



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 09:13 PM UTC

PDB ID : 6ZLO / pdb_00006zlo
EMDB ID : EMD-11270
Title : E2 core of the fungal Pyruvate dehydrogenase complex with asymmetric interior PX30 component
Authors : Forsberg, B.O.; Howard, R.J.; Aibara, S.; Mortesaei, N.; Lindahl, E.
Deposited on : 2020-06-30
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

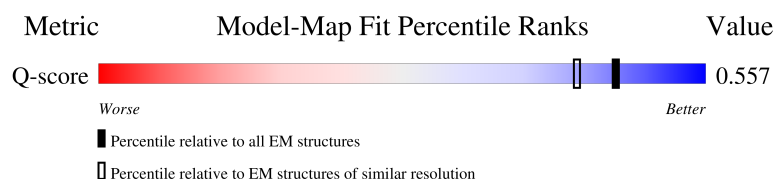
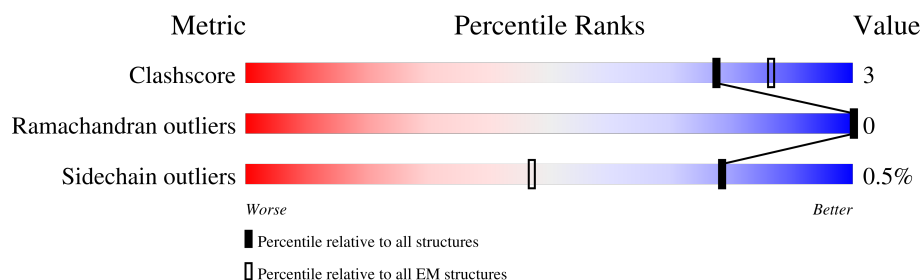
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	278	
1	AA	278	
1	AB	278	
1	B	278	

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Mol	Chain	Length	Quality of chain
1	BA	278	
1	BB	278	
1	C	278	
1	CA	278	
1	CB	278	
1	D	278	
1	DA	278	
1	DB	278	
1	E	278	
1	EA	278	
1	EB	278	
1	F	278	
1	FA	278	
1	FB	278	
1	G	278	
1	GA	278	
1	GB	278	
1	H	278	
1	HA	278	
1	HB	278	
1	I	278	
1	IA	278	
1	IB	278	
1	J	278	
1	JA	278	

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Mol	Chain	Length	Quality of chain
1	K	278	
1	KA	278	
1	L	278	
1	LA	278	
1	M	278	
1	MA	278	
1	N	278	
1	NA	278	
1	O	278	
1	OA	278	
1	P	278	
1	PA	278	
1	Q	278	
1	QA	278	
1	R	278	
1	RA	278	
1	S	278	
1	SA	278	
1	T	278	
1	TA	278	
1	UA	278	
1	V	278	
1	VA	278	
1	W	278	
1	WA	278	

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Mol	Chain	Length	Quality of chain
1	X	278	9% 77% 6% 17%
1	XA	278	9% 77% 6% 17%
1	Y	278	9% 77% 6% 17%
1	YA	278	8% 77% 6% 17%
1	Z	278	8% 77% 6% 17%
1	ZA	278	8% 76% 7% 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 105060 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 Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	B	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	C	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	D	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	E	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	F	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	G	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	H	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	I	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	J	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	K	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	L	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	M	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	N	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	O	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	P	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	R	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	S	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	T	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	V	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	W	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	X	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	Y	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	Z	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	AA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	BA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	CA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	DA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	EA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	FA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	GA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	HA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	IA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	JA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	KA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0
1	LA	232	Total 1751	C 1110	N 302	O 335	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	NA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	OA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	PA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	QA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	RA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	SA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	TA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	UA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	VA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	WA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	XA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	YA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	ZA	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	AB	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	BB	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	CB	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	DB	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	EB	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	FB	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	GB	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HB	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		
