UNP O66529
SA	123	GLU	GLN	conflict	UNP O66529
SA	127	CYS	ARG	conflict	UNP O66529
SA	131	GLU	LYS	conflict	UNP O66529
SA	155	LEU	-	expression tag	UNP O66529
SA	156	GLU	-	expression tag	UNP O66529
SA	157	HIS	-	expression tag	UNP O66529
SA	158	HIS	-	expression tag	UNP O66529
SA	159	HIS	-	expression tag	UNP O66529
SA	160	HIS	-	expression tag	UNP O66529
SA	161	HIS	-	expression tag	UNP O66529
SB	2	GLU	GLN	conflict	UNP O66529
SB	28	GLY	ASP	conflict	UNP O66529
SB	52	CYS	ARG	conflict	UNP O66529
SB	83	GLU	ARG	conflict	UNP O66529
SB	86	GLU	THR	conflict	UNP O66529
SB	112	SER	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
SB	115	ASP	VAL	conflict	UNP O66529
SB	118	ASP	ALA	conflict	UNP O66529
SB	120	GLU	THR	conflict	UNP O66529
SB	123	GLU	GLN	conflict	UNP O66529
SB	127	CYS	ARG	conflict	UNP O66529
SB	131	GLU	LYS	conflict	UNP O66529
SB	155	LEU	-	expression tag	UNP O66529
SB	156	GLU	-	expression tag	UNP O66529
SB	157	HIS	-	expression tag	UNP O66529
SB	158	HIS	-	expression tag	UNP O66529
SB	159	HIS	-	expression tag	UNP O66529
SB	160	HIS	-	expression tag	UNP O66529
SB	161	HIS	-	expression tag	UNP O66529
SC	2	GLU	GLN	conflict	UNP O66529
SC	28	GLY	ASP	conflict	UNP O66529
SC	52	CYS	ARG	conflict	UNP O66529
SC	83	GLU	ARG	conflict	UNP O66529
SC	86	GLU	THR	conflict	UNP O66529
SC	112	SER	THR	conflict	UNP O66529
SC	115	ASP	VAL	conflict	UNP O66529
SC	118	ASP	ALA	conflict	UNP O66529
SC	120	GLU	THR	conflict	UNP O66529
SC	123	GLU	GLN	conflict	UNP O66529
SC	127	CYS	ARG	conflict	UNP O66529
SC	131	GLU	LYS	conflict	UNP O66529
SC	155	LEU	-	expression tag	UNP O66529
SC	156	GLU	-	expression tag	UNP O66529
SC	157	HIS	-	expression tag	UNP O66529
SC	158	HIS	-	expression tag	UNP O66529
SC	159	HIS	-	expression tag	UNP O66529
SC	160	HIS	-	expression tag	UNP O66529
SC	161	HIS	-	expression tag	UNP O66529
SD	2	GLU	GLN	conflict	UNP O66529
SD	28	GLY	ASP	conflict	UNP O66529
SD	52	CYS	ARG	conflict	UNP O66529
SD	83	GLU	ARG	conflict	UNP O66529
SD	86	GLU	THR	conflict	UNP O66529
SD	112	SER	THR	conflict	UNP O66529
SD	115	ASP	VAL	conflict	UNP O66529
SD	118	ASP	ALA	conflict	UNP O66529
SD	120	GLU	THR	conflict	UNP O66529
SD	123	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
SD	127	CYS	ARG	conflict	UNP O66529
SD	131	GLU	LYS	conflict	UNP O66529
SD	155	LEU	-	expression tag	UNP O66529
SD	156	GLU	-	expression tag	UNP O66529
SD	157	HIS	-	expression tag	UNP O66529
SD	158	HIS	-	expression tag	UNP O66529
SD	159	HIS	-	expression tag	UNP O66529
SD	160	HIS	-	expression tag	UNP O66529
SD	161	HIS	-	expression tag	UNP O66529
SE	2	GLU	GLN	conflict	UNP O66529
SE	28	GLY	ASP	conflict	UNP O66529
SE	52	CYS	ARG	conflict	UNP O66529
SE	83	GLU	ARG	conflict	UNP O66529
SE	86	GLU	THR	conflict	UNP O66529
SE	112	SER	THR	conflict	UNP O66529
SE	115	ASP	VAL	conflict	UNP O66529
SE	118	ASP	ALA	conflict	UNP O66529
SE	120	GLU	THR	conflict	UNP O66529
SE	123	GLU	GLN	conflict	UNP O66529
SE	127	CYS	ARG	conflict	UNP O66529
SE	131	GLU	LYS	conflict	UNP O66529
SE	155	LEU	-	expression tag	UNP O66529
SE	156	GLU	-	expression tag	UNP O66529
SE	157	HIS	-	expression tag	UNP O66529
SE	158	HIS	-	expression tag	UNP O66529
SE	159	HIS	-	expression tag	UNP O66529
SE	160	HIS	-	expression tag	UNP O66529
SE	161	HIS	-	expression tag	UNP O66529
SX	2	GLU	GLN	conflict	UNP O66529
SX	28	GLY	ASP	conflict	UNP O66529
SX	52	CYS	ARG	conflict	UNP O66529
SX	83	GLU	ARG	conflict	UNP O66529
SX	86	GLU	THR	conflict	UNP O66529
SX	112	SER	THR	conflict	UNP O66529
SX	115	ASP	VAL	conflict	UNP O66529
SX	118	ASP	ALA	conflict	UNP O66529
SX	120	GLU	THR	conflict	UNP O66529
SX	123	GLU	GLN	conflict	UNP O66529
SX	127	CYS	ARG	conflict	UNP O66529
SX	131	GLU	LYS	conflict	UNP O66529
SX	155	LEU	-	expression tag	UNP O66529
SX	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
SX	157	HIS	-	expression tag	UNP O66529
SX	158	HIS	-	expression tag	UNP O66529
SX	159	HIS	-	expression tag	UNP O66529
SX	160	HIS	-	expression tag	UNP O66529
SX	161	HIS	-	expression tag	UNP O66529
TA	2	GLU	GLN	conflict	UNP O66529
TA	28	GLY	ASP	conflict	UNP O66529
TA	52	CYS	ARG	conflict	UNP O66529
TA	83	GLU	ARG	conflict	UNP O66529
TA	86	GLU	THR	conflict	UNP O66529
TA	112	SER	THR	conflict	UNP O66529
TA	115	ASP	VAL	conflict	UNP O66529
TA	118	ASP	ALA	conflict	UNP O66529
TA	120	GLU	THR	conflict	UNP O66529
TA	123	GLU	GLN	conflict	UNP O66529
TA	127	CYS	ARG	conflict	UNP O66529
TA	131	GLU	LYS	conflict	UNP O66529
TA	155	LEU	-	expression tag	UNP O66529
TA	156	GLU	-	expression tag	UNP O66529
TA	157	HIS	-	expression tag	UNP O66529
TA	158	HIS	-	expression tag	UNP O66529
TA	159	HIS	-	expression tag	UNP O66529
TA	160	HIS	-	expression tag	UNP O66529
TA	161	HIS	-	expression tag	UNP O66529
TB	2	GLU	GLN	conflict	UNP O66529
TB	28	GLY	ASP	conflict	UNP O66529
TB	52	CYS	ARG	conflict	UNP O66529
TB	83	GLU	ARG	conflict	UNP O66529
TB	86	GLU	THR	conflict	UNP O66529
TB	112	SER	THR	conflict	UNP O66529
TB	115	ASP	VAL	conflict	UNP O66529
TB	118	ASP	ALA	conflict	UNP O66529
TB	120	GLU	THR	conflict	UNP O66529
TB	123	GLU	GLN	conflict	UNP O66529
TB	127	CYS	ARG	conflict	UNP O66529
TB	131	GLU	LYS	conflict	UNP O66529
TB	155	LEU	-	expression tag	UNP O66529
TB	156	GLU	-	expression tag	UNP O66529
TB	157	HIS	-	expression tag	UNP O66529
TB	158	HIS	-	expression tag	UNP O66529
TB	159	HIS	-	expression tag	UNP O66529
TB	160	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
TB	161	HIS	-	expression tag	UNP O66529
TC	2	GLU	GLN	conflict	UNP O66529
TC	28	GLY	ASP	conflict	UNP O66529
TC	52	CYS	ARG	conflict	UNP O66529
TC	83	GLU	ARG	conflict	UNP O66529
TC	86	GLU	THR	conflict	UNP O66529
TC	112	SER	THR	conflict	UNP O66529
TC	115	ASP	VAL	conflict	UNP O66529
TC	118	ASP	ALA	conflict	UNP O66529
TC	120	GLU	THR	conflict	UNP O66529
TC	123	GLU	GLN	conflict	UNP O66529
TC	127	CYS	ARG	conflict	UNP O66529
TC	131	GLU	LYS	conflict	UNP O66529
TC	155	LEU	-	expression tag	UNP O66529
TC	156	GLU	-	expression tag	UNP O66529
TC	157	HIS	-	expression tag	UNP O66529
TC	158	HIS	-	expression tag	UNP O66529
TC	159	HIS	-	expression tag	UNP O66529
TC	160	HIS	-	expression tag	UNP O66529
TC	161	HIS	-	expression tag	UNP O66529
TD	2	GLU	GLN	conflict	UNP O66529
TD	28	GLY	ASP	conflict	UNP O66529
TD	52	CYS	ARG	conflict	UNP O66529
TD	83	GLU	ARG	conflict	UNP O66529
TD	86	GLU	THR	conflict	UNP O66529
TD	112	SER	THR	conflict	UNP O66529
TD	115	ASP	VAL	conflict	UNP O66529
TD	118	ASP	ALA	conflict	UNP O66529
TD	120	GLU	THR	conflict	UNP O66529
TD	123	GLU	GLN	conflict	UNP O66529
TD	127	CYS	ARG	conflict	UNP O66529
TD	131	GLU	LYS	conflict	UNP O66529
TD	155	LEU	-	expression tag	UNP O66529
TD	156	GLU	-	expression tag	UNP O66529
TD	157	HIS	-	expression tag	UNP O66529
TD	158	HIS	-	expression tag	UNP O66529
TD	159	HIS	-	expression tag	UNP O66529
TD	160	HIS	-	expression tag	UNP O66529
TD	161	HIS	-	expression tag	UNP O66529
TE	2	GLU	GLN	conflict	UNP O66529
TE	28	GLY	ASP	conflict	UNP O66529
TE	52	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
TE	83	GLU	ARG	conflict	UNP O66529
TE	86	GLU	THR	conflict	UNP O66529
TE	112	SER	THR	conflict	UNP O66529
TE	115	ASP	VAL	conflict	UNP O66529
TE	118	ASP	ALA	conflict	UNP O66529
TE	120	GLU	THR	conflict	UNP O66529
TE	123	GLU	GLN	conflict	UNP O66529
TE	127	CYS	ARG	conflict	UNP O66529
TE	131	GLU	LYS	conflict	UNP O66529
TE	155	LEU	-	expression tag	UNP O66529
TE	156	GLU	-	expression tag	UNP O66529
TE	157	HIS	-	expression tag	UNP O66529
TE	158	HIS	-	expression tag	UNP O66529
TE	159	HIS	-	expression tag	UNP O66529
TE	160	HIS	-	expression tag	UNP O66529
TE	161	HIS	-	expression tag	UNP O66529
TX	2	GLU	GLN	conflict	UNP O66529
TX	28	GLY	ASP	conflict	UNP O66529
TX	52	CYS	ARG	conflict	UNP O66529
TX	83	GLU	ARG	conflict	UNP O66529
TX	86	GLU	THR	conflict	UNP O66529
TX	112	SER	THR	conflict	UNP O66529
TX	115	ASP	VAL	conflict	UNP O66529
TX	118	ASP	ALA	conflict	UNP O66529
TX	120	GLU	THR	conflict	UNP O66529
TX	123	GLU	GLN	conflict	UNP O66529
TX	127	CYS	ARG	conflict	UNP O66529
TX	131	GLU	LYS	conflict	UNP O66529
TX	155	LEU	-	expression tag	UNP O66529
TX	156	GLU	-	expression tag	UNP O66529
TX	157	HIS	-	expression tag	UNP O66529
TX	158	HIS	-	expression tag	UNP O66529
TX	159	HIS	-	expression tag	UNP O66529
TX	160	HIS	-	expression tag	UNP O66529
TX	161	HIS	-	expression tag	UNP O66529
UA	2	GLU	GLN	conflict	UNP O66529
UA	28	GLY	ASP	conflict	UNP O66529
UA	52	CYS	ARG	conflict	UNP O66529
UA	83	GLU	ARG	conflict	UNP O66529
UA	86	GLU	THR	conflict	UNP O66529
UA	112	SER	THR	conflict	UNP O66529
UA	115	ASP	VAL	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
UA	118	ASP	ALA	conflict	UNP O66529
UA	120	GLU	THR	conflict	UNP O66529
UA	123	GLU	GLN	conflict	UNP O66529
UA	127	CYS	ARG	conflict	UNP O66529
UA	131	GLU	LYS	conflict	UNP O66529
UA	155	LEU	-	expression tag	UNP O66529
UA	156	GLU	-	expression tag	UNP O66529
UA	157	HIS	-	expression tag	UNP O66529
UA	158	HIS	-	expression tag	UNP O66529
UA	159	HIS	-	expression tag	UNP O66529
UA	160	HIS	-	expression tag	UNP O66529
UA	161	HIS	-	expression tag	UNP O66529
UB	2	GLU	GLN	conflict	UNP O66529
UB	28	GLY	ASP	conflict	UNP O66529
UB	52	CYS	ARG	conflict	UNP O66529
UB	83	GLU	ARG	conflict	UNP O66529
UB	86	GLU	THR	conflict	UNP O66529
UB	112	SER	THR	conflict	UNP O66529
UB	115	ASP	VAL	conflict	UNP O66529
UB	118	ASP	ALA	conflict	UNP O66529
UB	120	GLU	THR	conflict	UNP O66529
UB	123	GLU	GLN	conflict	UNP O66529
UB	127	CYS	ARG	conflict	UNP O66529
UB	131	GLU	LYS	conflict	UNP O66529
UB	155	LEU	-	expression tag	UNP O66529
UB	156	GLU	-	expression tag	UNP O66529
UB	157	HIS	-	expression tag	UNP O66529
UB	158	HIS	-	expression tag	UNP O66529
UB	159	HIS	-	expression tag	UNP O66529
UB	160	HIS	-	expression tag	UNP O66529
UB	161	HIS	-	expression tag	UNP O66529
UC	2	GLU	GLN	conflict	UNP O66529
UC	28	GLY	ASP	conflict	UNP O66529
UC	52	CYS	ARG	conflict	UNP O66529
UC	83	GLU	ARG	conflict	UNP O66529
UC	86	GLU	THR	conflict	UNP O66529
UC	112	SER	THR	conflict	UNP O66529
UC	115	ASP	VAL	conflict	UNP O66529
UC	118	ASP	ALA	conflict	UNP O66529
UC	120	GLU	THR	conflict	UNP O66529
UC	123	GLU	GLN	conflict	UNP O66529
UC	127	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
UC	131	GLU	LYS	conflict	UNP O66529
UC	155	LEU	-	expression tag	UNP O66529
UC	156	GLU	-	expression tag	UNP O66529
UC	157	HIS	-	expression tag	UNP O66529
UC	158	HIS	-	expression tag	UNP O66529
UC	159	HIS	-	expression tag	UNP O66529
UC	160	HIS	-	expression tag	UNP O66529
UC	161	HIS	-	expression tag	UNP O66529
UD	2	GLU	GLN	conflict	UNP O66529
UD	28	GLY	ASP	conflict	UNP O66529
UD	52	CYS	ARG	conflict	UNP O66529
UD	83	GLU	ARG	conflict	UNP O66529
UD	86	GLU	THR	conflict	UNP O66529
UD	112	SER	THR	conflict	UNP O66529
UD	115	ASP	VAL	conflict	UNP O66529
UD	118	ASP	ALA	conflict	UNP O66529
UD	120	GLU	THR	conflict	UNP O66529
UD	123	GLU	GLN	conflict	UNP O66529
UD	127	CYS	ARG	conflict	UNP O66529
UD	131	GLU	LYS	conflict	UNP O66529
UD	155	LEU	-	expression tag	UNP O66529
UD	156	GLU	-	expression tag	UNP O66529
UD	157	HIS	-	expression tag	UNP O66529
UD	158	HIS	-	expression tag	UNP O66529
UD	159	HIS	-	expression tag	UNP O66529
UD	160	HIS	-	expression tag	UNP O66529
UD	161	HIS	-	expression tag	UNP O66529
UE	2	GLU	GLN	conflict	UNP O66529
UE	28	GLY	ASP	conflict	UNP O66529
UE	52	CYS	ARG	conflict	UNP O66529
UE	83	GLU	ARG	conflict	UNP O66529
UE	86	GLU	THR	conflict	UNP O66529
UE	112	SER	THR	conflict	UNP O66529
UE	115	ASP	VAL	conflict	UNP O66529
UE	118	ASP	ALA	conflict	UNP O66529
UE	120	GLU	THR	conflict	UNP O66529
UE	123	GLU	GLN	conflict	UNP O66529
UE	127	CYS	ARG	conflict	UNP O66529
UE	131	GLU	LYS	conflict	UNP O66529
UE	155	LEU	-	expression tag	UNP O66529
UE	156	GLU	-	expression tag	UNP O66529
UE	157	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
UE	158	HIS	-	expression tag	UNP O66529
UE	159	HIS	-	expression tag	UNP O66529
UE	160	HIS	-	expression tag	UNP O66529
UE	161	HIS	-	expression tag	UNP O66529
UX	2	GLU	GLN	conflict	UNP O66529
UX	28	GLY	ASP	conflict	UNP O66529
UX	52	CYS	ARG	conflict	UNP O66529
UX	83	GLU	ARG	conflict	UNP O66529
UX	86	GLU	THR	conflict	UNP O66529
UX	112	SER	THR	conflict	UNP O66529
UX	115	ASP	VAL	conflict	UNP O66529
UX	118	ASP	ALA	conflict	UNP O66529
UX	120	GLU	THR	conflict	UNP O66529
UX	123	GLU	GLN	conflict	UNP O66529
UX	127	CYS	ARG	conflict	UNP O66529
UX	131	GLU	LYS	conflict	UNP O66529
UX	155	LEU	-	expression tag	UNP O66529
UX	156	GLU	-	expression tag	UNP O66529
UX	157	HIS	-	expression tag	UNP O66529
UX	158	HIS	-	expression tag	UNP O66529
UX	159	HIS	-	expression tag	UNP O66529
UX	160	HIS	-	expression tag	UNP O66529
UX	161	HIS	-	expression tag	UNP O66529
VA	2	GLU	GLN	conflict	UNP O66529
VA	28	GLY	ASP	conflict	UNP O66529
VA	52	CYS	ARG	conflict	UNP O66529
VA	83	GLU	ARG	conflict	UNP O66529
VA	86	GLU	THR	conflict	UNP O66529
VA	112	SER	THR	conflict	UNP O66529
VA	115	ASP	VAL	conflict	UNP O66529
VA	118	ASP	ALA	conflict	UNP O66529
VA	120	GLU	THR	conflict	UNP O66529
VA	123	GLU	GLN	conflict	UNP O66529
VA	127	CYS	ARG	conflict	UNP O66529
VA	131	GLU	LYS	conflict	UNP O66529
VA	155	LEU	-	expression tag	UNP O66529
VA	156	GLU	-	expression tag	UNP O66529
VA	157	HIS	-	expression tag	UNP O66529
VA	158	HIS	-	expression tag	UNP O66529
VA	159	HIS	-	expression tag	UNP O66529
VA	160	HIS	-	expression tag	UNP O66529
VA	161	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
VB	2	GLU	GLN	conflict	UNP O66529
VB	28	GLY	ASP	conflict	UNP O66529
VB	52	CYS	ARG	conflict	UNP O66529
VB	83	GLU	ARG	conflict	UNP O66529
VB	86	GLU	THR	conflict	UNP O66529
VB	112	SER	THR	conflict	UNP O66529
VB	115	ASP	VAL	conflict	UNP O66529
VB	118	ASP	ALA	conflict	UNP O66529
VB	120	GLU	THR	conflict	UNP O66529
VB	123	GLU	GLN	conflict	UNP O66529
VB	127	CYS	ARG	conflict	UNP O66529
VB	131	GLU	LYS	conflict	UNP O66529
VB	155	LEU	-	expression tag	UNP O66529
VB	156	GLU	-	expression tag	UNP O66529
VB	157	HIS	-	expression tag	UNP O66529
VB	158	HIS	-	expression tag	UNP O66529
VB	159	HIS	-	expression tag	UNP O66529
VB	160	HIS	-	expression tag	UNP O66529
VB	161	HIS	-	expression tag	UNP O66529
VC	2	GLU	GLN	conflict	UNP O66529
VC	28	GLY	ASP	conflict	UNP O66529
VC	52	CYS	ARG	conflict	UNP O66529
VC	83	GLU	ARG	conflict	UNP O66529
VC	86	GLU	THR	conflict	UNP O66529
VC	112	SER	THR	conflict	UNP O66529
VC	115	ASP	VAL	conflict	UNP O66529
VC	118	ASP	ALA	conflict	UNP O66529
VC	120	GLU	THR	conflict	UNP O66529
VC	123	GLU	GLN	conflict	UNP O66529
VC	127	CYS	ARG	conflict	UNP O66529
VC	131	GLU	LYS	conflict	UNP O66529
VC	155	LEU	-	expression tag	UNP O66529
VC	156	GLU	-	expression tag	UNP O66529
VC	157	HIS	-	expression tag	UNP O66529
VC	158	HIS	-	expression tag	UNP O66529
VC	159	HIS	-	expression tag	UNP O66529
VC	160	HIS	-	expression tag	UNP O66529
VC	161	HIS	-	expression tag	UNP O66529
VD	2	GLU	GLN	conflict	UNP O66529
VD	28	GLY	ASP	conflict	UNP O66529
VD	52	CYS	ARG	conflict	UNP O66529
VD	83	GLU	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
VD	86	GLU	THR	conflict	UNP O66529
VD	112	SER	THR	conflict	UNP O66529
VD	115	ASP	VAL	conflict	UNP O66529
VD	118	ASP	ALA	conflict	UNP O66529
VD	120	GLU	THR	conflict	UNP O66529
VD	123	GLU	GLN	conflict	UNP O66529
VD	127	CYS	ARG	conflict	UNP O66529
VD	131	GLU	LYS	conflict	UNP O66529
VD	155	LEU	-	expression tag	UNP O66529
VD	156	GLU	-	expression tag	UNP O66529
VD	157	HIS	-	expression tag	UNP O66529
VD	158	HIS	-	expression tag	UNP O66529
VD	159	HIS	-	expression tag	UNP O66529
VD	160	HIS	-	expression tag	UNP O66529
VD	161	HIS	-	expression tag	UNP O66529
VE	2	GLU	GLN	conflict	UNP O66529
VE	28	GLY	ASP	conflict	UNP O66529
VE	52	CYS	ARG	conflict	UNP O66529
VE	83	GLU	ARG	conflict	UNP O66529
VE	86	GLU	THR	conflict	UNP O66529
VE	112	SER	THR	conflict	UNP O66529
VE	115	ASP	VAL	conflict	UNP O66529
VE	118	ASP	ALA	conflict	UNP O66529
VE	120	GLU	THR	conflict	UNP O66529
VE	123	GLU	GLN	conflict	UNP O66529
VE	127	CYS	ARG	conflict	UNP O66529
VE	131	GLU	LYS	conflict	UNP O66529
VE	155	LEU	-	expression tag	UNP O66529
VE	156	GLU	-	expression tag	UNP O66529
VE	157	HIS	-	expression tag	UNP O66529
VE	158	HIS	-	expression tag	UNP O66529
VE	159	HIS	-	expression tag	UNP O66529
VE	160	HIS	-	expression tag	UNP O66529
VE	161	HIS	-	expression tag	UNP O66529
VX	2	GLU	GLN	conflict	UNP O66529
VX	28	GLY	ASP	conflict	UNP O66529
VX	52	CYS	ARG	conflict	UNP O66529
VX	83	GLU	ARG	conflict	UNP O66529
VX	86	GLU	THR	conflict	UNP O66529
VX	112	SER	THR	conflict	UNP O66529
VX	115	ASP	VAL	conflict	UNP O66529
VX	118	ASP	ALA	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
VX	120	GLU	THR	conflict	UNP O66529
VX	123	GLU	GLN	conflict	UNP O66529
VX	127	CYS	ARG	conflict	UNP O66529
VX	131	GLU	LYS	conflict	UNP O66529
VX	155	LEU	-	expression tag	UNP O66529
VX	156	GLU	-	expression tag	UNP O66529
VX	157	HIS	-	expression tag	UNP O66529
VX	158	HIS	-	expression tag	UNP O66529
VX	159	HIS	-	expression tag	UNP O66529
VX	160	HIS	-	expression tag	UNP O66529
VX	161	HIS	-	expression tag	UNP O66529
WA	2	GLU	GLN	conflict	UNP O66529
WA	28	GLY	ASP	conflict	UNP O66529
WA	52	CYS	ARG	conflict	UNP O66529
WA	83	GLU	ARG	conflict	UNP O66529
WA	86	GLU	THR	conflict	UNP O66529
WA	112	SER	THR	conflict	UNP O66529
WA	115	ASP	VAL	conflict	UNP O66529
WA	118	ASP	ALA	conflict	UNP O66529
WA	120	GLU	THR	conflict	UNP O66529
WA	123	GLU	GLN	conflict	UNP O66529
WA	127	CYS	ARG	conflict	UNP O66529
WA	131	GLU	LYS	conflict	UNP O66529
WA	155	LEU	-	expression tag	UNP O66529
WA	156	GLU	-	expression tag	UNP O66529
WA	157	HIS	-	expression tag	UNP O66529
WA	158	HIS	-	expression tag	UNP O66529
WA	159	HIS	-	expression tag	UNP O66529
WA	160	HIS	-	expression tag	UNP O66529
WA	161	HIS	-	expression tag	UNP O66529
WB	2	GLU	GLN	conflict	UNP O66529
WB	28	GLY	ASP	conflict	UNP O66529
WB	52	CYS	ARG	conflict	UNP O66529
WB	83	GLU	ARG	conflict	UNP O66529
WB	86	GLU	THR	conflict	UNP O66529
WB	112	SER	THR	conflict	UNP O66529
WB	115	ASP	VAL	conflict	UNP O66529
WB	118	ASP	ALA	conflict	UNP O66529
WB	120	GLU	THR	conflict	UNP O66529
WB	123	GLU	GLN	conflict	UNP O66529
WB	127	CYS	ARG	conflict	UNP O66529
WB	131	GLU	LYS	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
WB	155	LEU	-	expression tag	UNP O66529
WB	156	GLU	-	expression tag	UNP O66529
WB	157	HIS	-	expression tag	UNP O66529
WB	158	HIS	-	expression tag	UNP O66529
WB	159	HIS	-	expression tag	UNP O66529
WB	160	HIS	-	expression tag	UNP O66529
WB	161	HIS	-	expression tag	UNP O66529
WC	2	GLU	GLN	conflict	UNP O66529
WC	28	GLY	ASP	conflict	UNP O66529
WC	52	CYS	ARG	conflict	UNP O66529
WC	83	GLU	ARG	conflict	UNP O66529
WC	86	GLU	THR	conflict	UNP O66529
WC	112	SER	THR	conflict	UNP O66529
WC	115	ASP	VAL	conflict	UNP O66529
WC	118	ASP	ALA	conflict	UNP O66529
WC	120	GLU	THR	conflict	UNP O66529
WC	123	GLU	GLN	conflict	UNP O66529
WC	127	CYS	ARG	conflict	UNP O66529
WC	131	GLU	LYS	conflict	UNP O66529
WC	155	LEU	-	expression tag	UNP O66529
WC	156	GLU	-	expression tag	UNP O66529
WC	157	HIS	-	expression tag	UNP O66529
WC	158	HIS	-	expression tag	UNP O66529
WC	159	HIS	-	expression tag	UNP O66529
WC	160	HIS	-	expression tag	UNP O66529
WC	161	HIS	-	expression tag	UNP O66529
WD	2	GLU	GLN	conflict	UNP O66529
WD	28	GLY	ASP	conflict	UNP O66529
WD	52	CYS	ARG	conflict	UNP O66529
WD	83	GLU	ARG	conflict	UNP O66529
WD	86	GLU	THR	conflict	UNP O66529
WD	112	SER	THR	conflict	UNP O66529
WD	115	ASP	VAL	conflict	UNP O66529
WD	118	ASP	ALA	conflict	UNP O66529
WD	120	GLU	THR	conflict	UNP O66529
WD	123	GLU	GLN	conflict	UNP O66529
WD	127	CYS	ARG	conflict	UNP O66529
WD	131	GLU	LYS	conflict	UNP O66529
WD	155	LEU	-	expression tag	UNP O66529
WD	156	GLU	-	expression tag	UNP O66529
WD	157	HIS	-	expression tag	UNP O66529
WD	158	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
WD	159	HIS	-	expression tag	UNP O66529
WD	160	HIS	-	expression tag	UNP O66529
WD	161	HIS	-	expression tag	UNP O66529
WE	2	GLU	GLN	conflict	UNP O66529
WE	28	GLY	ASP	conflict	UNP O66529
WE	52	CYS	ARG	conflict	UNP O66529
WE	83	GLU	ARG	conflict	UNP O66529
WE	86	GLU	THR	conflict	UNP O66529
WE	112	SER	THR	conflict	UNP O66529
WE	115	ASP	VAL	conflict	UNP O66529
WE	118	ASP	ALA	conflict	UNP O66529
WE	120	GLU	THR	conflict	UNP O66529
WE	123	GLU	GLN	conflict	UNP O66529
WE	127	CYS	ARG	conflict	UNP O66529
WE	131	GLU	LYS	conflict	UNP O66529
WE	155	LEU	-	expression tag	UNP O66529
WE	156	GLU	-	expression tag	UNP O66529
WE	157	HIS	-	expression tag	UNP O66529
WE	158	HIS	-	expression tag	UNP O66529
WE	159	HIS	-	expression tag	UNP O66529
WE	160	HIS	-	expression tag	UNP O66529
WE	161	HIS	-	expression tag	UNP O66529
WX	2	GLU	GLN	conflict	UNP O66529
WX	28	GLY	ASP	conflict	UNP O66529
WX	52	CYS	ARG	conflict	UNP O66529
WX	83	GLU	ARG	conflict	UNP O66529
WX	86	GLU	THR	conflict	UNP O66529
WX	112	SER	THR	conflict	UNP O66529
WX	115	ASP	VAL	conflict	UNP O66529
WX	118	ASP	ALA	conflict	UNP O66529
WX	120	GLU	THR	conflict	UNP O66529
WX	123	GLU	GLN	conflict	UNP O66529
WX	127	CYS	ARG	conflict	UNP O66529
WX	131	GLU	LYS	conflict	UNP O66529
WX	155	LEU	-	expression tag	UNP O66529
WX	156	GLU	-	expression tag	UNP O66529
WX	157	HIS	-	expression tag	UNP O66529
WX	158	HIS	-	expression tag	UNP O66529
WX	159	HIS	-	expression tag	UNP O66529
WX	160	HIS	-	expression tag	UNP O66529
WX	161	HIS	-	expression tag	UNP O66529
XA	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
XA	28	GLY	ASP	conflict	UNP O66529
XA	52	CYS	ARG	conflict	UNP O66529
XA	83	GLU	ARG	conflict	UNP O66529
XA	86	GLU	THR	conflict	UNP O66529
XA	112	SER	THR	conflict	UNP O66529
XA	115	ASP	VAL	conflict	UNP O66529
XA	118	ASP	ALA	conflict	UNP O66529
XA	120	GLU	THR	conflict	UNP O66529
XA	123	GLU	GLN	conflict	UNP O66529
XA	127	CYS	ARG	conflict	UNP O66529
XA	131	GLU	LYS	conflict	UNP O66529
XA	155	LEU	-	expression tag	UNP O66529
XA	156	GLU	-	expression tag	UNP O66529
XA	157	HIS	-	expression tag	UNP O66529
XA	158	HIS	-	expression tag	UNP O66529
XA	159	HIS	-	expression tag	UNP O66529
XA	160	HIS	-	expression tag	UNP O66529
XA	161	HIS	-	expression tag	UNP O66529
XB	2	GLU	GLN	conflict	UNP O66529
XB	28	GLY	ASP	conflict	UNP O66529
XB	52	CYS	ARG	conflict	UNP O66529
XB	83	GLU	ARG	conflict	UNP O66529
XB	86	GLU	THR	conflict	UNP O66529
XB	112	SER	THR	conflict	UNP O66529
XB	115	ASP	VAL	conflict	UNP O66529
XB	118	ASP	ALA	conflict	UNP O66529
XB	120	GLU	THR	conflict	UNP O66529
XB	123	GLU	GLN	conflict	UNP O66529
XB	127	CYS	ARG	conflict	UNP O66529
XB	131	GLU	LYS	conflict	UNP O66529
XB	155	LEU	-	expression tag	UNP O66529
XB	156	GLU	-	expression tag	UNP O66529
XB	157	HIS	-	expression tag	UNP O66529
XB	158	HIS	-	expression tag	UNP O66529
XB	159	HIS	-	expression tag	UNP O66529
XB	160	HIS	-	expression tag	UNP O66529
XB	161	HIS	-	expression tag	UNP O66529
XC	2	GLU	GLN	conflict	UNP O66529
XC	28	GLY	ASP	conflict	UNP O66529
XC	52	CYS	ARG	conflict	UNP O66529
XC	83	GLU	ARG	conflict	UNP O66529
XC	86	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
XC	112	SER	THR	conflict	UNP O66529
XC	115	ASP	VAL	conflict	UNP O66529
XC	118	ASP	ALA	conflict	UNP O66529
XC	120	GLU	THR	conflict	UNP O66529
XC	123	GLU	GLN	conflict	UNP O66529
XC	127	CYS	ARG	conflict	UNP O66529
XC	131	GLU	LYS	conflict	UNP O66529
XC	155	LEU	-	expression tag	UNP O66529
XC	156	GLU	-	expression tag	UNP O66529
XC	157	HIS	-	expression tag	UNP O66529
XC	158	HIS	-	expression tag	UNP O66529
XC	159	HIS	-	expression tag	UNP O66529
XC	160	HIS	-	expression tag	UNP O66529
XC	161	HIS	-	expression tag	UNP O66529
XD	2	GLU	GLN	conflict	UNP O66529
XD	28	GLY	ASP	conflict	UNP O66529
XD	52	CYS	ARG	conflict	UNP O66529
XD	83	GLU	ARG	conflict	UNP O66529
XD	86	GLU	THR	conflict	UNP O66529
XD	112	SER	THR	conflict	UNP O66529
XD	115	ASP	VAL	conflict	UNP O66529
XD	118	ASP	ALA	conflict	UNP O66529
XD	120	GLU	THR	conflict	UNP O66529
XD	123	GLU	GLN	conflict	UNP O66529
XD	127	CYS	ARG	conflict	UNP O66529
XD	131	GLU	LYS	conflict	UNP O66529
XD	155	LEU	-	expression tag	UNP O66529
XD	156	GLU	-	expression tag	UNP O66529
XD	157	HIS	-	expression tag	UNP O66529
XD	158	HIS	-	expression tag	UNP O66529
XD	159	HIS	-	expression tag	UNP O66529
XD	160	HIS	-	expression tag	UNP O66529
XD	161	HIS	-	expression tag	UNP O66529
XE	2	GLU	GLN	conflict	UNP O66529
XE	28	GLY	ASP	conflict	UNP O66529
XE	52	CYS	ARG	conflict	UNP O66529
XE	83	GLU	ARG	conflict	UNP O66529
XE	86	GLU	THR	conflict	UNP O66529
XE	112	SER	THR	conflict	UNP O66529
XE	115	ASP	VAL	conflict	UNP O66529
XE	118	ASP	ALA	conflict	UNP O66529
XE	120	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
XE	123	GLU	GLN	conflict	UNP O66529
XE	127	CYS	ARG	conflict	UNP O66529
XE	131	GLU	LYS	conflict	UNP O66529
XE	155	LEU	-	expression tag	UNP O66529
XE	156	GLU	-	expression tag	UNP O66529
XE	157	HIS	-	expression tag	UNP O66529
XE	158	HIS	-	expression tag	UNP O66529
XE	159	HIS	-	expression tag	UNP O66529
XE	160	HIS	-	expression tag	UNP O66529
XE	161	HIS	-	expression tag	UNP O66529
XX	2	GLU	GLN	conflict	UNP O66529
XX	28	GLY	ASP	conflict	UNP O66529
XX	52	CYS	ARG	conflict	UNP O66529
XX	83	GLU	ARG	conflict	UNP O66529
XX	86	GLU	THR	conflict	UNP O66529
XX	112	SER	THR	conflict	UNP O66529
XX	115	ASP	VAL	conflict	UNP O66529
XX	118	ASP	ALA	conflict	UNP O66529
XX	120	GLU	THR	conflict	UNP O66529
XX	123	GLU	GLN	conflict	UNP O66529
XX	127	CYS	ARG	conflict	UNP O66529
XX	131	GLU	LYS	conflict	UNP O66529
XX	155	LEU	-	expression tag	UNP O66529
XX	156	GLU	-	expression tag	UNP O66529
XX	157	HIS	-	expression tag	UNP O66529
XX	158	HIS	-	expression tag	UNP O66529
XX	159	HIS	-	expression tag	UNP O66529
XX	160	HIS	-	expression tag	UNP O66529
XX	161	HIS	-	expression tag	UNP O66529
YA	2	GLU	GLN	conflict	UNP O66529
YA	28	GLY	ASP	conflict	UNP O66529
YA	52	CYS	ARG	conflict	UNP O66529
YA	83	GLU	ARG	conflict	UNP O66529
YA	86	GLU	THR	conflict	UNP O66529
YA	112	SER	THR	conflict	UNP O66529
YA	115	ASP	VAL	conflict	UNP O66529
YA	118	ASP	ALA	conflict	UNP O66529
YA	120	GLU	THR	conflict	UNP O66529
YA	123	GLU	GLN	conflict	UNP O66529
YA	127	CYS	ARG	conflict	UNP O66529
YA	131	GLU	LYS	conflict	UNP O66529
YA	155	LEU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
YA	156	GLU	-	expression tag	UNP O66529
YA	157	HIS	-	expression tag	UNP O66529
YA	158	HIS	-	expression tag	UNP O66529
YA	159	HIS	-	expression tag	UNP O66529
YA	160	HIS	-	expression tag	UNP O66529
YA	161	HIS	-	expression tag	UNP O66529
YB	2	GLU	GLN	conflict	UNP O66529
YB	28	GLY	ASP	conflict	UNP O66529
YB	52	CYS	ARG	conflict	UNP O66529
YB	83	GLU	ARG	conflict	UNP O66529
YB	86	GLU	THR	conflict	UNP O66529
YB	112	SER	THR	conflict	UNP O66529
YB	115	ASP	VAL	conflict	UNP O66529
YB	118	ASP	ALA	conflict	UNP O66529
YB	120	GLU	THR	conflict	UNP O66529
YB	123	GLU	GLN	conflict	UNP O66529
YB	127	CYS	ARG	conflict	UNP O66529
YB	131	GLU	LYS	conflict	UNP O66529
YB	155	LEU	-	expression tag	UNP O66529
YB	156	GLU	-	expression tag	UNP O66529
YB	157	HIS	-	expression tag	UNP O66529
YB	158	HIS	-	expression tag	UNP O66529
YB	159	HIS	-	expression tag	UNP O66529
YB	160	HIS	-	expression tag	UNP O66529
YB	161	HIS	-	expression tag	UNP O66529
YC	2	GLU	GLN	conflict	UNP O66529
YC	28	GLY	ASP	conflict	UNP O66529
YC	52	CYS	ARG	conflict	UNP O66529
YC	83	GLU	ARG	conflict	UNP O66529
YC	86	GLU	THR	conflict	UNP O66529
YC	112	SER	THR	conflict	UNP O66529
YC	115	ASP	VAL	conflict	UNP O66529
YC	118	ASP	ALA	conflict	UNP O66529
YC	120	GLU	THR	conflict	UNP O66529
YC	123	GLU	GLN	conflict	UNP O66529
YC	127	CYS	ARG	conflict	UNP O66529
YC	131	GLU	LYS	conflict	UNP O66529
YC	155	LEU	-	expression tag	UNP O66529
YC	156	GLU	-	expression tag	UNP O66529
YC	157	HIS	-	expression tag	UNP O66529
YC	158	HIS	-	expression tag	UNP O66529
YC	159	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
YC	160	HIS	-	expression tag	UNP O66529
YC	161	HIS	-	expression tag	UNP O66529
YD	2	GLU	GLN	conflict	UNP O66529
YD	28	GLY	ASP	conflict	UNP O66529
YD	52	CYS	ARG	conflict	UNP O66529
YD	83	GLU	ARG	conflict	UNP O66529
YD	86	GLU	THR	conflict	UNP O66529
YD	112	SER	THR	conflict	UNP O66529
YD	115	ASP	VAL	conflict	UNP O66529
YD	118	ASP	ALA	conflict	UNP O66529
YD	120	GLU	THR	conflict	UNP O66529
YD	123	GLU	GLN	conflict	UNP O66529
YD	127	CYS	ARG	conflict	UNP O66529
YD	131	GLU	LYS	conflict	UNP O66529
YD	155	LEU	-	expression tag	UNP O66529
YD	156	GLU	-	expression tag	UNP O66529
YD	157	HIS	-	expression tag	UNP O66529
YD	158	HIS	-	expression tag	UNP O66529
YD	159	HIS	-	expression tag	UNP O66529
YD	160	HIS	-	expression tag	UNP O66529
YD	161	HIS	-	expression tag	UNP O66529
YE	2	GLU	GLN	conflict	UNP O66529
YE	28	GLY	ASP	conflict	UNP O66529
YE	52	CYS	ARG	conflict	UNP O66529
YE	83	GLU	ARG	conflict	UNP O66529
YE	86	GLU	THR	conflict	UNP O66529
YE	112	SER	THR	conflict	UNP O66529
YE	115	ASP	VAL	conflict	UNP O66529
YE	118	ASP	ALA	conflict	UNP O66529
YE	120	GLU	THR	conflict	UNP O66529
YE	123	GLU	GLN	conflict	UNP O66529
YE	127	CYS	ARG	conflict	UNP O66529
YE	131	GLU	LYS	conflict	UNP O66529
YE	155	LEU	-	expression tag	UNP O66529
YE	156	GLU	-	expression tag	UNP O66529
YE	157	HIS	-	expression tag	UNP O66529
YE	158	HIS	-	expression tag	UNP O66529
YE	159	HIS	-	expression tag	UNP O66529
YE	160	HIS	-	expression tag	UNP O66529
YE	161	HIS	-	expression tag	UNP O66529
YX	2	GLU	GLN	conflict	UNP O66529
YX	28	GLY	ASP	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
YX	52	CYS	ARG	conflict	UNP O66529
YX	83	GLU	ARG	conflict	UNP O66529
YX	86	GLU	THR	conflict	UNP O66529
YX	112	SER	THR	conflict	UNP O66529
YX	115	ASP	VAL	conflict	UNP O66529
YX	118	ASP	ALA	conflict	UNP O66529
YX	120	GLU	THR	conflict	UNP O66529
YX	123	GLU	GLN	conflict	UNP O66529
YX	127	CYS	ARG	conflict	UNP O66529
YX	131	GLU	LYS	conflict	UNP O66529
YX	155	LEU	-	expression tag	UNP O66529
YX	156	GLU	-	expression tag	UNP O66529
YX	157	HIS	-	expression tag	UNP O66529
YX	158	HIS	-	expression tag	UNP O66529
YX	159	HIS	-	expression tag	UNP O66529
YX	160	HIS	-	expression tag	UNP O66529
YX	161	HIS	-	expression tag	UNP O66529
ZA	2	GLU	GLN	conflict	UNP O66529
ZA	28	GLY	ASP	conflict	UNP O66529
ZA	52	CYS	ARG	conflict	UNP O66529
ZA	83	GLU	ARG	conflict	UNP O66529
ZA	86	GLU	THR	conflict	UNP O66529
ZA	112	SER	THR	conflict	UNP O66529
ZA	115	ASP	VAL	conflict	UNP O66529
ZA	118	ASP	ALA	conflict	UNP O66529
ZA	120	GLU	THR	conflict	UNP O66529
ZA	123	GLU	GLN	conflict	UNP O66529
ZA	127	CYS	ARG	conflict	UNP O66529
ZA	131	GLU	LYS	conflict	UNP O66529
ZA	155	LEU	-	expression tag	UNP O66529
ZA	156	GLU	-	expression tag	UNP O66529
ZA	157	HIS	-	expression tag	UNP O66529
ZA	158	HIS	-	expression tag	UNP O66529
ZA	159	HIS	-	expression tag	UNP O66529
ZA	160	HIS	-	expression tag	UNP O66529
ZA	161	HIS	-	expression tag	UNP O66529
ZB	2	GLU	GLN	conflict	UNP O66529
ZB	28	GLY	ASP	conflict	UNP O66529
ZB	52	CYS	ARG	conflict	UNP O66529
ZB	83	GLU	ARG	conflict	UNP O66529
ZB	86	GLU	THR	conflict	UNP O66529
ZB	112	SER	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZB	115	ASP	VAL	conflict	UNP O66529
ZB	118	ASP	ALA	conflict	UNP O66529
ZB	120	GLU	THR	conflict	UNP O66529
ZB	123	GLU	GLN	conflict	UNP O66529
ZB	127	CYS	ARG	conflict	UNP O66529
ZB	131	GLU	LYS	conflict	UNP O66529
ZB	155	LEU	-	expression tag	UNP O66529
ZB	156	GLU	-	expression tag	UNP O66529
ZB	157	HIS	-	expression tag	UNP O66529
ZB	158	HIS	-	expression tag	UNP O66529
ZB	159	HIS	-	expression tag	UNP O66529
ZB	160	HIS	-	expression tag	UNP O66529
ZB	161	HIS	-	expression tag	UNP O66529
ZC	2	GLU	GLN	conflict	UNP O66529
ZC	28	GLY	ASP	conflict	UNP O66529
ZC	52	CYS	ARG	conflict	UNP O66529
ZC	83	GLU	ARG	conflict	UNP O66529
ZC	86	GLU	THR	conflict	UNP O66529
ZC	112	SER	THR	conflict	UNP O66529
ZC	115	ASP	VAL	conflict	UNP O66529
ZC	118	ASP	ALA	conflict	UNP O66529
ZC	120	GLU	THR	conflict	UNP O66529
ZC	123	GLU	GLN	conflict	UNP O66529
ZC	127	CYS	ARG	conflict	UNP O66529
ZC	131	GLU	LYS	conflict	UNP O66529
ZC	155	LEU	-	expression tag	UNP O66529
ZC	156	GLU	-	expression tag	UNP O66529
ZC	157	HIS	-	expression tag	UNP O66529
ZC	158	HIS	-	expression tag	UNP O66529
ZC	159	HIS	-	expression tag	UNP O66529
ZC	160	HIS	-	expression tag	UNP O66529
ZC	161	HIS	-	expression tag	UNP O66529
ZD	2	GLU	GLN	conflict	UNP O66529
ZD	28	GLY	ASP	conflict	UNP O66529
ZD	52	CYS	ARG	conflict	UNP O66529
ZD	83	GLU	ARG	conflict	UNP O66529
ZD	86	GLU	THR	conflict	UNP O66529
ZD	112	SER	THR	conflict	UNP O66529
ZD	115	ASP	VAL	conflict	UNP O66529
ZD	118	ASP	ALA	conflict	UNP O66529
ZD	120	GLU	THR	conflict	UNP O66529
ZD	123	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZD	127	CYS	ARG	conflict	UNP O66529
ZD	131	GLU	LYS	conflict	UNP O66529
ZD	155	LEU	-	expression tag	UNP O66529
ZD	156	GLU	-	expression tag	UNP O66529
ZD	157	HIS	-	expression tag	UNP O66529
ZD	158	HIS	-	expression tag	UNP O66529
ZD	159	HIS	-	expression tag	UNP O66529
ZD	160	HIS	-	expression tag	UNP O66529
ZD	161	HIS	-	expression tag	UNP O66529
ZE	2	GLU	GLN	conflict	UNP O66529
ZE	28	GLY	ASP	conflict	UNP O66529
ZE	52	CYS	ARG	conflict	UNP O66529
ZE	83	GLU	ARG	conflict	UNP O66529
ZE	86	GLU	THR	conflict	UNP O66529
ZE	112	SER	THR	conflict	UNP O66529
ZE	115	ASP	VAL	conflict	UNP O66529
ZE	118	ASP	ALA	conflict	UNP O66529
ZE	120	GLU	THR	conflict	UNP O66529
ZE	123	GLU	GLN	conflict	UNP O66529
ZE	127	CYS	ARG	conflict	UNP O66529
ZE	131	GLU	LYS	conflict	UNP O66529
ZE	155	LEU	-	expression tag	UNP O66529
ZE	156	GLU	-	expression tag	UNP O66529
ZE	157	HIS	-	expression tag	UNP O66529
ZE	158	HIS	-	expression tag	UNP O66529
ZE	159	HIS	-	expression tag	UNP O66529
ZE	160	HIS	-	expression tag	UNP O66529
ZE	161	HIS	-	expression tag	UNP O66529
ZX	2	GLU	GLN	conflict	UNP O66529
ZX	28	GLY	ASP	conflict	UNP O66529
ZX	52	CYS	ARG	conflict	UNP O66529
ZX	83	GLU	ARG	conflict	UNP O66529
ZX	86	GLU	THR	conflict	UNP O66529
ZX	112	SER	THR	conflict	UNP O66529
ZX	115	ASP	VAL	conflict	UNP O66529
ZX	118	ASP	ALA	conflict	UNP O66529
ZX	120	GLU	THR	conflict	UNP O66529
ZX	123	GLU	GLN	conflict	UNP O66529
ZX	127	CYS	ARG	conflict	UNP O66529
ZX	131	GLU	LYS	conflict	UNP O66529
ZX	155	LEU	-	expression tag	UNP O66529
ZX	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
ZX	157	HIS	-	expression tag	UNP O66529
ZX	158	HIS	-	expression tag	UNP O66529
ZX	159	HIS	-	expression tag	UNP O66529
ZX	160	HIS	-	expression tag	UNP O66529
ZX	161	HIS	-	expression tag	UNP O66529
aA	2	GLU	GLN	conflict	UNP O66529
aA	28	GLY	ASP	conflict	UNP O66529
aA	52	CYS	ARG	conflict	UNP O66529
aA	83	GLU	ARG	conflict	UNP O66529
aA	86	GLU	THR	conflict	UNP O66529
aA	112	SER	THR	conflict	UNP O66529
aA	115	ASP	VAL	conflict	UNP O66529
aA	118	ASP	ALA	conflict	UNP O66529
aA	120	GLU	THR	conflict	UNP O66529
aA	123	GLU	GLN	conflict	UNP O66529
aA	127	CYS	ARG	conflict	UNP O66529
aA	131	GLU	LYS	conflict	UNP O66529
aA	155	LEU	-	expression tag	UNP O66529
aA	156	GLU	-	expression tag	UNP O66529
aA	157	HIS	-	expression tag	UNP O66529
aA	158	HIS	-	expression tag	UNP O66529
aA	159	HIS	-	expression tag	UNP O66529
aA	160	HIS	-	expression tag	UNP O66529
aA	161	HIS	-	expression tag	UNP O66529
aB	2	GLU	GLN	conflict	UNP O66529
aB	28	GLY	ASP	conflict	UNP O66529
aB	52	CYS	ARG	conflict	UNP O66529
aB	83	GLU	ARG	conflict	UNP O66529
aB	86	GLU	THR	conflict	UNP O66529
aB	112	SER	THR	conflict	UNP O66529
aB	115	ASP	VAL	conflict	UNP O66529
aB	118	ASP	ALA	conflict	UNP O66529
aB	120	GLU	THR	conflict	UNP O66529
aB	123	GLU	GLN	conflict	UNP O66529
aB	127	CYS	ARG	conflict	UNP O66529
aB	131	GLU	LYS	conflict	UNP O66529
aB	155	LEU	-	expression tag	UNP O66529
aB	156	GLU	-	expression tag	UNP O66529
aB	157	HIS	-	expression tag	UNP O66529
aB	158	HIS	-	expression tag	UNP O66529
aB	159	HIS	-	expression tag	UNP O66529
aB	160	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
aB	161	HIS	-	expression tag	UNP O66529
aC	2	GLU	GLN	conflict	UNP O66529
aC	28	GLY	ASP	conflict	UNP O66529
aC	52	CYS	ARG	conflict	UNP O66529
aC	83	GLU	ARG	conflict	UNP O66529
aC	86	GLU	THR	conflict	UNP O66529
aC	112	SER	THR	conflict	UNP O66529
aC	115	ASP	VAL	conflict	UNP O66529
aC	118	ASP	ALA	conflict	UNP O66529
aC	120	GLU	THR	conflict	UNP O66529
aC	123	GLU	GLN	conflict	UNP O66529
aC	127	CYS	ARG	conflict	UNP O66529
aC	131	GLU	LYS	conflict	UNP O66529
aC	155	LEU	-	expression tag	UNP O66529
aC	156	GLU	-	expression tag	UNP O66529
aC	157	HIS	-	expression tag	UNP O66529
aC	158	HIS	-	expression tag	UNP O66529
aC	159	HIS	-	expression tag	UNP O66529
aC	160	HIS	-	expression tag	UNP O66529
aC	161	HIS	-	expression tag	UNP O66529
aD	2	GLU	GLN	conflict	UNP O66529
aD	28	GLY	ASP	conflict	UNP O66529
aD	52	CYS	ARG	conflict	UNP O66529
aD	83	GLU	ARG	conflict	UNP O66529
aD	86	GLU	THR	conflict	UNP O66529
aD	112	SER	THR	conflict	UNP O66529
aD	115	ASP	VAL	conflict	UNP O66529
aD	118	ASP	ALA	conflict	UNP O66529
aD	120	GLU	THR	conflict	UNP O66529
aD	123	GLU	GLN	conflict	UNP O66529
aD	127	CYS	ARG	conflict	UNP O66529
aD	131	GLU	LYS	conflict	UNP O66529
aD	155	LEU	-	expression tag	UNP O66529
aD	156	GLU	-	expression tag	UNP O66529
aD	157	HIS	-	expression tag	UNP O66529
aD	158	HIS	-	expression tag	UNP O66529
aD	159	HIS	-	expression tag	UNP O66529
aD	160	HIS	-	expression tag	UNP O66529
aD	161	HIS	-	expression tag	UNP O66529
aE	2	GLU	GLN	conflict	UNP O66529
aE	28	GLY	ASP	conflict	UNP O66529
aE	52	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
aE	83	GLU	ARG	conflict	UNP O66529
aE	86	GLU	THR	conflict	UNP O66529
aE	112	SER	THR	conflict	UNP O66529
aE	115	ASP	VAL	conflict	UNP O66529
aE	118	ASP	ALA	conflict	UNP O66529
aE	120	GLU	THR	conflict	UNP O66529
aE	123	GLU	GLN	conflict	UNP O66529
aE	127	CYS	ARG	conflict	UNP O66529
aE	131	GLU	LYS	conflict	UNP O66529
aE	155	LEU	-	expression tag	UNP O66529
aE	156	GLU	-	expression tag	UNP O66529
aE	157	HIS	-	expression tag	UNP O66529
aE	158	HIS	-	expression tag	UNP O66529
aE	159	HIS	-	expression tag	UNP O66529
aE	160	HIS	-	expression tag	UNP O66529
aE	161	HIS	-	expression tag	UNP O66529
aX	2	GLU	GLN	conflict	UNP O66529
aX	28	GLY	ASP	conflict	UNP O66529
aX	52	CYS	ARG	conflict	UNP O66529
aX	83	GLU	ARG	conflict	UNP O66529
aX	86	GLU	THR	conflict	UNP O66529
aX	112	SER	THR	conflict	UNP O66529
aX	115	ASP	VAL	conflict	UNP O66529
aX	118	ASP	ALA	conflict	UNP O66529
aX	120	GLU	THR	conflict	UNP O66529
aX	123	GLU	GLN	conflict	UNP O66529
aX	127	CYS	ARG	conflict	UNP O66529
aX	131	GLU	LYS	conflict	UNP O66529
aX	155	LEU	-	expression tag	UNP O66529
aX	156	GLU	-	expression tag	UNP O66529
aX	157	HIS	-	expression tag	UNP O66529
aX	158	HIS	-	expression tag	UNP O66529
aX	159	HIS	-	expression tag	UNP O66529
aX	160	HIS	-	expression tag	UNP O66529
aX	161	HIS	-	expression tag	UNP O66529
bA	2	GLU	GLN	conflict	UNP O66529
bA	28	GLY	ASP	conflict	UNP O66529
bA	52	CYS	ARG	conflict	UNP O66529
bA	83	GLU	ARG	conflict	UNP O66529
bA	86	GLU	THR	conflict	UNP O66529
bA	112	SER	THR	conflict	UNP O66529
bA	115	ASP	VAL	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
bA	118	ASP	ALA	conflict	UNP O66529
bA	120	GLU	THR	conflict	UNP O66529
bA	123	GLU	GLN	conflict	UNP O66529
bA	127	CYS	ARG	conflict	UNP O66529
bA	131	GLU	LYS	conflict	UNP O66529
bA	155	LEU	-	expression tag	UNP O66529
bA	156	GLU	-	expression tag	UNP O66529
bA	157	HIS	-	expression tag	UNP O66529
bA	158	HIS	-	expression tag	UNP O66529
bA	159	HIS	-	expression tag	UNP O66529
bA	160	HIS	-	expression tag	UNP O66529
bA	161	HIS	-	expression tag	UNP O66529
bB	2	GLU	GLN	conflict	UNP O66529
bB	28	GLY	ASP	conflict	UNP O66529
bB	52	CYS	ARG	conflict	UNP O66529
bB	83	GLU	ARG	conflict	UNP O66529
bB	86	GLU	THR	conflict	UNP O66529
bB	112	SER	THR	conflict	UNP O66529
bB	115	ASP	VAL	conflict	UNP O66529
bB	118	ASP	ALA	conflict	UNP O66529
bB	120	GLU	THR	conflict	UNP O66529
bB	123	GLU	GLN	conflict	UNP O66529
bB	127	CYS	ARG	conflict	UNP O66529
bB	131	GLU	LYS	conflict	UNP O66529
bB	155	LEU	-	expression tag	UNP O66529
bB	156	GLU	-	expression tag	UNP O66529
bB	157	HIS	-	expression tag	UNP O66529
bB	158	HIS	-	expression tag	UNP O66529
bB	159	HIS	-	expression tag	UNP O66529
bB	160	HIS	-	expression tag	UNP O66529
bB	161	HIS	-	expression tag	UNP O66529
bC	2	GLU	GLN	conflict	UNP O66529
bC	28	GLY	ASP	conflict	UNP O66529
bC	52	CYS	ARG	conflict	UNP O66529
bC	83	GLU	ARG	conflict	UNP O66529
bC	86	GLU	THR	conflict	UNP O66529
bC	112	SER	THR	conflict	UNP O66529
bC	115	ASP	VAL	conflict	UNP O66529
bC	118	ASP	ALA	conflict	UNP O66529
bC	120	GLU	THR	conflict	UNP O66529
bC	123	GLU	GLN	conflict	UNP O66529
bC	127	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
bC	131	GLU	LYS	conflict	UNP O66529
bC	155	LEU	-	expression tag	UNP O66529
bC	156	GLU	-	expression tag	UNP O66529
bC	157	HIS	-	expression tag	UNP O66529
bC	158	HIS	-	expression tag	UNP O66529
bC	159	HIS	-	expression tag	UNP O66529
bC	160	HIS	-	expression tag	UNP O66529
bC	161	HIS	-	expression tag	UNP O66529
bD	2	GLU	GLN	conflict	UNP O66529
bD	28	GLY	ASP	conflict	UNP O66529
bD	52	CYS	ARG	conflict	UNP O66529
bD	83	GLU	ARG	conflict	UNP O66529
bD	86	GLU	THR	conflict	UNP O66529
bD	112	SER	THR	conflict	UNP O66529
bD	115	ASP	VAL	conflict	UNP O66529
bD	118	ASP	ALA	conflict	UNP O66529
bD	120	GLU	THR	conflict	UNP O66529
bD	123	GLU	GLN	conflict	UNP O66529
bD	127	CYS	ARG	conflict	UNP O66529
bD	131	GLU	LYS	conflict	UNP O66529
bD	155	LEU	-	expression tag	UNP O66529
bD	156	GLU	-	expression tag	UNP O66529
bD	157	HIS	-	expression tag	UNP O66529
bD	158	HIS	-	expression tag	UNP O66529
bD	159	HIS	-	expression tag	UNP O66529
bD	160	HIS	-	expression tag	UNP O66529
bD	161	HIS	-	expression tag	UNP O66529
bE	2	GLU	GLN	conflict	UNP O66529
bE	28	GLY	ASP	conflict	UNP O66529
bE	52	CYS	ARG	conflict	UNP O66529
bE	83	GLU	ARG	conflict	UNP O66529
bE	86	GLU	THR	conflict	UNP O66529
bE	112	SER	THR	conflict	UNP O66529
bE	115	ASP	VAL	conflict	UNP O66529
bE	118	ASP	ALA	conflict	UNP O66529
bE	120	GLU	THR	conflict	UNP O66529
bE	123	GLU	GLN	conflict	UNP O66529
bE	127	CYS	ARG	conflict	UNP O66529
bE	131	GLU	LYS	conflict	UNP O66529
bE	155	LEU	-	expression tag	UNP O66529
bE	156	GLU	-	expression tag	UNP O66529
bE	157	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
bE	158	HIS	-	expression tag	UNP O66529
bE	159	HIS	-	expression tag	UNP O66529
bE	160	HIS	-	expression tag	UNP O66529
bE	161	HIS	-	expression tag	UNP O66529
bX	2	GLU	GLN	conflict	UNP O66529
bX	28	GLY	ASP	conflict	UNP O66529
bX	52	CYS	ARG	conflict	UNP O66529
bX	83	GLU	ARG	conflict	UNP O66529
bX	86	GLU	THR	conflict	UNP O66529
bX	112	SER	THR	conflict	UNP O66529
bX	115	ASP	VAL	conflict	UNP O66529
bX	118	ASP	ALA	conflict	UNP O66529
bX	120	GLU	THR	conflict	UNP O66529
bX	123	GLU	GLN	conflict	UNP O66529
bX	127	CYS	ARG	conflict	UNP O66529
bX	131	GLU	LYS	conflict	UNP O66529
bX	155	LEU	-	expression tag	UNP O66529
bX	156	GLU	-	expression tag	UNP O66529
bX	157	HIS	-	expression tag	UNP O66529
bX	158	HIS	-	expression tag	UNP O66529
bX	159	HIS	-	expression tag	UNP O66529
bX	160	HIS	-	expression tag	UNP O66529
bX	161	HIS	-	expression tag	UNP O66529
cA	2	GLU	GLN	conflict	UNP O66529
cA	28	GLY	ASP	conflict	UNP O66529
cA	52	CYS	ARG	conflict	UNP O66529
cA	83	GLU	ARG	conflict	UNP O66529
cA	86	GLU	THR	conflict	UNP O66529
cA	112	SER	THR	conflict	UNP O66529
cA	115	ASP	VAL	conflict	UNP O66529
cA	118	ASP	ALA	conflict	UNP O66529
cA	120	GLU	THR	conflict	UNP O66529
cA	123	GLU	GLN	conflict	UNP O66529
cA	127	CYS	ARG	conflict	UNP O66529
cA	131	GLU	LYS	conflict	UNP O66529
cA	155	LEU	-	expression tag	UNP O66529
cA	156	GLU	-	expression tag	UNP O66529
cA	157	HIS	-	expression tag	UNP O66529
cA	158	HIS	-	expression tag	UNP O66529
cA	159	HIS	-	expression tag	UNP O66529
cA	160	HIS	-	expression tag	UNP O66529
cA	161	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
cB	2	GLU	GLN	conflict	UNP O66529
cB	28	GLY	ASP	conflict	UNP O66529
cB	52	CYS	ARG	conflict	UNP O66529
cB	83	GLU	ARG	conflict	UNP O66529
cB	86	GLU	THR	conflict	UNP O66529
cB	112	SER	THR	conflict	UNP O66529
cB	115	ASP	VAL	conflict	UNP O66529
cB	118	ASP	ALA	conflict	UNP O66529
cB	120	GLU	THR	conflict	UNP O66529
cB	123	GLU	GLN	conflict	UNP O66529
cB	127	CYS	ARG	conflict	UNP O66529
cB	131	GLU	LYS	conflict	UNP O66529
cB	155	LEU	-	expression tag	UNP O66529
cB	156	GLU	-	expression tag	UNP O66529
cB	157	HIS	-	expression tag	UNP O66529
cB	158	HIS	-	expression tag	UNP O66529
cB	159	HIS	-	expression tag	UNP O66529
cB	160	HIS	-	expression tag	UNP O66529
cB	161	HIS	-	expression tag	UNP O66529
cC	2	GLU	GLN	conflict	UNP O66529
cC	28	GLY	ASP	conflict	UNP O66529
cC	52	CYS	ARG	conflict	UNP O66529
cC	83	GLU	ARG	conflict	UNP O66529
cC	86	GLU	THR	conflict	UNP O66529
cC	112	SER	THR	conflict	UNP O66529
cC	115	ASP	VAL	conflict	UNP O66529
cC	118	ASP	ALA	conflict	UNP O66529
cC	120	GLU	THR	conflict	UNP O66529
cC	123	GLU	GLN	conflict	UNP O66529
cC	127	CYS	ARG	conflict	UNP O66529
cC	131	GLU	LYS	conflict	UNP O66529
cC	155	LEU	-	expression tag	UNP O66529
cC	156	GLU	-	expression tag	UNP O66529
cC	157	HIS	-	expression tag	UNP O66529
cC	158	HIS	-	expression tag	UNP O66529
cC	159	HIS	-	expression tag	UNP O66529
cC	160	HIS	-	expression tag	UNP O66529
cC	161	HIS	-	expression tag	UNP O66529
cD	2	GLU	GLN	conflict	UNP O66529
cD	28	GLY	ASP	conflict	UNP O66529
cD	52	CYS	ARG	conflict	UNP O66529
cD	83	GLU	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
cD	86	GLU	THR	conflict	UNP O66529
cD	112	SER	THR	conflict	UNP O66529
cD	115	ASP	VAL	conflict	UNP O66529
cD	118	ASP	ALA	conflict	UNP O66529
cD	120	GLU	THR	conflict	UNP O66529
cD	123	GLU	GLN	conflict	UNP O66529
cD	127	CYS	ARG	conflict	UNP O66529
cD	131	GLU	LYS	conflict	UNP O66529
cD	155	LEU	-	expression tag	UNP O66529
cD	156	GLU	-	expression tag	UNP O66529
cD	157	HIS	-	expression tag	UNP O66529
cD	158	HIS	-	expression tag	UNP O66529
cD	159	HIS	-	expression tag	UNP O66529
cD	160	HIS	-	expression tag	UNP O66529
cD	161	HIS	-	expression tag	UNP O66529
cE	2	GLU	GLN	conflict	UNP O66529
cE	28	GLY	ASP	conflict	UNP O66529
cE	52	CYS	ARG	conflict	UNP O66529
cE	83	GLU	ARG	conflict	UNP O66529
cE	86	GLU	THR	conflict	UNP O66529
cE	112	SER	THR	conflict	UNP O66529
cE	115	ASP	VAL	conflict	UNP O66529
cE	118	ASP	ALA	conflict	UNP O66529
cE	120	GLU	THR	conflict	UNP O66529
cE	123	GLU	GLN	conflict	UNP O66529
cE	127	CYS	ARG	conflict	UNP O66529
cE	131	GLU	LYS	conflict	UNP O66529
cE	155	LEU	-	expression tag	UNP O66529
cE	156	GLU	-	expression tag	UNP O66529
cE	157	HIS	-	expression tag	UNP O66529
cE	158	HIS	-	expression tag	UNP O66529
cE	159	HIS	-	expression tag	UNP O66529
cE	160	HIS	-	expression tag	UNP O66529
cE	161	HIS	-	expression tag	UNP O66529
cX	2	GLU	GLN	conflict	UNP O66529
cX	28	GLY	ASP	conflict	UNP O66529
cX	52	CYS	ARG	conflict	UNP O66529
cX	83	GLU	ARG	conflict	UNP O66529
cX	86	GLU	THR	conflict	UNP O66529
cX	112	SER	THR	conflict	UNP O66529
cX	115	ASP	VAL	conflict	UNP O66529
cX	118	ASP	ALA	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
cX	120	GLU	THR	conflict	UNP O66529
cX	123	GLU	GLN	conflict	UNP O66529
cX	127	CYS	ARG	conflict	UNP O66529
cX	131	GLU	LYS	conflict	UNP O66529
cX	155	LEU	-	expression tag	UNP O66529
cX	156	GLU	-	expression tag	UNP O66529
cX	157	HIS	-	expression tag	UNP O66529
cX	158	HIS	-	expression tag	UNP O66529
cX	159	HIS	-	expression tag	UNP O66529
cX	160	HIS	-	expression tag	UNP O66529
cX	161	HIS	-	expression tag	UNP O66529
dA	2	GLU	GLN	conflict	UNP O66529
dA	28	GLY	ASP	conflict	UNP O66529
dA	52	CYS	ARG	conflict	UNP O66529
dA	83	GLU	ARG	conflict	UNP O66529
dA	86	GLU	THR	conflict	UNP O66529
dA	112	SER	THR	conflict	UNP O66529
dA	115	ASP	VAL	conflict	UNP O66529
dA	118	ASP	ALA	conflict	UNP O66529
dA	120	GLU	THR	conflict	UNP O66529
dA	123	GLU	GLN	conflict	UNP O66529
dA	127	CYS	ARG	conflict	UNP O66529
dA	131	GLU	LYS	conflict	UNP O66529
dA	155	LEU	-	expression tag	UNP O66529
dA	156	GLU	-	expression tag	UNP O66529
dA	157	HIS	-	expression tag	UNP O66529
dA	158	HIS	-	expression tag	UNP O66529
dA	159	HIS	-	expression tag	UNP O66529
dA	160	HIS	-	expression tag	UNP O66529
dA	161	HIS	-	expression tag	UNP O66529
dB	2	GLU	GLN	conflict	UNP O66529
dB	28	GLY	ASP	conflict	UNP O66529
dB	52	CYS	ARG	conflict	UNP O66529
dB	83	GLU	ARG	conflict	UNP O66529
dB	86	GLU	THR	conflict	UNP O66529
dB	112	SER	THR	conflict	UNP O66529
dB	115	ASP	VAL	conflict	UNP O66529
dB	118	ASP	ALA	conflict	UNP O66529
dB	120	GLU	THR	conflict	UNP O66529
dB	123	GLU	GLN	conflict	UNP O66529
dB	127	CYS	ARG	conflict	UNP O66529
dB	131	GLU	LYS	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
dB	155	LEU	-	expression tag	UNP O66529
dB	156	GLU	-	expression tag	UNP O66529
dB	157	HIS	-	expression tag	UNP O66529
dB	158	HIS	-	expression tag	UNP O66529
dB	159	HIS	-	expression tag	UNP O66529
dB	160	HIS	-	expression tag	UNP O66529
dB	161	HIS	-	expression tag	UNP O66529
dC	2	GLU	GLN	conflict	UNP O66529
dC	28	GLY	ASP	conflict	UNP O66529
dC	52	CYS	ARG	conflict	UNP O66529
dC	83	GLU	ARG	conflict	UNP O66529
dC	86	GLU	THR	conflict	UNP O66529
dC	112	SER	THR	conflict	UNP O66529
dC	115	ASP	VAL	conflict	UNP O66529
dC	118	ASP	ALA	conflict	UNP O66529
dC	120	GLU	THR	conflict	UNP O66529
dC	123	GLU	GLN	conflict	UNP O66529
dC	127	CYS	ARG	conflict	UNP O66529
dC	131	GLU	LYS	conflict	UNP O66529
dC	155	LEU	-	expression tag	UNP O66529
dC	156	GLU	-	expression tag	UNP O66529
dC	157	HIS	-	expression tag	UNP O66529
dC	158	HIS	-	expression tag	UNP O66529
dC	159	HIS	-	expression tag	UNP O66529
dC	160	HIS	-	expression tag	UNP O66529
dC	161	HIS	-	expression tag	UNP O66529
dD	2	GLU	GLN	conflict	UNP O66529
dD	28	GLY	ASP	conflict	UNP O66529
dD	52	CYS	ARG	conflict	UNP O66529
dD	83	GLU	ARG	conflict	UNP O66529
dD	86	GLU	THR	conflict	UNP O66529
dD	112	SER	THR	conflict	UNP O66529
dD	115	ASP	VAL	conflict	UNP O66529
dD	118	ASP	ALA	conflict	UNP O66529
dD	120	GLU	THR	conflict	UNP O66529
dD	123	GLU	GLN	conflict	UNP O66529
dD	127	CYS	ARG	conflict	UNP O66529
dD	131	GLU	LYS	conflict	UNP O66529
dD	155	LEU	-	expression tag	UNP O66529
dD	156	GLU	-	expression tag	UNP O66529
dD	157	HIS	-	expression tag	UNP O66529
dD	158	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
dD	159	HIS	-	expression tag	UNP O66529
dD	160	HIS	-	expression tag	UNP O66529
dD	161	HIS	-	expression tag	UNP O66529
dE	2	GLU	GLN	conflict	UNP O66529
dE	28	GLY	ASP	conflict	UNP O66529
dE	52	CYS	ARG	conflict	UNP O66529
dE	83	GLU	ARG	conflict	UNP O66529
dE	86	GLU	THR	conflict	UNP O66529
dE	112	SER	THR	conflict	UNP O66529
dE	115	ASP	VAL	conflict	UNP O66529
dE	118	ASP	ALA	conflict	UNP O66529
dE	120	GLU	THR	conflict	UNP O66529
dE	123	GLU	GLN	conflict	UNP O66529
dE	127	CYS	ARG	conflict	UNP O66529
dE	131	GLU	LYS	conflict	UNP O66529
dE	155	LEU	-	expression tag	UNP O66529
dE	156	GLU	-	expression tag	UNP O66529
dE	157	HIS	-	expression tag	UNP O66529
dE	158	HIS	-	expression tag	UNP O66529
dE	159	HIS	-	expression tag	UNP O66529
dE	160	HIS	-	expression tag	UNP O66529
dE	161	HIS	-	expression tag	UNP O66529
dX	2	GLU	GLN	conflict	UNP O66529
dX	28	GLY	ASP	conflict	UNP O66529
dX	52	CYS	ARG	conflict	UNP O66529
dX	83	GLU	ARG	conflict	UNP O66529
dX	86	GLU	THR	conflict	UNP O66529
dX	112	SER	THR	conflict	UNP O66529
dX	115	ASP	VAL	conflict	UNP O66529
dX	118	ASP	ALA	conflict	UNP O66529
dX	120	GLU	THR	conflict	UNP O66529
dX	123	GLU	GLN	conflict	UNP O66529
dX	127	CYS	ARG	conflict	UNP O66529
dX	131	GLU	LYS	conflict	UNP O66529
dX	155	LEU	-	expression tag	UNP O66529
dX	156	GLU	-	expression tag	UNP O66529
dX	157	HIS	-	expression tag	UNP O66529
dX	158	HIS	-	expression tag	UNP O66529
dX	159	HIS	-	expression tag	UNP O66529
dX	160	HIS	-	expression tag	UNP O66529
dX	161	HIS	-	expression tag	UNP O66529
eA	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
eA	28	GLY	ASP	conflict	UNP O66529
eA	52	CYS	ARG	conflict	UNP O66529
eA	83	GLU	ARG	conflict	UNP O66529
eA	86	GLU	THR	conflict	UNP O66529
eA	112	SER	THR	conflict	UNP O66529
eA	115	ASP	VAL	conflict	UNP O66529
eA	118	ASP	ALA	conflict	UNP O66529
eA	120	GLU	THR	conflict	UNP O66529
eA	123	GLU	GLN	conflict	UNP O66529
eA	127	CYS	ARG	conflict	UNP O66529
eA	131	GLU	LYS	conflict	UNP O66529
eA	155	LEU	-	expression tag	UNP O66529
eA	156	GLU	-	expression tag	UNP O66529
eA	157	HIS	-	expression tag	UNP O66529
eA	158	HIS	-	expression tag	UNP O66529
eA	159	HIS	-	expression tag	UNP O66529
eA	160	HIS	-	expression tag	UNP O66529
eA	161	HIS	-	expression tag	UNP O66529
eB	2	GLU	GLN	conflict	UNP O66529
eB	28	GLY	ASP	conflict	UNP O66529
eB	52	CYS	ARG	conflict	UNP O66529
eB	83	GLU	ARG	conflict	UNP O66529
eB	86	GLU	THR	conflict	UNP O66529
eB	112	SER	THR	conflict	UNP O66529
eB	115	ASP	VAL	conflict	UNP O66529
eB	118	ASP	ALA	conflict	UNP O66529
eB	120	GLU	THR	conflict	UNP O66529
eB	123	GLU	GLN	conflict	UNP O66529
eB	127	CYS	ARG	conflict	UNP O66529
eB	131	GLU	LYS	conflict	UNP O66529
eB	155	LEU	-	expression tag	UNP O66529
eB	156	GLU	-	expression tag	UNP O66529
eB	157	HIS	-	expression tag	UNP O66529
eB	158	HIS	-	expression tag	UNP O66529
eB	159	HIS	-	expression tag	UNP O66529
eB	160	HIS	-	expression tag	UNP O66529
eB	161	HIS	-	expression tag	UNP O66529
eC	2	GLU	GLN	conflict	UNP O66529
eC	28	GLY	ASP	conflict	UNP O66529
eC	52	CYS	ARG	conflict	UNP O66529
eC	83	GLU	ARG	conflict	UNP O66529
eC	86	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
eC	112	SER	THR	conflict	UNP O66529
eC	115	ASP	VAL	conflict	UNP O66529
eC	118	ASP	ALA	conflict	UNP O66529
eC	120	GLU	THR	conflict	UNP O66529
eC	123	GLU	GLN	conflict	UNP O66529
eC	127	CYS	ARG	conflict	UNP O66529
eC	131	GLU	LYS	conflict	UNP O66529
eC	155	LEU	-	expression tag	UNP O66529
eC	156	GLU	-	expression tag	UNP O66529
eC	157	HIS	-	expression tag	UNP O66529
eC	158	HIS	-	expression tag	UNP O66529
eC	159	HIS	-	expression tag	UNP O66529
eC	160	HIS	-	expression tag	UNP O66529
eC	161	HIS	-	expression tag	UNP O66529
eD	2	GLU	GLN	conflict	UNP O66529
eD	28	GLY	ASP	conflict	UNP O66529
eD	52	CYS	ARG	conflict	UNP O66529
eD	83	GLU	ARG	conflict	UNP O66529
eD	86	GLU	THR	conflict	UNP O66529
eD	112	SER	THR	conflict	UNP O66529
eD	115	ASP	VAL	conflict	UNP O66529
eD	118	ASP	ALA	conflict	UNP O66529
eD	120	GLU	THR	conflict	UNP O66529
eD	123	GLU	GLN	conflict	UNP O66529
eD	127	CYS	ARG	conflict	UNP O66529
eD	131	GLU	LYS	conflict	UNP O66529
eD	155	LEU	-	expression tag	UNP O66529
eD	156	GLU	-	expression tag	UNP O66529
eD	157	HIS	-	expression tag	UNP O66529
eD	158	HIS	-	expression tag	UNP O66529
eD	159	HIS	-	expression tag	UNP O66529
eD	160	HIS	-	expression tag	UNP O66529
eD	161	HIS	-	expression tag	UNP O66529
eE	2	GLU	GLN	conflict	UNP O66529
eE	28	GLY	ASP	conflict	UNP O66529
eE	52	CYS	ARG	conflict	UNP O66529
eE	83	GLU	ARG	conflict	UNP O66529
eE	86	GLU	THR	conflict	UNP O66529
eE	112	SER	THR	conflict	UNP O66529
eE	115	ASP	VAL	conflict	UNP O66529
eE	118	ASP	ALA	conflict	UNP O66529
eE	120	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
eE	123	GLU	GLN	conflict	UNP O66529
eE	127	CYS	ARG	conflict	UNP O66529
eE	131	GLU	LYS	conflict	UNP O66529
eE	155	LEU	-	expression tag	UNP O66529
eE	156	GLU	-	expression tag	UNP O66529
eE	157	HIS	-	expression tag	UNP O66529
eE	158	HIS	-	expression tag	UNP O66529
eE	159	HIS	-	expression tag	UNP O66529
eE	160	HIS	-	expression tag	UNP O66529
eE	161	HIS	-	expression tag	UNP O66529
eX	2	GLU	GLN	conflict	UNP O66529
eX	28	GLY	ASP	conflict	UNP O66529
eX	52	CYS	ARG	conflict	UNP O66529
eX	83	GLU	ARG	conflict	UNP O66529
eX	86	GLU	THR	conflict	UNP O66529
eX	112	SER	THR	conflict	UNP O66529
eX	115	ASP	VAL	conflict	UNP O66529
eX	118	ASP	ALA	conflict	UNP O66529
eX	120	GLU	THR	conflict	UNP O66529
eX	123	GLU	GLN	conflict	UNP O66529
eX	127	CYS	ARG	conflict	UNP O66529
eX	131	GLU	LYS	conflict	UNP O66529
eX	155	LEU	-	expression tag	UNP O66529
eX	156	GLU	-	expression tag	UNP O66529
eX	157	HIS	-	expression tag	UNP O66529
eX	158	HIS	-	expression tag	UNP O66529
eX	159	HIS	-	expression tag	UNP O66529
eX	160	HIS	-	expression tag	UNP O66529
eX	161	HIS	-	expression tag	UNP O66529
fA	2	GLU	GLN	conflict	UNP O66529
fA	28	GLY	ASP	conflict	UNP O66529
fA	52	CYS	ARG	conflict	UNP O66529
fA	83	GLU	ARG	conflict	UNP O66529
fA	86	GLU	THR	conflict	UNP O66529
fA	112	SER	THR	conflict	UNP O66529
fA	115	ASP	VAL	conflict	UNP O66529
fA	118	ASP	ALA	conflict	UNP O66529
fA	120	GLU	THR	conflict	UNP O66529
fA	123	GLU	GLN	conflict	UNP O66529
fA	127	CYS	ARG	conflict	UNP O66529
fA	131	GLU	LYS	conflict	UNP O66529
fA	155	LEU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
fA	156	GLU	-	expression tag	UNP O66529
fA	157	HIS	-	expression tag	UNP O66529
fA	158	HIS	-	expression tag	UNP O66529
fA	159	HIS	-	expression tag	UNP O66529
fA	160	HIS	-	expression tag	UNP O66529
fA	161	HIS	-	expression tag	UNP O66529
fB	2	GLU	GLN	conflict	UNP O66529
fB	28	GLY	ASP	conflict	UNP O66529
fB	52	CYS	ARG	conflict	UNP O66529
fB	83	GLU	ARG	conflict	UNP O66529
fB	86	GLU	THR	conflict	UNP O66529
fB	112	SER	THR	conflict	UNP O66529
fB	115	ASP	VAL	conflict	UNP O66529
fB	118	ASP	ALA	conflict	UNP O66529
fB	120	GLU	THR	conflict	UNP O66529
fB	123	GLU	GLN	conflict	UNP O66529
fB	127	CYS	ARG	conflict	UNP O66529
fB	131	GLU	LYS	conflict	UNP O66529
fB	155	LEU	-	expression tag	UNP O66529
fB	156	GLU	-	expression tag	UNP O66529
fB	157	HIS	-	expression tag	UNP O66529
fB	158	HIS	-	expression tag	UNP O66529
fB	159	HIS	-	expression tag	UNP O66529
fB	160	HIS	-	expression tag	UNP O66529
fB	161	HIS	-	expression tag	UNP O66529
fC	2	GLU	GLN	conflict	UNP O66529
fC	28	GLY	ASP	conflict	UNP O66529
fC	52	CYS	ARG	conflict	UNP O66529
fC	83	GLU	ARG	conflict	UNP O66529
fC	86	GLU	THR	conflict	UNP O66529
fC	112	SER	THR	conflict	UNP O66529
fC	115	ASP	VAL	conflict	UNP O66529
fC	118	ASP	ALA	conflict	UNP O66529
fC	120	GLU	THR	conflict	UNP O66529
fC	123	GLU	GLN	conflict	UNP O66529
fC	127	CYS	ARG	conflict	UNP O66529
fC	131	GLU	LYS	conflict	UNP O66529
fC	155	LEU	-	expression tag	UNP O66529
fC	156	GLU	-	expression tag	UNP O66529
fC	157	HIS	-	expression tag	UNP O66529
fC	158	HIS	-	expression tag	UNP O66529
fC	159	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
fC	160	HIS	-	expression tag	UNP O66529
fC	161	HIS	-	expression tag	UNP O66529
fD	2	GLU	GLN	conflict	UNP O66529
fD	28	GLY	ASP	conflict	UNP O66529
fD	52	CYS	ARG	conflict	UNP O66529
fD	83	GLU	ARG	conflict	UNP O66529
fD	86	GLU	THR	conflict	UNP O66529
fD	112	SER	THR	conflict	UNP O66529
fD	115	ASP	VAL	conflict	UNP O66529
fD	118	ASP	ALA	conflict	UNP O66529
fD	120	GLU	THR	conflict	UNP O66529
fD	123	GLU	GLN	conflict	UNP O66529
fD	127	CYS	ARG	conflict	UNP O66529
fD	131	GLU	LYS	conflict	UNP O66529
fD	155	LEU	-	expression tag	UNP O66529
fD	156	GLU	-	expression tag	UNP O66529
fD	157	HIS	-	expression tag	UNP O66529
fD	158	HIS	-	expression tag	UNP O66529
fD	159	HIS	-	expression tag	UNP O66529
fD	160	HIS	-	expression tag	UNP O66529
fD	161	HIS	-	expression tag	UNP O66529
fE	2	GLU	GLN	conflict	UNP O66529
fE	28	GLY	ASP	conflict	UNP O66529
fE	52	CYS	ARG	conflict	UNP O66529
fE	83	GLU	ARG	conflict	UNP O66529
fE	86	GLU	THR	conflict	UNP O66529
fE	112	SER	THR	conflict	UNP O66529
fE	115	ASP	VAL	conflict	UNP O66529
fE	118	ASP	ALA	conflict	UNP O66529
fE	120	GLU	THR	conflict	UNP O66529
fE	123	GLU	GLN	conflict	UNP O66529
fE	127	CYS	ARG	conflict	UNP O66529
fE	131	GLU	LYS	conflict	UNP O66529
fE	155	LEU	-	expression tag	UNP O66529
fE	156	GLU	-	expression tag	UNP O66529
fE	157	HIS	-	expression tag	UNP O66529
fE	158	HIS	-	expression tag	UNP O66529
fE	159	HIS	-	expression tag	UNP O66529
fE	160	HIS	-	expression tag	UNP O66529
fE	161	HIS	-	expression tag	UNP O66529
fX	2	GLU	GLN	conflict	UNP O66529
fX	28	GLY	ASP	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
fX	52	CYS	ARG	conflict	UNP O66529
fX	83	GLU	ARG	conflict	UNP O66529
fX	86	GLU	THR	conflict	UNP O66529
fX	112	SER	THR	conflict	UNP O66529
fX	115	ASP	VAL	conflict	UNP O66529
fX	118	ASP	ALA	conflict	UNP O66529
fX	120	GLU	THR	conflict	UNP O66529
fX	123	GLU	GLN	conflict	UNP O66529
fX	127	CYS	ARG	conflict	UNP O66529
fX	131	GLU	LYS	conflict	UNP O66529
fX	155	LEU	-	expression tag	UNP O66529
fX	156	GLU	-	expression tag	UNP O66529
fX	157	HIS	-	expression tag	UNP O66529
fX	158	HIS	-	expression tag	UNP O66529
fX	159	HIS	-	expression tag	UNP O66529
fX	160	HIS	-	expression tag	UNP O66529
fX	161	HIS	-	expression tag	UNP O66529
gA	2	GLU	GLN	conflict	UNP O66529
gA	28	GLY	ASP	conflict	UNP O66529
gA	52	CYS	ARG	conflict	UNP O66529
gA	83	GLU	ARG	conflict	UNP O66529
gA	86	GLU	THR	conflict	UNP O66529
gA	112	SER	THR	conflict	UNP O66529
gA	115	ASP	VAL	conflict	UNP O66529
gA	118	ASP	ALA	conflict	UNP O66529
gA	120	GLU	THR	conflict	UNP O66529
gA	123	GLU	GLN	conflict	UNP O66529
gA	127	CYS	ARG	conflict	UNP O66529
gA	131	GLU	LYS	conflict	UNP O66529
gA	155	LEU	-	expression tag	UNP O66529
gA	156	GLU	-	expression tag	UNP O66529
gA	157	HIS	-	expression tag	UNP O66529
gA	158	HIS	-	expression tag	UNP O66529
gA	159	HIS	-	expression tag	UNP O66529
gA	160	HIS	-	expression tag	UNP O66529
gA	161	HIS	-	expression tag	UNP O66529
gB	2	GLU	GLN	conflict	UNP O66529
gB	28	GLY	ASP	conflict	UNP O66529
gB	52	CYS	ARG	conflict	UNP O66529
gB	83	GLU	ARG	conflict	UNP O66529
gB	86	GLU	THR	conflict	UNP O66529
gB	112	SER	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
gB	115	ASP	VAL	conflict	UNP O66529
gB	118	ASP	ALA	conflict	UNP O66529
gB	120	GLU	THR	conflict	UNP O66529
gB	123	GLU	GLN	conflict	UNP O66529
gB	127	CYS	ARG	conflict	UNP O66529
gB	131	GLU	LYS	conflict	UNP O66529
gB	155	LEU	-	expression tag	UNP O66529
gB	156	GLU	-	expression tag	UNP O66529
gB	157	HIS	-	expression tag	UNP O66529
gB	158	HIS	-	expression tag	UNP O66529
gB	159	HIS	-	expression tag	UNP O66529
gB	160	HIS	-	expression tag	UNP O66529
gB	161	HIS	-	expression tag	UNP O66529
gC	2	GLU	GLN	conflict	UNP O66529
gC	28	GLY	ASP	conflict	UNP O66529
gC	52	CYS	ARG	conflict	UNP O66529
gC	83	GLU	ARG	conflict	UNP O66529
gC	86	GLU	THR	conflict	UNP O66529
gC	112	SER	THR	conflict	UNP O66529
gC	115	ASP	VAL	conflict	UNP O66529
gC	118	ASP	ALA	conflict	UNP O66529
gC	120	GLU	THR	conflict	UNP O66529
gC	123	GLU	GLN	conflict	UNP O66529
gC	127	CYS	ARG	conflict	UNP O66529
gC	131	GLU	LYS	conflict	UNP O66529
gC	155	LEU	-	expression tag	UNP O66529
gC	156	GLU	-	expression tag	UNP O66529
gC	157	HIS	-	expression tag	UNP O66529
gC	158	HIS	-	expression tag	UNP O66529
gC	159	HIS	-	expression tag	UNP O66529
gC	160	HIS	-	expression tag	UNP O66529
gC	161	HIS	-	expression tag	UNP O66529
gD	2	GLU	GLN	conflict	UNP O66529
gD	28	GLY	ASP	conflict	UNP O66529
gD	52	CYS	ARG	conflict	UNP O66529
gD	83	GLU	ARG	conflict	UNP O66529
gD	86	GLU	THR	conflict	UNP O66529
gD	112	SER	THR	conflict	UNP O66529
gD	115	ASP	VAL	conflict	UNP O66529
gD	118	ASP	ALA	conflict	UNP O66529
gD	120	GLU	THR	conflict	UNP O66529
gD	123	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
gD	127	CYS	ARG	conflict	UNP O66529
gD	131	GLU	LYS	conflict	UNP O66529
gD	155	LEU	-	expression tag	UNP O66529
gD	156	GLU	-	expression tag	UNP O66529
gD	157	HIS	-	expression tag	UNP O66529
gD	158	HIS	-	expression tag	UNP O66529
gD	159	HIS	-	expression tag	UNP O66529
gD	160	HIS	-	expression tag	UNP O66529
gD	161	HIS	-	expression tag	UNP O66529
gE	2	GLU	GLN	conflict	UNP O66529
gE	28	GLY	ASP	conflict	UNP O66529
gE	52	CYS	ARG	conflict	UNP O66529
gE	83	GLU	ARG	conflict	UNP O66529
gE	86	GLU	THR	conflict	UNP O66529
gE	112	SER	THR	conflict	UNP O66529
gE	115	ASP	VAL	conflict	UNP O66529
gE	118	ASP	ALA	conflict	UNP O66529
gE	120	GLU	THR	conflict	UNP O66529
gE	123	GLU	GLN	conflict	UNP O66529
gE	127	CYS	ARG	conflict	UNP O66529
gE	131	GLU	LYS	conflict	UNP O66529
gE	155	LEU	-	expression tag	UNP O66529
gE	156	GLU	-	expression tag	UNP O66529
gE	157	HIS	-	expression tag	UNP O66529
gE	158	HIS	-	expression tag	UNP O66529
gE	159	HIS	-	expression tag	UNP O66529
gE	160	HIS	-	expression tag	UNP O66529
gE	161	HIS	-	expression tag	UNP O66529
gX	2	GLU	GLN	conflict	UNP O66529
gX	28	GLY	ASP	conflict	UNP O66529
gX	52	CYS	ARG	conflict	UNP O66529
gX	83	GLU	ARG	conflict	UNP O66529
gX	86	GLU	THR	conflict	UNP O66529
gX	112	SER	THR	conflict	UNP O66529
gX	115	ASP	VAL	conflict	UNP O66529
gX	118	ASP	ALA	conflict	UNP O66529
gX	120	GLU	THR	conflict	UNP O66529
gX	123	GLU	GLN	conflict	UNP O66529
gX	127	CYS	ARG	conflict	UNP O66529
gX	131	GLU	LYS	conflict	UNP O66529
gX	155	LEU	-	expression tag	UNP O66529
gX	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
gX	157	HIS	-	expression tag	UNP O66529
gX	158	HIS	-	expression tag	UNP O66529
gX	159	HIS	-	expression tag	UNP O66529
gX	160	HIS	-	expression tag	UNP O66529
gX	161	HIS	-	expression tag	UNP O66529
hA	2	GLU	GLN	conflict	UNP O66529
hA	28	GLY	ASP	conflict	UNP O66529
hA	52	CYS	ARG	conflict	UNP O66529
hA	83	GLU	ARG	conflict	UNP O66529
hA	86	GLU	THR	conflict	UNP O66529
hA	112	SER	THR	conflict	UNP O66529
hA	115	ASP	VAL	conflict	UNP O66529
hA	118	ASP	ALA	conflict	UNP O66529
hA	120	GLU	THR	conflict	UNP O66529
hA	123	GLU	GLN	conflict	UNP O66529
hA	127	CYS	ARG	conflict	UNP O66529
hA	131	GLU	LYS	conflict	UNP O66529
hA	155	LEU	-	expression tag	UNP O66529
hA	156	GLU	-	expression tag	UNP O66529
hA	157	HIS	-	expression tag	UNP O66529
hA	158	HIS	-	expression tag	UNP O66529
hA	159	HIS	-	expression tag	UNP O66529
hA	160	HIS	-	expression tag	UNP O66529
hA	161	HIS	-	expression tag	UNP O66529
hB	2	GLU	GLN	conflict	UNP O66529
hB	28	GLY	ASP	conflict	UNP O66529
hB	52	CYS	ARG	conflict	UNP O66529
hB	83	GLU	ARG	conflict	UNP O66529
hB	86	GLU	THR	conflict	UNP O66529
hB	112	SER	THR	conflict	UNP O66529
hB	115	ASP	VAL	conflict	UNP O66529
hB	118	ASP	ALA	conflict	UNP O66529
hB	120	GLU	THR	conflict	UNP O66529
hB	123	GLU	GLN	conflict	UNP O66529
hB	127	CYS	ARG	conflict	UNP O66529
hB	131	GLU	LYS	conflict	UNP O66529
hB	155	LEU	-	expression tag	UNP O66529
hB	156	GLU	-	expression tag	UNP O66529
hB	157	HIS	-	expression tag	UNP O66529
hB	158	HIS	-	expression tag	UNP O66529
hB	159	HIS	-	expression tag	UNP O66529
hB	160	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
hB	161	HIS	-	expression tag	UNP O66529
hC	2	GLU	GLN	conflict	UNP O66529
hC	28	GLY	ASP	conflict	UNP O66529
hC	52	CYS	ARG	conflict	UNP O66529
hC	83	GLU	ARG	conflict	UNP O66529
hC	86	GLU	THR	conflict	UNP O66529
hC	112	SER	THR	conflict	UNP O66529
hC	115	ASP	VAL	conflict	UNP O66529
hC	118	ASP	ALA	conflict	UNP O66529
hC	120	GLU	THR	conflict	UNP O66529
hC	123	GLU	GLN	conflict	UNP O66529
hC	127	CYS	ARG	conflict	UNP O66529
hC	131	GLU	LYS	conflict	UNP O66529
hC	155	LEU	-	expression tag	UNP O66529
hC	156	GLU	-	expression tag	UNP O66529
hC	157	HIS	-	expression tag	UNP O66529
hC	158	HIS	-	expression tag	UNP O66529
hC	159	HIS	-	expression tag	UNP O66529
hC	160	HIS	-	expression tag	UNP O66529
hC	161	HIS	-	expression tag	UNP O66529
hD	2	GLU	GLN	conflict	UNP O66529
hD	28	GLY	ASP	conflict	UNP O66529
hD	52	CYS	ARG	conflict	UNP O66529
hD	83	GLU	ARG	conflict	UNP O66529
hD	86	GLU	THR	conflict	UNP O66529
hD	112	SER	THR	conflict	UNP O66529
hD	115	ASP	VAL	conflict	UNP O66529
hD	118	ASP	ALA	conflict	UNP O66529
hD	120	GLU	THR	conflict	UNP O66529
hD	123	GLU	GLN	conflict	UNP O66529
hD	127	CYS	ARG	conflict	UNP O66529
hD	131	GLU	LYS	conflict	UNP O66529
hD	155	LEU	-	expression tag	UNP O66529
hD	156	GLU	-	expression tag	UNP O66529
hD	157	HIS	-	expression tag	UNP O66529
hD	158	HIS	-	expression tag	UNP O66529
hD	159	HIS	-	expression tag	UNP O66529
hD	160	HIS	-	expression tag	UNP O66529
hD	161	HIS	-	expression tag	UNP O66529
hE	2	GLU	GLN	conflict	UNP O66529
hE	28	GLY	ASP	conflict	UNP O66529
hE	52	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
hE	83	GLU	ARG	conflict	UNP O66529
hE	86	GLU	THR	conflict	UNP O66529
hE	112	SER	THR	conflict	UNP O66529
hE	115	ASP	VAL	conflict	UNP O66529
hE	118	ASP	ALA	conflict	UNP O66529
hE	120	GLU	THR	conflict	UNP O66529
hE	123	GLU	GLN	conflict	UNP O66529
hE	127	CYS	ARG	conflict	UNP O66529
hE	131	GLU	LYS	conflict	UNP O66529
hE	155	LEU	-	expression tag	UNP O66529
hE	156	GLU	-	expression tag	UNP O66529
hE	157	HIS	-	expression tag	UNP O66529
hE	158	HIS	-	expression tag	UNP O66529
hE	159	HIS	-	expression tag	UNP O66529
hE	160	HIS	-	expression tag	UNP O66529
hE	161	HIS	-	expression tag	UNP O66529
hX	2	GLU	GLN	conflict	UNP O66529
hX	28	GLY	ASP	conflict	UNP O66529
hX	52	CYS	ARG	conflict	UNP O66529
hX	83	GLU	ARG	conflict	UNP O66529
hX	86	GLU	THR	conflict	UNP O66529
hX	112	SER	THR	conflict	UNP O66529
hX	115	ASP	VAL	conflict	UNP O66529
hX	118	ASP	ALA	conflict	UNP O66529
hX	120	GLU	THR	conflict	UNP O66529
hX	123	GLU	GLN	conflict	UNP O66529
hX	127	CYS	ARG	conflict	UNP O66529
hX	131	GLU	LYS	conflict	UNP O66529
hX	155	LEU	-	expression tag	UNP O66529
hX	156	GLU	-	expression tag	UNP O66529
hX	157	HIS	-	expression tag	UNP O66529
hX	158	HIS	-	expression tag	UNP O66529
hX	159	HIS	-	expression tag	UNP O66529
hX	160	HIS	-	expression tag	UNP O66529
hX	161	HIS	-	expression tag	UNP O66529
iA	2	GLU	GLN	conflict	UNP O66529
iA	28	GLY	ASP	conflict	UNP O66529
iA	52	CYS	ARG	conflict	UNP O66529
iA	83	GLU	ARG	conflict	UNP O66529
iA	86	GLU	THR	conflict	UNP O66529
iA	112	SER	THR	conflict	UNP O66529
iA	115	ASP	VAL	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
iA	118	ASP	ALA	conflict	UNP O66529
iA	120	GLU	THR	conflict	UNP O66529
iA	123	GLU	GLN	conflict	UNP O66529
iA	127	CYS	ARG	conflict	UNP O66529
iA	131	GLU	LYS	conflict	UNP O66529
iA	155	LEU	-	expression tag	UNP O66529
iA	156	GLU	-	expression tag	UNP O66529
iA	157	HIS	-	expression tag	UNP O66529
iA	158	HIS	-	expression tag	UNP O66529
iA	159	HIS	-	expression tag	UNP O66529
iA	160	HIS	-	expression tag	UNP O66529
iA	161	HIS	-	expression tag	UNP O66529
iB	2	GLU	GLN	conflict	UNP O66529
iB	28	GLY	ASP	conflict	UNP O66529
iB	52	CYS	ARG	conflict	UNP O66529
iB	83	GLU	ARG	conflict	UNP O66529
iB	86	GLU	THR	conflict	UNP O66529
iB	112	SER	THR	conflict	UNP O66529
iB	115	ASP	VAL	conflict	UNP O66529
iB	118	ASP	ALA	conflict	UNP O66529
iB	120	GLU	THR	conflict	UNP O66529
iB	123	GLU	GLN	conflict	UNP O66529
iB	127	CYS	ARG	conflict	UNP O66529
iB	131	GLU	LYS	conflict	UNP O66529
iB	155	LEU	-	expression tag	UNP O66529
iB	156	GLU	-	expression tag	UNP O66529
iB	157	HIS	-	expression tag	UNP O66529
iB	158	HIS	-	expression tag	UNP O66529
iB	159	HIS	-	expression tag	UNP O66529
iB	160	HIS	-	expression tag	UNP O66529
iB	161	HIS	-	expression tag	UNP O66529
iC	2	GLU	GLN	conflict	UNP O66529
iC	28	GLY	ASP	conflict	UNP O66529
iC	52	CYS	ARG	conflict	UNP O66529
iC	83	GLU	ARG	conflict	UNP O66529
iC	86	GLU	THR	conflict	UNP O66529
iC	112	SER	THR	conflict	UNP O66529
iC	115	ASP	VAL	conflict	UNP O66529
iC	118	ASP	ALA	conflict	UNP O66529
iC	120	GLU	THR	conflict	UNP O66529
iC	123	GLU	GLN	conflict	UNP O66529
iC	127	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
iC	131	GLU	LYS	conflict	UNP O66529
iC	155	LEU	-	expression tag	UNP O66529
iC	156	GLU	-	expression tag	UNP O66529
iC	157	HIS	-	expression tag	UNP O66529
iC	158	HIS	-	expression tag	UNP O66529
iC	159	HIS	-	expression tag	UNP O66529
iC	160	HIS	-	expression tag	UNP O66529
iC	161	HIS	-	expression tag	UNP O66529
iD	2	GLU	GLN	conflict	UNP O66529
iD	28	GLY	ASP	conflict	UNP O66529
iD	52	CYS	ARG	conflict	UNP O66529
iD	83	GLU	ARG	conflict	UNP O66529
iD	86	GLU	THR	conflict	UNP O66529
iD	112	SER	THR	conflict	UNP O66529
iD	115	ASP	VAL	conflict	UNP O66529
iD	118	ASP	ALA	conflict	UNP O66529
iD	120	GLU	THR	conflict	UNP O66529
iD	123	GLU	GLN	conflict	UNP O66529
iD	127	CYS	ARG	conflict	UNP O66529
iD	131	GLU	LYS	conflict	UNP O66529
iD	155	LEU	-	expression tag	UNP O66529
iD	156	GLU	-	expression tag	UNP O66529
iD	157	HIS	-	expression tag	UNP O66529
iD	158	HIS	-	expression tag	UNP O66529
iD	159	HIS	-	expression tag	UNP O66529
iD	160	HIS	-	expression tag	UNP O66529
iD	161	HIS	-	expression tag	UNP O66529
iE	2	GLU	GLN	conflict	UNP O66529
iE	28	GLY	ASP	conflict	UNP O66529
iE	52	CYS	ARG	conflict	UNP O66529
iE	83	GLU	ARG	conflict	UNP O66529
iE	86	GLU	THR	conflict	UNP O66529
iE	112	SER	THR	conflict	UNP O66529
iE	115	ASP	VAL	conflict	UNP O66529
iE	118	ASP	ALA	conflict	UNP O66529
iE	120	GLU	THR	conflict	UNP O66529
iE	123	GLU	GLN	conflict	UNP O66529
iE	127	CYS	ARG	conflict	UNP O66529
iE	131	GLU	LYS	conflict	UNP O66529
iE	155	LEU	-	expression tag	UNP O66529
iE	156	GLU	-	expression tag	UNP O66529
iE	157	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
iE	158	HIS	-	expression tag	UNP O66529
iE	159	HIS	-	expression tag	UNP O66529
iE	160	HIS	-	expression tag	UNP O66529
iE	161	HIS	-	expression tag	UNP O66529
iX	2	GLU	GLN	conflict	UNP O66529
iX	28	GLY	ASP	conflict	UNP O66529
iX	52	CYS	ARG	conflict	UNP O66529
iX	83	GLU	ARG	conflict	UNP O66529
iX	86	GLU	THR	conflict	UNP O66529
iX	112	SER	THR	conflict	UNP O66529
iX	115	ASP	VAL	conflict	UNP O66529
iX	118	ASP	ALA	conflict	UNP O66529
iX	120	GLU	THR	conflict	UNP O66529
iX	123	GLU	GLN	conflict	UNP O66529
iX	127	CYS	ARG	conflict	UNP O66529
iX	131	GLU	LYS	conflict	UNP O66529
iX	155	LEU	-	expression tag	UNP O66529
iX	156	GLU	-	expression tag	UNP O66529
iX	157	HIS	-	expression tag	UNP O66529
iX	158	HIS	-	expression tag	UNP O66529
iX	159	HIS	-	expression tag	UNP O66529
iX	160	HIS	-	expression tag	UNP O66529
iX	161	HIS	-	expression tag	UNP O66529
jA	2	GLU	GLN	conflict	UNP O66529
jA	28	GLY	ASP	conflict	UNP O66529
jA	52	CYS	ARG	conflict	UNP O66529
jA	83	GLU	ARG	conflict	UNP O66529
jA	86	GLU	THR	conflict	UNP O66529
jA	112	SER	THR	conflict	UNP O66529
jA	115	ASP	VAL	conflict	UNP O66529
jA	118	ASP	ALA	conflict	UNP O66529
jA	120	GLU	THR	conflict	UNP O66529
jA	123	GLU	GLN	conflict	UNP O66529
jA	127	CYS	ARG	conflict	UNP O66529
jA	131	GLU	LYS	conflict	UNP O66529
jA	155	LEU	-	expression tag	UNP O66529
jA	156	GLU	-	expression tag	UNP O66529
jA	157	HIS	-	expression tag	UNP O66529
jA	158	HIS	-	expression tag	UNP O66529
jA	159	HIS	-	expression tag	UNP O66529
jA	160	HIS	-	expression tag	UNP O66529
jA	161	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
jB	2	GLU	GLN	conflict	UNP O66529
jB	28	GLY	ASP	conflict	UNP O66529
jB	52	CYS	ARG	conflict	UNP O66529
jB	83	GLU	ARG	conflict	UNP O66529
jB	86	GLU	THR	conflict	UNP O66529
jB	112	SER	THR	conflict	UNP O66529
jB	115	ASP	VAL	conflict	UNP O66529
jB	118	ASP	ALA	conflict	UNP O66529
jB	120	GLU	THR	conflict	UNP O66529
jB	123	GLU	GLN	conflict	UNP O66529
jB	127	CYS	ARG	conflict	UNP O66529
jB	131	GLU	LYS	conflict	UNP O66529
jB	155	LEU	-	expression tag	UNP O66529
jB	156	GLU	-	expression tag	UNP O66529
jB	157	HIS	-	expression tag	UNP O66529
jB	158	HIS	-	expression tag	UNP O66529
jB	159	HIS	-	expression tag	UNP O66529
jB	160	HIS	-	expression tag	UNP O66529
jB	161	HIS	-	expression tag	UNP O66529
jC	2	GLU	GLN	conflict	UNP O66529
jC	28	GLY	ASP	conflict	UNP O66529
jC	52	CYS	ARG	conflict	UNP O66529
jC	83	GLU	ARG	conflict	UNP O66529
jC	86	GLU	THR	conflict	UNP O66529
jC	112	SER	THR	conflict	UNP O66529
jC	115	ASP	VAL	conflict	UNP O66529
jC	118	ASP	ALA	conflict	UNP O66529
jC	120	GLU	THR	conflict	UNP O66529
jC	123	GLU	GLN	conflict	UNP O66529
jC	127	CYS	ARG	conflict	UNP O66529
jC	131	GLU	LYS	conflict	UNP O66529
jC	155	LEU	-	expression tag	UNP O66529
jC	156	GLU	-	expression tag	UNP O66529
jC	157	HIS	-	expression tag	UNP O66529
jC	158	HIS	-	expression tag	UNP O66529
jC	159	HIS	-	expression tag	UNP O66529
jC	160	HIS	-	expression tag	UNP O66529
jC	161	HIS	-	expression tag	UNP O66529
jD	2	GLU	GLN	conflict	UNP O66529
jD	28	GLY	ASP	conflict	UNP O66529
jD	52	CYS	ARG	conflict	UNP O66529
jD	83	GLU	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
jD	86	GLU	THR	conflict	UNP O66529
jD	112	SER	THR	conflict	UNP O66529
jD	115	ASP	VAL	conflict	UNP O66529
jD	118	ASP	ALA	conflict	UNP O66529
jD	120	GLU	THR	conflict	UNP O66529
jD	123	GLU	GLN	conflict	UNP O66529
jD	127	CYS	ARG	conflict	UNP O66529
jD	131	GLU	LYS	conflict	UNP O66529
jD	155	LEU	-	expression tag	UNP O66529
jD	156	GLU	-	expression tag	UNP O66529
jD	157	HIS	-	expression tag	UNP O66529
jD	158	HIS	-	expression tag	UNP O66529
jD	159	HIS	-	expression tag	UNP O66529
jD	160	HIS	-	expression tag	UNP O66529
jD	161	HIS	-	expression tag	UNP O66529
jE	2	GLU	GLN	conflict	UNP O66529
jE	28	GLY	ASP	conflict	UNP O66529
jE	52	CYS	ARG	conflict	UNP O66529
jE	83	GLU	ARG	conflict	UNP O66529
jE	86	GLU	THR	conflict	UNP O66529
jE	112	SER	THR	conflict	UNP O66529
jE	115	ASP	VAL	conflict	UNP O66529
jE	118	ASP	ALA	conflict	UNP O66529
jE	120	GLU	THR	conflict	UNP O66529
jE	123	GLU	GLN	conflict	UNP O66529
jE	127	CYS	ARG	conflict	UNP O66529
jE	131	GLU	LYS	conflict	UNP O66529
jE	155	LEU	-	expression tag	UNP O66529
jE	156	GLU	-	expression tag	UNP O66529
jE	157	HIS	-	expression tag	UNP O66529
jE	158	HIS	-	expression tag	UNP O66529
jE	159	HIS	-	expression tag	UNP O66529
jE	160	HIS	-	expression tag	UNP O66529
jE	161	HIS	-	expression tag	UNP O66529
jX	2	GLU	GLN	conflict	UNP O66529
jX	28	GLY	ASP	conflict	UNP O66529
jX	52	CYS	ARG	conflict	UNP O66529
jX	83	GLU	ARG	conflict	UNP O66529
jX	86	GLU	THR	conflict	UNP O66529
jX	112	SER	THR	conflict	UNP O66529
jX	115	ASP	VAL	conflict	UNP O66529
jX	118	ASP	ALA	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
jX	120	GLU	THR	conflict	UNP O66529
jX	123	GLU	GLN	conflict	UNP O66529
jX	127	CYS	ARG	conflict	UNP O66529
jX	131	GLU	LYS	conflict	UNP O66529
jX	155	LEU	-	expression tag	UNP O66529
jX	156	GLU	-	expression tag	UNP O66529
jX	157	HIS	-	expression tag	UNP O66529
jX	158	HIS	-	expression tag	UNP O66529
jX	159	HIS	-	expression tag	UNP O66529
jX	160	HIS	-	expression tag	UNP O66529
jX	161	HIS	-	expression tag	UNP O66529
kA	2	GLU	GLN	conflict	UNP O66529
kA	28	GLY	ASP	conflict	UNP O66529
kA	52	CYS	ARG	conflict	UNP O66529
kA	83	GLU	ARG	conflict	UNP O66529
kA	86	GLU	THR	conflict	UNP O66529
kA	112	SER	THR	conflict	UNP O66529
kA	115	ASP	VAL	conflict	UNP O66529
kA	118	ASP	ALA	conflict	UNP O66529
kA	120	GLU	THR	conflict	UNP O66529
kA	123	GLU	GLN	conflict	UNP O66529
kA	127	CYS	ARG	conflict	UNP O66529
kA	131	GLU	LYS	conflict	UNP O66529
kA	155	LEU	-	expression tag	UNP O66529
kA	156	GLU	-	expression tag	UNP O66529
kA	157	HIS	-	expression tag	UNP O66529
kA	158	HIS	-	expression tag	UNP O66529
kA	159	HIS	-	expression tag	UNP O66529
kA	160	HIS	-	expression tag	UNP O66529
kA	161	HIS	-	expression tag	UNP O66529
kB	2	GLU	GLN	conflict	UNP O66529
kB	28	GLY	ASP	conflict	UNP O66529
kB	52	CYS	ARG	conflict	UNP O66529
kB	83	GLU	ARG	conflict	UNP O66529
kB	86	GLU	THR	conflict	UNP O66529
kB	112	SER	THR	conflict	UNP O66529
kB	115	ASP	VAL	conflict	UNP O66529
kB	118	ASP	ALA	conflict	UNP O66529
kB	120	GLU	THR	conflict	UNP O66529
kB	123	GLU	GLN	conflict	UNP O66529
kB	127	CYS	ARG	conflict	UNP O66529
kB	131	GLU	LYS	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
kB	155	LEU	-	expression tag	UNP O66529
kB	156	GLU	-	expression tag	UNP O66529
kB	157	HIS	-	expression tag	UNP O66529
kB	158	HIS	-	expression tag	UNP O66529
kB	159	HIS	-	expression tag	UNP O66529
kB	160	HIS	-	expression tag	UNP O66529
kB	161	HIS	-	expression tag	UNP O66529
kC	2	GLU	GLN	conflict	UNP O66529
kC	28	GLY	ASP	conflict	UNP O66529
kC	52	CYS	ARG	conflict	UNP O66529
kC	83	GLU	ARG	conflict	UNP O66529
kC	86	GLU	THR	conflict	UNP O66529
kC	112	SER	THR	conflict	UNP O66529
kC	115	ASP	VAL	conflict	UNP O66529
kC	118	ASP	ALA	conflict	UNP O66529
kC	120	GLU	THR	conflict	UNP O66529
kC	123	GLU	GLN	conflict	UNP O66529
kC	127	CYS	ARG	conflict	UNP O66529
kC	131	GLU	LYS	conflict	UNP O66529
kC	155	LEU	-	expression tag	UNP O66529
kC	156	GLU	-	expression tag	UNP O66529
kC	157	HIS	-	expression tag	UNP O66529
kC	158	HIS	-	expression tag	UNP O66529
kC	159	HIS	-	expression tag	UNP O66529
kC	160	HIS	-	expression tag	UNP O66529
kC	161	HIS	-	expression tag	UNP O66529
kD	2	GLU	GLN	conflict	UNP O66529
kD	28	GLY	ASP	conflict	UNP O66529
kD	52	CYS	ARG	conflict	UNP O66529
kD	83	GLU	ARG	conflict	UNP O66529
kD	86	GLU	THR	conflict	UNP O66529
kD	112	SER	THR	conflict	UNP O66529
kD	115	ASP	VAL	conflict	UNP O66529
kD	118	ASP	ALA	conflict	UNP O66529
kD	120	GLU	THR	conflict	UNP O66529
kD	123	GLU	GLN	conflict	UNP O66529
kD	127	CYS	ARG	conflict	UNP O66529
kD	131	GLU	LYS	conflict	UNP O66529
kD	155	LEU	-	expression tag	UNP O66529
kD	156	GLU	-	expression tag	UNP O66529
kD	157	HIS	-	expression tag	UNP O66529
kD	158	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
kD	159	HIS	-	expression tag	UNP O66529
kD	160	HIS	-	expression tag	UNP O66529
kD	161	HIS	-	expression tag	UNP O66529
kE	2	GLU	GLN	conflict	UNP O66529
kE	28	GLY	ASP	conflict	UNP O66529
kE	52	CYS	ARG	conflict	UNP O66529
kE	83	GLU	ARG	conflict	UNP O66529
kE	86	GLU	THR	conflict	UNP O66529
kE	112	SER	THR	conflict	UNP O66529
kE	115	ASP	VAL	conflict	UNP O66529
kE	118	ASP	ALA	conflict	UNP O66529
kE	120	GLU	THR	conflict	UNP O66529
kE	123	GLU	GLN	conflict	UNP O66529
kE	127	CYS	ARG	conflict	UNP O66529
kE	131	GLU	LYS	conflict	UNP O66529
kE	155	LEU	-	expression tag	UNP O66529
kE	156	GLU	-	expression tag	UNP O66529
kE	157	HIS	-	expression tag	UNP O66529
kE	158	HIS	-	expression tag	UNP O66529
kE	159	HIS	-	expression tag	UNP O66529
kE	160	HIS	-	expression tag	UNP O66529
kE	161	HIS	-	expression tag	UNP O66529
kX	2	GLU	GLN	conflict	UNP O66529
kX	28	GLY	ASP	conflict	UNP O66529
kX	52	CYS	ARG	conflict	UNP O66529
kX	83	GLU	ARG	conflict	UNP O66529
kX	86	GLU	THR	conflict	UNP O66529
kX	112	SER	THR	conflict	UNP O66529
kX	115	ASP	VAL	conflict	UNP O66529
kX	118	ASP	ALA	conflict	UNP O66529
kX	120	GLU	THR	conflict	UNP O66529
kX	123	GLU	GLN	conflict	UNP O66529
kX	127	CYS	ARG	conflict	UNP O66529
kX	131	GLU	LYS	conflict	UNP O66529
kX	155	LEU	-	expression tag	UNP O66529
kX	156	GLU	-	expression tag	UNP O66529
kX	157	HIS	-	expression tag	UNP O66529
kX	158	HIS	-	expression tag	UNP O66529
kX	159	HIS	-	expression tag	UNP O66529
kX	160	HIS	-	expression tag	UNP O66529
kX	161	HIS	-	expression tag	UNP O66529
lA	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1A	28	GLY	ASP	conflict	UNP O66529
1A	52	CYS	ARG	conflict	UNP O66529
1A	83	GLU	ARG	conflict	UNP O66529
1A	86	GLU	THR	conflict	UNP O66529
1A	112	SER	THR	conflict	UNP O66529
1A	115	ASP	VAL	conflict	UNP O66529
1A	118	ASP	ALA	conflict	UNP O66529
1A	120	GLU	THR	conflict	UNP O66529
1A	123	GLU	GLN	conflict	UNP O66529
1A	127	CYS	ARG	conflict	UNP O66529
1A	131	GLU	LYS	conflict	UNP O66529
1A	155	LEU	-	expression tag	UNP O66529
1A	156	GLU	-	expression tag	UNP O66529
1A	157	HIS	-	expression tag	UNP O66529
1A	158	HIS	-	expression tag	UNP O66529
1A	159	HIS	-	expression tag	UNP O66529
1A	160	HIS	-	expression tag	UNP O66529
1A	161	HIS	-	expression tag	UNP O66529
1B	2	GLU	GLN	conflict	UNP O66529
1B	28	GLY	ASP	conflict	UNP O66529
1B	52	CYS	ARG	conflict	UNP O66529
1B	83	GLU	ARG	conflict	UNP O66529
1B	86	GLU	THR	conflict	UNP O66529
1B	112	SER	THR	conflict	UNP O66529
1B	115	ASP	VAL	conflict	UNP O66529
1B	118	ASP	ALA	conflict	UNP O66529
1B	120	GLU	THR	conflict	UNP O66529
1B	123	GLU	GLN	conflict	UNP O66529
1B	127	CYS	ARG	conflict	UNP O66529
1B	131	GLU	LYS	conflict	UNP O66529
1B	155	LEU	-	expression tag	UNP O66529
1B	156	GLU	-	expression tag	UNP O66529
1B	157	HIS	-	expression tag	UNP O66529
1B	158	HIS	-	expression tag	UNP O66529
1B	159	HIS	-	expression tag	UNP O66529
1B	160	HIS	-	expression tag	UNP O66529
1B	161	HIS	-	expression tag	UNP O66529
1C	2	GLU	GLN	conflict	UNP O66529
1C	28	GLY	ASP	conflict	UNP O66529
1C	52	CYS	ARG	conflict	UNP O66529
1C	83	GLU	ARG	conflict	UNP O66529
1C	86	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1C	112	SER	THR	conflict	UNP O66529
1C	115	ASP	VAL	conflict	UNP O66529
1C	118	ASP	ALA	conflict	UNP O66529
1C	120	GLU	THR	conflict	UNP O66529
1C	123	GLU	GLN	conflict	UNP O66529
1C	127	CYS	ARG	conflict	UNP O66529
1C	131	GLU	LYS	conflict	UNP O66529
1C	155	LEU	-	expression tag	UNP O66529
1C	156	GLU	-	expression tag	UNP O66529
1C	157	HIS	-	expression tag	UNP O66529
1C	158	HIS	-	expression tag	UNP O66529
1C	159	HIS	-	expression tag	UNP O66529
1C	160	HIS	-	expression tag	UNP O66529
1C	161	HIS	-	expression tag	UNP O66529
1D	2	GLU	GLN	conflict	UNP O66529
1D	28	GLY	ASP	conflict	UNP O66529
1D	52	CYS	ARG	conflict	UNP O66529
1D	83	GLU	ARG	conflict	UNP O66529
1D	86	GLU	THR	conflict	UNP O66529
1D	112	SER	THR	conflict	UNP O66529
1D	115	ASP	VAL	conflict	UNP O66529
1D	118	ASP	ALA	conflict	UNP O66529
1D	120	GLU	THR	conflict	UNP O66529
1D	123	GLU	GLN	conflict	UNP O66529
1D	127	CYS	ARG	conflict	UNP O66529
1D	131	GLU	LYS	conflict	UNP O66529
1D	155	LEU	-	expression tag	UNP O66529
1D	156	GLU	-	expression tag	UNP O66529
1D	157	HIS	-	expression tag	UNP O66529
1D	158	HIS	-	expression tag	UNP O66529
1D	159	HIS	-	expression tag	UNP O66529
1D	160	HIS	-	expression tag	UNP O66529
1D	161	HIS	-	expression tag	UNP O66529
1E	2	GLU	GLN	conflict	UNP O66529
1E	28	GLY	ASP	conflict	UNP O66529
1E	52	CYS	ARG	conflict	UNP O66529
1E	83	GLU	ARG	conflict	UNP O66529
1E	86	GLU	THR	conflict	UNP O66529
1E	112	SER	THR	conflict	UNP O66529
1E	115	ASP	VAL	conflict	UNP O66529
1E	118	ASP	ALA	conflict	UNP O66529
1E	120	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
lE	123	GLU	GLN	conflict	UNP O66529
lE	127	CYS	ARG	conflict	UNP O66529
lE	131	GLU	LYS	conflict	UNP O66529
lE	155	LEU	-	expression tag	UNP O66529
lE	156	GLU	-	expression tag	UNP O66529
lE	157	HIS	-	expression tag	UNP O66529
lE	158	HIS	-	expression tag	UNP O66529
lE	159	HIS	-	expression tag	UNP O66529
lE	160	HIS	-	expression tag	UNP O66529
lE	161	HIS	-	expression tag	UNP O66529
lX	2	GLU	GLN	conflict	UNP O66529
lX	28	GLY	ASP	conflict	UNP O66529
lX	52	CYS	ARG	conflict	UNP O66529
lX	83	GLU	ARG	conflict	UNP O66529
lX	86	GLU	THR	conflict	UNP O66529
lX	112	SER	THR	conflict	UNP O66529
lX	115	ASP	VAL	conflict	UNP O66529
lX	118	ASP	ALA	conflict	UNP O66529
lX	120	GLU	THR	conflict	UNP O66529
lX	123	GLU	GLN	conflict	UNP O66529
lX	127	CYS	ARG	conflict	UNP O66529
lX	131	GLU	LYS	conflict	UNP O66529
lX	155	LEU	-	expression tag	UNP O66529
lX	156	GLU	-	expression tag	UNP O66529
lX	157	HIS	-	expression tag	UNP O66529
lX	158	HIS	-	expression tag	UNP O66529
lX	159	HIS	-	expression tag	UNP O66529
lX	160	HIS	-	expression tag	UNP O66529
lX	161	HIS	-	expression tag	UNP O66529
mA	2	GLU	GLN	conflict	UNP O66529
mA	28	GLY	ASP	conflict	UNP O66529
mA	52	CYS	ARG	conflict	UNP O66529
mA	83	GLU	ARG	conflict	UNP O66529
mA	86	GLU	THR	conflict	UNP O66529
mA	112	SER	THR	conflict	UNP O66529
mA	115	ASP	VAL	conflict	UNP O66529
mA	118	ASP	ALA	conflict	UNP O66529
mA	120	GLU	THR	conflict	UNP O66529
mA	123	GLU	GLN	conflict	UNP O66529
mA	127	CYS	ARG	conflict	UNP O66529
mA	131	GLU	LYS	conflict	UNP O66529
mA	155	LEU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
mA	156	GLU	-	expression tag	UNP O66529
mA	157	HIS	-	expression tag	UNP O66529
mA	158	HIS	-	expression tag	UNP O66529
mA	159	HIS	-	expression tag	UNP O66529
mA	160	HIS	-	expression tag	UNP O66529
mA	161	HIS	-	expression tag	UNP O66529
mB	2	GLU	GLN	conflict	UNP O66529
mB	28	GLY	ASP	conflict	UNP O66529
mB	52	CYS	ARG	conflict	UNP O66529
mB	83	GLU	ARG	conflict	UNP O66529
mB	86	GLU	THR	conflict	UNP O66529
mB	112	SER	THR	conflict	UNP O66529
mB	115	ASP	VAL	conflict	UNP O66529
mB	118	ASP	ALA	conflict	UNP O66529
mB	120	GLU	THR	conflict	UNP O66529
mB	123	GLU	GLN	conflict	UNP O66529
mB	127	CYS	ARG	conflict	UNP O66529
mB	131	GLU	LYS	conflict	UNP O66529
mB	155	LEU	-	expression tag	UNP O66529
mB	156	GLU	-	expression tag	UNP O66529
mB	157	HIS	-	expression tag	UNP O66529
mB	158	HIS	-	expression tag	UNP O66529
mB	159	HIS	-	expression tag	UNP O66529
mB	160	HIS	-	expression tag	UNP O66529
mB	161	HIS	-	expression tag	UNP O66529
mC	2	GLU	GLN	conflict	UNP O66529
mC	28	GLY	ASP	conflict	UNP O66529
mC	52	CYS	ARG	conflict	UNP O66529
mC	83	GLU	ARG	conflict	UNP O66529
mC	86	GLU	THR	conflict	UNP O66529
mC	112	SER	THR	conflict	UNP O66529
mC	115	ASP	VAL	conflict	UNP O66529
mC	118	ASP	ALA	conflict	UNP O66529
mC	120	GLU	THR	conflict	UNP O66529
mC	123	GLU	GLN	conflict	UNP O66529
mC	127	CYS	ARG	conflict	UNP O66529
mC	131	GLU	LYS	conflict	UNP O66529
mC	155	LEU	-	expression tag	UNP O66529
mC	156	GLU	-	expression tag	UNP O66529
mC	157	HIS	-	expression tag	UNP O66529
mC	158	HIS	-	expression tag	UNP O66529
mC	159	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
mC	160	HIS	-	expression tag	UNP O66529
mC	161	HIS	-	expression tag	UNP O66529
mD	2	GLU	GLN	conflict	UNP O66529
mD	28	GLY	ASP	conflict	UNP O66529
mD	52	CYS	ARG	conflict	UNP O66529
mD	83	GLU	ARG	conflict	UNP O66529
mD	86	GLU	THR	conflict	UNP O66529
mD	112	SER	THR	conflict	UNP O66529
mD	115	ASP	VAL	conflict	UNP O66529
mD	118	ASP	ALA	conflict	UNP O66529
mD	120	GLU	THR	conflict	UNP O66529
mD	123	GLU	GLN	conflict	UNP O66529
mD	127	CYS	ARG	conflict	UNP O66529
mD	131	GLU	LYS	conflict	UNP O66529
mD	155	LEU	-	expression tag	UNP O66529
mD	156	GLU	-	expression tag	UNP O66529
mD	157	HIS	-	expression tag	UNP O66529
mD	158	HIS	-	expression tag	UNP O66529
mD	159	HIS	-	expression tag	UNP O66529
mD	160	HIS	-	expression tag	UNP O66529
mD	161	HIS	-	expression tag	UNP O66529
mE	2	GLU	GLN	conflict	UNP O66529
mE	28	GLY	ASP	conflict	UNP O66529
mE	52	CYS	ARG	conflict	UNP O66529
mE	83	GLU	ARG	conflict	UNP O66529
mE	86	GLU	THR	conflict	UNP O66529
mE	112	SER	THR	conflict	UNP O66529
mE	115	ASP	VAL	conflict	UNP O66529
mE	118	ASP	ALA	conflict	UNP O66529
mE	120	GLU	THR	conflict	UNP O66529
mE	123	GLU	GLN	conflict	UNP O66529
mE	127	CYS	ARG	conflict	UNP O66529
mE	131	GLU	LYS	conflict	UNP O66529
mE	155	LEU	-	expression tag	UNP O66529
mE	156	GLU	-	expression tag	UNP O66529
mE	157	HIS	-	expression tag	UNP O66529
mE	158	HIS	-	expression tag	UNP O66529
mE	159	HIS	-	expression tag	UNP O66529
mE	160	HIS	-	expression tag	UNP O66529
mE	161	HIS	-	expression tag	UNP O66529
mX	2	GLU	GLN	conflict	UNP O66529
mX	28	GLY	ASP	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
mX	52	CYS	ARG	conflict	UNP O66529
mX	83	GLU	ARG	conflict	UNP O66529
mX	86	GLU	THR	conflict	UNP O66529
mX	112	SER	THR	conflict	UNP O66529
mX	115	ASP	VAL	conflict	UNP O66529
mX	118	ASP	ALA	conflict	UNP O66529
mX	120	GLU	THR	conflict	UNP O66529
mX	123	GLU	GLN	conflict	UNP O66529
mX	127	CYS	ARG	conflict	UNP O66529
mX	131	GLU	LYS	conflict	UNP O66529
mX	155	LEU	-	expression tag	UNP O66529
mX	156	GLU	-	expression tag	UNP O66529
mX	157	HIS	-	expression tag	UNP O66529
mX	158	HIS	-	expression tag	UNP O66529
mX	159	HIS	-	expression tag	UNP O66529
mX	160	HIS	-	expression tag	UNP O66529
mX	161	HIS	-	expression tag	UNP O66529
nA	2	GLU	GLN	conflict	UNP O66529
nA	28	GLY	ASP	conflict	UNP O66529
nA	52	CYS	ARG	conflict	UNP O66529
nA	83	GLU	ARG	conflict	UNP O66529
nA	86	GLU	THR	conflict	UNP O66529
nA	112	SER	THR	conflict	UNP O66529