1	IB	232	Total	C	N	O	S	0	0
			1751	1110	302	335	4		

There are 2760 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	MET	-	initiating methionine	UNP P20285
A	182	ARG	-	expression tag	UNP P20285
A	183	GLY	-	expression tag	UNP P20285
A	184	SER	-	expression tag	UNP P20285
A	185	HIS	-	expression tag	UNP P20285
A	186	HIS	-	expression tag	UNP P20285
A	187	HIS	-	expression tag	UNP P20285
A	188	HIS	-	expression tag	UNP P20285
A	189	HIS	-	expression tag	UNP P20285
A	190	HIS	-	expression tag	UNP P20285
A	191	GLY	-	expression tag	UNP P20285
A	192	MET	-	expression tag	UNP P20285
A	193	ALA	-	expression tag	UNP P20285
A	194	SER	-	expression tag	UNP P20285
A	195	MET	-	expression tag	UNP P20285
A	196	THR	-	expression tag	UNP P20285
A	197	GLY	-	expression tag	UNP P20285
A	198	GLY	-	expression tag	UNP P20285
A	199	GLN	-	expression tag	UNP P20285
A	200	GLN	-	expression tag	UNP P20285
A	201	MET	-	expression tag	UNP P20285
A	202	GLY	-	expression tag	UNP P20285
A	203	ARG	-	expression tag	UNP P20285
A	204	ASP	-	expression tag	UNP P20285
A	205	LEU	-	expression tag	UNP P20285
A	206	TYR	-	expression tag	UNP P20285
A	207	ASP	-	expression tag	UNP P20285
A	208	ASP	-	expression tag	UNP P20285
A	209	ASP	-	expression tag	UNP P20285
A	210	ASP	-	expression tag	UNP P20285
A	211	LYS	-	expression tag	UNP P20285
A	212	ASP	-	expression tag	UNP P20285
A	213	ARG	-	expression tag	UNP P20285
A	214	TRP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
A	215	GLY	-	expression tag	UNP P20285
A	216	SER	-	expression tag	UNP P20285
A	217	LEU	-	expression tag	UNP P20285
A	218	VAL	-	expression tag	UNP P20285
A	219	PRO	-	expression tag	UNP P20285
A	220	ARG	-	expression tag	UNP P20285
A	221	GLY	-	expression tag	UNP P20285
A	222	SER	-	expression tag	UNP P20285
A	223	HIS	-	expression tag	UNP P20285
A	224	MET	-	expression tag	UNP P20285
A	225	ALA	-	expression tag	UNP P20285
A	226	ALA	-	expression tag	UNP P20285
B	181	MET	-	initiating methionine	UNP P20285
B	182	ARG	-	expression tag	UNP P20285
B	183	GLY	-	expression tag	UNP P20285
B	184	SER	-	expression tag	UNP P20285
B	185	HIS	-	expression tag	UNP P20285
B	186	HIS	-	expression tag	UNP P20285
B	187	HIS	-	expression tag	UNP P20285
B	188	HIS	-	expression tag	UNP P20285
B	189	HIS	-	expression tag	UNP P20285
B	190	HIS	-	expression tag	UNP P20285
B	191	GLY	-	expression tag	UNP P20285
B	192	MET	-	expression tag	UNP P20285
B	193	ALA	-	expression tag	UNP P20285
B	194	SER	-	expression tag	UNP P20285
B	195	MET	-	expression tag	UNP P20285
B	196	THR	-	expression tag	UNP P20285
B	197	GLY	-	expression tag	UNP P20285
B	198	GLY	-	expression tag	UNP P20285
B	199	GLN	-	expression tag	UNP P20285
B	200	GLN	-	expression tag	UNP P20285
B	201	MET	-	expression tag	UNP P20285
B	202	GLY	-	expression tag	UNP P20285
B	203	ARG	-	expression tag	UNP P20285
B	204	ASP	-	expression tag	UNP P20285
B	205	LEU	-	expression tag	UNP P20285
B	206	TYR	-	expression tag	UNP P20285
B	207	ASP	-	expression tag	UNP P20285
B	208	ASP	-	expression tag	UNP P20285
B	209	ASP	-	expression tag	UNP P20285
B	210	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
B	211	LYS	-	expression tag	UNP P20285
B	212	ASP	-	expression tag	UNP P20285
B	213	ARG	-	expression tag	UNP P20285
B	214	TRP	-	expression tag	UNP P20285
B	215	GLY	-	expression tag	UNP P20285
B	216	SER	-	expression tag	UNP P20285
B	217	LEU	-	expression tag	UNP P20285
B	218	VAL	-	expression tag	UNP P20285
B	219	PRO	-	expression tag	UNP P20285
B	220	ARG	-	expression tag	UNP P20285
B	221	GLY	-	expression tag	UNP P20285
B	222	SER	-	expression tag	UNP P20285
B	223	HIS	-	expression tag	UNP P20285
B	224	MET	-	expression tag	UNP P20285
B	225	ALA	-	expression tag	UNP P20285
B	226	ALA	-	expression tag	UNP P20285
C	181	MET	-	initiating methionine	UNP P20285
C	182	ARG	-	expression tag	UNP P20285
C	183	GLY	-	expression tag	UNP P20285
C	184	SER	-	expression tag	UNP P20285
C	185	HIS	-	expression tag	UNP P20285
C	186	HIS	-	expression tag	UNP P20285
C	187	HIS	-	expression tag	UNP P20285
C	188	HIS	-	expression tag	UNP P20285
C	189	HIS	-	expression tag	UNP P20285
C	190	HIS	-	expression tag	UNP P20285
C	191	GLY	-	expression tag	UNP P20285
C	192	MET	-	expression tag	UNP P20285
C	193	ALA	-	expression tag	UNP P20285
C	194	SER	-	expression tag	UNP P20285
C	195	MET	-	expression tag	UNP P20285
C	196	THR	-	expression tag	UNP P20285
C	197	GLY	-	expression tag	UNP P20285
C	198	GLY	-	expression tag	UNP P20285
C	199	GLN	-	expression tag	UNP P20285
C	200	GLN	-	expression tag	UNP P20285
C	201	MET	-	expression tag	UNP P20285
C	202	GLY	-	expression tag	UNP P20285
C	203	ARG	-	expression tag	UNP P20285
C	204	ASP	-	expression tag	UNP P20285
C	205	LEU	-	expression tag	UNP P20285
C	206	TYR	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
C	207	ASP	-	expression tag	UNP P20285
C	208	ASP	-	expression tag	UNP P20285
C	209	ASP	-	expression tag	UNP P20285
C	210	ASP	-	expression tag	UNP P20285
C	211	LYS	-	expression tag	UNP P20285
C	212	ASP	-	expression tag	UNP P20285
C	213	ARG	-	expression tag	UNP P20285
C	214	TRP	-	expression tag	UNP P20285
C	215	GLY	-	expression tag	UNP P20285
C	216	SER	-	expression tag	UNP P20285
C	217	LEU	-	expression tag	UNP P20285
C	218	VAL	-	expression tag	UNP P20285
C	219	PRO	-	expression tag	UNP P20285
C	220	ARG	-	expression tag	UNP P20285
C	221	GLY	-	expression tag	UNP P20285
C	222	SER	-	expression tag	UNP P20285
C	223	HIS	-	expression tag	UNP P20285
C	224	MET	-	expression tag	UNP P20285
C	225	ALA	-	expression tag	UNP P20285
C	226	ALA	-	expression tag	UNP P20285
D	181	MET	-	initiating methionine	UNP P20285
D	182	ARG	-	expression tag	UNP P20285
D	183	GLY	-	expression tag	UNP P20285
D	184	SER	-	expression tag	UNP P20285
D	185	HIS	-	expression tag	UNP P20285
D	186	HIS	-	expression tag	UNP P20285
D	187	HIS	-	expression tag	UNP P20285
D	188	HIS	-	expression tag	UNP P20285
D	189	HIS	-	expression tag	UNP P20285
D	190	HIS	-	expression tag	UNP P20285
D	191	GLY	-	expression tag	UNP P20285
D	192	MET	-	expression tag	UNP P20285
D	193	ALA	-	expression tag	UNP P20285
D	194	SER	-	expression tag	UNP P20285
D	195	MET	-	expression tag	UNP P20285
D	196	THR	-	expression tag	UNP P20285
D	197	GLY	-	expression tag	UNP P20285
D	198	GLY	-	expression tag	UNP P20285
D	199	GLN	-	expression tag	UNP P20285
D	200	GLN	-	expression tag	UNP P20285
D	201	MET	-	expression tag	UNP P20285
D	202	GLY	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
D	203	ARG	-	expression tag	UNP P20285
D	204	ASP	-	expression tag	UNP P20285
D	205	LEU	-	expression tag	UNP P20285
D	206	TYR	-	expression tag	UNP P20285
D	207	ASP	-	expression tag	UNP P20285
D	208	ASP	-	expression tag	UNP P20285
D	209	ASP	-	expression tag	UNP P20285
D	210	ASP	-	expression tag	UNP P20285
D	211	LYS	-	expression tag	UNP P20285
D	212	ASP	-	expression tag	UNP P20285
D	213	ARG	-	expression tag	UNP P20285
D	214	TRP	-	expression tag	UNP P20285
D	215	GLY	-	expression tag	UNP P20285
D	216	SER	-	expression tag	UNP P20285
D	217	LEU	-	expression tag	UNP P20285
D	218	VAL	-	expression tag	UNP P20285
D	219	PRO	-	expression tag	UNP P20285
D	220	ARG	-	expression tag	UNP P20285
D	221	GLY	-	expression tag	UNP P20285
D	222	SER	-	expression tag	UNP P20285
D	223	HIS	-	expression tag	UNP P20285
D	224	MET	-	expression tag	UNP P20285
D	225	ALA	-	expression tag	UNP P20285
D	226	ALA	-	expression tag	UNP P20285
E	181	MET	-	initiating methionine	UNP P20285
E	182	ARG	-	expression tag	UNP P20285
E	183	GLY	-	expression tag	UNP P20285
E	184	SER	-	expression tag	UNP P20285
E	185	HIS	-	expression tag	UNP P20285
E	186	HIS	-	expression tag	UNP P20285
E	187	HIS	-	expression tag	UNP P20285
E	188	HIS	-	expression tag	UNP P20285
E	189	HIS	-	expression tag	UNP P20285
E	190	HIS	-	expression tag	UNP P20285
E	191	GLY	-	expression tag	UNP P20285
E	192	MET	-	expression tag	UNP P20285
E	193	ALA	-	expression tag	UNP P20285
E	194	SER	-	expression tag	UNP P20285
E	195	MET	-	expression tag	UNP P20285
E	196	THR	-	expression tag	UNP P20285
E	197	GLY	-	expression tag	UNP P20285
E	198	GLY	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
E	199	GLN	-	expression tag	UNP P20285
E	200	GLN	-	expression tag	UNP P20285
E	201	MET	-	expression tag	UNP P20285
E	202	GLY	-	expression tag	UNP P20285
E	203	ARG	-	expression tag	UNP P20285
E	204	ASP	-	expression tag	UNP P20285
E	205	LEU	-	expression tag	UNP P20285
E	206	TYR	-	expression tag	UNP P20285
E	207	ASP	-	expression tag	UNP P20285
E	208	ASP	-	expression tag	UNP P20285
E	209	ASP	-	expression tag	UNP P20285
E	210	ASP	-	expression tag	UNP P20285
E	211	LYS	-	expression tag	UNP P20285
E	212	ASP	-	expression tag	UNP P20285
E	213	ARG	-	expression tag	UNP P20285
E	214	TRP	-	expression tag	UNP P20285
E	215	GLY	-	expression tag	UNP P20285
E	216	SER	-	expression tag	UNP P20285
E	217	LEU	-	expression tag	UNP P20285
E	218	VAL	-	expression tag	UNP P20285
E	219	PRO	-	expression tag	UNP P20285
E	220	ARG	-	expression tag	UNP P20285
E	221	GLY	-	expression tag	UNP P20285
E	222	SER	-	expression tag	UNP P20285