nA	115	ASP	VAL	conflict	UNP O66529
nA	118	ASP	ALA	conflict	UNP O66529
nA	120	GLU	THR	conflict	UNP O66529
nA	123	GLU	GLN	conflict	UNP O66529
nA	127	CYS	ARG	conflict	UNP O66529
nA	131	GLU	LYS	conflict	UNP O66529
nA	155	LEU	-	expression tag	UNP O66529
nA	156	GLU	-	expression tag	UNP O66529
nA	157	HIS	-	expression tag	UNP O66529
nA	158	HIS	-	expression tag	UNP O66529
nA	159	HIS	-	expression tag	UNP O66529
nA	160	HIS	-	expression tag	UNP O66529
nA	161	HIS	-	expression tag	UNP O66529
nB	2	GLU	GLN	conflict	UNP O66529
nB	28	GLY	ASP	conflict	UNP O66529
nB	52	CYS	ARG	conflict	UNP O66529
nB	83	GLU	ARG	conflict	UNP O66529
nB	86	GLU	THR	conflict	UNP O66529
nB	112	SER	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
nB	115	ASP	VAL	conflict	UNP O66529
nB	118	ASP	ALA	conflict	UNP O66529
nB	120	GLU	THR	conflict	UNP O66529
nB	123	GLU	GLN	conflict	UNP O66529
nB	127	CYS	ARG	conflict	UNP O66529
nB	131	GLU	LYS	conflict	UNP O66529
nB	155	LEU	-	expression tag	UNP O66529
nB	156	GLU	-	expression tag	UNP O66529
nB	157	HIS	-	expression tag	UNP O66529
nB	158	HIS	-	expression tag	UNP O66529
nB	159	HIS	-	expression tag	UNP O66529
nB	160	HIS	-	expression tag	UNP O66529
nB	161	HIS	-	expression tag	UNP O66529
nC	2	GLU	GLN	conflict	UNP O66529
nC	28	GLY	ASP	conflict	UNP O66529
nC	52	CYS	ARG	conflict	UNP O66529
nC	83	GLU	ARG	conflict	UNP O66529
nC	86	GLU	THR	conflict	UNP O66529
nC	112	SER	THR	conflict	UNP O66529
nC	115	ASP	VAL	conflict	UNP O66529
nC	118	ASP	ALA	conflict	UNP O66529
nC	120	GLU	THR	conflict	UNP O66529
nC	123	GLU	GLN	conflict	UNP O66529
nC	127	CYS	ARG	conflict	UNP O66529
nC	131	GLU	LYS	conflict	UNP O66529
nC	155	LEU	-	expression tag	UNP O66529
nC	156	GLU	-	expression tag	UNP O66529
nC	157	HIS	-	expression tag	UNP O66529
nC	158	HIS	-	expression tag	UNP O66529
nC	159	HIS	-	expression tag	UNP O66529
nC	160	HIS	-	expression tag	UNP O66529
nC	161	HIS	-	expression tag	UNP O66529
nD	2	GLU	GLN	conflict	UNP O66529
nD	28	GLY	ASP	conflict	UNP O66529
nD	52	CYS	ARG	conflict	UNP O66529
nD	83	GLU	ARG	conflict	UNP O66529
nD	86	GLU	THR	conflict	UNP O66529
nD	112	SER	THR	conflict	UNP O66529
nD	115	ASP	VAL	conflict	UNP O66529
nD	118	ASP	ALA	conflict	UNP O66529
nD	120	GLU	THR	conflict	UNP O66529
nD	123	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
nD	127	CYS	ARG	conflict	UNP O66529
nD	131	GLU	LYS	conflict	UNP O66529
nD	155	LEU	-	expression tag	UNP O66529
nD	156	GLU	-	expression tag	UNP O66529
nD	157	HIS	-	expression tag	UNP O66529
nD	158	HIS	-	expression tag	UNP O66529
nD	159	HIS	-	expression tag	UNP O66529
nD	160	HIS	-	expression tag	UNP O66529
nD	161	HIS	-	expression tag	UNP O66529
nE	2	GLU	GLN	conflict	UNP O66529
nE	28	GLY	ASP	conflict	UNP O66529
nE	52	CYS	ARG	conflict	UNP O66529
nE	83	GLU	ARG	conflict	UNP O66529
nE	86	GLU	THR	conflict	UNP O66529
nE	112	SER	THR	conflict	UNP O66529
nE	115	ASP	VAL	conflict	UNP O66529
nE	118	ASP	ALA	conflict	UNP O66529
nE	120	GLU	THR	conflict	UNP O66529
nE	123	GLU	GLN	conflict	UNP O66529
nE	127	CYS	ARG	conflict	UNP O66529
nE	131	GLU	LYS	conflict	UNP O66529
nE	155	LEU	-	expression tag	UNP O66529
nE	156	GLU	-	expression tag	UNP O66529
nE	157	HIS	-	expression tag	UNP O66529
nE	158	HIS	-	expression tag	UNP O66529
nE	159	HIS	-	expression tag	UNP O66529
nE	160	HIS	-	expression tag	UNP O66529
nE	161	HIS	-	expression tag	UNP O66529
nX	2	GLU	GLN	conflict	UNP O66529
nX	28	GLY	ASP	conflict	UNP O66529
nX	52	CYS	ARG	conflict	UNP O66529
nX	83	GLU	ARG	conflict	UNP O66529
nX	86	GLU	THR	conflict	UNP O66529
nX	112	SER	THR	conflict	UNP O66529
nX	115	ASP	VAL	conflict	UNP O66529
nX	118	ASP	ALA	conflict	UNP O66529
nX	120	GLU	THR	conflict	UNP O66529
nX	123	GLU	GLN	conflict	UNP O66529
nX	127	CYS	ARG	conflict	UNP O66529
nX	131	GLU	LYS	conflict	UNP O66529
nX	155	LEU	-	expression tag	UNP O66529
nX	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
nX	157	HIS	-	expression tag	UNP O66529
nX	158	HIS	-	expression tag	UNP O66529
nX	159	HIS	-	expression tag	UNP O66529
nX	160	HIS	-	expression tag	UNP O66529
nX	161	HIS	-	expression tag	UNP O66529
oA	2	GLU	GLN	conflict	UNP O66529
oA	28	GLY	ASP	conflict	UNP O66529
oA	52	CYS	ARG	conflict	UNP O66529
oA	83	GLU	ARG	conflict	UNP O66529
oA	86	GLU	THR	conflict	UNP O66529
oA	112	SER	THR	conflict	UNP O66529
oA	115	ASP	VAL	conflict	UNP O66529
oA	118	ASP	ALA	conflict	UNP O66529
oA	120	GLU	THR	conflict	UNP O66529
oA	123	GLU	GLN	conflict	UNP O66529
oA	127	CYS	ARG	conflict	UNP O66529
oA	131	GLU	LYS	conflict	UNP O66529
oA	155	LEU	-	expression tag	UNP O66529
oA	156	GLU	-	expression tag	UNP O66529
oA	157	HIS	-	expression tag	UNP O66529
oA	158	HIS	-	expression tag	UNP O66529
oA	159	HIS	-	expression tag	UNP O66529
oA	160	HIS	-	expression tag	UNP O66529
oA	161	HIS	-	expression tag	UNP O66529
oB	2	GLU	GLN	conflict	UNP O66529
oB	28	GLY	ASP	conflict	UNP O66529
oB	52	CYS	ARG	conflict	UNP O66529
oB	83	GLU	ARG	conflict	UNP O66529
oB	86	GLU	THR	conflict	UNP O66529
oB	112	SER	THR	conflict	UNP O66529
oB	115	ASP	VAL	conflict	UNP O66529
oB	118	ASP	ALA	conflict	UNP O66529
oB	120	GLU	THR	conflict	UNP O66529
oB	123	GLU	GLN	conflict	UNP O66529
oB	127	CYS	ARG	conflict	UNP O66529
oB	131	GLU	LYS	conflict	UNP O66529
oB	155	LEU	-	expression tag	UNP O66529
oB	156	GLU	-	expression tag	UNP O66529
oB	157	HIS	-	expression tag	UNP O66529
oB	158	HIS	-	expression tag	UNP O66529
oB	159	HIS	-	expression tag	UNP O66529
oB	160	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
oB	161	HIS	-	expression tag	UNP O66529
oC	2	GLU	GLN	conflict	UNP O66529
oC	28	GLY	ASP	conflict	UNP O66529
oC	52	CYS	ARG	conflict	UNP O66529
oC	83	GLU	ARG	conflict	UNP O66529
oC	86	GLU	THR	conflict	UNP O66529
oC	112	SER	THR	conflict	UNP O66529
oC	115	ASP	VAL	conflict	UNP O66529
oC	118	ASP	ALA	conflict	UNP O66529
oC	120	GLU	THR	conflict	UNP O66529
oC	123	GLU	GLN	conflict	UNP O66529
oC	127	CYS	ARG	conflict	UNP O66529
oC	131	GLU	LYS	conflict	UNP O66529
oC	155	LEU	-	expression tag	UNP O66529
oC	156	GLU	-	expression tag	UNP O66529
oC	157	HIS	-	expression tag	UNP O66529
oC	158	HIS	-	expression tag	UNP O66529
oC	159	HIS	-	expression tag	UNP O66529
oC	160	HIS	-	expression tag	UNP O66529
oC	161	HIS	-	expression tag	UNP O66529
oD	2	GLU	GLN	conflict	UNP O66529
oD	28	GLY	ASP	conflict	UNP O66529
oD	52	CYS	ARG	conflict	UNP O66529
oD	83	GLU	ARG	conflict	UNP O66529
oD	86	GLU	THR	conflict	UNP O66529
oD	112	SER	THR	conflict	UNP O66529
oD	115	ASP	VAL	conflict	UNP O66529
oD	118	ASP	ALA	conflict	UNP O66529
oD	120	GLU	THR	conflict	UNP O66529
oD	123	GLU	GLN	conflict	UNP O66529
oD	127	CYS	ARG	conflict	UNP O66529
oD	131	GLU	LYS	conflict	UNP O66529
oD	155	LEU	-	expression tag	UNP O66529
oD	156	GLU	-	expression tag	UNP O66529
oD	157	HIS	-	expression tag	UNP O66529
oD	158	HIS	-	expression tag	UNP O66529
oD	159	HIS	-	expression tag	UNP O66529
oD	160	HIS	-	expression tag	UNP O66529
oD	161	HIS	-	expression tag	UNP O66529
oE	2	GLU	GLN	conflict	UNP O66529
oE	28	GLY	ASP	conflict	UNP O66529
oE	52	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
oE	83	GLU	ARG	conflict	UNP O66529
oE	86	GLU	THR	conflict	UNP O66529
oE	112	SER	THR	conflict	UNP O66529
oE	115	ASP	VAL	conflict	UNP O66529
oE	118	ASP	ALA	conflict	UNP O66529
oE	120	GLU	THR	conflict	UNP O66529
oE	123	GLU	GLN	conflict	UNP O66529
oE	127	CYS	ARG	conflict	UNP O66529
oE	131	GLU	LYS	conflict	UNP O66529
oE	155	LEU	-	expression tag	UNP O66529
oE	156	GLU	-	expression tag	UNP O66529
oE	157	HIS	-	expression tag	UNP O66529
oE	158	HIS	-	expression tag	UNP O66529
oE	159	HIS	-	expression tag	UNP O66529
oE	160	HIS	-	expression tag	UNP O66529
oE	161	HIS	-	expression tag	UNP O66529
oX	2	GLU	GLN	conflict	UNP O66529
oX	28	GLY	ASP	conflict	UNP O66529
oX	52	CYS	ARG	conflict	UNP O66529
oX	83	GLU	ARG	conflict	UNP O66529
oX	86	GLU	THR	conflict	UNP O66529
oX	112	SER	THR	conflict	UNP O66529
oX	115	ASP	VAL	conflict	UNP O66529
oX	118	ASP	ALA	conflict	UNP O66529
oX	120	GLU	THR	conflict	UNP O66529
oX	123	GLU	GLN	conflict	UNP O66529
oX	127	CYS	ARG	conflict	UNP O66529
oX	131	GLU	LYS	conflict	UNP O66529
oX	155	LEU	-	expression tag	UNP O66529
oX	156	GLU	-	expression tag	UNP O66529
oX	157	HIS	-	expression tag	UNP O66529
oX	158	HIS	-	expression tag	UNP O66529
oX	159	HIS	-	expression tag	UNP O66529
oX	160	HIS	-	expression tag	UNP O66529
oX	161	HIS	-	expression tag	UNP O66529
pA	2	GLU	GLN	conflict	UNP O66529
pA	28	GLY	ASP	conflict	UNP O66529
pA	52	CYS	ARG	conflict	UNP O66529
pA	83	GLU	ARG	conflict	UNP O66529
pA	86	GLU	THR	conflict	UNP O66529
pA	112	SER	THR	conflict	UNP O66529
pA	115	ASP	VAL	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
pA	118	ASP	ALA	conflict	UNP O66529
pA	120	GLU	THR	conflict	UNP O66529
pA	123	GLU	GLN	conflict	UNP O66529
pA	127	CYS	ARG	conflict	UNP O66529
pA	131	GLU	LYS	conflict	UNP O66529
pA	155	LEU	-	expression tag	UNP O66529
pA	156	GLU	-	expression tag	UNP O66529
pA	157	HIS	-	expression tag	UNP O66529
pA	158	HIS	-	expression tag	UNP O66529
pA	159	HIS	-	expression tag	UNP O66529
pA	160	HIS	-	expression tag	UNP O66529
pA	161	HIS	-	expression tag	UNP O66529
pB	2	GLU	GLN	conflict	UNP O66529
pB	28	GLY	ASP	conflict	UNP O66529
pB	52	CYS	ARG	conflict	UNP O66529
pB	83	GLU	ARG	conflict	UNP O66529
pB	86	GLU	THR	conflict	UNP O66529
pB	112	SER	THR	conflict	UNP O66529
pB	115	ASP	VAL	conflict	UNP O66529
pB	118	ASP	ALA	conflict	UNP O66529
pB	120	GLU	THR	conflict	UNP O66529
pB	123	GLU	GLN	conflict	UNP O66529
pB	127	CYS	ARG	conflict	UNP O66529
pB	131	GLU	LYS	conflict	UNP O66529
pB	155	LEU	-	expression tag	UNP O66529
pB	156	GLU	-	expression tag	UNP O66529
pB	157	HIS	-	expression tag	UNP O66529
pB	158	HIS	-	expression tag	UNP O66529
pB	159	HIS	-	expression tag	UNP O66529
pB	160	HIS	-	expression tag	UNP O66529
pB	161	HIS	-	expression tag	UNP O66529
pC	2	GLU	GLN	conflict	UNP O66529
pC	28	GLY	ASP	conflict	UNP O66529
pC	52	CYS	ARG	conflict	UNP O66529
pC	83	GLU	ARG	conflict	UNP O66529
pC	86	GLU	THR	conflict	UNP O66529
pC	112	SER	THR	conflict	UNP O66529
pC	115	ASP	VAL	conflict	UNP O66529
pC	118	ASP	ALA	conflict	UNP O66529
pC	120	GLU	THR	conflict	UNP O66529
pC	123	GLU	GLN	conflict	UNP O66529
pC	127	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
pC	131	GLU	LYS	conflict	UNP O66529
pC	155	LEU	-	expression tag	UNP O66529
pC	156	GLU	-	expression tag	UNP O66529
pC	157	HIS	-	expression tag	UNP O66529
pC	158	HIS	-	expression tag	UNP O66529
pC	159	HIS	-	expression tag	UNP O66529
pC	160	HIS	-	expression tag	UNP O66529
pC	161	HIS	-	expression tag	UNP O66529
pD	2	GLU	GLN	conflict	UNP O66529
pD	28	GLY	ASP	conflict	UNP O66529
pD	52	CYS	ARG	conflict	UNP O66529
pD	83	GLU	ARG	conflict	UNP O66529
pD	86	GLU	THR	conflict	UNP O66529
pD	112	SER	THR	conflict	UNP O66529
pD	115	ASP	VAL	conflict	UNP O66529
pD	118	ASP	ALA	conflict	UNP O66529
pD	120	GLU	THR	conflict	UNP O66529
pD	123	GLU	GLN	conflict	UNP O66529
pD	127	CYS	ARG	conflict	UNP O66529
pD	131	GLU	LYS	conflict	UNP O66529
pD	155	LEU	-	expression tag	UNP O66529
pD	156	GLU	-	expression tag	UNP O66529
pD	157	HIS	-	expression tag	UNP O66529
pD	158	HIS	-	expression tag	UNP O66529
pD	159	HIS	-	expression tag	UNP O66529
pD	160	HIS	-	expression tag	UNP O66529
pD	161	HIS	-	expression tag	UNP O66529
pE	2	GLU	GLN	conflict	UNP O66529
pE	28	GLY	ASP	conflict	UNP O66529
pE	52	CYS	ARG	conflict	UNP O66529
pE	83	GLU	ARG	conflict	UNP O66529
pE	86	GLU	THR	conflict	UNP O66529
pE	112	SER	THR	conflict	UNP O66529
pE	115	ASP	VAL	conflict	UNP O66529
pE	118	ASP	ALA	conflict	UNP O66529
pE	120	GLU	THR	conflict	UNP O66529
pE	123	GLU	GLN	conflict	UNP O66529
pE	127	CYS	ARG	conflict	UNP O66529
pE	131	GLU	LYS	conflict	UNP O66529
pE	155	LEU	-	expression tag	UNP O66529
pE	156	GLU	-	expression tag	UNP O66529
pE	157	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
pE	158	HIS	-	expression tag	UNP O66529
pE	159	HIS	-	expression tag	UNP O66529
pE	160	HIS	-	expression tag	UNP O66529
pE	161	HIS	-	expression tag	UNP O66529
pX	2	GLU	GLN	conflict	UNP O66529
pX	28	GLY	ASP	conflict	UNP O66529
pX	52	CYS	ARG	conflict	UNP O66529
pX	83	GLU	ARG	conflict	UNP O66529
pX	86	GLU	THR	conflict	UNP O66529
pX	112	SER	THR	conflict	UNP O66529
pX	115	ASP	VAL	conflict	UNP O66529
pX	118	ASP	ALA	conflict	UNP O66529
pX	120	GLU	THR	conflict	UNP O66529
pX	123	GLU	GLN	conflict	UNP O66529
pX	127	CYS	ARG	conflict	UNP O66529
pX	131	GLU	LYS	conflict	UNP O66529
pX	155	LEU	-	expression tag	UNP O66529
pX	156	GLU	-	expression tag	UNP O66529
pX	157	HIS	-	expression tag	UNP O66529
pX	158	HIS	-	expression tag	UNP O66529
pX	159	HIS	-	expression tag	UNP O66529
pX	160	HIS	-	expression tag	UNP O66529
pX	161	HIS	-	expression tag	UNP O66529
qA	2	GLU	GLN	conflict	UNP O66529
qA	28	GLY	ASP	conflict	UNP O66529
qA	52	CYS	ARG	conflict	UNP O66529
qA	83	GLU	ARG	conflict	UNP O66529
qA	86	GLU	THR	conflict	UNP O66529
qA	112	SER	THR	conflict	UNP O66529
qA	115	ASP	VAL	conflict	UNP O66529
qA	118	ASP	ALA	conflict	UNP O66529
qA	120	GLU	THR	conflict	UNP O66529
qA	123	GLU	GLN	conflict	UNP O66529
qA	127	CYS	ARG	conflict	UNP O66529
qA	131	GLU	LYS	conflict	UNP O66529
qA	155	LEU	-	expression tag	UNP O66529
qA	156	GLU	-	expression tag	UNP O66529
qA	157	HIS	-	expression tag	UNP O66529
qA	158	HIS	-	expression tag	UNP O66529
qA	159	HIS	-	expression tag	UNP O66529
qA	160	HIS	-	expression tag	UNP O66529
qA	161	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
qB	2	GLU	GLN	conflict	UNP O66529
qB	28	GLY	ASP	conflict	UNP O66529
qB	52	CYS	ARG	conflict	UNP O66529
qB	83	GLU	ARG	conflict	UNP O66529
qB	86	GLU	THR	conflict	UNP O66529
qB	112	SER	THR	conflict	UNP O66529
qB	115	ASP	VAL	conflict	UNP O66529
qB	118	ASP	ALA	conflict	UNP O66529
qB	120	GLU	THR	conflict	UNP O66529
qB	123	GLU	GLN	conflict	UNP O66529
qB	127	CYS	ARG	conflict	UNP O66529
qB	131	GLU	LYS	conflict	UNP O66529
qB	155	LEU	-	expression tag	UNP O66529
qB	156	GLU	-	expression tag	UNP O66529
qB	157	HIS	-	expression tag	UNP O66529
qB	158	HIS	-	expression tag	UNP O66529
qB	159	HIS	-	expression tag	UNP O66529
qB	160	HIS	-	expression tag	UNP O66529
qB	161	HIS	-	expression tag	UNP O66529
qC	2	GLU	GLN	conflict	UNP O66529
qC	28	GLY	ASP	conflict	UNP O66529
qC	52	CYS	ARG	conflict	UNP O66529
qC	83	GLU	ARG	conflict	UNP O66529
qC	86	GLU	THR	conflict	UNP O66529
qC	112	SER	THR	conflict	UNP O66529
qC	115	ASP	VAL	conflict	UNP O66529
qC	118	ASP	ALA	conflict	UNP O66529
qC	120	GLU	THR	conflict	UNP O66529
qC	123	GLU	GLN	conflict	UNP O66529
qC	127	CYS	ARG	conflict	UNP O66529
qC	131	GLU	LYS	conflict	UNP O66529
qC	155	LEU	-	expression tag	UNP O66529
qC	156	GLU	-	expression tag	UNP O66529
qC	157	HIS	-	expression tag	UNP O66529
qC	158	HIS	-	expression tag	UNP O66529
qC	159	HIS	-	expression tag	UNP O66529
qC	160	HIS	-	expression tag	UNP O66529
qC	161	HIS	-	expression tag	UNP O66529
qD	2	GLU	GLN	conflict	UNP O66529
qD	28	GLY	ASP	conflict	UNP O66529
qD	52	CYS	ARG	conflict	UNP O66529
qD	83	GLU	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
qD	86	GLU	THR	conflict	UNP O66529
qD	112	SER	THR	conflict	UNP O66529
qD	115	ASP	VAL	conflict	UNP O66529
qD	118	ASP	ALA	conflict	UNP O66529
qD	120	GLU	THR	conflict	UNP O66529
qD	123	GLU	GLN	conflict	UNP O66529
qD	127	CYS	ARG	conflict	UNP O66529
qD	131	GLU	LYS	conflict	UNP O66529
qD	155	LEU	-	expression tag	UNP O66529
qD	156	GLU	-	expression tag	UNP O66529
qD	157	HIS	-	expression tag	UNP O66529
qD	158	HIS	-	expression tag	UNP O66529
qD	159	HIS	-	expression tag	UNP O66529
qD	160	HIS	-	expression tag	UNP O66529
qD	161	HIS	-	expression tag	UNP O66529
qE	2	GLU	GLN	conflict	UNP O66529
qE	28	GLY	ASP	conflict	UNP O66529
qE	52	CYS	ARG	conflict	UNP O66529
qE	83	GLU	ARG	conflict	UNP O66529
qE	86	GLU	THR	conflict	UNP O66529
qE	112	SER	THR	conflict	UNP O66529
qE	115	ASP	VAL	conflict	UNP O66529
qE	118	ASP	ALA	conflict	UNP O66529
qE	120	GLU	THR	conflict	UNP O66529
qE	123	GLU	GLN	conflict	UNP O66529
qE	127	CYS	ARG	conflict	UNP O66529
qE	131	GLU	LYS	conflict	UNP O66529
qE	155	LEU	-	expression tag	UNP O66529
qE	156	GLU	-	expression tag	UNP O66529
qE	157	HIS	-	expression tag	UNP O66529
qE	158	HIS	-	expression tag	UNP O66529
qE	159	HIS	-	expression tag	UNP O66529
qE	160	HIS	-	expression tag	UNP O66529
qE	161	HIS	-	expression tag	UNP O66529
qX	2	GLU	GLN	conflict	UNP O66529
qX	28	GLY	ASP	conflict	UNP O66529
qX	52	CYS	ARG	conflict	UNP O66529
qX	83	GLU	ARG	conflict	UNP O66529
qX	86	GLU	THR	conflict	UNP O66529
qX	112	SER	THR	conflict	UNP O66529
qX	115	ASP	VAL	conflict	UNP O66529
qX	118	ASP	ALA	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
qX	120	GLU	THR	conflict	UNP O66529
qX	123	GLU	GLN	conflict	UNP O66529
qX	127	CYS	ARG	conflict	UNP O66529
qX	131	GLU	LYS	conflict	UNP O66529
qX	155	LEU	-	expression tag	UNP O66529
qX	156	GLU	-	expression tag	UNP O66529
qX	157	HIS	-	expression tag	UNP O66529
qX	158	HIS	-	expression tag	UNP O66529
qX	159	HIS	-	expression tag	UNP O66529
qX	160	HIS	-	expression tag	UNP O66529
qX	161	HIS	-	expression tag	UNP O66529
rA	2	GLU	GLN	conflict	UNP O66529
rA	28	GLY	ASP	conflict	UNP O66529
rA	52	CYS	ARG	conflict	UNP O66529
rA	83	GLU	ARG	conflict	UNP O66529
rA	86	GLU	THR	conflict	UNP O66529
rA	112	SER	THR	conflict	UNP O66529
rA	115	ASP	VAL	conflict	UNP O66529
rA	118	ASP	ALA	conflict	UNP O66529
rA	120	GLU	THR	conflict	UNP O66529
rA	123	GLU	GLN	conflict	UNP O66529
rA	127	CYS	ARG	conflict	UNP O66529
rA	131	GLU	LYS	conflict	UNP O66529
rA	155	LEU	-	expression tag	UNP O66529
rA	156	GLU	-	expression tag	UNP O66529
rA	157	HIS	-	expression tag	UNP O66529
rA	158	HIS	-	expression tag	UNP O66529
rA	159	HIS	-	expression tag	UNP O66529
rA	160	HIS	-	expression tag	UNP O66529
rA	161	HIS	-	expression tag	UNP O66529
rB	2	GLU	GLN	conflict	UNP O66529
rB	28	GLY	ASP	conflict	UNP O66529
rB	52	CYS	ARG	conflict	UNP O66529
rB	83	GLU	ARG	conflict	UNP O66529
rB	86	GLU	THR	conflict	UNP O66529
rB	112	SER	THR	conflict	UNP O66529
rB	115	ASP	VAL	conflict	UNP O66529
rB	118	ASP	ALA	conflict	UNP O66529
rB	120	GLU	THR	conflict	UNP O66529
rB	123	GLU	GLN	conflict	UNP O66529
rB	127	CYS	ARG	conflict	UNP O66529
rB	131	GLU	LYS	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
rB	155	LEU	-	expression tag	UNP O66529
rB	156	GLU	-	expression tag	UNP O66529
rB	157	HIS	-	expression tag	UNP O66529
rB	158	HIS	-	expression tag	UNP O66529
rB	159	HIS	-	expression tag	UNP O66529
rB	160	HIS	-	expression tag	UNP O66529
rB	161	HIS	-	expression tag	UNP O66529
rC	2	GLU	GLN	conflict	UNP O66529
rC	28	GLY	ASP	conflict	UNP O66529
rC	52	CYS	ARG	conflict	UNP O66529
rC	83	GLU	ARG	conflict	UNP O66529
rC	86	GLU	THR	conflict	UNP O66529
rC	112	SER	THR	conflict	UNP O66529
rC	115	ASP	VAL	conflict	UNP O66529
rC	118	ASP	ALA	conflict	UNP O66529
rC	120	GLU	THR	conflict	UNP O66529
rC	123	GLU	GLN	conflict	UNP O66529
rC	127	CYS	ARG	conflict	UNP O66529
rC	131	GLU	LYS	conflict	UNP O66529
rC	155	LEU	-	expression tag	UNP O66529
rC	156	GLU	-	expression tag	UNP O66529
rC	157	HIS	-	expression tag	UNP O66529
rC	158	HIS	-	expression tag	UNP O66529
rC	159	HIS	-	expression tag	UNP O66529
rC	160	HIS	-	expression tag	UNP O66529
rC	161	HIS	-	expression tag	UNP O66529
rD	2	GLU	GLN	conflict	UNP O66529
rD	28	GLY	ASP	conflict	UNP O66529
rD	52	CYS	ARG	conflict	UNP O66529
rD	83	GLU	ARG	conflict	UNP O66529
rD	86	GLU	THR	conflict	UNP O66529
rD	112	SER	THR	conflict	UNP O66529
rD	115	ASP	VAL	conflict	UNP O66529
rD	118	ASP	ALA	conflict	UNP O66529
rD	120	GLU	THR	conflict	UNP O66529
rD	123	GLU	GLN	conflict	UNP O66529
rD	127	CYS	ARG	conflict	UNP O66529
rD	131	GLU	LYS	conflict	UNP O66529
rD	155	LEU	-	expression tag	UNP O66529
rD	156	GLU	-	expression tag	UNP O66529
rD	157	HIS	-	expression tag	UNP O66529
rD	158	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
rD	159	HIS	-	expression tag	UNP O66529
rD	160	HIS	-	expression tag	UNP O66529
rD	161	HIS	-	expression tag	UNP O66529
rE	2	GLU	GLN	conflict	UNP O66529
rE	28	GLY	ASP	conflict	UNP O66529
rE	52	CYS	ARG	conflict	UNP O66529
rE	83	GLU	ARG	conflict	UNP O66529
rE	86	GLU	THR	conflict	UNP O66529
rE	112	SER	THR	conflict	UNP O66529
rE	115	ASP	VAL	conflict	UNP O66529
rE	118	ASP	ALA	conflict	UNP O66529
rE	120	GLU	THR	conflict	UNP O66529
rE	123	GLU	GLN	conflict	UNP O66529
rE	127	CYS	ARG	conflict	UNP O66529
rE	131	GLU	LYS	conflict	UNP O66529
rE	155	LEU	-	expression tag	UNP O66529
rE	156	GLU	-	expression tag	UNP O66529
rE	157	HIS	-	expression tag	UNP O66529
rE	158	HIS	-	expression tag	UNP O66529
rE	159	HIS	-	expression tag	UNP O66529
rE	160	HIS	-	expression tag	UNP O66529
rE	161	HIS	-	expression tag	UNP O66529
rX	2	GLU	GLN	conflict	UNP O66529
rX	28	GLY	ASP	conflict	UNP O66529
rX	52	CYS	ARG	conflict	UNP O66529
rX	83	GLU	ARG	conflict	UNP O66529
rX	86	GLU	THR	conflict	UNP O66529
rX	112	SER	THR	conflict	UNP O66529
rX	115	ASP	VAL	conflict	UNP O66529
rX	118	ASP	ALA	conflict	UNP O66529
rX	120	GLU	THR	conflict	UNP O66529
rX	123	GLU	GLN	conflict	UNP O66529
rX	127	CYS	ARG	conflict	UNP O66529
rX	131	GLU	LYS	conflict	UNP O66529
rX	155	LEU	-	expression tag	UNP O66529
rX	156	GLU	-	expression tag	UNP O66529
rX	157	HIS	-	expression tag	UNP O66529
rX	158	HIS	-	expression tag	UNP O66529
rX	159	HIS	-	expression tag	UNP O66529
rX	160	HIS	-	expression tag	UNP O66529
rX	161	HIS	-	expression tag	UNP O66529
sA	2	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
sA	28	GLY	ASP	conflict	UNP O66529
sA	52	CYS	ARG	conflict	UNP O66529
sA	83	GLU	ARG	conflict	UNP O66529
sA	86	GLU	THR	conflict	UNP O66529
sA	112	SER	THR	conflict	UNP O66529
sA	115	ASP	VAL	conflict	UNP O66529
sA	118	ASP	ALA	conflict	UNP O66529
sA	120	GLU	THR	conflict	UNP O66529
sA	123	GLU	GLN	conflict	UNP O66529
sA	127	CYS	ARG	conflict	UNP O66529
sA	131	GLU	LYS	conflict	UNP O66529
sA	155	LEU	-	expression tag	UNP O66529
sA	156	GLU	-	expression tag	UNP O66529
sA	157	HIS	-	expression tag	UNP O66529
sA	158	HIS	-	expression tag	UNP O66529
sA	159	HIS	-	expression tag	UNP O66529
sA	160	HIS	-	expression tag	UNP O66529
sA	161	HIS	-	expression tag	UNP O66529
sB	2	GLU	GLN	conflict	UNP O66529
sB	28	GLY	ASP	conflict	UNP O66529
sB	52	CYS	ARG	conflict	UNP O66529
sB	83	GLU	ARG	conflict	UNP O66529
sB	86	GLU	THR	conflict	UNP O66529
sB	112	SER	THR	conflict	UNP O66529
sB	115	ASP	VAL	conflict	UNP O66529
sB	118	ASP	ALA	conflict	UNP O66529
sB	120	GLU	THR	conflict	UNP O66529
sB	123	GLU	GLN	conflict	UNP O66529
sB	127	CYS	ARG	conflict	UNP O66529
sB	131	GLU	LYS	conflict	UNP O66529
sB	155	LEU	-	expression tag	UNP O66529
sB	156	GLU	-	expression tag	UNP O66529
sB	157	HIS	-	expression tag	UNP O66529
sB	158	HIS	-	expression tag	UNP O66529
sB	159	HIS	-	expression tag	UNP O66529
sB	160	HIS	-	expression tag	UNP O66529
sB	161	HIS	-	expression tag	UNP O66529
sC	2	GLU	GLN	conflict	UNP O66529
sC	28	GLY	ASP	conflict	UNP O66529
sC	52	CYS	ARG	conflict	UNP O66529
sC	83	GLU	ARG	conflict	UNP O66529
sC	86	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
sC	112	SER	THR	conflict	UNP O66529
sC	115	ASP	VAL	conflict	UNP O66529
sC	118	ASP	ALA	conflict	UNP O66529
sC	120	GLU	THR	conflict	UNP O66529
sC	123	GLU	GLN	conflict	UNP O66529
sC	127	CYS	ARG	conflict	UNP O66529
sC	131	GLU	LYS	conflict	UNP O66529
sC	155	LEU	-	expression tag	UNP O66529
sC	156	GLU	-	expression tag	UNP O66529
sC	157	HIS	-	expression tag	UNP O66529
sC	158	HIS	-	expression tag	UNP O66529
sC	159	HIS	-	expression tag	UNP O66529
sC	160	HIS	-	expression tag	UNP O66529
sC	161	HIS	-	expression tag	UNP O66529
sD	2	GLU	GLN	conflict	UNP O66529
sD	28	GLY	ASP	conflict	UNP O66529
sD	52	CYS	ARG	conflict	UNP O66529
sD	83	GLU	ARG	conflict	UNP O66529
sD	86	GLU	THR	conflict	UNP O66529
sD	112	SER	THR	conflict	UNP O66529
sD	115	ASP	VAL	conflict	UNP O66529
sD	118	ASP	ALA	conflict	UNP O66529
sD	120	GLU	THR	conflict	UNP O66529
sD	123	GLU	GLN	conflict	UNP O66529
sD	127	CYS	ARG	conflict	UNP O66529
sD	131	GLU	LYS	conflict	UNP O66529
sD	155	LEU	-	expression tag	UNP O66529
sD	156	GLU	-	expression tag	UNP O66529
sD	157	HIS	-	expression tag	UNP O66529
sD	158	HIS	-	expression tag	UNP O66529
sD	159	HIS	-	expression tag	UNP O66529
sD	160	HIS	-	expression tag	UNP O66529
sD	161	HIS	-	expression tag	UNP O66529
sE	2	GLU	GLN	conflict	UNP O66529
sE	28	GLY	ASP	conflict	UNP O66529
sE	52	CYS	ARG	conflict	UNP O66529
sE	83	GLU	ARG	conflict	UNP O66529
sE	86	GLU	THR	conflict	UNP O66529
sE	112	SER	THR	conflict	UNP O66529
sE	115	ASP	VAL	conflict	UNP O66529
sE	118	ASP	ALA	conflict	UNP O66529
sE	120	GLU	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
sE	123	GLU	GLN	conflict	UNP O66529
sE	127	CYS	ARG	conflict	UNP O66529
sE	131	GLU	LYS	conflict	UNP O66529
sE	155	LEU	-	expression tag	UNP O66529
sE	156	GLU	-	expression tag	UNP O66529
sE	157	HIS	-	expression tag	UNP O66529
sE	158	HIS	-	expression tag	UNP O66529
sE	159	HIS	-	expression tag	UNP O66529
sE	160	HIS	-	expression tag	UNP O66529
sE	161	HIS	-	expression tag	UNP O66529
sX	2	GLU	GLN	conflict	UNP O66529
sX	28	GLY	ASP	conflict	UNP O66529
sX	52	CYS	ARG	conflict	UNP O66529
sX	83	GLU	ARG	conflict	UNP O66529
sX	86	GLU	THR	conflict	UNP O66529
sX	112	SER	THR	conflict	UNP O66529
sX	115	ASP	VAL	conflict	UNP O66529
sX	118	ASP	ALA	conflict	UNP O66529
sX	120	GLU	THR	conflict	UNP O66529
sX	123	GLU	GLN	conflict	UNP O66529
sX	127	CYS	ARG	conflict	UNP O66529
sX	131	GLU	LYS	conflict	UNP O66529
sX	155	LEU	-	expression tag	UNP O66529
sX	156	GLU	-	expression tag	UNP O66529
sX	157	HIS	-	expression tag	UNP O66529
sX	158	HIS	-	expression tag	UNP O66529
sX	159	HIS	-	expression tag	UNP O66529
sX	160	HIS	-	expression tag	UNP O66529
sX	161	HIS	-	expression tag	UNP O66529
tA	2	GLU	GLN	conflict	UNP O66529
tA	28	GLY	ASP	conflict	UNP O66529
tA	52	CYS	ARG	conflict	UNP O66529
tA	83	GLU	ARG	conflict	UNP O66529
tA	86	GLU	THR	conflict	UNP O66529
tA	112	SER	THR	conflict	UNP O66529
tA	115	ASP	VAL	conflict	UNP O66529
tA	118	ASP	ALA	conflict	UNP O66529
tA	120	GLU	THR	conflict	UNP O66529
tA	123	GLU	GLN	conflict	UNP O66529
tA	127	CYS	ARG	conflict	UNP O66529
tA	131	GLU	LYS	conflict	UNP O66529
tA	155	LEU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
tA	156	GLU	-	expression tag	UNP O66529
tA	157	HIS	-	expression tag	UNP O66529
tA	158	HIS	-	expression tag	UNP O66529
tA	159	HIS	-	expression tag	UNP O66529
tA	160	HIS	-	expression tag	UNP O66529
tA	161	HIS	-	expression tag	UNP O66529
tB	2	GLU	GLN	conflict	UNP O66529
tB	28	GLY	ASP	conflict	UNP O66529
tB	52	CYS	ARG	conflict	UNP O66529
tB	83	GLU	ARG	conflict	UNP O66529
tB	86	GLU	THR	conflict	UNP O66529
tB	112	SER	THR	conflict	UNP O66529
tB	115	ASP	VAL	conflict	UNP O66529
tB	118	ASP	ALA	conflict	UNP O66529
tB	120	GLU	THR	conflict	UNP O66529
tB	123	GLU	GLN	conflict	UNP O66529
tB	127	CYS	ARG	conflict	UNP O66529
tB	131	GLU	LYS	conflict	UNP O66529
tB	155	LEU	-	expression tag	UNP O66529
tB	156	GLU	-	expression tag	UNP O66529
tB	157	HIS	-	expression tag	UNP O66529
tB	158	HIS	-	expression tag	UNP O66529
tB	159	HIS	-	expression tag	UNP O66529
tB	160	HIS	-	expression tag	UNP O66529
tB	161	HIS	-	expression tag	UNP O66529
tC	2	GLU	GLN	conflict	UNP O66529
tC	28	GLY	ASP	conflict	UNP O66529
tC	52	CYS	ARG	conflict	UNP O66529
tC	83	GLU	ARG	conflict	UNP O66529
tC	86	GLU	THR	conflict	UNP O66529
tC	112	SER	THR	conflict	UNP O66529
tC	115	ASP	VAL	conflict	UNP O66529
tC	118	ASP	ALA	conflict	UNP O66529
tC	120	GLU	THR	conflict	UNP O66529
tC	123	GLU	GLN	conflict	UNP O66529
tC	127	CYS	ARG	conflict	UNP O66529
tC	131	GLU	LYS	conflict	UNP O66529
tC	155	LEU	-	expression tag	UNP O66529
tC	156	GLU	-	expression tag	UNP O66529
tC	157	HIS	-	expression tag	UNP O66529
tC	158	HIS	-	expression tag	UNP O66529
tC	159	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
tC	160	HIS	-	expression tag	UNP O66529
tC	161	HIS	-	expression tag	UNP O66529
tD	2	GLU	GLN	conflict	UNP O66529
tD	28	GLY	ASP	conflict	UNP O66529
tD	52	CYS	ARG	conflict	UNP O66529
tD	83	GLU	ARG	conflict	UNP O66529
tD	86	GLU	THR	conflict	UNP O66529
tD	112	SER	THR	conflict	UNP O66529
tD	115	ASP	VAL	conflict	UNP O66529
tD	118	ASP	ALA	conflict	UNP O66529
tD	120	GLU	THR	conflict	UNP O66529
tD	123	GLU	GLN	conflict	UNP O66529
tD	127	CYS	ARG	conflict	UNP O66529
tD	131	GLU	LYS	conflict	UNP O66529
tD	155	LEU	-	expression tag	UNP O66529
tD	156	GLU	-	expression tag	UNP O66529
tD	157	HIS	-	expression tag	UNP O66529
tD	158	HIS	-	expression tag	UNP O66529
tD	159	HIS	-	expression tag	UNP O66529
tD	160	HIS	-	expression tag	UNP O66529
tD	161	HIS	-	expression tag	UNP O66529
tE	2	GLU	GLN	conflict	UNP O66529
tE	28	GLY	ASP	conflict	UNP O66529
tE	52	CYS	ARG	conflict	UNP O66529
tE	83	GLU	ARG	conflict	UNP O66529
tE	86	GLU	THR	conflict	UNP O66529
tE	112	SER	THR	conflict	UNP O66529
tE	115	ASP	VAL	conflict	UNP O66529
tE	118	ASP	ALA	conflict	UNP O66529
tE	120	GLU	THR	conflict	UNP O66529
tE	123	GLU	GLN	conflict	UNP O66529
tE	127	CYS	ARG	conflict	UNP O66529
tE	131	GLU	LYS	conflict	UNP O66529
tE	155	LEU	-	expression tag	UNP O66529
tE	156	GLU	-	expression tag	UNP O66529
tE	157	HIS	-	expression tag	UNP O66529
tE	158	HIS	-	expression tag	UNP O66529
tE	159	HIS	-	expression tag	UNP O66529
tE	160	HIS	-	expression tag	UNP O66529
tE	161	HIS	-	expression tag	UNP O66529
tX	2	GLU	GLN	conflict	UNP O66529
tX	28	GLY	ASP	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
tX	52	CYS	ARG	conflict	UNP O66529
tX	83	GLU	ARG	conflict	UNP O66529
tX	86	GLU	THR	conflict	UNP O66529
tX	112	SER	THR	conflict	UNP O66529
tX	115	ASP	VAL	conflict	UNP O66529
tX	118	ASP	ALA	conflict	UNP O66529
tX	120	GLU	THR	conflict	UNP O66529
tX	123	GLU	GLN	conflict	UNP O66529
tX	127	CYS	ARG	conflict	UNP O66529
tX	131	GLU	LYS	conflict	UNP O66529
tX	155	LEU	-	expression tag	UNP O66529
tX	156	GLU	-	expression tag	UNP O66529
tX	157	HIS	-	expression tag	UNP O66529
tX	158	HIS	-	expression tag	UNP O66529
tX	159	HIS	-	expression tag	UNP O66529
tX	160	HIS	-	expression tag	UNP O66529
tX	161	HIS	-	expression tag	UNP O66529
uA	2	GLU	GLN	conflict	UNP O66529
uA	28	GLY	ASP	conflict	UNP O66529
uA	52	CYS	ARG	conflict	UNP O66529
uA	83	GLU	ARG	conflict	UNP O66529
uA	86	GLU	THR	conflict	UNP O66529
uA	112	SER	THR	conflict	UNP O66529
uA	115	ASP	VAL	conflict	UNP O66529
uA	118	ASP	ALA	conflict	UNP O66529
uA	120	GLU	THR	conflict	UNP O66529
uA	123	GLU	GLN	conflict	UNP O66529
uA	127	CYS	ARG	conflict	UNP O66529
uA	131	GLU	LYS	conflict	UNP O66529
uA	155	LEU	-	expression tag	UNP O66529
uA	156	GLU	-	expression tag	UNP O66529
uA	157	HIS	-	expression tag	UNP O66529
uA	158	HIS	-	expression tag	UNP O66529
uA	159	HIS	-	expression tag	UNP O66529
uA	160	HIS	-	expression tag	UNP O66529
uA	161	HIS	-	expression tag	UNP O66529
uB	2	GLU	GLN	conflict	UNP O66529
uB	28	GLY	ASP	conflict	UNP O66529
uB	52	CYS	ARG	conflict	UNP O66529
uB	83	GLU	ARG	conflict	UNP O66529
uB	86	GLU	THR	conflict	UNP O66529
uB	112	SER	THR	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
uB	115	ASP	VAL	conflict	UNP O66529
uB	118	ASP	ALA	conflict	UNP O66529
uB	120	GLU	THR	conflict	UNP O66529
uB	123	GLU	GLN	conflict	UNP O66529
uB	127	CYS	ARG	conflict	UNP O66529
uB	131	GLU	LYS	conflict	UNP O66529
uB	155	LEU	-	expression tag	UNP O66529
uB	156	GLU	-	expression tag	UNP O66529
uB	157	HIS	-	expression tag	UNP O66529
uB	158	HIS	-	expression tag	UNP O66529
uB	159	HIS	-	expression tag	UNP O66529
uB	160	HIS	-	expression tag	UNP O66529
uB	161	HIS	-	expression tag	UNP O66529
uC	2	GLU	GLN	conflict	UNP O66529
uC	28	GLY	ASP	conflict	UNP O66529
uC	52	CYS	ARG	conflict	UNP O66529
uC	83	GLU	ARG	conflict	UNP O66529
uC	86	GLU	THR	conflict	UNP O66529
uC	112	SER	THR	conflict	UNP O66529
uC	115	ASP	VAL	conflict	UNP O66529
uC	118	ASP	ALA	conflict	UNP O66529
uC	120	GLU	THR	conflict	UNP O66529
uC	123	GLU	GLN	conflict	UNP O66529
uC	127	CYS	ARG	conflict	UNP O66529
uC	131	GLU	LYS	conflict	UNP O66529
uC	155	LEU	-	expression tag	UNP O66529
uC	156	GLU	-	expression tag	UNP O66529
uC	157	HIS	-	expression tag	UNP O66529
uC	158	HIS	-	expression tag	UNP O66529
uC	159	HIS	-	expression tag	UNP O66529
uC	160	HIS	-	expression tag	UNP O66529
uC	161	HIS	-	expression tag	UNP O66529
uD	2	GLU	GLN	conflict	UNP O66529
uD	28	GLY	ASP	conflict	UNP O66529
uD	52	CYS	ARG	conflict	UNP O66529
uD	83	GLU	ARG	conflict	UNP O66529
uD	86	GLU	THR	conflict	UNP O66529
uD	112	SER	THR	conflict	UNP O66529
uD	115	ASP	VAL	conflict	UNP O66529
uD	118	ASP	ALA	conflict	UNP O66529
uD	120	GLU	THR	conflict	UNP O66529
uD	123	GLU	GLN	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
uD	127	CYS	ARG	conflict	UNP O66529
uD	131	GLU	LYS	conflict	UNP O66529
uD	155	LEU	-	expression tag	UNP O66529
uD	156	GLU	-	expression tag	UNP O66529
uD	157	HIS	-	expression tag	UNP O66529
uD	158	HIS	-	expression tag	UNP O66529
uD	159	HIS	-	expression tag	UNP O66529
uD	160	HIS	-	expression tag	UNP O66529
uD	161	HIS	-	expression tag	UNP O66529
uE	2	GLU	GLN	conflict	UNP O66529
uE	28	GLY	ASP	conflict	UNP O66529
uE	52	CYS	ARG	conflict	UNP O66529
uE	83	GLU	ARG	conflict	UNP O66529
uE	86	GLU	THR	conflict	UNP O66529
uE	112	SER	THR	conflict	UNP O66529
uE	115	ASP	VAL	conflict	UNP O66529
uE	118	ASP	ALA	conflict	UNP O66529
uE	120	GLU	THR	conflict	UNP O66529
uE	123	GLU	GLN	conflict	UNP O66529
uE	127	CYS	ARG	conflict	UNP O66529
uE	131	GLU	LYS	conflict	UNP O66529
uE	155	LEU	-	expression tag	UNP O66529
uE	156	GLU	-	expression tag	UNP O66529
uE	157	HIS	-	expression tag	UNP O66529
uE	158	HIS	-	expression tag	UNP O66529
uE	159	HIS	-	expression tag	UNP O66529
uE	160	HIS	-	expression tag	UNP O66529
uE	161	HIS	-	expression tag	UNP O66529
uX	2	GLU	GLN	conflict	UNP O66529
uX	28	GLY	ASP	conflict	UNP O66529
uX	52	CYS	ARG	conflict	UNP O66529
uX	83	GLU	ARG	conflict	UNP O66529
uX	86	GLU	THR	conflict	UNP O66529
uX	112	SER	THR	conflict	UNP O66529
uX	115	ASP	VAL	conflict	UNP O66529
uX	118	ASP	ALA	conflict	UNP O66529
uX	120	GLU	THR	conflict	UNP O66529
uX	123	GLU	GLN	conflict	UNP O66529
uX	127	CYS	ARG	conflict	UNP O66529
uX	131	GLU	LYS	conflict	UNP O66529
uX	155	LEU	-	expression tag	UNP O66529
uX	156	GLU	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
uX	157	HIS	-	expression tag	UNP O66529
uX	158	HIS	-	expression tag	UNP O66529
uX	159	HIS	-	expression tag	UNP O66529
uX	160	HIS	-	expression tag	UNP O66529
uX	161	HIS	-	expression tag	UNP O66529
vA	2	GLU	GLN	conflict	UNP O66529
vA	28	GLY	ASP	conflict	UNP O66529
vA	52	CYS	ARG	conflict	UNP O66529
vA	83	GLU	ARG	conflict	UNP O66529
vA	86	GLU	THR	conflict	UNP O66529
vA	112	SER	THR	conflict	UNP O66529
vA	115	ASP	VAL	conflict	UNP O66529
vA	118	ASP	ALA	conflict	UNP O66529
vA	120	GLU	THR	conflict	UNP O66529
vA	123	GLU	GLN	conflict	UNP O66529
vA	127	CYS	ARG	conflict	UNP O66529
vA	131	GLU	LYS	conflict	UNP O66529
vA	155	LEU	-	expression tag	UNP O66529
vA	156	GLU	-	expression tag	UNP O66529
vA	157	HIS	-	expression tag	UNP O66529
vA	158	HIS	-	expression tag	UNP O66529
vA	159	HIS	-	expression tag	UNP O66529
vA	160	HIS	-	expression tag	UNP O66529
vA	161	HIS	-	expression tag	UNP O66529
vB	2	GLU	GLN	conflict	UNP O66529
vB	28	GLY	ASP	conflict	UNP O66529
vB	52	CYS	ARG	conflict	UNP O66529
vB	83	GLU	ARG	conflict	UNP O66529
vB	86	GLU	THR	conflict	UNP O66529
vB	112	SER	THR	conflict	UNP O66529
vB	115	ASP	VAL	conflict	UNP O66529
vB	118	ASP	ALA	conflict	UNP O66529
vB	120	GLU	THR	conflict	UNP O66529
vB	123	GLU	GLN	conflict	UNP O66529
vB	127	CYS	ARG	conflict	UNP O66529
vB	131	GLU	LYS	conflict	UNP O66529
vB	155	LEU	-	expression tag	UNP O66529
vB	156	GLU	-	expression tag	UNP O66529
vB	157	HIS	-	expression tag	UNP O66529
vB	158	HIS	-	expression tag	UNP O66529
vB	159	HIS	-	expression tag	UNP O66529
vB	160	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
vB	161	HIS	-	expression tag	UNP O66529
vC	2	GLU	GLN	conflict	UNP O66529
vC	28	GLY	ASP	conflict	UNP O66529
vC	52	CYS	ARG	conflict	UNP O66529
vC	83	GLU	ARG	conflict	UNP O66529
vC	86	GLU	THR	conflict	UNP O66529
vC	112	SER	THR	conflict	UNP O66529
vC	115	ASP	VAL	conflict	UNP O66529
vC	118	ASP	ALA	conflict	UNP O66529
vC	120	GLU	THR	conflict	UNP O66529
vC	123	GLU	GLN	conflict	UNP O66529
vC	127	CYS	ARG	conflict	UNP O66529
vC	131	GLU	LYS	conflict	UNP O66529
vC	155	LEU	-	expression tag	UNP O66529
vC	156	GLU	-	expression tag	UNP O66529
vC	157	HIS	-	expression tag	UNP O66529
vC	158	HIS	-	expression tag	UNP O66529
vC	159	HIS	-	expression tag	UNP O66529
vC	160	HIS	-	expression tag	UNP O66529
vC	161	HIS	-	expression tag	UNP O66529
vD	2	GLU	GLN	conflict	UNP O66529
vD	28	GLY	ASP	conflict	UNP O66529
vD	52	CYS	ARG	conflict	UNP O66529
vD	83	GLU	ARG	conflict	UNP O66529
vD	86	GLU	THR	conflict	UNP O66529
vD	112	SER	THR	conflict	UNP O66529
vD	115	ASP	VAL	conflict	UNP O66529
vD	118	ASP	ALA	conflict	UNP O66529
vD	120	GLU	THR	conflict	UNP O66529
vD	123	GLU	GLN	conflict	UNP O66529
vD	127	CYS	ARG	conflict	UNP O66529
vD	131	GLU	LYS	conflict	UNP O66529
vD	155	LEU	-	expression tag	UNP O66529
vD	156	GLU	-	expression tag	UNP O66529
vD	157	HIS	-	expression tag	UNP O66529
vD	158	HIS	-	expression tag	UNP O66529
vD	159	HIS	-	expression tag	UNP O66529
vD	160	HIS	-	expression tag	UNP O66529
vD	161	HIS	-	expression tag	UNP O66529
vE	2	GLU	GLN	conflict	UNP O66529
vE	28	GLY	ASP	conflict	UNP O66529
vE	52	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
vE	83	GLU	ARG	conflict	UNP O66529
vE	86	GLU	THR	conflict	UNP O66529
vE	112	SER	THR	conflict	UNP O66529
vE	115	ASP	VAL	conflict	UNP O66529
vE	118	ASP	ALA	conflict	UNP O66529
vE	120	GLU	THR	conflict	UNP O66529
vE	123	GLU	GLN	conflict	UNP O66529
vE	127	CYS	ARG	conflict	UNP O66529
vE	131	GLU	LYS	conflict	UNP O66529
vE	155	LEU	-	expression tag	UNP O66529
vE	156	GLU	-	expression tag	UNP O66529
vE	157	HIS	-	expression tag	UNP O66529
vE	158	HIS	-	expression tag	UNP O66529
vE	159	HIS	-	expression tag	UNP O66529
vE	160	HIS	-	expression tag	UNP O66529
vE	161	HIS	-	expression tag	UNP O66529
vX	2	GLU	GLN	conflict	UNP O66529
vX	28	GLY	ASP	conflict	UNP O66529
vX	52	CYS	ARG	conflict	UNP O66529
vX	83	GLU	ARG	conflict	UNP O66529
vX	86	GLU	THR	conflict	UNP O66529
vX	112	SER	THR	conflict	UNP O66529
vX	115	ASP	VAL	conflict	UNP O66529
vX	118	ASP	ALA	conflict	UNP O66529
vX	120	GLU	THR	conflict	UNP O66529
vX	123	GLU	GLN	conflict	UNP O66529
vX	127	CYS	ARG	conflict	UNP O66529
vX	131	GLU	LYS	conflict	UNP O66529
vX	155	LEU	-	expression tag	UNP O66529
vX	156	GLU	-	expression tag	UNP O66529
vX	157	HIS	-	expression tag	UNP O66529
vX	158	HIS	-	expression tag	UNP O66529
vX	159	HIS	-	expression tag	UNP O66529
vX	160	HIS	-	expression tag	UNP O66529
vX	161	HIS	-	expression tag	UNP O66529
wA	2	GLU	GLN	conflict	UNP O66529
wA	28	GLY	ASP	conflict	UNP O66529
wA	52	CYS	ARG	conflict	UNP O66529
wA	83	GLU	ARG	conflict	UNP O66529
wA	86	GLU	THR	conflict	UNP O66529
wA	112	SER	THR	conflict	UNP O66529
wA	115	ASP	VAL	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
wA	118	ASP	ALA	conflict	UNP O66529
wA	120	GLU	THR	conflict	UNP O66529
wA	123	GLU	GLN	conflict	UNP O66529
wA	127	CYS	ARG	conflict	UNP O66529
wA	131	GLU	LYS	conflict	UNP O66529
wA	155	LEU	-	expression tag	UNP O66529
wA	156	GLU	-	expression tag	UNP O66529
wA	157	HIS	-	expression tag	UNP O66529
wA	158	HIS	-	expression tag	UNP O66529
wA	159	HIS	-	expression tag	UNP O66529
wA	160	HIS	-	expression tag	UNP O66529
wA	161	HIS	-	expression tag	UNP O66529
wB	2	GLU	GLN	conflict	UNP O66529
wB	28	GLY	ASP	conflict	UNP O66529
wB	52	CYS	ARG	conflict	UNP O66529
wB	83	GLU	ARG	conflict	UNP O66529
wB	86	GLU	THR	conflict	UNP O66529
wB	112	SER	THR	conflict	UNP O66529
wB	115	ASP	VAL	conflict	UNP O66529
wB	118	ASP	ALA	conflict	UNP O66529
wB	120	GLU	THR	conflict	UNP O66529
wB	123	GLU	GLN	conflict	UNP O66529
wB	127	CYS	ARG	conflict	UNP O66529
wB	131	GLU	LYS	conflict	UNP O66529
wB	155	LEU	-	expression tag	UNP O66529
wB	156	GLU	-	expression tag	UNP O66529
wB	157	HIS	-	expression tag	UNP O66529
wB	158	HIS	-	expression tag	UNP O66529
wB	159	HIS	-	expression tag	UNP O66529
wB	160	HIS	-	expression tag	UNP O66529
wB	161	HIS	-	expression tag	UNP O66529
wC	2	GLU	GLN	conflict	UNP O66529
wC	28	GLY	ASP	conflict	UNP O66529
wC	52	CYS	ARG	conflict	UNP O66529
wC	83	GLU	ARG	conflict	UNP O66529
wC	86	GLU	THR	conflict	UNP O66529
wC	112	SER	THR	conflict	UNP O66529
wC	115	ASP	VAL	conflict	UNP O66529
wC	118	ASP	ALA	conflict	UNP O66529
wC	120	GLU	THR	conflict	UNP O66529
wC	123	GLU	GLN	conflict	UNP O66529
wC	127	CYS	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
wC	131	GLU	LYS	conflict	UNP O66529
wC	155	LEU	-	expression tag	UNP O66529
wC	156	GLU	-	expression tag	UNP O66529
wC	157	HIS	-	expression tag	UNP O66529
wC	158	HIS	-	expression tag	UNP O66529
wC	159	HIS	-	expression tag	UNP O66529
wC	160	HIS	-	expression tag	UNP O66529
wC	161	HIS	-	expression tag	UNP O66529
wD	2	GLU	GLN	conflict	UNP O66529
wD	28	GLY	ASP	conflict	UNP O66529
wD	52	CYS	ARG	conflict	UNP O66529
wD	83	GLU	ARG	conflict	UNP O66529
wD	86	GLU	THR	conflict	UNP O66529
wD	112	SER	THR	conflict	UNP O66529
wD	115	ASP	VAL	conflict	UNP O66529
wD	118	ASP	ALA	conflict	UNP O66529
wD	120	GLU	THR	conflict	UNP O66529
wD	123	GLU	GLN	conflict	UNP O66529
wD	127	CYS	ARG	conflict	UNP O66529
wD	131	GLU	LYS	conflict	UNP O66529
wD	155	LEU	-	expression tag	UNP O66529
wD	156	GLU	-	expression tag	UNP O66529
wD	157	HIS	-	expression tag	UNP O66529
wD	158	HIS	-	expression tag	UNP O66529
wD	159	HIS	-	expression tag	UNP O66529
wD	160	HIS	-	expression tag	UNP O66529
wD	161	HIS	-	expression tag	UNP O66529
wE	2	GLU	GLN	conflict	UNP O66529
wE	28	GLY	ASP	conflict	UNP O66529
wE	52	CYS	ARG	conflict	UNP O66529
wE	83	GLU	ARG	conflict	UNP O66529
wE	86	GLU	THR	conflict	UNP O66529
wE	112	SER	THR	conflict	UNP O66529
wE	115	ASP	VAL	conflict	UNP O66529
wE	118	ASP	ALA	conflict	UNP O66529
wE	120	GLU	THR	conflict	UNP O66529
wE	123	GLU	GLN	conflict	UNP O66529
wE	127	CYS	ARG	conflict	UNP O66529
wE	131	GLU	LYS	conflict	UNP O66529
wE	155	LEU	-	expression tag	UNP O66529
wE	156	GLU	-	expression tag	UNP O66529
wE	157	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
wE	158	HIS	-	expression tag	UNP O66529
wE	159	HIS	-	expression tag	UNP O66529
wE	160	HIS	-	expression tag	UNP O66529
wE	161	HIS	-	expression tag	UNP O66529
wX	2	GLU	GLN	conflict	UNP O66529
wX	28	GLY	ASP	conflict	UNP O66529
wX	52	CYS	ARG	conflict	UNP O66529
wX	83	GLU	ARG	conflict	UNP O66529
wX	86	GLU	THR	conflict	UNP O66529
wX	112	SER	THR	conflict	UNP O66529
wX	115	ASP	VAL	conflict	UNP O66529
wX	118	ASP	ALA	conflict	UNP O66529
wX	120	GLU	THR	conflict	UNP O66529
wX	123	GLU	GLN	conflict	UNP O66529
wX	127	CYS	ARG	conflict	UNP O66529
wX	131	GLU	LYS	conflict	UNP O66529
wX	155	LEU	-	expression tag	UNP O66529
wX	156	GLU	-	expression tag	UNP O66529
wX	157	HIS	-	expression tag	UNP O66529
wX	158	HIS	-	expression tag	UNP O66529
wX	159	HIS	-	expression tag	UNP O66529
wX	160	HIS	-	expression tag	UNP O66529
wX	161	HIS	-	expression tag	UNP O66529
xA	2	GLU	GLN	conflict	UNP O66529
xA	28	GLY	ASP	conflict	UNP O66529
xA	52	CYS	ARG	conflict	UNP O66529
xA	83	GLU	ARG	conflict	UNP O66529
xA	86	GLU	THR	conflict	UNP O66529
xA	112	SER	THR	conflict	UNP O66529
xA	115	ASP	VAL	conflict	UNP O66529
xA	118	ASP	ALA	conflict	UNP O66529
xA	120	GLU	THR	conflict	UNP O66529
xA	123	GLU	GLN	conflict	UNP O66529
xA	127	CYS	ARG	conflict	UNP O66529
xA	131	GLU	LYS	conflict	UNP O66529
xA	155	LEU	-	expression tag	UNP O66529
xA	156	GLU	-	expression tag	UNP O66529
xA	157	HIS	-	expression tag	UNP O66529
xA	158	HIS	-	expression tag	UNP O66529
xA	159	HIS	-	expression tag	UNP O66529
xA	160	HIS	-	expression tag	UNP O66529
xA	161	HIS	-	expression tag	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
xB	2	GLU	GLN	conflict	UNP O66529
xB	28	GLY	ASP	conflict	UNP O66529
xB	52	CYS	ARG	conflict	UNP O66529
xB	83	GLU	ARG	conflict	UNP O66529
xB	86	GLU	THR	conflict	UNP O66529
xB	112	SER	THR	conflict	UNP O66529
xB	115	ASP	VAL	conflict	UNP O66529
xB	118	ASP	ALA	conflict	UNP O66529
xB	120	GLU	THR	conflict	UNP O66529
xB	123	GLU	GLN	conflict	UNP O66529
xB	127	CYS	ARG	conflict	UNP O66529
xB	131	GLU	LYS	conflict	UNP O66529
xB	155	LEU	-	expression tag	UNP O66529
xB	156	GLU	-	expression tag	UNP O66529
xB	157	HIS	-	expression tag	UNP O66529
xB	158	HIS	-	expression tag	UNP O66529
xB	159	HIS	-	expression tag	UNP O66529
xB	160	HIS	-	expression tag	UNP O66529
xB	161	HIS	-	expression tag	UNP O66529
xC	2	GLU	GLN	conflict	UNP O66529
xC	28	GLY	ASP	conflict	UNP O66529
xC	52	CYS	ARG	conflict	UNP O66529
xC	83	GLU	ARG	conflict	UNP O66529
xC	86	GLU	THR	conflict	UNP O66529
xC	112	SER	THR	conflict	UNP O66529
xC	115	ASP	VAL	conflict	UNP O66529
xC	118	ASP	ALA	conflict	UNP O66529
xC	120	GLU	THR	conflict	UNP O66529
xC	123	GLU	GLN	conflict	UNP O66529
xC	127	CYS	ARG	conflict	UNP O66529
xC	131	GLU	LYS	conflict	UNP O66529
xC	155	LEU	-	expression tag	UNP O66529
xC	156	GLU	-	expression tag	UNP O66529
xC	157	HIS	-	expression tag	UNP O66529
xC	158	HIS	-	expression tag	UNP O66529
xC	159	HIS	-	expression tag	UNP O66529
xC	160	HIS	-	expression tag	UNP O66529
xC	161	HIS	-	expression tag	UNP O66529
xD	2	GLU	GLN	conflict	UNP O66529
xD	28	GLY	ASP	conflict	UNP O66529
xD	52	CYS	ARG	conflict	UNP O66529
xD	83	GLU	ARG	conflict	UNP O66529