E	223	HIS	-	expression tag	UNP P20285
E	224	MET	-	expression tag	UNP P20285
E	225	ALA	-	expression tag	UNP P20285
E	226	ALA	-	expression tag	UNP P20285
F	181	MET	-	initiating methionine	UNP P20285
F	182	ARG	-	expression tag	UNP P20285
F	183	GLY	-	expression tag	UNP P20285
F	184	SER	-	expression tag	UNP P20285
F	185	HIS	-	expression tag	UNP P20285
F	186	HIS	-	expression tag	UNP P20285
F	187	HIS	-	expression tag	UNP P20285
F	188	HIS	-	expression tag	UNP P20285
F	189	HIS	-	expression tag	UNP P20285
F	190	HIS	-	expression tag	UNP P20285
F	191	GLY	-	expression tag	UNP P20285
F	192	MET	-	expression tag	UNP P20285
F	193	ALA	-	expression tag	UNP P20285
F	194	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
F	195	MET	-	expression tag	UNP P20285
F	196	THR	-	expression tag	UNP P20285
F	197	GLY	-	expression tag	UNP P20285
F	198	GLY	-	expression tag	UNP P20285
F	199	GLN	-	expression tag	UNP P20285
F	200	GLN	-	expression tag	UNP P20285
F	201	MET	-	expression tag	UNP P20285
F	202	GLY	-	expression tag	UNP P20285
F	203	ARG	-	expression tag	UNP P20285
F	204	ASP	-	expression tag	UNP P20285
F	205	LEU	-	expression tag	UNP P20285
F	206	TYR	-	expression tag	UNP P20285
F	207	ASP	-	expression tag	UNP P20285
F	208	ASP	-	expression tag	UNP P20285
F	209	ASP	-	expression tag	UNP P20285
F	210	ASP	-	expression tag	UNP P20285
F	211	LYS	-	expression tag	UNP P20285
F	212	ASP	-	expression tag	UNP P20285
F	213	ARG	-	expression tag	UNP P20285
F	214	TRP	-	expression tag	UNP P20285
F	215	GLY	-	expression tag	UNP P20285
F	216	SER	-	expression tag	UNP P20285
F	217	LEU	-	expression tag	UNP P20285
F	218	VAL	-	expression tag	UNP P20285
F	219	PRO	-	expression tag	UNP P20285
F	220	ARG	-	expression tag	UNP P20285
F	221	GLY	-	expression tag	UNP P20285
F	222	SER	-	expression tag	UNP P20285
F	223	HIS	-	expression tag	UNP P20285
F	224	MET	-	expression tag	UNP P20285
F	225	ALA	-	expression tag	UNP P20285
F	226	ALA	-	expression tag	UNP P20285
G	181	MET	-	initiating methionine	UNP P20285
G	182	ARG	-	expression tag	UNP P20285
G	183	GLY	-	expression tag	UNP P20285
G	184	SER	-	expression tag	UNP P20285
G	185	HIS	-	expression tag	UNP P20285
G	186	HIS	-	expression tag	UNP P20285
G	187	HIS	-	expression tag	UNP P20285
G	188	HIS	-	expression tag	UNP P20285
G	189	HIS	-	expression tag	UNP P20285
G	190	HIS	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	-	expression tag	UNP P20285
G	192	MET	-	expression tag	UNP P20285
G	193	ALA	-	expression tag	UNP P20285
G	194	SER	-	expression tag	UNP P20285
G	195	MET	-	expression tag	UNP P20285
G	196	THR	-	expression tag	UNP P20285
G	197	GLY	-	expression tag	UNP P20285
G	198	GLY	-	expression tag	UNP P20285
G	199	GLN	-	expression tag	UNP P20285
G	200	GLN	-	expression tag	UNP P20285
G	201	MET	-	expression tag	UNP P20285
G	202	GLY	-	expression tag	UNP P20285
G	203	ARG	-	expression tag	UNP P20285
G	204	ASP	-	expression tag	UNP P20285
G	205	LEU	-	expression tag	UNP P20285
G	206	TYR	-	expression tag	UNP P20285
G	207	ASP	-	expression tag	UNP P20285
G	208	ASP	-	expression tag	UNP P20285
G	209	ASP	-	expression tag	UNP P20285
G	210	ASP	-	expression tag	UNP P20285
G	211	LYS	-	expression tag	UNP P20285
G	212	ASP	-	expression tag	UNP P20285
G	213	ARG	-	expression tag	UNP P20285
G	214	TRP	-	expression tag	UNP P20285
G	215	GLY	-	expression tag	UNP P20285
G	216	SER	-	expression tag	UNP P20285
G	217	LEU	-	expression tag	UNP P20285
G	218	VAL	-	expression tag	UNP P20285
G	219	PRO	-	expression tag	UNP P20285
G	220	ARG	-	expression tag	UNP P20285
G	221	GLY	-	expression tag	UNP P20285
G	222	SER	-	expression tag	UNP P20285
G	223	HIS	-	expression tag	UNP P20285
G	224	MET	-	expression tag	UNP P20285
G	225	ALA	-	expression tag	UNP P20285
G	226	ALA	-	expression tag	UNP P20285
H	181	MET	-	initiating methionine	UNP P20285
H	182	ARG	-	expression tag	UNP P20285
H	183	GLY	-	expression tag	UNP P20285
H	184	SER	-	expression tag	UNP P20285
H	185	HIS	-	expression tag	UNP P20285
H	186	HIS	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
H	187	HIS	-	expression tag	UNP P20285
H	188	HIS	-	expression tag	UNP P20285
H	189	HIS	-	expression tag	UNP P20285
H	190	HIS	-	expression tag	UNP P20285
H	191	GLY	-	expression tag	UNP P20285
H	192	MET	-	expression tag	UNP P20285
H	193	ALA	-	expression tag	UNP P20285
H	194	SER	-	expression tag	UNP P20285
H	195	MET	-	expression tag	UNP P20285
H	196	THR	-	expression tag	UNP P20285
H	197	GLY	-	expression tag	UNP P20285
H	198	GLY	-	expression tag	UNP P20285
H	199	GLN	-	expression tag	UNP P20285
H	200	GLN	-	expression tag	UNP P20285
H	201	MET	-	expression tag	UNP P20285
H	202	GLY	-	expression tag	UNP P20285
H	203	ARG	-	expression tag	UNP P20285
H	204	ASP	-	expression tag	UNP P20285
H	205	LEU	-	expression tag	UNP P20285
H	206	TYR	-	expression tag	UNP P20285
H	207	ASP	-	expression tag	UNP P20285
H	208	ASP	-	expression tag	UNP P20285
H	209	ASP	-	expression tag	UNP P20285
H	210	ASP	-	expression tag	UNP P20285
H	211	LYS	-	expression tag	UNP P20285
H	212	ASP	-	expression tag	UNP P20285
H	213	ARG	-	expression tag	UNP P20285
H	214	TRP	-	expression tag	UNP P20285
H	215	GLY	-	expression tag	UNP P20285
H	216	SER	-	expression tag	UNP P20285
H	217	LEU	-	expression tag	UNP P20285
H	218	VAL	-	expression tag	UNP P20285
H	219	PRO	-	expression tag	UNP P20285
H	220	ARG	-	expression tag	UNP P20285
H	221	GLY	-	expression tag	UNP P20285
H	222	SER	-	expression tag	UNP P20285
H	223	HIS	-	expression tag	UNP P20285
H	224	MET	-	expression tag	UNP P20285
H	225	ALA	-	expression tag	UNP P20285
H	226	ALA	-	expression tag	UNP P20285
I	181	MET	-	initiating methionine	UNP P20285
I	182	ARG	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
I	183	GLY	-	expression tag	UNP P20285
I	184	SER	-	expression tag	UNP P20285
I	185	HIS	-	expression tag	UNP P20285
I	186	HIS	-	expression tag	UNP P20285
I	187	HIS	-	expression tag	UNP P20285
I	188	HIS	-	expression tag	UNP P20285
I	189	HIS	-	expression tag	UNP P20285
I	190	HIS	-	expression tag	UNP P20285
I	191	GLY	-	expression tag	UNP P20285
I	192	MET	-	expression tag	UNP P20285
I	193	ALA	-	expression tag	UNP P20285
I	194	SER	-	expression tag	UNP P20285
I	195	MET	-	expression tag	UNP P20285
I	196	THR	-	expression tag	UNP P20285
I	197	GLY	-	expression tag	UNP P20285
I	198	GLY	-	expression tag	UNP P20285
I	199	GLN	-	expression tag	UNP P20285
I	200	GLN	-	expression tag	UNP P20285
I	201	MET	-	expression tag	UNP P20285
I	202	GLY	-	expression tag	UNP P20285
I	203	ARG	-	expression tag	UNP P20285
I	204	ASP	-	expression tag	UNP P20285
I	205	LEU	-	expression tag	UNP P20285
I	206	TYR	-	expression tag	UNP P20285
I	207	ASP	-	expression tag	UNP P20285
I	208	ASP	-	expression tag	UNP P20285
I	209	ASP	-	expression tag	UNP P20285
I	210	ASP	-	expression tag	UNP P20285
I	211	LYS	-	expression tag	UNP P20285
I	212	ASP	-	expression tag	UNP P20285
I	213	ARG	-	expression tag	UNP P20285
I	214	TRP	-	expression tag	UNP P20285
I	215	GLY	-	expression tag	UNP P20285
I	216	SER	-	expression tag	UNP P20285
I	217	LEU	-	expression tag	UNP P20285
I	218	VAL	-	expression tag	UNP P20285
I	219	PRO	-	expression tag	UNP P20285
I	220	ARG	-	expression tag	UNP P20285
I	221	GLY	-	expression tag	UNP P20285
I	222	SER	-	expression tag	UNP P20285
I	223	HIS	-	expression tag	UNP P20285
I	224	MET	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
I	225	ALA	-	expression tag	UNP P20285
I	226	ALA	-	expression tag	UNP P20285
J	181	MET	-	initiating methionine	UNP P20285
J	182	ARG	-	expression tag	UNP P20285
J	183	GLY	-	expression tag	UNP P20285
J	184	SER	-	expression tag	UNP P20285
J	185	HIS	-	expression tag	UNP P20285
J	186	HIS	-	expression tag	UNP P20285
J	187	HIS	-	expression tag	UNP P20285
J	188	HIS	-	expression tag	UNP P20285
J	189	HIS	-	expression tag	UNP P20285
J	190	HIS	-	expression tag	UNP P20285
J	191	GLY	-	expression tag	UNP P20285
J	192	MET	-	expression tag	UNP P20285
J	193	ALA	-	expression tag	UNP P20285
J	194	SER	-	expression tag	UNP P20285
J	195	MET	-	expression tag	UNP P20285
J	196	THR	-	expression tag	UNP P20285
J	197	GLY	-	expression tag	UNP P20285
J	198	GLY	-	expression tag	UNP P20285
J	199	GLN	-	expression tag	UNP P20285
J	200	GLN	-	expression tag	UNP P20285
J	201	MET	-	expression tag	UNP P20285
J	202	GLY	-	expression tag	UNP P20285
J	203	ARG	-	expression tag	UNP P20285
J	204	ASP	-	expression tag	UNP P20285
J	205	LEU	-	expression tag	UNP P20285
J	206	TYR	-	expression tag	UNP P20285
J	207	ASP	-	expression tag	UNP P20285
J	208	ASP	-	expression tag	UNP P20285
J	209	ASP	-	expression tag	UNP P20285
J	210	ASP	-	expression tag	UNP P20285
J	211	LYS	-	expression tag	UNP P20285
J	212	ASP	-	expression tag	UNP P20285
J	213	ARG	-	expression tag	UNP P20285
J	214	TRP	-	expression tag	UNP P20285
J	215	GLY	-	expression tag	UNP P20285
J	216	SER	-	expression tag	UNP P20285
J	217	LEU	-	expression tag	UNP P20285
J	218	VAL	-	expression tag	UNP P20285
J	219	PRO	-	expression tag	UNP P20285
J	220	ARG	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
J	221	GLY	-	expression tag	UNP P20285
J	222	SER	-	expression tag	UNP P20285
J	223	HIS	-	expression tag	UNP P20285
J	224	MET	-	expression tag	UNP P20285
J	225	ALA	-	expression tag	UNP P20285
J	226	ALA	-	expression tag	UNP P20285
K	181	MET	-	initiating methionine	UNP P20285