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
xD	86	GLU	THR	conflict	UNP O66529
xD	112	SER	THR	conflict	UNP O66529
xD	115	ASP	VAL	conflict	UNP O66529
xD	118	ASP	ALA	conflict	UNP O66529
xD	120	GLU	THR	conflict	UNP O66529
xD	123	GLU	GLN	conflict	UNP O66529
xD	127	CYS	ARG	conflict	UNP O66529
xD	131	GLU	LYS	conflict	UNP O66529
xD	155	LEU	-	expression tag	UNP O66529
xD	156	GLU	-	expression tag	UNP O66529
xD	157	HIS	-	expression tag	UNP O66529
xD	158	HIS	-	expression tag	UNP O66529
xD	159	HIS	-	expression tag	UNP O66529
xD	160	HIS	-	expression tag	UNP O66529
xD	161	HIS	-	expression tag	UNP O66529
xE	2	GLU	GLN	conflict	UNP O66529
xE	28	GLY	ASP	conflict	UNP O66529
xE	52	CYS	ARG	conflict	UNP O66529
xE	83	GLU	ARG	conflict	UNP O66529
xE	86	GLU	THR	conflict	UNP O66529
xE	112	SER	THR	conflict	UNP O66529
xE	115	ASP	VAL	conflict	UNP O66529
xE	118	ASP	ALA	conflict	UNP O66529
xE	120	GLU	THR	conflict	UNP O66529
xE	123	GLU	GLN	conflict	UNP O66529
xE	127	CYS	ARG	conflict	UNP O66529
xE	131	GLU	LYS	conflict	UNP O66529
xE	155	LEU	-	expression tag	UNP O66529
xE	156	GLU	-	expression tag	UNP O66529
xE	157	HIS	-	expression tag	UNP O66529
xE	158	HIS	-	expression tag	UNP O66529
xE	159	HIS	-	expression tag	UNP O66529
xE	160	HIS	-	expression tag	UNP O66529
xE	161	HIS	-	expression tag	UNP O66529
xX	2	GLU	GLN	conflict	UNP O66529
xX	28	GLY	ASP	conflict	UNP O66529
xX	52	CYS	ARG	conflict	UNP O66529
xX	83	GLU	ARG	conflict	UNP O66529
xX	86	GLU	THR	conflict	UNP O66529
xX	112	SER	THR	conflict	UNP O66529
xX	115	ASP	VAL	conflict	UNP O66529
xX	118	ASP	ALA	conflict	UNP O66529