K	182	ARG	-	expression tag	UNP P20285
K	183	GLY	-	expression tag	UNP P20285
K	184	SER	-	expression tag	UNP P20285
K	185	HIS	-	expression tag	UNP P20285
K	186	HIS	-	expression tag	UNP P20285
K	187	HIS	-	expression tag	UNP P20285
K	188	HIS	-	expression tag	UNP P20285
K	189	HIS	-	expression tag	UNP P20285
K	190	HIS	-	expression tag	UNP P20285
K	191	GLY	-	expression tag	UNP P20285
K	192	MET	-	expression tag	UNP P20285
K	193	ALA	-	expression tag	UNP P20285
K	194	SER	-	expression tag	UNP P20285
K	195	MET	-	expression tag	UNP P20285
K	196	THR	-	expression tag	UNP P20285
K	197	GLY	-	expression tag	UNP P20285
K	198	GLY	-	expression tag	UNP P20285
K	199	GLN	-	expression tag	UNP P20285
K	200	GLN	-	expression tag	UNP P20285
K	201	MET	-	expression tag	UNP P20285
K	202	GLY	-	expression tag	UNP P20285
K	203	ARG	-	expression tag	UNP P20285
K	204	ASP	-	expression tag	UNP P20285
K	205	LEU	-	expression tag	UNP P20285
K	206	TYR	-	expression tag	UNP P20285
K	207	ASP	-	expression tag	UNP P20285
K	208	ASP	-	expression tag	UNP P20285
K	209	ASP	-	expression tag	UNP P20285
K	210	ASP	-	expression tag	UNP P20285
K	211	LYS	-	expression tag	UNP P20285
K	212	ASP	-	expression tag	UNP P20285
K	213	ARG	-	expression tag	UNP P20285
K	214	TRP	-	expression tag	UNP P20285
K	215	GLY	-	expression tag	UNP P20285
K	216	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
K	217	LEU	-	expression tag	UNP P20285
K	218	VAL	-	expression tag	UNP P20285
K	219	PRO	-	expression tag	UNP P20285
K	220	ARG	-	expression tag	UNP P20285
K	221	GLY	-	expression tag	UNP P20285
K	222	SER	-	expression tag	UNP P20285
K	223	HIS	-	expression tag	UNP P20285
K	224	MET	-	expression tag	UNP P20285
K	225	ALA	-	expression tag	UNP P20285
K	226	ALA	-	expression tag	UNP P20285
L	181	MET	-	initiating methionine	UNP P20285
L	182	ARG	-	expression tag	UNP P20285
L	183	GLY	-	expression tag	UNP P20285
L	184	SER	-	expression tag	UNP P20285
L	185	HIS	-	expression tag	UNP P20285
L	186	HIS	-	expression tag	UNP P20285
L	187	HIS	-	expression tag	UNP P20285
L	188	HIS	-	expression tag	UNP P20285
L	189	HIS	-	expression tag	UNP P20285
L	190	HIS	-	expression tag	UNP P20285
L	191	GLY	-	expression tag	UNP P20285
L	192	MET	-	expression tag	UNP P20285
L	193	ALA	-	expression tag	UNP P20285
L	194	SER	-	expression tag	UNP P20285
L	195	MET	-	expression tag	UNP P20285
L	196	THR	-	expression tag	UNP P20285
L	197	GLY	-	expression tag	UNP P20285
L	198	GLY	-	expression tag	UNP P20285
L	199	GLN	-	expression tag	UNP P20285
L	200	GLN	-	expression tag	UNP P20285
L	201	MET	-	expression tag	UNP P20285
L	202	GLY	-	expression tag	UNP P20285
L	203	ARG	-	expression tag	UNP P20285
L	204	ASP	-	expression tag	UNP P20285
L	205	LEU	-	expression tag	UNP P20285
L	206	TYR	-	expression tag	UNP P20285
L	207	ASP	-	expression tag	UNP P20285
L	208	ASP	-	expression tag	UNP P20285
L	209	ASP	-	expression tag	UNP P20285
L	210	ASP	-	expression tag	UNP P20285
L	211	LYS	-	expression tag	UNP P20285
L	212	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
L	213	ARG	-	expression tag	UNP P20285
L	214	TRP	-	expression tag	UNP P20285
L	215	GLY	-	expression tag	UNP P20285
L	216	SER	-	expression tag	UNP P20285
L	217	LEU	-	expression tag	UNP P20285
L	218	VAL	-	expression tag	UNP P20285
L	219	PRO	-	expression tag	UNP P20285
L	220	ARG	-	expression tag	UNP P20285
L	221	GLY	-	expression tag	UNP P20285
L	222	SER	-	expression tag	UNP P20285
L	223	HIS	-	expression tag	UNP P20285
L	224	MET	-	expression tag	UNP P20285
L	225	ALA	-	expression tag	UNP P20285
L	226	ALA	-	expression tag	UNP P20285
M	181	MET	-	initiating methionine	UNP P20285
M	182	ARG	-	expression tag	UNP P20285
M	183	GLY	-	expression tag	UNP P20285
M	184	SER	-	expression tag	UNP P20285
M	185	HIS	-	expression tag	UNP P20285
M	186	HIS	-	expression tag	UNP P20285
M	187	HIS	-	expression tag	UNP P20285
M	188	HIS	-	expression tag	UNP P20285
M	189	HIS	-	expression tag	UNP P20285
M	190	HIS	-	expression tag	UNP P20285
M	191	GLY	-	expression tag	UNP P20285
M	192	MET	-	expression tag	UNP P20285
M	193	ALA	-	expression tag	UNP P20285
M	194	SER	-	expression tag	UNP P20285
M	195	MET	-	expression tag	UNP P20285
M	196	THR	-	expression tag	UNP P20285
M	197	GLY	-	expression tag	UNP P20285
M	198	GLY	-	expression tag	UNP P20285
M	199	GLN	-	expression tag	UNP P20285
M	200	GLN	-	expression tag	UNP P20285
M	201	MET	-	expression tag	UNP P20285
M	202	GLY	-	expression tag	UNP P20285
M	203	ARG	-	expression tag	UNP P20285
M	204	ASP	-	expression tag	UNP P20285
M	205	LEU	-	expression tag	UNP P20285
M	206	TYR	-	expression tag	UNP P20285
M	207	ASP	-	expression tag	UNP P20285
M	208	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
M	209	ASP	-	expression tag	UNP P20285
M	210	ASP	-	expression tag	UNP P20285
M	211	LYS	-	expression tag	UNP P20285
M	212	ASP	-	expression tag	UNP P20285
M	213	ARG	-	expression tag	UNP P20285
M	214	TRP	-	expression tag	UNP P20285
M	215	GLY	-	expression tag	UNP P20285
M	216	SER	-	expression tag	UNP P20285
M	217	LEU	-	expression tag	UNP P20285
M	218	VAL	-	expression tag	UNP P20285
M	219	PRO	-	expression tag	UNP P20285
M	220	ARG	-	expression tag	UNP P20285
M	221	GLY	-	expression tag	UNP P20285
M	222	SER	-	expression tag	UNP P20285
M	223	HIS	-	expression tag	UNP P20285
M	224	MET	-	expression tag	UNP P20285
M	225	ALA	-	expression tag	UNP P20285
M	226	ALA	-	expression tag	UNP P20285
N	181	MET	-	initiating methionine	UNP P20285
N	182	ARG	-	expression tag	UNP P20285
N	183	GLY	-	expression tag	UNP P20285
N	184	SER	-	expression tag	UNP P20285
N	185	HIS	-	expression tag	UNP P20285
N	186	HIS	-	expression tag	UNP P20285
N	187	HIS	-	expression tag	UNP P20285
N	188	HIS	-	expression tag	UNP P20285
N	189	HIS	-	expression tag	UNP P20285
N	190	HIS	-	expression tag	UNP P20285
N	191	GLY	-	expression tag	UNP P20285
N	192	MET	-	expression tag	UNP P20285
N	193	ALA	-	expression tag	UNP P20285
N	194	SER	-	expression tag	UNP P20285
N	195	MET	-	expression tag	UNP P20285
N	196	THR	-	expression tag	UNP P20285
N	197	GLY	-	expression tag	UNP P20285
N	198	GLY	-	expression tag	UNP P20285
N	199	GLN	-	expression tag	UNP P20285
N	200	GLN	-	expression tag	UNP P20285
N	201	MET	-	expression tag	UNP P20285
N	202	GLY	-	expression tag	UNP P20285
N	203	ARG	-	expression tag	UNP P20285
N	204	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
N	205	LEU	-	expression tag	UNP P20285
N	206	TYR	-	expression tag	UNP P20285
N	207	ASP	-	expression tag	UNP P20285
N	208	ASP	-	expression tag	UNP P20285
N	209	ASP	-	expression tag	UNP P20285
N	210	ASP	-	expression tag	UNP P20285
N	211	LYS	-	expression tag	UNP P20285
N	212	ASP	-	expression tag	UNP P20285
N	213	ARG	-	expression tag	UNP P20285
N	214	TRP	-	expression tag	UNP P20285
N	215	GLY	-	expression tag	UNP P20285
N	216	SER	-	expression tag	UNP P20285
N	217	LEU	-	expression tag	UNP P20285
N	218	VAL	-	expression tag	UNP P20285
N	219	PRO	-	expression tag	UNP P20285
N	220	ARG	-	expression tag	UNP P20285
N	221	GLY	-	expression tag	UNP P20285
N	222	SER	-	expression tag	UNP P20285
N	223	HIS	-	expression tag	UNP P20285
N	224	MET	-	expression tag	UNP P20285
N	225	ALA	-	expression tag	UNP P20285
N	226	ALA	-	expression tag	UNP P20285
O	181	MET	-	initiating methionine	UNP P20285
O	182	ARG	-	expression tag	UNP P20285
O	183	GLY	-	expression tag	UNP P20285
O	184	SER	-	expression tag	UNP P20285
O	185	HIS	-	expression tag	UNP P20285
O	186	HIS	-	expression tag	UNP P20285
O	187	HIS	-	expression tag	UNP P20285
O	188	HIS	-	expression tag	UNP P20285
O	189	HIS	-	expression tag	UNP P20285
O	190	HIS	-	expression tag	UNP P20285
O	191	GLY	-	expression tag	UNP P20285
O	192	MET	-	expression tag	UNP P20285
O	193	ALA	-	expression tag	UNP P20285
O	194	SER	-	expression tag	UNP P20285
O	195	MET	-	expression tag	UNP P20285
O	196	THR	-	expression tag	UNP P20285
O	197	GLY	-	expression tag	UNP P20285
O	198	GLY	-	expression tag	UNP P20285
O	199	GLN	-	expression tag	UNP P20285
O	200	GLN	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
O	201	MET	-	expression tag	UNP P20285
O	202	GLY	-	expression tag	UNP P20285
O	203	ARG	-	expression tag	UNP P20285
O	204	ASP	-	expression tag	UNP P20285
O	205	LEU	-	expression tag	UNP P20285
O	206	TYR	-	expression tag	UNP P20285
O	207	ASP	-	expression tag	UNP P20285
O	208	ASP	-	expression tag	UNP P20285
O	209	ASP	-	expression tag	UNP P20285
O	210	ASP	-	expression tag	UNP P20285
O	211	LYS	-	expression tag	UNP P20285
O	212	ASP	-	expression tag	UNP P20285
O	213	ARG	-	expression tag	UNP P20285
O	214	TRP	-	expression tag	UNP P20285
O	215	GLY	-	expression tag	UNP P20285
O	216	SER	-	expression tag	UNP P20285
O	217	LEU	-	expression tag	UNP P20285
O	218	VAL	-	expression tag	UNP P20285
O	219	PRO	-	expression tag	UNP P20285
O	220	ARG	-	expression tag	UNP P20285
O	221	GLY	-	expression tag	UNP P20285
O	222	SER	-	expression tag	UNP P20285
O	223	HIS	-	expression tag	UNP P20285
O	224	MET	-	expression tag	UNP P20285
O	225	ALA	-	expression tag	UNP P20285
O	226	ALA	-	expression tag	UNP P20285
P	181	MET	-	initiating methionine	UNP P20285
P	182	ARG	-	expression tag	UNP P20285
P	183	GLY	-	expression tag	UNP P20285
P	184	SER	-	expression tag	UNP P20285
P	185	HIS	-	expression tag	UNP P20285
P	186	HIS	-	expression tag	UNP P20285
P	187	HIS	-	expression tag	UNP P20285