Continued on next page...

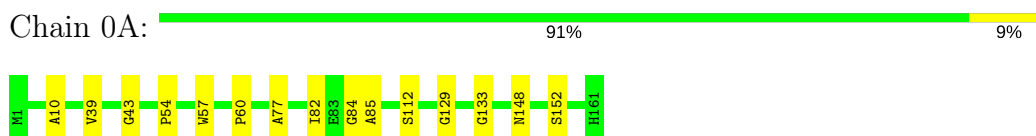
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
xX	120	GLU	THR	conflict	UNP O66529
xX	123	GLU	GLN	conflict	UNP O66529
xX	127	CYS	ARG	conflict	UNP O66529
xX	131	GLU	LYS	conflict	UNP O66529
xX	155	LEU	-	expression tag	UNP O66529
xX	156	GLU	-	expression tag	UNP O66529
xX	157	HIS	-	expression tag	UNP O66529
xX	158	HIS	-	expression tag	UNP O66529
xX	159	HIS	-	expression tag	UNP O66529
xX	160	HIS	-	expression tag	UNP O66529
xX	161	HIS	-	expression tag	UNP O66529

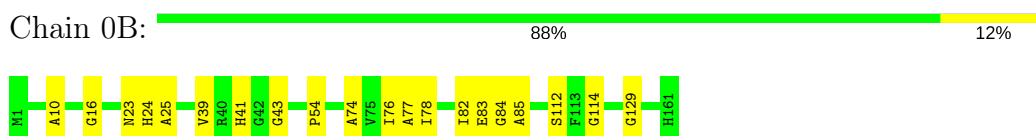
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

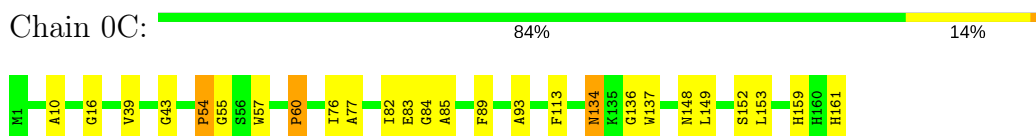
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



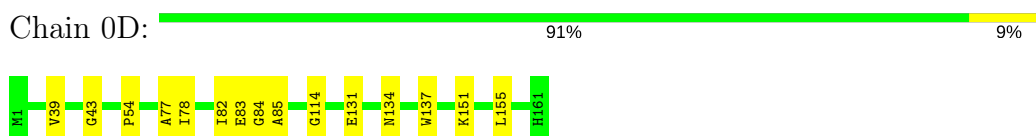
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



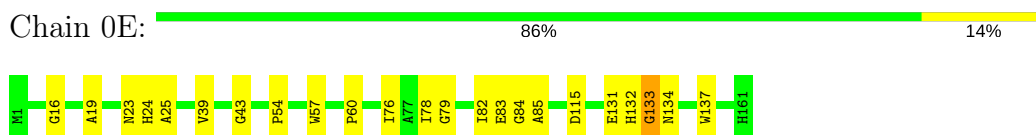
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

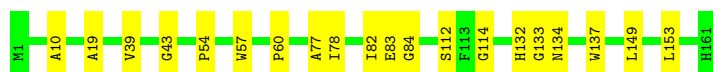


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase





- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 1A: 91% 9%



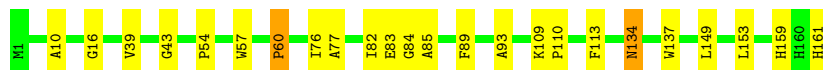
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 1B: 88% 12%



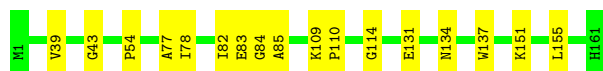
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 1C: 85% 14%



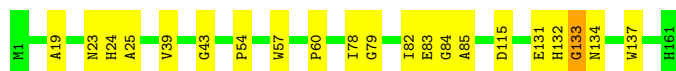
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 1D: 89% 11%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 1E: 87% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 1X: 88% 12%

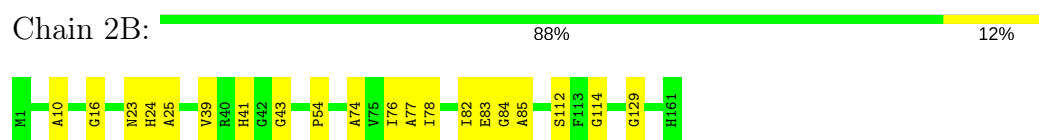


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

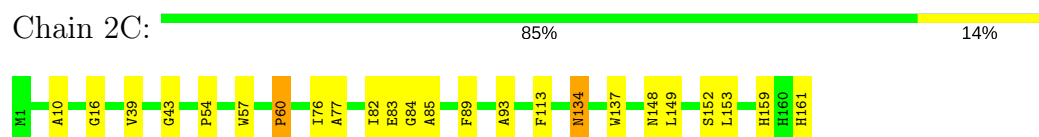
Chain 2A: 89% 11%



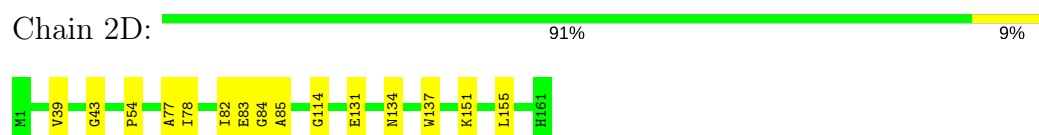
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



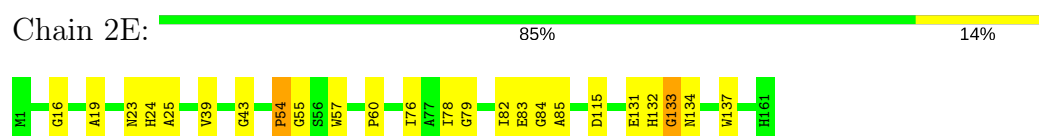
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



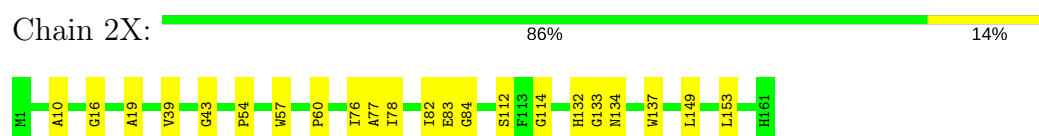
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



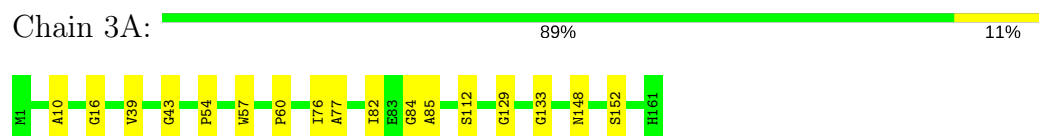
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



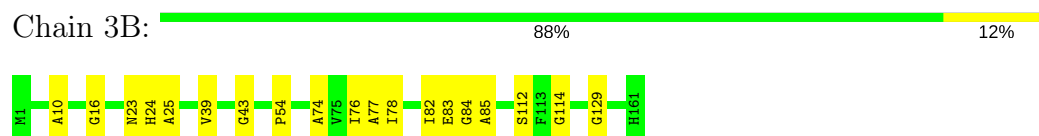
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

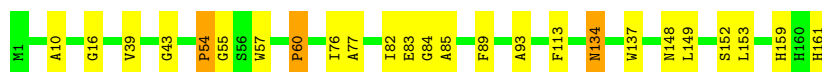


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



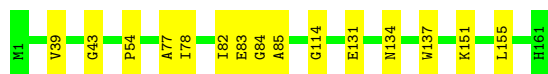
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 3C:  84% 14%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 3D:  91% 9%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 3E:  85% 14%




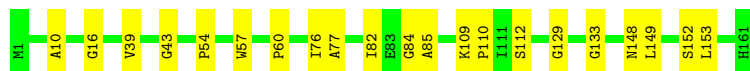
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 3X:  88% 12%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 4A:  87% 13%




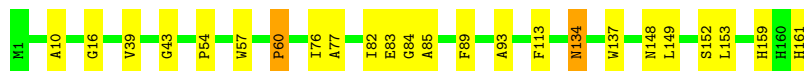
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 4B:  87% 12%



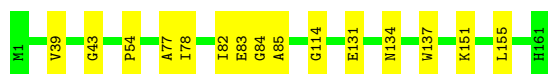
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 4C:  85% 14%



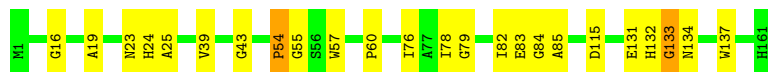
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 4D:  91% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 4E: 85% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 4X: 88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 5A: 88% 12%



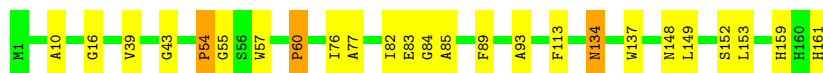
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 5B: 87% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 5C: 84% 14%



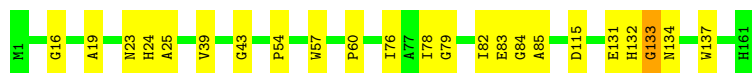
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 5D: 91% 9%

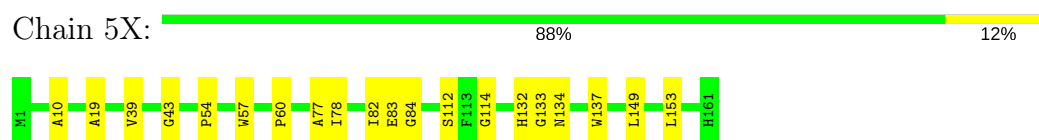


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

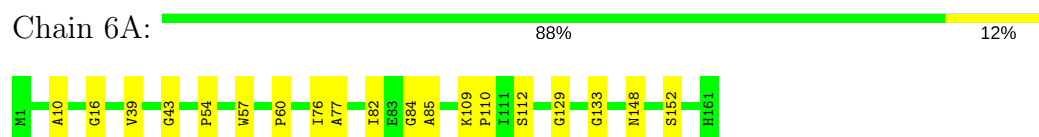
Chain 5E: 86% 14%



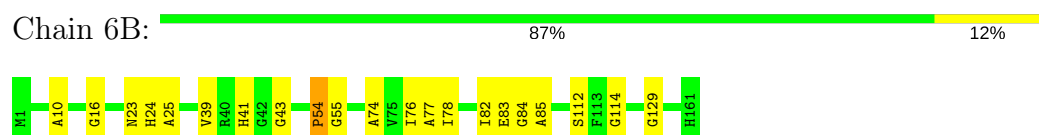
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



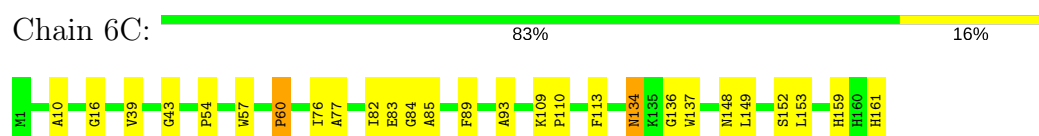
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



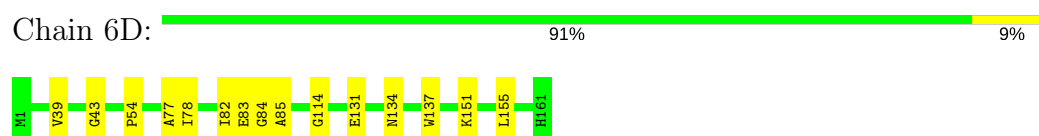
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



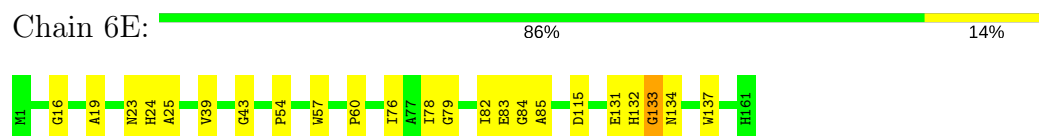
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



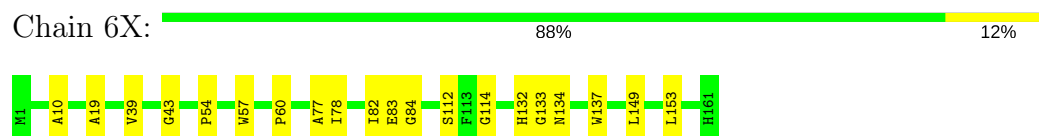
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



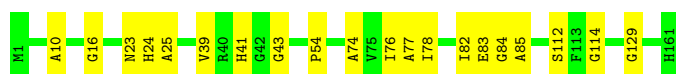
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 7A:  88% 12%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 7B:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 7C:  83% 16%




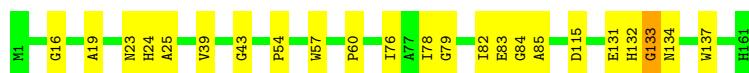
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 7D:  91% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 7E:  86% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 7X:  88% 12%




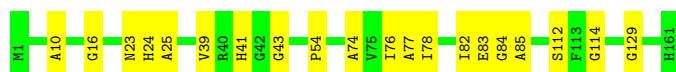
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 8A:  91% 9%



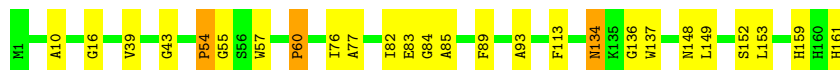
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 8B:  88% 12%



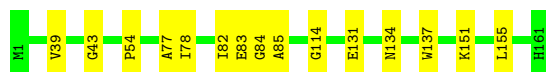
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 8C: 84% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 8D: 91% 9%



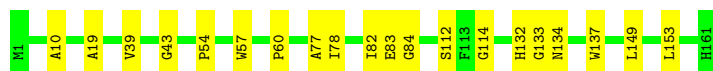
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 8E: 86% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 8X: 88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 9A: 89% 11%



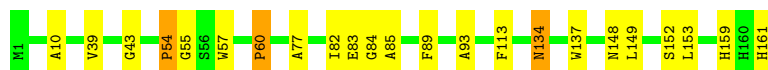
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 9B: 88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 9C: 86% 12%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 9D:  91% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 9E:  85% 14%



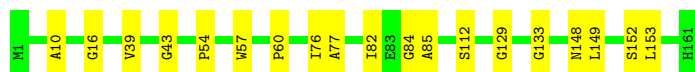
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain 9X:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AA:  88% 12%




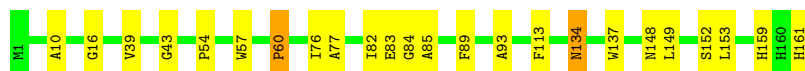
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AB:  87% 12%



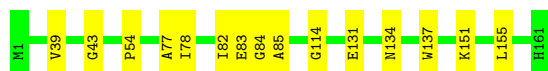
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AC:  85% 14%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AD:  91% 9%



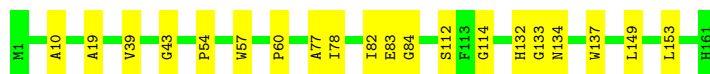
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AE:  84% 15%



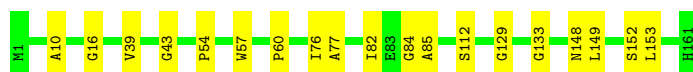
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AX:  88% 12%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BA:  88% 12%




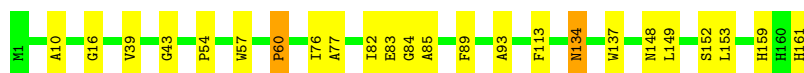
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BB:  87% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BC:  85% 14%




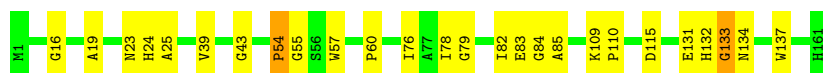
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BD:  91% 9%



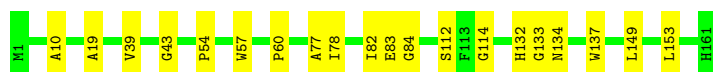
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BE:  84% 15%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BX:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CA: 87% 13%



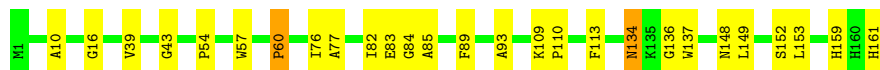
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CB: 87% 12%



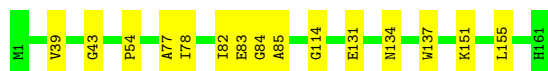
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CC: 83% 16%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CD: 91% 9%



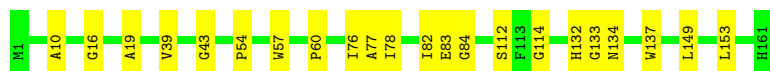
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CE: 86% 14%



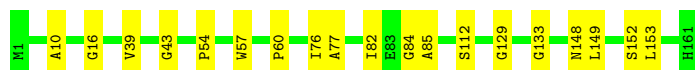
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CX: 86% 14%



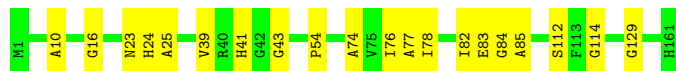
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DA: 88% 12%




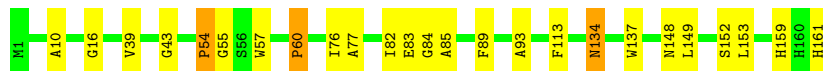
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DB:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DC:  84% 14%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DD:  91% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DE:  85% 14%




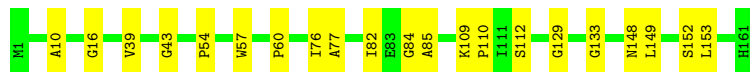
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain DX:  88% 12%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EA:  87% 13%




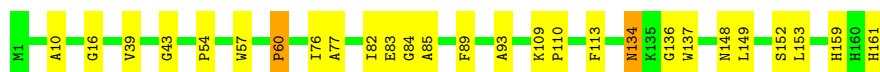
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EB:  87% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EC:  83% 16%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ED:  91% 9%



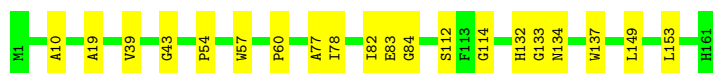
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EE:  86% 14%




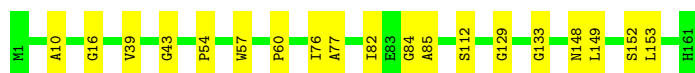
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain EX:  88% 12%



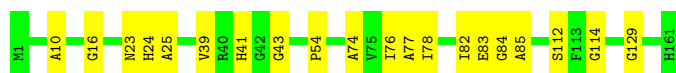
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FA:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FB:  88% 12%



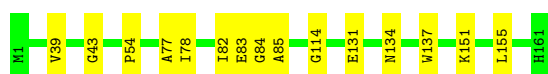
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FC:  84% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FD:  91% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FE: 86% 14%



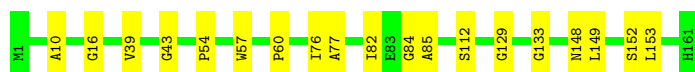
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain FX: 88% 12%



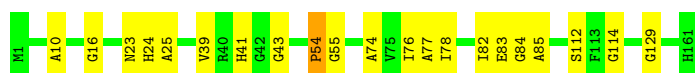
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GA: 88% 12%



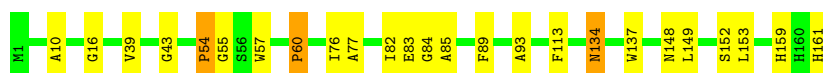
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GB: 87% 12%



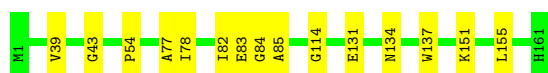
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GC: 84% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GD: 91% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GE: 85% 14%




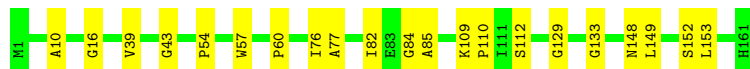
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain GX:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HA:  87% 13%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HB:  87% 12%



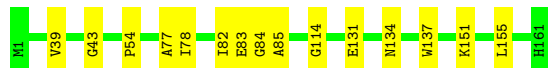
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HC:  82% 17%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HD:  91% 9%




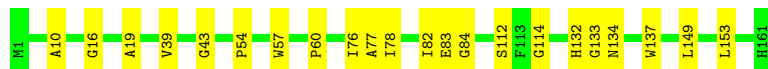
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HE:  84% 15%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain HX:  86% 14%




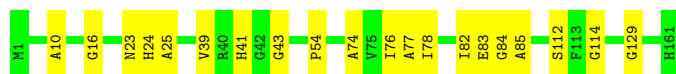
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IA:  89% 11%




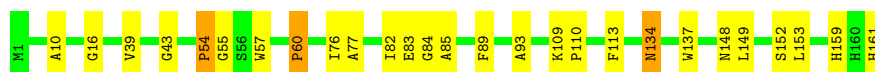
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IB:  88% 12%



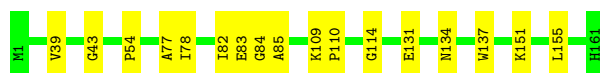
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IC:  83% 15% .




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ID:  89% 11%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IE:  86% 14% .



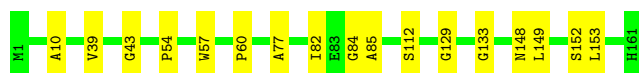
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IX:  86% 14%




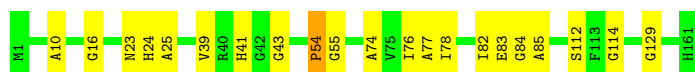
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JA:  89% 11%



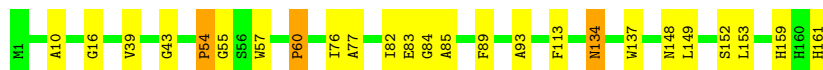
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JB:  87% 12% .



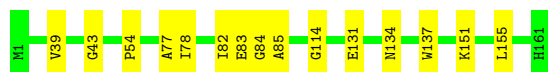
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JC: 84% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JD: 91% 9%



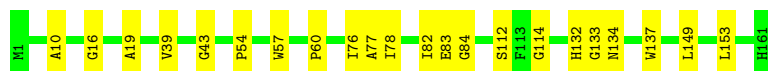
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JE: 85% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain JX: 86% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KA: 87% 13%



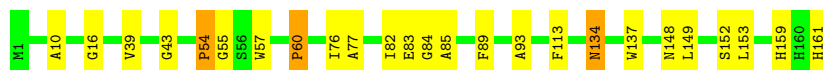
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KB: 88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KC: 84% 14%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KD:  91% 9%



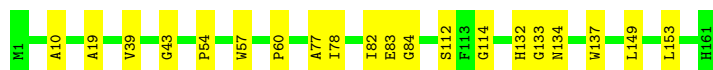
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KE:  85% 14%



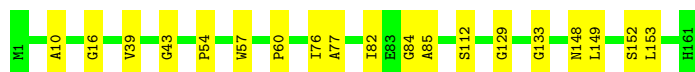
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain KX:  88% 12%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LA:  88% 12%




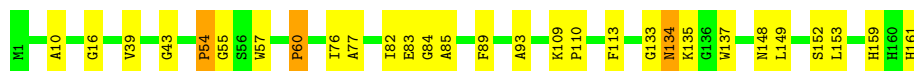
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LB:  87% 12%



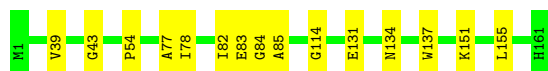
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LC:  82% 16%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LD:  91% 9%



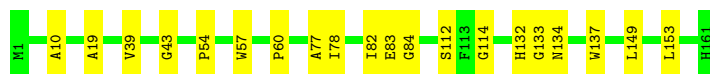
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LE:  86% 14%



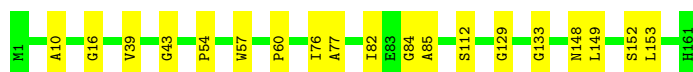
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain LX:  88% 12%



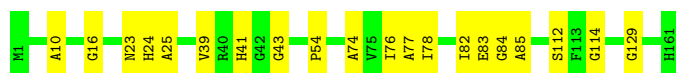
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MA:  88% 12%




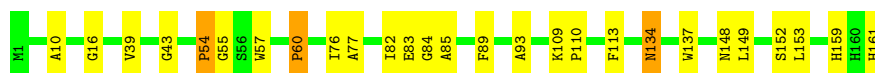
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MB:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MC:  83% 15%




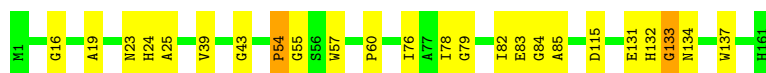
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MD:  91% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ME:  85% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain MX:  88% 12%



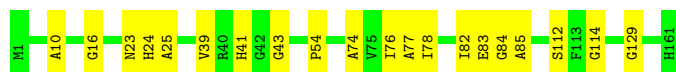
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NA: 89% 11%



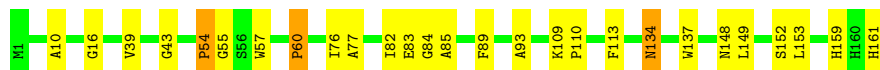
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NB: 88% 12%



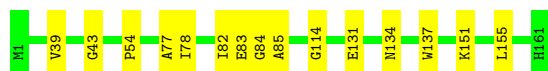
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NC: 83% 15%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ND: 91% 9%



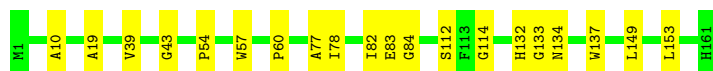
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NE: 86% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain NX: 88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OA: 89% 11%



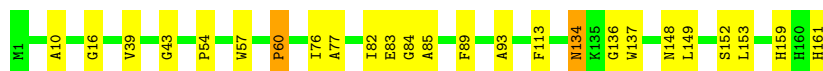
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OB:  87% 12%



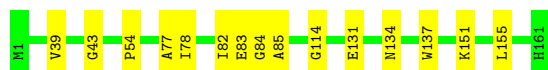
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OC:  84% 14%




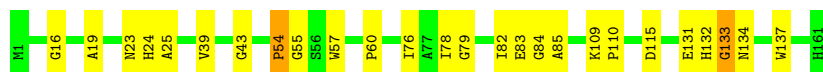
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OD:  91% 9%



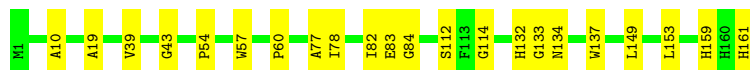
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OE:  84% 15%




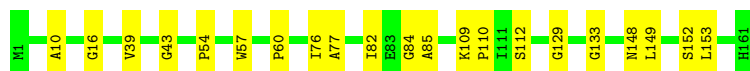
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain OX:  86% 14%




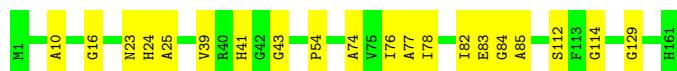
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain PA:  87% 13%

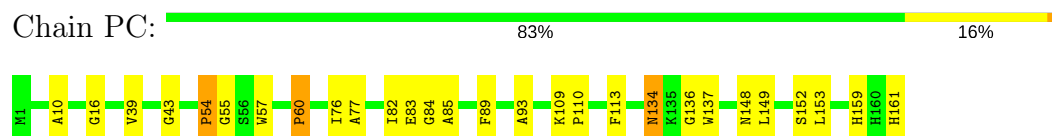


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

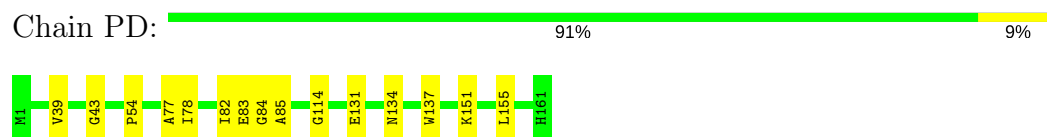
Chain PB:  88% 12%



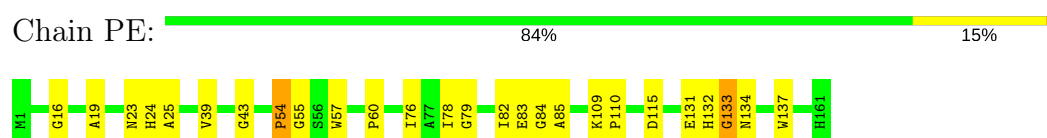
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



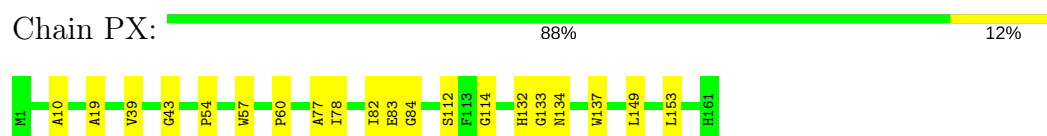
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



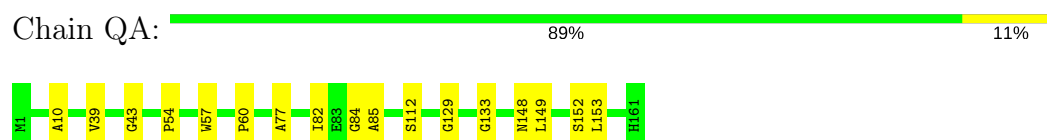
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



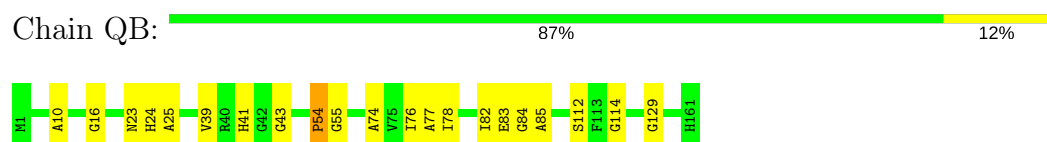
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



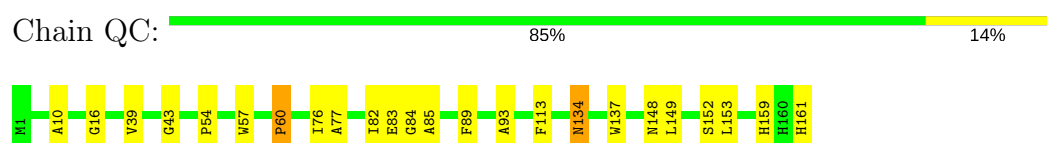
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

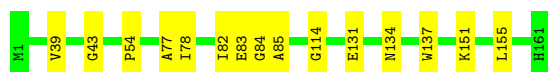


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase





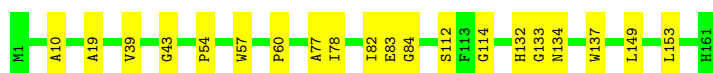
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain QE: 85% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain QX: 88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain RA: 89% 11%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain RB: 87% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain RC: 83% 15%



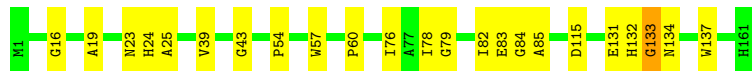
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain RD: 91% 9%

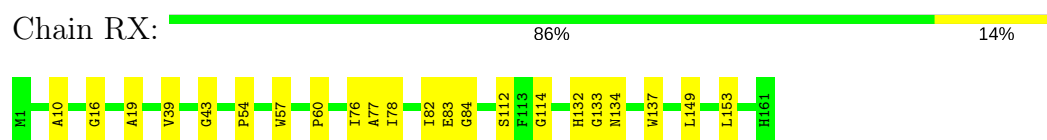


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

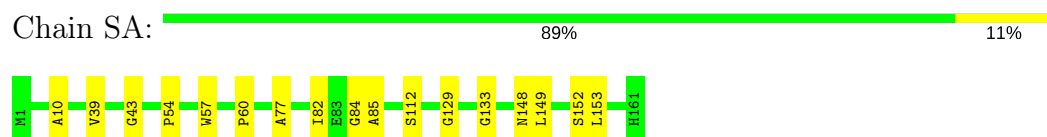
Chain RE: 86% 14%



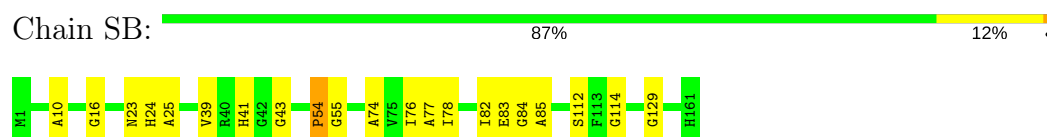
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



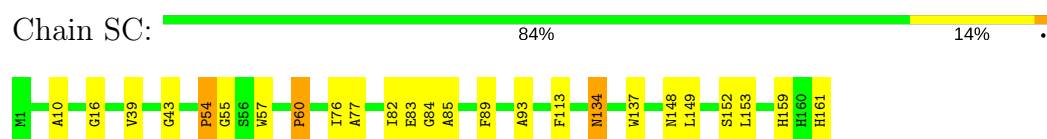
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



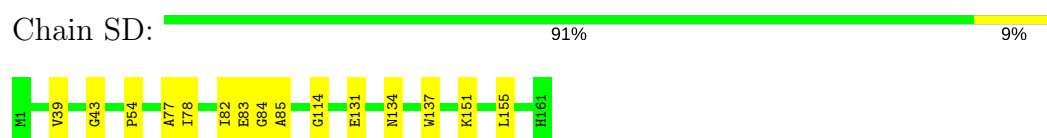
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



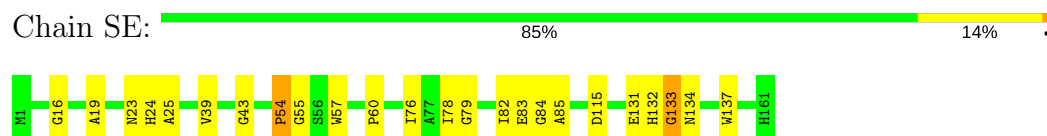
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



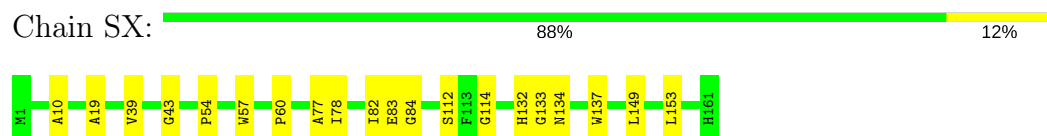
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase




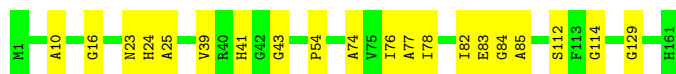
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TA:  89% 11%



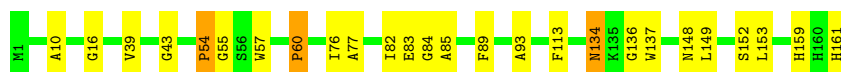
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TB:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TC:  84% 14% .




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TD:  91% 9%



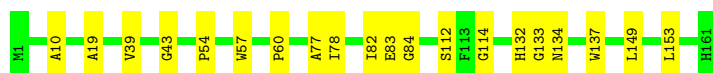
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TE:  85% 14% .



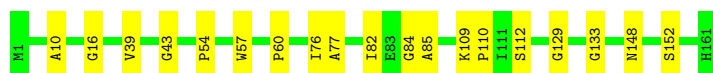
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain TX:  88% 12%



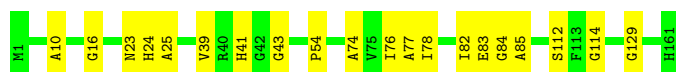
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UA:  88% 12%



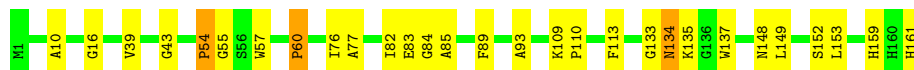
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UB:  88% 12%



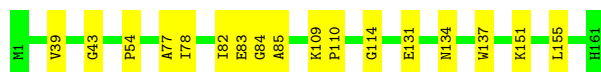
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UC: 82% 16%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UD: 89% 11%



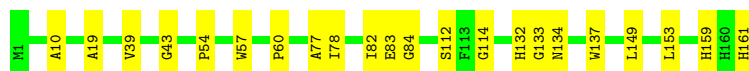
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UE: 85% 14%



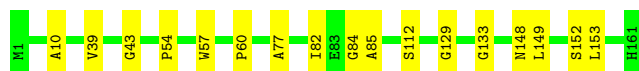
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain UX: 86% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VA: 89% 11%



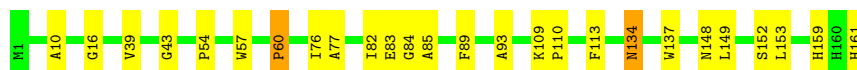
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VB: 88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VC: 84% 15%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VD:  91% 9%



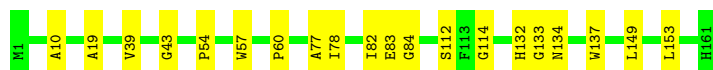
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VE:  85% 14%



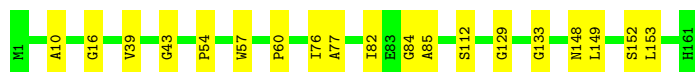
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain VX:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WA:  88% 12%




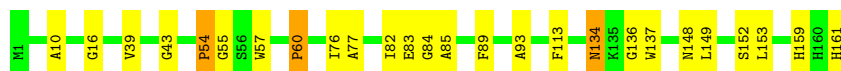
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WB:  88% 12%



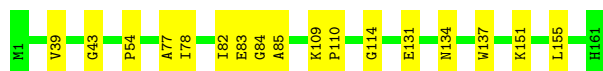
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WC:  84% 14%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WD:  89% 11%



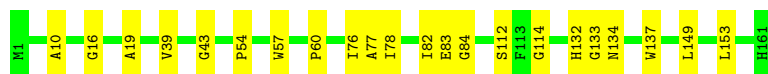
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WE:  85% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain WX:  86% 14%



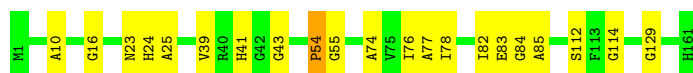
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XA:  89% 11%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XB:  87% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XC:  84% 15%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XD:  91% 9%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XE:  85% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain XX:  88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YA: 89% 11%



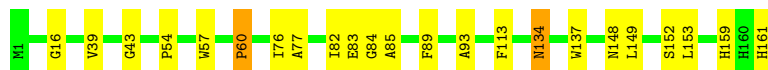
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YB: 88% 12%



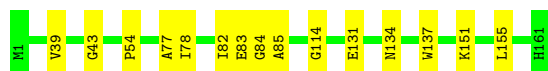
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YC: 86% 13%



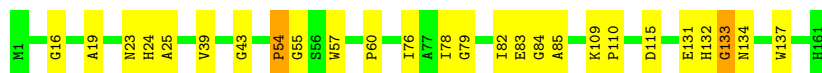
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YD: 91% 9%



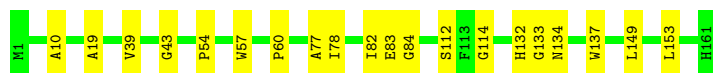
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YE: 84% 15%



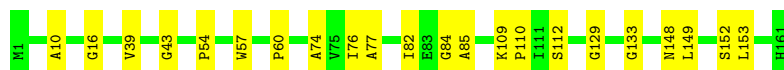
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain YX: 88% 12%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZA: 86% 14%




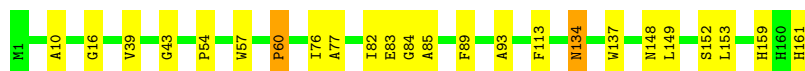
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZB:  87% 12%



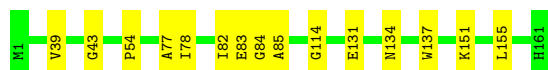
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZC:  85% 14%




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZD:  91% 9%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZE:  85% 14%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ZX:  88% 12%



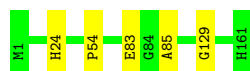
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain aA:  98%




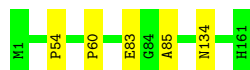
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain aB:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain aC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain aD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain aE:  96%



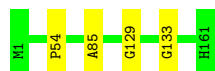
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain aX:  98%



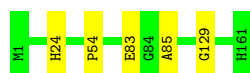
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain bA:  98%



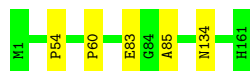
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain bB:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain bC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain bD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain bE:  96%



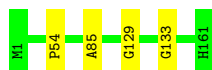
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain bX:  98%



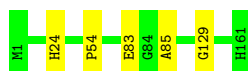
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain cA:  98%



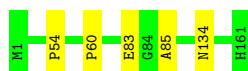
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain cB:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain cC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain cD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain cE:  96%



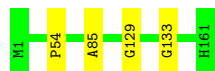
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain cX:  98%



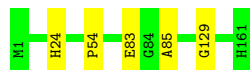
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain dA:  98%



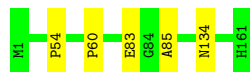
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain dB:  97%



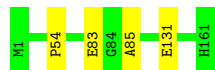
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain dC:  97%



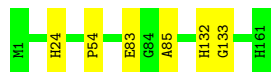
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain dD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain dE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain dX:  98%



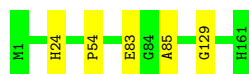
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain eA:  98% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain eB:  97% .



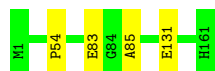
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain eC:  97% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain eD:  98% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain eE:  96% .



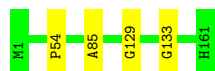
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain eX:  98% .



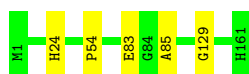
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain fA:  98% .



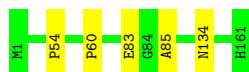
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain fB:  97% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain fC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain fD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain fE:  96%



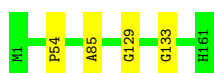
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain fX:  98%



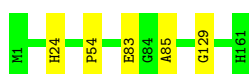
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain gA:  98%



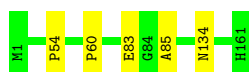
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain gB:  97%



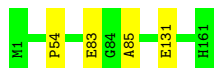
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain gC:  97%



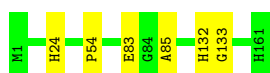
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain gD: 98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain gE: 96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain gX: 98%



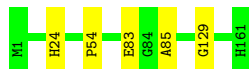
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain hA: 98%



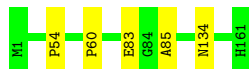
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain hB: 97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain hC: 97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain hD: 98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain hE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain hX:  98%



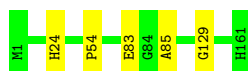
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain iA:  98%



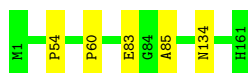
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain iB:  97%



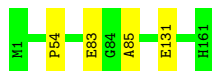
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain iC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain iD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain iE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain iX:  98%



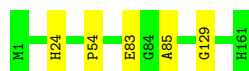
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain jA:  98%



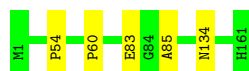
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain jB:  97%



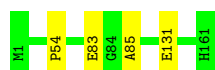
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain jC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain jD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain jE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain jX:  98%



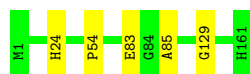
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain kA:  98% .



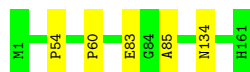
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain kB:  97% .



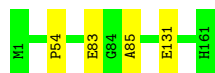
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain kC:  97% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain kD:  98% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain kE:  96% .



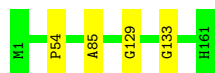
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain kX:  98% .



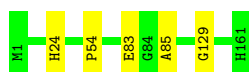
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain lA:  98% .



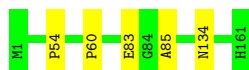
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain lB:  97% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain ID:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain IX:  98%



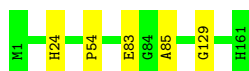
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain mA:  98%



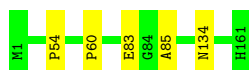
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain mB:  97%



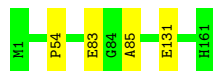
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain mC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain mD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain mE:  96%



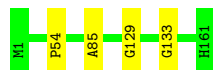
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain mX:  98%



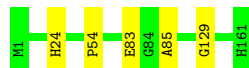
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain nA:  98%



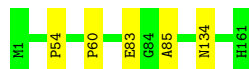
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain nB:  97%



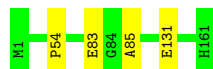
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain nC:  97%

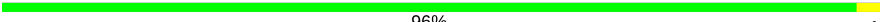


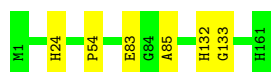
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain nD:  98%



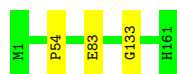
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain nE:  96% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain nX:  98% .



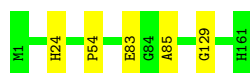
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain oA:  98% .



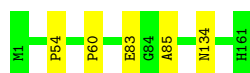
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain oB:  97% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain oC:  97% .



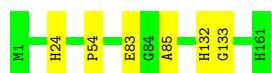
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain oD:  98% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain oE:  96% .



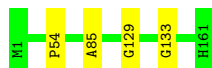
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain oX:  98% .



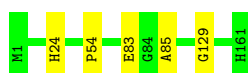
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain pA:  98%



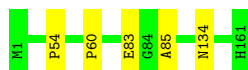
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain pB:  97%



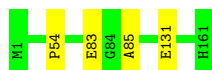
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain pC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain pD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain pE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain pX:  98%



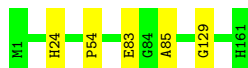
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain qA:  98%



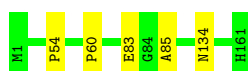
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain qB:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain qC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain qD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain qE:  96%



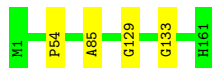
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain qX:  98%



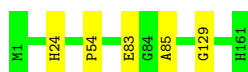
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain rA:  98%



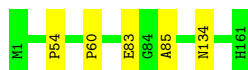
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain rB:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain rC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain rD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain rE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain rX:  98%



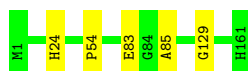
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain sA:  98%



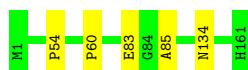
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain sB:  97%



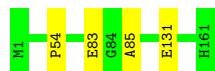
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain sC:  97%



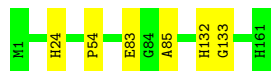
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain sD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain sE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain sX:  98%



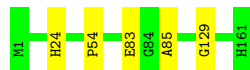
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain tA:  98%



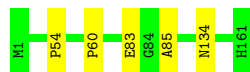
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain tB:  97%



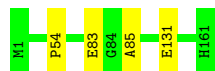
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain tC:  97%



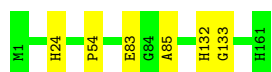
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain tD:  98%



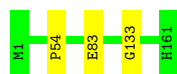
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain tE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain tX:  98%



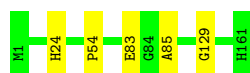
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain uA:  98%



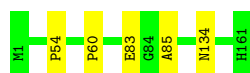
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain uB:  97%



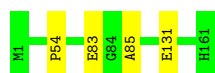
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain uC:  97%



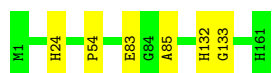
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain uD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain uE:  96%



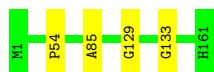
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain uX:  98%



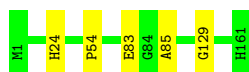
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain vA:  98%



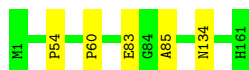
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain vB:  97%



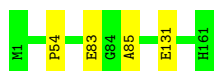
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain vC:  97%



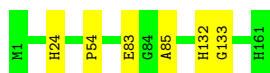
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain vD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain vE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain vX:  98%



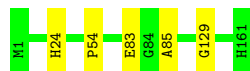
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain wA:  98%



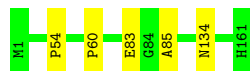
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain wB:  97%



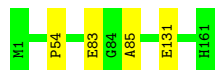
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain wC:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain wD:  98%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain wE:  96%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain wX:  98%



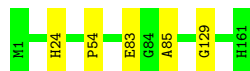
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain xA:  98%



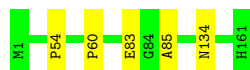
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain xB:  97%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain xC:  97% .



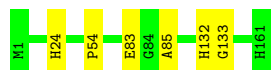
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain xD:  98% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain xE:  96% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain xX:  98% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	0A	0.35	0/800	0.56	0/1112
1	0B	0.34	0/800	0.54	0/1112
1	0C	0.39	0/800	0.61	0/1112
1	0D	0.33	0/800	0.55	0/1112
1	0E	0.33	0/800	0.54	0/1112
1	0X	0.34	0/800	0.56	0/1112
1	1A	0.35	0/800	0.56	0/1112
1	1B	0.34	0/800	0.54	0/1112
1	1C	0.39	0/800	0.61	0/1112
1	1D	0.33	0/800	0.55	0/1112
1	1E	0.33	0/800	0.54	0/1112
1	1X	0.34	0/800	0.56	0/1112
1	2A	0.34	0/800	0.56	0/1112
1	2B	0.34	0/800	0.54	0/1112
1	2C	0.39	0/800	0.61	0/1112
1	2D	0.33	0/800	0.55	0/1112
1	2E	0.33	0/800	0.54	0/1112
1	2X	0.34	0/800	0.56	0/1112
1	3A	0.35	0/800	0.56	0/1112
1	3B	0.34	0/800	0.54	0/1112
1	3C	0.39	0/800	0.61	0/1112
1	3D	0.33	0/800	0.55	0/1112
1	3E	0.33	0/800	0.54	0/1112
1	3X	0.34	0/800	0.56	0/1112
1	4A	0.35	0/800	0.56	0/1112
1	4B	0.34	0/800	0.54	0/1112
1	4C	0.39	0/800	0.61	0/1112
1	4D	0.33	0/800	0.55	0/1112
1	4E	0.33	0/800	0.54	0/1112
1	4X	0.34	0/800	0.56	0/1112
1	5A	0.35	0/800	0.56	0/1112
1	5B	0.34	0/800	0.54	0/1112
1	5C	0.39	0/800	0.61	0/1112
1	5D	0.33	0/800	0.55	0/1112

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	5E	0.33	0/800	0.54	0/1112
1	5X	0.34	0/800	0.56	0/1112
1	6A	0.34	0/800	0.56	0/1112
1	6B	0.34	0/800	0.54	0/1112
1	6C	0.39	0/800	0.61	0/1112
1	6D	0.33	0/800	0.55	0/1112
1	6E	0.33	0/800	0.54	0/1112
1	6X	0.34	0/800	0.56	0/1112
1	7A	0.35	0/800	0.56	0/1112
1	7B	0.34	0/800	0.54	0/1112
1	7C	0.39	0/800	0.61	0/1112
1	7D	0.33	0/800	0.55	0/1112
1	7E	0.33	0/800	0.54	0/1112
1	7X	0.34	0/800	0.56	0/1112
1	8A	0.35	0/800	0.56	0/1112
1	8B	0.34	0/800	0.54	0/1112
1	8C	0.39	0/800	0.61	0/1112
1	8D	0.33	0/800	0.55	0/1112
1	8E	0.33	0/800	0.54	0/1112
1	8X	0.34	0/800	0.56	0/1112
1	9A	0.35	0/800	0.56	0/1112
1	9B	0.34	0/800	0.53	0/1112
1	9C	0.39	0/800	0.61	0/1112
1	9D	0.33	0/800	0.55	0/1112
1	9E	0.33	0/800	0.54	0/1112
1	9X	0.34	0/800	0.56	0/1112
1	AA	0.34	0/800	0.56	0/1112
1	AB	0.34	0/800	0.54	0/1112
1	AC	0.39	0/800	0.61	0/1112
1	AD	0.33	0/800	0.55	0/1112
1	AE	0.33	0/800	0.54	0/1112
1	AX	0.34	0/800	0.56	0/1112
1	BA	0.34	0/800	0.56	0/1112
1	BB	0.34	0/800	0.54	0/1112
1	BC	0.39	0/800	0.61	0/1112
1	BD	0.33	0/800	0.55	0/1112
1	BE	0.33	0/800	0.54	0/1112
1	BX	0.34	0/800	0.56	0/1112
1	CA	0.35	0/800	0.56	0/1112
1	CB	0.34	0/800	0.53	0/1112
1	CC	0.39	0/800	0.61	0/1112
1	CD	0.33	0/800	0.55	0/1112
1	CE	0.33	0/800	0.54	0/1112

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	CX	0.34	0/800	0.56	0/1112
1	DA	0.35	0/800	0.56	0/1112
1	DB	0.34	0/800	0.54	0/1112
1	DC	0.39	0/800	0.61	0/1112
1	DD	0.33	0/800	0.55	0/1112
1	DE	0.33	0/800	0.54	0/1112
1	DX	0.34	0/800	0.56	0/1112
1	EA	0.35	0/800	0.56	0/1112
1	EB	0.34	0/800	0.54	0/1112
1	EC	0.39	0/800	0.61	0/1112
1	ED	0.33	0/800	0.55	0/1112
1	EE	0.33	0/800	0.54	0/1112
1	EX	0.34	0/800	0.56	0/1112
1	FA	0.35	0/800	0.56	0/1112
1	FB	0.34	0/800	0.54	0/1112
1	FC	0.39	0/800	0.61	0/1112
1	FD	0.33	0/800	0.55	0/1112
1	FE	0.33	0/800	0.54	0/1112
1	FX	0.34	0/800	0.56	0/1112
1	GA	0.35	0/800	0.56	0/1112
1	GB	0.34	0/800	0.54	0/1112
1	GC	0.39	0/800	0.61	0/1112
1	GD	0.33	0/800	0.55	0/1112
1	GE	0.33	0/800	0.54	0/1112
1	GX	0.34	0/800	0.56	0/1112
1	HA	0.35	0/800	0.56	0/1112
1	HB	0.34	0/800	0.53	0/1112
1	HC	0.39	0/800	0.61	0/1112
1	HD	0.33	0/800	0.55	0/1112
1	HE	0.33	0/800	0.54	0/1112
1	HX	0.34	0/800	0.56	0/1112
1	IA	0.35	0/800	0.56	0/1112
1	IB	0.34	0/800	0.54	0/1112
1	IC	0.39	0/800	0.61	0/1112
1	ID	0.33	0/800	0.55	0/1112
1	IE	0.33	0/800	0.54	0/1112
1	IX	0.34	0/800	0.56	0/1112
1	JA	0.35	0/800	0.56	0/1112
1	JB	0.34	0/800	0.53	0/1112
1	JC	0.39	0/800	0.61	0/1112
1	JD	0.33	0/800	0.55	0/1112
1	JE	0.33	0/800	0.54	0/1112
1	JX	0.34	0/800	0.56	0/1112

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	KA	0.35	0/800	0.56	0/1112
1	KB	0.34	0/800	0.54	0/1112
1	KC	0.39	0/800	0.61	0/1112
1	KD	0.33	0/800	0.55	0/1112
1	KE	0.33	0/800	0.54	0/1112
1	KX	0.34	0/800	0.56	0/1112
1	LA	0.35	0/800	0.56	0/1112
1	LB	0.34	0/800	0.54	0/1112
1	LC	0.39	0/800	0.61	0/1112
1	LD	0.33	0/800	0.55	0/1112
1	LE	0.33	0/800	0.54	0/1112
1	LX	0.34	0/800	0.56	0/1112
1	MA	0.35	0/800	0.56	0/1112
1	MB	0.34	0/800	0.54	0/1112
1	MC	0.39	0/800	0.61	0/1112
1	MD	0.33	0/800	0.55	0/1112
1	ME	0.33	0/800	0.54	0/1112
1	MX	0.34	0/800	0.56	0/1112
1	NA	0.35	0/800	0.56	0/1112
1	NB	0.34	0/800	0.54	0/1112
1	NC	0.39	0/800	0.61	0/1112
1	ND	0.33	0/800	0.55	0/1112
1	NE	0.33	0/800	0.54	0/1112
1	NX	0.34	0/800	0.56	0/1112
1	OA	0.35	0/800	0.56	0/1112
1	OB	0.34	0/800	0.54	0/1112
1	OC	0.39	0/800	0.61	0/1112
1	OD	0.33	0/800	0.55	0/1112
1	OE	0.33	0/800	0.54	0/1112
1	OX	0.34	0/800	0.56	0/1112
1	PA	0.34	0/800	0.56	0/1112
1	PB	0.34	0/800	0.54	0/1112
1	PC	0.39	0/800	0.61	0/1112
1	PD	0.33	0/800	0.55	0/1112
1	PE	0.33	0/800	0.54	0/1112
1	PX	0.34	0/800	0.56	0/1112
1	QA	0.35	0/800	0.56	0/1112
1	QB	0.34	0/800	0.53	0/1112
1	QC	0.39	0/800	0.61	0/1112
1	QD	0.33	0/800	0.55	0/1112
1	QE	0.33	0/800	0.54	0/1112
1	QX	0.34	0/800	0.56	0/1112
1	RA	0.35	0/800	0.56	0/1112

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	RB	0.34	0/800	0.54	0/1112
1	RC	0.39	0/800	0.61	0/1112
1	RD	0.33	0/800	0.55	0/1112
1	RE	0.33	0/800	0.54	0/1112
1	RX	0.34	0/800	0.56	0/1112
1	SA	0.35	0/800	0.56	0/1112
1	SB	0.34	0/800	0.54	0/1112
1	SC	0.39	0/800	0.61	0/1112
1	SD	0.33	0/800	0.55	0/1112
1	SE	0.33	0/800	0.54	0/1112
1	SX	0.34	0/800	0.56	0/1112
1	TA	0.34	0/800	0.56	0/1112
1	TB	0.34	0/800	0.54	0/1112
1	TC	0.39	0/800	0.61	0/1112
1	TD	0.33	0/800	0.55	0/1112
1	TE	0.33	0/800	0.54	0/1112
1	TX	0.34	0/800	0.56	0/1112
1	UA	0.35	0/800	0.56	0/1112
1	UB	0.34	0/800	0.54	0/1112
1	UC	0.39	0/800	0.61	0/1112
1	UD	0.33	0/800	0.55	0/1112
1	UE	0.33	0/800	0.54	0/1112
1	UX	0.34	0/800	0.56	0/1112
1	VA	0.35	0/800	0.56	0/1112
1	VB	0.34	0/800	0.54	0/1112
1	VC	0.39	0/800	0.61	0/1112
1	VD	0.33	0/800	0.55	0/1112
1	VE	0.33	0/800	0.54	0/1112
1	VX	0.34	0/800	0.56	0/1112
1	WA	0.34	0/800	0.56	0/1112
1	WB	0.34	0/800	0.54	0/1112
1	WC	0.39	0/800	0.61	0/1112
1	WD	0.33	0/800	0.55	0/1112
1	WE	0.33	0/800	0.54	0/1112
1	WX	0.34	0/800	0.56	0/1112
1	XA	0.35	0/800	0.56	0/1112
1	XB	0.34	0/800	0.53	0/1112
1	XC	0.39	0/800	0.61	0/1112
1	XD	0.33	0/800	0.55	0/1112
1	XE	0.33	0/800	0.54	0/1112
1	XX	0.34	0/800	0.56	0/1112
1	YA	0.35	0/800	0.56	0/1112
1	YB	0.34	0/800	0.53	0/1112

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	YC	0.39	0/800	0.61	0/1112
1	YD	0.33	0/800	0.55	0/1112
1	YE	0.33	0/800	0.54	0/1112
1	YX	0.34	0/800	0.56	0/1112
1	ZA	0.35	0/800	0.56	0/1112
1	ZB	0.34	0/800	0.54	0/1112
1	ZC	0.39	0/800	0.61	0/1112
1	ZD	0.33	0/800	0.55	0/1112
1	ZE	0.33	0/800	0.54	0/1112
1	ZX	0.34	0/800	0.56	0/1112
1	aA	0.35	0/800	0.56	0/1112
1	aB	0.34	0/800	0.54	0/1112
1	aC	0.39	0/800	0.61	0/1112
1	aD	0.33	0/800	0.55	0/1112
1	aE	0.33	0/800	0.54	0/1112
1	aX	0.34	0/800	0.56	0/1112
1	bA	0.35	0/800	0.56	0/1112
1	bB	0.34	0/800	0.54	0/1112
1	bC	0.39	0/800	0.61	0/1112
1	bD	0.33	0/800	0.55	0/1112
1	bE	0.33	0/800	0.54	0/1112
1	bX	0.34	0/800	0.56	0/1112
1	cA	0.35	0/800	0.56	0/1112
1	cB	0.34	0/800	0.53	0/1112
1	cC	0.39	0/800	0.61	0/1112
1	cD	0.33	0/800	0.55	0/1112
1	cE	0.33	0/800	0.54	0/1112
1	cX	0.34	0/800	0.56	0/1112
1	dA	0.35	0/800	0.56	0/1112
1	dB	0.34	0/800	0.54	0/1112
1	dC	0.39	0/800	0.61	0/1112
1	dD	0.33	0/800	0.55	0/1112
1	dE	0.33	0/800	0.54	0/1112
1	dX	0.34	0/800	0.56	0/1112
1	eA	0.34	0/800	0.56	0/1112
1	eB	0.34	0/800	0.54	0/1112
1	eC	0.39	0/800	0.61	0/1112
1	eD	0.33	0/800	0.55	0/1112
1	eE	0.33	0/800	0.54	0/1112
1	eX	0.34	0/800	0.56	0/1112
1	fA	0.34	0/800	0.56	0/1112
1	fB	0.34	0/800	0.54	0/1112
1	fC	0.39	0/800	0.61	0/1112

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	fD	0.33	0/800	0.55	0/1112
1	fE	0.33	0/800	0.54	0/1112
1	fX	0.34	0/800	0.56	0/1112
1	gA	0.35	0/800	0.56	0/1112
1	gB	0.34	0/800	0.53	0/1112
1	gC	0.39	0/800	0.61	0/1112
1	gD	0.33	0/800	0.55	0/1112
1	gE	0.33	0/800	0.54	0/1112
1	gX	0.34	0/800	0.56	0/1112
1	hA	0.35	0/800	0.56	0/1112
1	hB	0.34	0/800	0.54	0/1112
1	hC	0.39	0/800	0.61	0/1112
1	hD	0.33	0/800	0.55	0/1112
1	hE	0.33	0/800	0.54	0/1112
1	hX	0.34	0/800	0.56	0/1112
1	iA	0.35	0/800	0.56	0/1112
1	iB	0.34	0/800	0.54	0/1112
1	iC	0.39	0/800	0.61	0/1112
1	iD	0.33	0/800	0.55	0/1112
1	iE	0.33	0/800	0.54	0/1112
1	iX	0.34	0/800	0.56	0/1112
1	jA	0.34	0/800	0.56	0/1112
1	jB	0.34	0/800	0.54	0/1112
1	jC	0.39	0/800	0.61	0/1112
1	jD	0.33	0/800	0.55	0/1112
1	jE	0.33	0/800	0.54	0/1112
1	jX	0.34	0/800	0.56	0/1112
1	kA	0.35	0/800	0.56	0/1112
1	kB	0.34	0/800	0.54	0/1112
1	kC	0.39	0/800	0.61	0/1112
1	kD	0.33	0/800	0.55	0/1112
1	kE	0.33	0/800	0.54	0/1112
1	kX	0.34	0/800	0.56	0/1112
1	lA	0.35	0/800	0.56	0/1112
1	lB	0.34	0/800	0.54	0/1112
1	lC	0.39	0/800	0.61	0/1112
1	lD	0.33	0/800	0.55	0/1112
1	lE	0.33	0/800	0.54	0/1112
1	lX	0.34	0/800	0.56	0/1112
1	mA	0.35	0/800	0.56	0/1112
1	mB	0.34	0/800	0.54	0/1112
1	mC	0.39	0/800	0.61	0/1112
1	mD	0.33	0/800	0.55	0/1112

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	mE	0.33	0/800	0.54	0/1112
1	mX	0.34	0/800	0.56	0/1112
1	nA	0.35	0/800	0.56	0/1112
1	nB	0.34	0/800	0.54	0/1112
1	nC	0.39	0/800	0.61	0/1112
1	nD	0.33	0/800	0.55	0/1112
1	nE	0.33	0/800	0.54	0/1112
1	nX	0.34	0/800	0.56	0/1112
1	oA	0.35	0/800	0.56	0/1112
1	oB	0.34	0/800	0.53	0/1112
1	oC	0.39	0/800	0.61	0/1112
1	oD	0.33	0/800	0.55	0/1112
1	oE	0.33	0/800	0.54	0/1112
1	oX	0.34	0/800	0.56	0/1112
1	pA	0.35	0/800	0.56	0/1112
1	pB	0.34	0/800	0.54	0/1112
1	pC	0.39	0/800	0.61	0/1112
1	pD	0.33	0/800	0.55	0/1112
1	pE	0.33	0/800	0.54	0/1112
1	pX	0.34	0/800	0.56	0/1112
1	qA	0.35	0/800	0.56	0/1112
1	qB	0.34	0/800	0.54	0/1112
1	qC	0.39	0/800	0.61	0/1112
1	qD	0.33	0/800	0.55	0/1112
1	qE	0.33	0/800	0.54	0/1112
1	qX	0.34	0/800	0.56	0/1112
1	rA	0.34	0/800	0.56	0/1112
1	rB	0.34	0/800	0.54	0/1112
1	rC	0.39	0/800	0.61	0/1112
1	rD	0.33	0/800	0.55	0/1112
1	rE	0.33	0/800	0.54	0/1112
1	rX	0.34	0/800	0.56	0/1112
1	sA	0.35	0/800	0.56	0/1112
1	sB	0.34	0/800	0.53	0/1112
1	sC	0.39	0/800	0.61	0/1112
1	sD	0.33	0/800	0.55	0/1112
1	sE	0.33	0/800	0.54	0/1112
1	sX	0.34	0/800	0.56	0/1112
1	tA	0.35	0/800	0.56	0/1112
1	tB	0.34	0/800	0.54	0/1112
1	tC	0.39	0/800	0.61	0/1112
1	tD	0.33	0/800	0.55	0/1112
1	tE	0.33	0/800	0.54	0/1112

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	tX	0.34	0/800	0.56	0/1112
1	uA	0.35	0/800	0.56	0/1112
1	uB	0.34	0/800	0.54	0/1112
1	uC	0.39	0/800	0.61	0/1112
1	uD	0.33	0/800	0.55	0/1112
1	uE	0.33	0/800	0.54	0/1112
1	uX	0.34	0/800	0.56	0/1112
1	vA	0.35	0/800	0.56	0/1112
1	vB	0.34	0/800	0.53	0/1112
1	vC	0.39	0/800	0.61	0/1112
1	vD	0.33	0/800	0.55	0/1112
1	vE	0.33	0/800	0.54	0/1112
1	vX	0.34	0/800	0.56	0/1112
1	wA	0.35	0/800	0.56	0/1112
1	wB	0.34	0/800	0.54	0/1112
1	wC	0.39	0/800	0.61	0/1112
1	wD	0.33	0/800	0.55	0/1112
1	wE	0.33	0/800	0.54	0/1112
1	wX	0.34	0/800	0.56	0/1112
1	xA	0.34	0/800	0.56	0/1112
1	xB	0.34	0/800	0.54	0/1112
1	xC	0.39	0/800	0.61	0/1112
1	xD	0.33	0/800	0.55	0/1112
1	xE	0.33	0/800	0.54	0/1112
1	XX	0.34	0/800	0.56	0/1112
All	All	0.35	0/288000	0.56	0/400320

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0A	797	0	414	6	0
1	0B	797	0	414	10	0
1	0C	797	0	414	14	0
1	0D	797	0	414	8	0
1	0E	797	0	414	10	0
1	0X	797	0	414	11	0
1	1A	797	0	414	6	0
1	1B	797	0	414	10	0
1	1C	797	0	414	12	0
1	1D	797	0	414	9	0
1	1E	797	0	414	9	0
1	1X	797	0	414	11	0
1	2A	797	0	414	7	0
1	2B	797	0	414	11	0
1	2C	797	0	414	12	0
1	2D	797	0	414	8	0
1	2E	797	0	414	11	0
1	2X	797	0	414	12	0
1	3A	797	0	414	7	0
1	3B	797	0	414	10	0
1	3C	797	0	414	13	0
1	3D	797	0	414	8	0
1	3E	797	0	414	11	0
1	3X	797	0	414	11	0
1	4A	797	0	414	9	0
1	4B	797	0	414	11	0
1	4C	797	0	414	12	0
1	4D	797	0	414	8	0
1	4E	797	0	414	11	0
1	4X	797	0	414	11	0
1	5A	797	0	414	8	0
1	5B	797	0	414	11	0
1	5C	797	0	414	13	0
1	5D	797	0	414	8	0
1	5E	797	0	414	10	0
1	5X	797	0	414	11	0
1	6A	797	0	414	8	0
1	6B	797	0	414	11	0
1	6C	797	0	414	14	0
1	6D	797	0	414	8	0
1	6E	797	0	414	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6X	797	0	414	11	0
1	7A	797	0	414	8	0
1	7B	797	0	414	10	0
1	7C	797	0	414	14	0
1	7D	797	0	414	8	0
1	7E	797	0	414	10	0
1	7X	797	0	414	11	0
1	8A	797	0	414	6	0
1	8B	797	0	414	10	0
1	8C	797	0	414	14	0
1	8D	797	0	414	8	0
1	8E	797	0	414	10	0
1	8X	797	0	414	11	0
1	9A	797	0	414	7	0
1	9B	797	0	414	11	0
1	9C	797	0	414	12	0
1	9D	797	0	414	8	0
1	9E	797	0	414	11	0
1	9X	797	0	414	11	0
1	AA	797	0	414	8	0
1	AB	797	0	414	12	0
1	AC	797	0	414	13	0
1	AD	797	0	414	8	0
1	AE	797	0	414	12	0
1	AX	797	0	414	11	0
1	BA	797	0	414	8	0
1	BB	797	0	414	12	0
1	BC	797	0	414	13	0
1	BD	797	0	414	8	0
1	BE	797	0	414	12	0
1	BX	797	0	414	11	0
1	CA	797	0	414	9	0
1	CB	797	0	414	12	0
1	CC	797	0	414	14	0
1	CD	797	0	414	8	0
1	CE	797	0	414	10	0
1	CX	797	0	414	12	0
1	DA	797	0	414	8	0
1	DB	797	0	414	11	0
1	DC	797	0	414	14	0
1	DD	797	0	414	8	0
1	DE	797	0	414	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DX	797	0	414	11	0
1	EA	797	0	414	9	0
1	EB	797	0	414	11	0
1	EC	797	0	414	14	0
1	ED	797	0	414	8	0
1	EE	797	0	414	10	0
1	EX	797	0	414	11	0
1	FA	797	0	414	8	0
1	FB	797	0	414	11	0
1	FC	797	0	414	15	0
1	FD	797	0	414	8	0
1	FE	797	0	414	10	0
1	FX	797	0	414	11	0
1	GA	797	0	414	8	0
1	GB	797	0	414	12	0
1	GC	797	0	414	14	0
1	GD	797	0	414	8	0
1	GE	797	0	414	11	0
1	GX	797	0	414	11	0
1	HA	797	0	414	9	0
1	HB	797	0	414	11	0
1	HC	797	0	414	15	0
1	HD	797	0	414	8	0
1	HE	797	0	414	12	0
1	HX	797	0	414	12	0
1	IA	797	0	414	7	0
1	IB	797	0	414	11	0
1	IC	797	0	414	14	0
1	ID	797	0	414	9	0
1	IE	797	0	414	10	0
1	IX	797	0	414	12	0
1	JA	797	0	414	7	0
1	JB	797	0	414	12	0
1	JC	797	0	414	13	0
1	JD	797	0	414	8	0
1	JE	797	0	414	11	0
1	JX	797	0	414	12	0
1	KA	797	0	414	9	0
1	KB	797	0	414	11	0
1	KC	797	0	414	14	0
1	KD	797	0	414	8	0
1	KE	797	0	414	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	KX	797	0	414	11	0
1	LA	797	0	414	8	0
1	LB	797	0	414	11	0
1	LC	797	0	414	15	0
1	LD	797	0	414	8	0
1	LE	797	0	414	10	0
1	LX	797	0	414	11	0
1	MA	797	0	414	8	0
1	MB	797	0	414	11	0
1	MC	797	0	414	14	0
1	MD	797	0	414	8	0
1	ME	797	0	414	11	0
1	MX	797	0	414	11	0
1	NA	797	0	414	7	0
1	NB	797	0	414	10	0
1	NC	797	0	414	14	0
1	ND	797	0	414	8	0
1	NE	797	0	414	10	0
1	NX	797	0	414	11	0
1	OA	797	0	414	7	0
1	OB	797	0	414	12	0
1	OC	797	0	414	13	0
1	OD	797	0	414	8	0
1	OE	797	0	414	12	0
1	OX	797	0	414	12	0
1	PA	797	0	414	9	0
1	PB	797	0	414	11	0
1	PC	797	0	414	15	0
1	PD	797	0	414	8	0
1	PE	797	0	414	12	0
1	PX	797	0	414	11	0
1	QA	797	0	414	7	0
1	QB	797	0	414	12	0
1	QC	797	0	414	12	0
1	QD	797	0	414	8	0
1	QE	797	0	414	11	0
1	QX	797	0	414	11	0
1	RA	797	0	414	7	0
1	RB	797	0	414	12	0
1	RC	797	0	414	14	0
1	RD	797	0	414	8	0
1	RE	797	0	414	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RX	797	0	414	12	0
1	SA	797	0	414	7	0
1	SB	797	0	414	12	0
1	SC	797	0	414	14	0
1	SD	797	0	414	8	0
1	SE	797	0	414	11	0
1	SX	797	0	414	11	0
1	TA	797	0	414	7	0
1	TB	797	0	414	11	0
1	TC	797	0	414	15	0
1	TD	797	0	414	8	0
1	TE	797	0	414	11	0
1	TX	797	0	414	11	0
1	UA	797	0	414	8	0
1	UB	797	0	414	10	0
1	UC	797	0	414	15	0
1	UD	797	0	414	9	0
1	UE	797	0	414	11	0
1	UX	797	0	414	12	0
1	VA	797	0	414	7	0
1	VB	797	0	414	10	0
1	VC	797	0	414	13	0
1	VD	797	0	414	8	0
1	VE	797	0	414	11	0
1	VX	797	0	414	11	0
1	WA	797	0	414	8	0
1	WB	797	0	414	11	0
1	WC	797	0	414	14	0
1	WD	797	0	414	9	0
1	WE	797	0	414	11	0
1	WX	797	0	414	12	0
1	XA	797	0	414	7	0
1	XB	797	0	414	12	0
1	XC	797	0	414	13	0
1	XD	797	0	414	8	0
1	XE	797	0	414	11	0
1	XX	797	0	414	11	0
1	YA	797	0	414	7	0
1	YB	797	0	414	11	0
1	YC	797	0	414	11	0
1	YD	797	0	414	8	0
1	YE	797	0	414	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	YX	797	0	414	11	0
1	ZA	797	0	414	10	0
1	ZB	797	0	414	11	0
1	ZC	797	0	414	12	0
1	ZD	797	0	414	8	0
1	ZE	797	0	414	11	0
1	ZX	797	0	414	11	0
1	aA	797	0	414	0	0
1	aB	797	0	414	0	0
1	aC	797	0	414	0	0
1	aD	797	0	414	0	0
1	aE	797	0	414	0	0
1	aX	797	0	414	0	0
1	bA	797	0	414	0	0
1	bB	797	0	414	0	0
1	bC	797	0	414	0	0
1	bD	797	0	414	0	0
1	bE	797	0	414	0	0
1	bX	797	0	414	0	0
1	cA	797	0	414	0	0
1	cB	797	0	414	0	0
1	cC	797	0	414	0	0
1	cD	797	0	414	0	0
1	cE	797	0	414	0	0
1	cX	797	0	414	0	0
1	dA	797	0	414	0	0
1	dB	797	0	414	0	0
1	dC	797	0	414	0	0
1	dD	797	0	414	0	0
1	dE	797	0	414	0	0
1	dX	797	0	414	0	0
1	eA	797	0	414	0	0
1	eB	797	0	414	0	0
1	eC	797	0	414	0	0
1	eD	797	0	414	0	0
1	eE	797	0	414	0	0
1	eX	797	0	414	0	0
1	fA	797	0	414	0	0
1	fB	797	0	414	0	0
1	fC	797	0	414	0	0
1	fD	797	0	414	0	0
1	fE	797	0	414	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	fX	797	0	414	0	0
1	gA	797	0	414	0	0
1	gB	797	0	414	0	0
1	gC	797	0	414	0	0
1	gD	797	0	414	0	0
1	gE	797	0	414	0	0
1	gX	797	0	414	0	0
1	hA	797	0	414	0	0
1	hB	797	0	414	0	0
1	hC	797	0	414	0	0
1	hD	797	0	414	0	0
1	hE	797	0	414	0	0
1	hX	797	0	414	0	0
1	iA	797	0	414	0	0
1	iB	797	0	414	0	0
1	iC	797	0	414	0	0
1	iD	797	0	414	0	0
1	iE	797	0	414	0	0
1	iX	797	0	414	0	0
1	jA	797	0	414	0	0
1	jB	797	0	414	0	0
1	jC	797	0	414	0	0
1	jD	797	0	414	0	0
1	jE	797	0	414	0	0
1	jX	797	0	414	0	0
1	kA	797	0	414	0	0
1	kB	797	0	414	0	0
1	kC	797	0	414	0	0
1	kD	797	0	414	0	0
1	kE	797	0	414	0	0
1	kX	797	0	414	0	0
1	lA	797	0	414	0	0
1	lB	797	0	414	0	0
1	lC	797	0	414	0	0
1	lD	797	0	414	0	0
1	lE	797	0	414	0	0
1	lX	797	0	414	0	0
1	mA	797	0	414	0	0
1	mB	797	0	414	0	0
1	mC	797	0	414	0	0
1	mD	797	0	414	0	0
1	mE	797	0	414	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	mX	797	0	414	0	0
1	nA	797	0	414	0	0
1	nB	797	0	414	0	0
1	nC	797	0	414	0	0
1	nD	797	0	414	0	0
1	nE	797	0	414	0	0
1	nX	797	0	414	0	0
1	oA	797	0	414	0	0
1	oB	797	0	414	0	0
1	oC	797	0	414	0	0
1	oD	797	0	414	0	0
1	oE	797	0	414	0	0
1	oX	797	0	414	0	0
1	pA	797	0	414	0	0
1	pB	797	0	414	0	0
1	pC	797	0	414	0	0
1	pD	797	0	414	0	0
1	pE	797	0	414	0	0
1	pX	797	0	414	0	0
1	qA	797	0	414	0	0
1	qB	797	0	414	0	0
1	qC	797	0	414	0	0
1	qD	797	0	414	0	0
1	qE	797	0	414	0	0
1	qX	797	0	414	0	0
1	rA	797	0	414	0	0
1	rB	797	0	414	0	0
1	rC	797	0	414	0	0
1	rD	797	0	414	0	0
1	rE	797	0	414	0	0
1	rX	797	0	414	0	0
1	sA	797	0	414	0	0
1	sB	797	0	414	0	0
1	sC	797	0	414	0	0
1	sD	797	0	414	0	0
1	sE	797	0	414	0	0
1	sX	797	0	414	0	0
1	tA	797	0	414	0	0
1	tB	797	0	414	0	0
1	tC	797	0	414	0	0
1	tD	797	0	414	0	0
1	tE	797	0	414	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	tX	797	0	414	0	0
1	uA	797	0	414	0	0
1	uB	797	0	414	0	0
1	uC	797	0	414	0	0
1	uD	797	0	414	0	0
1	uE	797	0	414	0	0
1	uX	797	0	414	0	0
1	vA	797	0	414	0	0
1	vB	797	0	414	0	0
1	vC	797	0	414	0	0
1	vD	797	0	414	0	0
1	vE	797	0	414	0	0
1	vX	797	0	414	0	0
1	wA	797	0	414	0	0
1	wB	797	0	414	0	0
1	wC	797	0	414	0	0
1	wD	797	0	414	0	0
1	wE	797	0	414	0	0
1	wX	797	0	414	0	0
1	xA	797	0	414	0	0
1	xB	797	0	414	0	0
1	xC	797	0	414	0	0
1	xD	797	0	414	0	0
1	xE	797	0	414	0	0
1	XX	797	0	414	0	0
All	All	286920	0	149040	2246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 2246 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IE:19:ALA:HA	1:IE:78:ILE:O	1.91	0.71
1:4E:19:ALA:HA	1:4E:78:ILE:O	1.91	0.71
1:JE:19:ALA:HA	1:JE:78:ILE:O	1.91	0.71
1:OE:19:ALA:HA	1:OE:78:ILE:O	1.91	0.71
1:RE:19:ALA:HA	1:RE:78:ILE:O	1.91	0.71

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	0B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	0C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	0D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	0E	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	0X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	1A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	1B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	1C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	1D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	1E	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	1X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	2A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	2B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	2C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	2D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	2E	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	2X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	3A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	3B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	3C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	3D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	3E	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	3X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	4A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	4C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	4D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	4E	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	4X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	5A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	5B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	5C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	5D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	5E	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	5X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	6A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	6B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	6C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	6D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	6E	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	6X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	7A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	7B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	7C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	7D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	7E	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	7X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	8A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	8B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	8C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	8D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	8E	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	8X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	9A	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	9B	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9C	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	9D	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	9E	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	9X	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	AA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	AB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	AC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	AD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	AE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	AX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	BA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	BB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	BC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	BD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	BE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	BX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	CA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	CB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	CC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	CD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	CE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	CX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	DA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	DB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	DC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	DD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	DE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	DX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	EA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	EB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	EC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ED	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	EE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	EX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	FA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	FB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	FC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	FD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	FE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	FX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	GA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	GB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	GC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	GD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	GE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	GX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	HA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	HB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	HC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	HD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	HE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	HX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	IA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	IB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	IC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	ID	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	IE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	IX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	JA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	JB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	JC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	JD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	JX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	KA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	KB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	KC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	KD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	KE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	KX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	LA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	LB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	LC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	LD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	LE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	LX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	MA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	MB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	MC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	MD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	ME	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	MX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	NA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	NB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	NC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	ND	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	NE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	NX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	OA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	OB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	OC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	OD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	OE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	PA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	PB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	PC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	PD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	PE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	PX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	QA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	QB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	QC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	QD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	QE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	QX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	RA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	RB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	RC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	RD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	RE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	RX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	SA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	SB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	SC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	SD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	SE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	SX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	TA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	TB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	TC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	TD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	TE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	TX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	UB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	UC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	UD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	UE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	UX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	VA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	VB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	VC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	VD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	VE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	VX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	WA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	WB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	WC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	WD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	WE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	WX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	XA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	XB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	XC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	XD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	XE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	XX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	YA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	YB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	YC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	YD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	YE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	YX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	ZA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ZB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	ZC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	ZD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	ZE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	ZX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	aA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	aB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	aC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	aD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	aE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	aX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	bA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	bB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	bC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	bD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	bE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	bX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	cA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	cB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	cC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	cD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	cE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	cX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	dA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	dB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	dC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	dD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	dE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	dX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	eA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	eB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	eC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	eD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	eE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	eX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	fA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	fB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	fC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	fD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	fE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	fX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	gA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	gB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	gC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	gD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	gE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	gX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	hA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	hB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	hC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	hD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	hE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	hX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	iA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	iB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	iC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	iD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	iE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	iX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	jA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	jB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	jC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	jD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	jE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	jX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	kA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	kB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	kC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	kD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	kE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	kX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	lA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	lB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	lC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	lD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	lE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	lX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	mA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	mB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	mC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	mD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	mE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	mX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	nA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	nB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	nC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	nD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	nE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	nX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	oA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	oB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	oC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	oD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	oE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	oX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	pA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	pB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	pC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	pD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	pE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	pX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	qA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	qB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	qC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	qD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	qE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	qX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	rA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	rB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	rC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	rD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	rE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	rX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	sA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	sB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	sC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	sD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	sE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	sX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	tA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	tB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	tC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	tD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	tE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	tX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	uA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	uB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	uC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	uD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	uE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	uX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	vA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	vB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	vC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	vD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	vE	159/161 (99%)	143 (90%)	10 (6%)	6 (4%)	3	30
1	vX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	wA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	wB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	wC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	wD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	wE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	wX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
1	xA	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	xB	159/161 (99%)	145 (91%)	9 (6%)	5 (3%)	4	34
1	xC	159/161 (99%)	142 (89%)	12 (8%)	5 (3%)	4	34
1	xD	159/161 (99%)	144 (91%)	11 (7%)	4 (2%)	6	38
1	xE	159/161 (99%)	142 (89%)	11 (7%)	6 (4%)	3	30
1	XX	159/161 (99%)	142 (89%)	14 (9%)	3 (2%)	9	44
All	All	57240/57960 (99%)	51576 (90%)	4044 (7%)	1620 (3%)	9	37

5 of 1620 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0B	54	PRO
1	0B	83	GLU
1	0C	54	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0C	83	GLU
1	0E	54	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0A	4/127 (3%)	4 (100%)	0	100	100
1	0B	4/127 (3%)	4 (100%)	0	100	100
1	0C	4/127 (3%)	4 (100%)	0	100	100
1	0D	4/127 (3%)	4 (100%)	0	100	100
1	0E	4/127 (3%)	4 (100%)	0	100	100
1	0X	4/127 (3%)	4 (100%)	0	100	100
1	1A	4/127 (3%)	4 (100%)	0	100	100
1	1B	4/127 (3%)	4 (100%)	0	100	100
1	1C	4/127 (3%)	4 (100%)	0	100	100
1	1D	4/127 (3%)	4 (100%)	0	100	100
1	1E	4/127 (3%)	4 (100%)	0	100	100
1	1X	4/127 (3%)	4 (100%)	0	100	100
1	2A	4/127 (3%)	4 (100%)	0	100	100
1	2B	4/127 (3%)	4 (100%)	0	100	100
1	2C	4/127 (3%)	4 (100%)	0	100	100
1	2D	4/127 (3%)	4 (100%)	0	100	100
1	2E	4/127 (3%)	4 (100%)	0	100	100
1	2X	4/127 (3%)	4 (100%)	0	100	100
1	3A	4/127 (3%)	4 (100%)	0	100	100
1	3B	4/127 (3%)	4 (100%)	0	100	100
1	3C	4/127 (3%)	4 (100%)	0	100	100
1	3D	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3E	4/127 (3%)	4 (100%)	0	100	100
1	3X	4/127 (3%)	4 (100%)	0	100	100
1	4A	4/127 (3%)	4 (100%)	0	100	100
1	4B	4/127 (3%)	4 (100%)	0	100	100
1	4C	4/127 (3%)	4 (100%)	0	100	100
1	4D	4/127 (3%)	4 (100%)	0	100	100
1	4E	4/127 (3%)	4 (100%)	0	100	100
1	4X	4/127 (3%)	4 (100%)	0	100	100
1	5A	4/127 (3%)	4 (100%)	0	100	100
1	5B	4/127 (3%)	4 (100%)	0	100	100
1	5C	4/127 (3%)	4 (100%)	0	100	100
1	5D	4/127 (3%)	4 (100%)	0	100	100
1	5E	4/127 (3%)	4 (100%)	0	100	100
1	5X	4/127 (3%)	4 (100%)	0	100	100
1	6A	4/127 (3%)	4 (100%)	0	100	100
1	6B	4/127 (3%)	4 (100%)	0	100	100
1	6C	4/127 (3%)	4 (100%)	0	100	100
1	6D	4/127 (3%)	4 (100%)	0	100	100
1	6E	4/127 (3%)	4 (100%)	0	100	100
1	6X	4/127 (3%)	4 (100%)	0	100	100
1	7A	4/127 (3%)	4 (100%)	0	100	100
1	7B	4/127 (3%)	4 (100%)	0	100	100
1	7C	4/127 (3%)	4 (100%)	0	100	100
1	7D	4/127 (3%)	4 (100%)	0	100	100
1	7E	4/127 (3%)	4 (100%)	0	100	100
1	7X	4/127 (3%)	4 (100%)	0	100	100
1	8A	4/127 (3%)	4 (100%)	0	100	100
1	8B	4/127 (3%)	4 (100%)	0	100	100
1	8C	4/127 (3%)	4 (100%)	0	100	100
1	8D	4/127 (3%)	4 (100%)	0	100	100
1	8E	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8X	4/127 (3%)	4 (100%)	0	100	100
1	9A	4/127 (3%)	4 (100%)	0	100	100
1	9B	4/127 (3%)	4 (100%)	0	100	100
1	9C	4/127 (3%)	4 (100%)	0	100	100
1	9D	4/127 (3%)	4 (100%)	0	100	100
1	9E	4/127 (3%)	4 (100%)	0	100	100
1	9X	4/127 (3%)	4 (100%)	0	100	100
1	AA	4/127 (3%)	4 (100%)	0	100	100
1	AB	4/127 (3%)	4 (100%)	0	100	100
1	AC	4/127 (3%)	4 (100%)	0	100	100
1	AD	4/127 (3%)	4 (100%)	0	100	100
1	AE	4/127 (3%)	4 (100%)	0	100	100
1	AX	4/127 (3%)	4 (100%)	0	100	100
1	BA	4/127 (3%)	4 (100%)	0	100	100
1	BB	4/127 (3%)	4 (100%)	0	100	100
1	BC	4/127 (3%)	4 (100%)	0	100	100
1	BD	4/127 (3%)	4 (100%)	0	100	100
1	BE	4/127 (3%)	4 (100%)	0	100	100
1	BX	4/127 (3%)	4 (100%)	0	100	100
1	CA	4/127 (3%)	4 (100%)	0	100	100
1	CB	4/127 (3%)	4 (100%)	0	100	100
1	CC	4/127 (3%)	4 (100%)	0	100	100
1	CD	4/127 (3%)	4 (100%)	0	100	100
1	CE	4/127 (3%)	4 (100%)	0	100	100
1	CX	4/127 (3%)	4 (100%)	0	100	100
1	DA	4/127 (3%)	4 (100%)	0	100	100
1	DB	4/127 (3%)	4 (100%)	0	100	100
1	DC	4/127 (3%)	4 (100%)	0	100	100
1	DD	4/127 (3%)	4 (100%)	0	100	100
1	DE	4/127 (3%)	4 (100%)	0	100	100
1	DX	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EA	4/127 (3%)	4 (100%)	0	100	100
1	EB	4/127 (3%)	4 (100%)	0	100	100
1	EC	4/127 (3%)	4 (100%)	0	100	100
1	ED	4/127 (3%)	4 (100%)	0	100	100
1	EE	4/127 (3%)	4 (100%)	0	100	100
1	EX	4/127 (3%)	4 (100%)	0	100	100
1	FA	4/127 (3%)	4 (100%)	0	100	100
1	FB	4/127 (3%)	4 (100%)	0	100	100
1	FC	4/127 (3%)	4 (100%)	0	100	100
1	FD	4/127 (3%)	4 (100%)	0	100	100
1	FE	4/127 (3%)	4 (100%)	0	100	100
1	FX	4/127 (3%)	4 (100%)	0	100	100
1	GA	4/127 (3%)	4 (100%)	0	100	100
1	GB	4/127 (3%)	4 (100%)	0	100	100
1	GC	4/127 (3%)	4 (100%)	0	100	100
1	GD	4/127 (3%)	4 (100%)	0	100	100
1	GE	4/127 (3%)	4 (100%)	0	100	100
1	GX	4/127 (3%)	4 (100%)	0	100	100
1	HA	4/127 (3%)	4 (100%)	0	100	100
1	HB	4/127 (3%)	4 (100%)	0	100	100
1	HC	4/127 (3%)	4 (100%)	0	100	100
1	HD	4/127 (3%)	4 (100%)	0	100	100
1	HE	4/127 (3%)	4 (100%)	0	100	100
1	HX	4/127 (3%)	4 (100%)	0	100	100
1	IA	4/127 (3%)	4 (100%)	0	100	100
1	IB	4/127 (3%)	4 (100%)	0	100	100
1	IC	4/127 (3%)	4 (100%)	0	100	100
1	ID	4/127 (3%)	4 (100%)	0	100	100
1	IE	4/127 (3%)	4 (100%)	0	100	100
1	IX	4/127 (3%)	4 (100%)	0	100	100
1	JA	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JB	4/127 (3%)	4 (100%)	0	100	100
1	JC	4/127 (3%)	4 (100%)	0	100	100
1	JD	4/127 (3%)	4 (100%)	0	100	100
1	JE	4/127 (3%)	4 (100%)	0	100	100
1	JX	4/127 (3%)	4 (100%)	0	100	100
1	KA	4/127 (3%)	4 (100%)	0	100	100
1	KB	4/127 (3%)	4 (100%)	0	100	100
1	KC	4/127 (3%)	4 (100%)	0	100	100
1	KD	4/127 (3%)	4 (100%)	0	100	100
1	KE	4/127 (3%)	4 (100%)	0	100	100
1	KX	4/127 (3%)	4 (100%)	0	100	100
1	LA	4/127 (3%)	4 (100%)	0	100	100
1	LB	4/127 (3%)	4 (100%)	0	100	100
1	LC	4/127 (3%)	4 (100%)	0	100	100
1	LD	4/127 (3%)	4 (100%)	0	100	100
1	LE	4/127 (3%)	4 (100%)	0	100	100
1	LX	4/127 (3%)	4 (100%)	0	100	100
1	MA	4/127 (3%)	4 (100%)	0	100	100
1	MB	4/127 (3%)	4 (100%)	0	100	100
1	MC	4/127 (3%)	4 (100%)	0	100	100
1	MD	4/127 (3%)	4 (100%)	0	100	100
1	ME	4/127 (3%)	4 (100%)	0	100	100
1	MX	4/127 (3%)	4 (100%)	0	100	100
1	NA	4/127 (3%)	4 (100%)	0	100	100
1	NB	4/127 (3%)	4 (100%)	0	100	100
1	NC	4/127 (3%)	4 (100%)	0	100	100
1	ND	4/127 (3%)	4 (100%)	0	100	100
1	NE	4/127 (3%)	4 (100%)	0	100	100
1	NX	4/127 (3%)	4 (100%)	0	100	100
1	OA	4/127 (3%)	4 (100%)	0	100	100
1	OB	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	OC	4/127 (3%)	4 (100%)	0	100	100
1	OD	4/127 (3%)	4 (100%)	0	100	100
1	OE	4/127 (3%)	4 (100%)	0	100	100
1	OX	4/127 (3%)	4 (100%)	0	100	100
1	PA	4/127 (3%)	4 (100%)	0	100	100
1	PB	4/127 (3%)	4 (100%)	0	100	100
1	PC	4/127 (3%)	4 (100%)	0	100	100
1	PD	4/127 (3%)	4 (100%)	0	100	100
1	PE	4/127 (3%)	4 (100%)	0	100	100
1	PX	4/127 (3%)	4 (100%)	0	100	100
1	QA	4/127 (3%)	4 (100%)	0	100	100
1	QB	4/127 (3%)	4 (100%)	0	100	100
1	QC	4/127 (3%)	4 (100%)	0	100	100
1	QD	4/127 (3%)	4 (100%)	0	100	100
1	QE	4/127 (3%)	4 (100%)	0	100	100
1	QX	4/127 (3%)	4 (100%)	0	100	100
1	RA	4/127 (3%)	4 (100%)	0	100	100
1	RB	4/127 (3%)	4 (100%)	0	100	100
1	RC	4/127 (3%)	4 (100%)	0	100	100
1	RD	4/127 (3%)	4 (100%)	0	100	100
1	RE	4/127 (3%)	4 (100%)	0	100	100
1	RX	4/127 (3%)	4 (100%)	0	100	100
1	SA	4/127 (3%)	4 (100%)	0	100	100
1	SB	4/127 (3%)	4 (100%)	0	100	100
1	SC	4/127 (3%)	4 (100%)	0	100	100
1	SD	4/127 (3%)	4 (100%)	0	100	100
1	SE	4/127 (3%)	4 (100%)	0	100	100
1	SX	4/127 (3%)	4 (100%)	0	100	100
1	TA	4/127 (3%)	4 (100%)	0	100	100
1	TB	4/127 (3%)	4 (100%)	0	100	100
1	TC	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	TD	4/127 (3%)	4 (100%)	0	100	100
1	TE	4/127 (3%)	4 (100%)	0	100	100
1	TX	4/127 (3%)	4 (100%)	0	100	100
1	UA	4/127 (3%)	4 (100%)	0	100	100
1	UB	4/127 (3%)	4 (100%)	0	100	100
1	UC	4/127 (3%)	4 (100%)	0	100	100
1	UD	4/127 (3%)	4 (100%)	0	100	100
1	UE	4/127 (3%)	4 (100%)	0	100	100
1	UX	4/127 (3%)	4 (100%)	0	100	100
1	VA	4/127 (3%)	4 (100%)	0	100	100
1	VB	4/127 (3%)	4 (100%)	0	100	100
1	VC	4/127 (3%)	4 (100%)	0	100	100
1	VD	4/127 (3%)	4 (100%)	0	100	100
1	VE	4/127 (3%)	4 (100%)	0	100	100
1	VX	4/127 (3%)	4 (100%)	0	100	100
1	WA	4/127 (3%)	4 (100%)	0	100	100
1	WB	4/127 (3%)	4 (100%)	0	100	100
1	WC	4/127 (3%)	4 (100%)	0	100	100
1	WD	4/127 (3%)	4 (100%)	0	100	100
1	WE	4/127 (3%)	4 (100%)	0	100	100
1	WX	4/127 (3%)	4 (100%)	0	100	100
1	XA	4/127 (3%)	4 (100%)	0	100	100
1	XB	4/127 (3%)	4 (100%)	0	100	100
1	XC	4/127 (3%)	4 (100%)	0	100	100
1	XD	4/127 (3%)	4 (100%)	0	100	100
1	XE	4/127 (3%)	4 (100%)	0	100	100
1	XX	4/127 (3%)	4 (100%)	0	100	100
1	YA	4/127 (3%)	4 (100%)	0	100	100
1	YB	4/127 (3%)	4 (100%)	0	100	100
1	YC	4/127 (3%)	4 (100%)	0	100	100
1	YD	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	YE	4/127 (3%)	4 (100%)	0	100	100
1	YX	4/127 (3%)	4 (100%)	0	100	100
1	ZA	4/127 (3%)	4 (100%)	0	100	100
1	ZB	4/127 (3%)	4 (100%)	0	100	100
1	ZC	4/127 (3%)	4 (100%)	0	100	100
1	ZD	4/127 (3%)	4 (100%)	0	100	100
1	ZE	4/127 (3%)	4 (100%)	0	100	100
1	ZX	4/127 (3%)	4 (100%)	0	100	100
1	aA	4/127 (3%)	4 (100%)	0	100	100
1	aB	4/127 (3%)	4 (100%)	0	100	100
1	aC	4/127 (3%)	4 (100%)	0	100	100
1	aD	4/127 (3%)	4 (100%)	0	100	100
1	aE	4/127 (3%)	4 (100%)	0	100	100
1	aX	4/127 (3%)	4 (100%)	0	100	100
1	bA	4/127 (3%)	4 (100%)	0	100	100
1	bB	4/127 (3%)	4 (100%)	0	100	100
1	bC	4/127 (3%)	4 (100%)	0	100	100
1	bD	4/127 (3%)	4 (100%)	0	100	100
1	bE	4/127 (3%)	4 (100%)	0	100	100
1	bX	4/127 (3%)	4 (100%)	0	100	100
1	cA	4/127 (3%)	4 (100%)	0	100	100
1	cB	4/127 (3%)	4 (100%)	0	100	100
1	cC	4/127 (3%)	4 (100%)	0	100	100
1	cD	4/127 (3%)	4 (100%)	0	100	100
1	cE	4/127 (3%)	4 (100%)	0	100	100
1	cX	4/127 (3%)	4 (100%)	0	100	100
1	dA	4/127 (3%)	4 (100%)	0	100	100
1	dB	4/127 (3%)	4 (100%)	0	100	100
1	dC	4/127 (3%)	4 (100%)	0	100	100
1	dD	4/127 (3%)	4 (100%)	0	100	100
1	dE	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	dX	4/127 (3%)	4 (100%)	0	100	100
1	eA	4/127 (3%)	4 (100%)	0	100	100
1	eB	4/127 (3%)	4 (100%)	0	100	100
1	eC	4/127 (3%)	4 (100%)	0	100	100
1	eD	4/127 (3%)	4 (100%)	0	100	100
1	eE	4/127 (3%)	4 (100%)	0	100	100
1	eX	4/127 (3%)	4 (100%)	0	100	100
1	fA	4/127 (3%)	4 (100%)	0	100	100
1	fB	4/127 (3%)	4 (100%)	0	100	100
1	fC	4/127 (3%)	4 (100%)	0	100	100
1	fD	4/127 (3%)	4 (100%)	0	100	100
1	fE	4/127 (3%)	4 (100%)	0	100	100
1	fX	4/127 (3%)	4 (100%)	0	100	100
1	gA	4/127 (3%)	4 (100%)	0	100	100
1	gB	4/127 (3%)	4 (100%)	0	100	100
1	gC	4/127 (3%)	4 (100%)	0	100	100
1	gD	4/127 (3%)	4 (100%)	0	100	100
1	gE	4/127 (3%)	4 (100%)	0	100	100
1	gX	4/127 (3%)	4 (100%)	0	100	100
1	hA	4/127 (3%)	4 (100%)	0	100	100
1	hB	4/127 (3%)	4 (100%)	0	100	100
1	hC	4/127 (3%)	4 (100%)	0	100	100
1	hD	4/127 (3%)	4 (100%)	0	100	100
1	hE	4/127 (3%)	4 (100%)	0	100	100
1	hX	4/127 (3%)	4 (100%)	0	100	100
1	iA	4/127 (3%)	4 (100%)	0	100	100
1	iB	4/127 (3%)	4 (100%)	0	100	100
1	iC	4/127 (3%)	4 (100%)	0	100	100
1	iD	4/127 (3%)	4 (100%)	0	100	100
1	iE	4/127 (3%)	4 (100%)	0	100	100
1	iX	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	jA	4/127 (3%)	4 (100%)	0	100	100
1	jB	4/127 (3%)	4 (100%)	0	100	100
1	jC	4/127 (3%)	4 (100%)	0	100	100
1	jD	4/127 (3%)	4 (100%)	0	100	100
1	jE	4/127 (3%)	4 (100%)	0	100	100
1	jX	4/127 (3%)	4 (100%)	0	100	100
1	kA	4/127 (3%)	4 (100%)	0	100	100
1	kB	4/127 (3%)	4 (100%)	0	100	100
1	kC	4/127 (3%)	4 (100%)	0	100	100
1	kD	4/127 (3%)	4 (100%)	0	100	100
1	kE	4/127 (3%)	4 (100%)	0	100	100
1	kX	4/127 (3%)	4 (100%)	0	100	100
1	lA	4/127 (3%)	4 (100%)	0	100	100
1	lB	4/127 (3%)	4 (100%)	0	100	100
1	lC	4/127 (3%)	4 (100%)	0	100	100
1	lD	4/127 (3%)	4 (100%)	0	100	100
1	lE	4/127 (3%)	4 (100%)	0	100	100
1	lX	4/127 (3%)	4 (100%)	0	100	100
1	mA	4/127 (3%)	4 (100%)	0	100	100
1	mB	4/127 (3%)	4 (100%)	0	100	100
1	mC	4/127 (3%)	4 (100%)	0	100	100
1	mD	4/127 (3%)	4 (100%)	0	100	100
1	mE	4/127 (3%)	4 (100%)	0	100	100
1	mX	4/127 (3%)	4 (100%)	0	100	100
1	nA	4/127 (3%)	4 (100%)	0	100	100
1	nB	4/127 (3%)	4 (100%)	0	100	100
1	nC	4/127 (3%)	4 (100%)	0	100	100
1	nD	4/127 (3%)	4 (100%)	0	100	100
1	nE	4/127 (3%)	4 (100%)	0	100	100
1	nX	4/127 (3%)	4 (100%)	0	100	100
1	oA	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	oB	4/127 (3%)	4 (100%)	0	100	100
1	oC	4/127 (3%)	4 (100%)	0	100	100
1	oD	4/127 (3%)	4 (100%)	0	100	100
1	oE	4/127 (3%)	4 (100%)	0	100	100
1	oX	4/127 (3%)	4 (100%)	0	100	100
1	pA	4/127 (3%)	4 (100%)	0	100	100
1	pB	4/127 (3%)	4 (100%)	0	100	100
1	pC	4/127 (3%)	4 (100%)	0	100	100
1	pD	4/127 (3%)	4 (100%)	0	100	100
1	pE	4/127 (3%)	4 (100%)	0	100	100
1	pX	4/127 (3%)	4 (100%)	0	100	100
1	qA	4/127 (3%)	4 (100%)	0	100	100
1	qB	4/127 (3%)	4 (100%)	0	100	100
1	qC	4/127 (3%)	4 (100%)	0	100	100
1	qD	4/127 (3%)	4 (100%)	0	100	100
1	qE	4/127 (3%)	4 (100%)	0	100	100
1	qX	4/127 (3%)	4 (100%)	0	100	100
1	rA	4/127 (3%)	4 (100%)	0	100	100
1	rB	4/127 (3%)	4 (100%)	0	100	100
1	rC	4/127 (3%)	4 (100%)	0	100	100
1	rD	4/127 (3%)	4 (100%)	0	100	100
1	rE	4/127 (3%)	4 (100%)	0	100	100
1	rX	4/127 (3%)	4 (100%)	0	100	100
1	sA	4/127 (3%)	4 (100%)	0	100	100
1	sB	4/127 (3%)	4 (100%)	0	100	100
1	sC	4/127 (3%)	4 (100%)	0	100	100
1	sD	4/127 (3%)	4 (100%)	0	100	100
1	sE	4/127 (3%)	4 (100%)	0	100	100
1	sX	4/127 (3%)	4 (100%)	0	100	100
1	tA	4/127 (3%)	4 (100%)	0	100	100
1	tB	4/127 (3%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	tC	4/127 (3%)	4 (100%)	0	100	100
1	tD	4/127 (3%)	4 (100%)	0	100	100
1	tE	4/127 (3%)	4 (100%)	0	100	100
1	tX	4/127 (3%)	4 (100%)	0	100	100
1	uA	4/127 (3%)	4 (100%)	0	100	100
1	uB	4/127 (3%)	4 (100%)	0	100	100
1	uC	4/127 (3%)	4 (100%)	0	100	100
1	uD	4/127 (3%)	4 (100%)	0	100	100
1	uE	4/127 (3%)	4 (100%)	0	100	100
1	uX	4/127 (3%)	4 (100%)	0	100	100
1	vA	4/127 (3%)	4 (100%)	0	100	100
1	vB	4/127 (3%)	4 (100%)	0	100	100
1	vC	4/127 (3%)	4 (100%)	0	100	100
1	vD	4/127 (3%)	4 (100%)	0	100	100
1	vE	4/127 (3%)	4 (100%)	0	100	100
1	vX	4/127 (3%)	4 (100%)	0	100	100
1	wA	4/127 (3%)	4 (100%)	0	100	100
1	wB	4/127 (3%)	4 (100%)	0	100	100
1	wC	4/127 (3%)	4 (100%)	0	100	100
1	wD	4/127 (3%)	4 (100%)	0	100	100
1	wE	4/127 (3%)	4 (100%)	0	100	100
1	wX	4/127 (3%)	4 (100%)	0	100	100
1	xA	4/127 (3%)	4 (100%)	0	100	100
1	xB	4/127 (3%)	4 (100%)	0	100	100
1	xC	4/127 (3%)	4 (100%)	0	100	100
1	xD	4/127 (3%)	4 (100%)	0	100	100
1	xE	4/127 (3%)	4 (100%)	0	100	100
1	XX	4/127 (3%)	4 (100%)	0	100	100
All	All	1440/45720 (3%)	1440 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.