P	188	HIS	-	expression tag	UNP P20285
P	189	HIS	-	expression tag	UNP P20285
P	190	HIS	-	expression tag	UNP P20285
P	191	GLY	-	expression tag	UNP P20285
P	192	MET	-	expression tag	UNP P20285
P	193	ALA	-	expression tag	UNP P20285
P	194	SER	-	expression tag	UNP P20285
P	195	MET	-	expression tag	UNP P20285
P	196	THR	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
P	197	GLY	-	expression tag	UNP P20285
P	198	GLY	-	expression tag	UNP P20285
P	199	GLN	-	expression tag	UNP P20285
P	200	GLN	-	expression tag	UNP P20285
P	201	MET	-	expression tag	UNP P20285
P	202	GLY	-	expression tag	UNP P20285
P	203	ARG	-	expression tag	UNP P20285
P	204	ASP	-	expression tag	UNP P20285
P	205	LEU	-	expression tag	UNP P20285
P	206	TYR	-	expression tag	UNP P20285
P	207	ASP	-	expression tag	UNP P20285
P	208	ASP	-	expression tag	UNP P20285
P	209	ASP	-	expression tag	UNP P20285
P	210	ASP	-	expression tag	UNP P20285
P	211	LYS	-	expression tag	UNP P20285
P	212	ASP	-	expression tag	UNP P20285
P	213	ARG	-	expression tag	UNP P20285
P	214	TRP	-	expression tag	UNP P20285
P	215	GLY	-	expression tag	UNP P20285
P	216	SER	-	expression tag	UNP P20285
P	217	LEU	-	expression tag	UNP P20285
P	218	VAL	-	expression tag	UNP P20285
P	219	PRO	-	expression tag	UNP P20285
P	220	ARG	-	expression tag	UNP P20285
P	221	GLY	-	expression tag	UNP P20285
P	222	SER	-	expression tag	UNP P20285
P	223	HIS	-	expression tag	UNP P20285
P	224	MET	-	expression tag	UNP P20285
P	225	ALA	-	expression tag	UNP P20285
P	226	ALA	-	expression tag	UNP P20285
Q	181	MET	-	initiating methionine	UNP P20285
Q	182	ARG	-	expression tag	UNP P20285
Q	183	GLY	-	expression tag	UNP P20285
Q	184	SER	-	expression tag	UNP P20285
Q	185	HIS	-	expression tag	UNP P20285
Q	186	HIS	-	expression tag	UNP P20285
Q	187	HIS	-	expression tag	UNP P20285
Q	188	HIS	-	expression tag	UNP P20285
Q	189	HIS	-	expression tag	UNP P20285
Q	190	HIS	-	expression tag	UNP P20285
Q	191	GLY	-	expression tag	UNP P20285
Q	192	MET	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	193	ALA	-	expression tag	UNP P20285
Q	194	SER	-	expression tag	UNP P20285
Q	195	MET	-	expression tag	UNP P20285
Q	196	THR	-	expression tag	UNP P20285
Q	197	GLY	-	expression tag	UNP P20285
Q	198	GLY	-	expression tag	UNP P20285
Q	199	GLN	-	expression tag	UNP P20285
Q	200	GLN	-	expression tag	UNP P20285
Q	201	MET	-	expression tag	UNP P20285
Q	202	GLY	-	expression tag	UNP P20285
Q	203	ARG	-	expression tag	UNP P20285
Q	204	ASP	-	expression tag	UNP P20285
Q	205	LEU	-	expression tag	UNP P20285
Q	206	TYR	-	expression tag	UNP P20285
Q	207	ASP	-	expression tag	UNP P20285
Q	208	ASP	-	expression tag	UNP P20285
Q	209	ASP	-	expression tag	UNP P20285
Q	210	ASP	-	expression tag	UNP P20285
Q	211	LYS	-	expression tag	UNP P20285
Q	212	ASP	-	expression tag	UNP P20285
Q	213	ARG	-	expression tag	UNP P20285
Q	214	TRP	-	expression tag	UNP P20285
Q	215	GLY	-	expression tag	UNP P20285
Q	216	SER	-	expression tag	UNP P20285
Q	217	LEU	-	expression tag	UNP P20285
Q	218	VAL	-	expression tag	UNP P20285
Q	219	PRO	-	expression tag	UNP P20285
Q	220	ARG	-	expression tag	UNP P20285
Q	221	GLY	-	expression tag	UNP P20285
Q	222	SER	-	expression tag	UNP P20285
Q	223	HIS	-	expression tag	UNP P20285
Q	224	MET	-	expression tag	UNP P20285
Q	225	ALA	-	expression tag	UNP P20285
Q	226	ALA	-	expression tag	UNP P20285
R	181	MET	-	initiating methionine	UNP P20285
R	182	ARG	-	expression tag	UNP P20285
R	183	GLY	-	expression tag	UNP P20285
R	184	SER	-	expression tag	UNP P20285
R	185	HIS	-	expression tag	UNP P20285
R	186	HIS	-	expression tag	UNP P20285
R	187	HIS	-	expression tag	UNP P20285
R	188	HIS	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
R	189	HIS	-	expression tag	UNP P20285
R	190	HIS	-	expression tag	UNP P20285
R	191	GLY	-	expression tag	UNP P20285
R	192	MET	-	expression tag	UNP P20285
R	193	ALA	-	expression tag	UNP P20285
R	194	SER	-	expression tag	UNP P20285
R	195	MET	-	expression tag	UNP P20285
R	196	THR	-	expression tag	UNP P20285
R	197	GLY	-	expression tag	UNP P20285
R	198	GLY	-	expression tag	UNP P20285
R	199	GLN	-	expression tag	UNP P20285
R	200	GLN	-	expression tag	UNP P20285
R	201	MET	-	expression tag	UNP P20285
R	202	GLY	-	expression tag	UNP P20285
R	203	ARG	-	expression tag	UNP P20285
R	204	ASP	-	expression tag	UNP P20285
R	205	LEU	-	expression tag	UNP P20285
R	206	TYR	-	expression tag	UNP P20285
R	207	ASP	-	expression tag	UNP P20285
R	208	ASP	-	expression tag	UNP P20285
R	209	ASP	-	expression tag	UNP P20285
R	210	ASP	-	expression tag	UNP P20285
R	211	LYS	-	expression tag	UNP P20285
R	212	ASP	-	expression tag	UNP P20285
R	213	ARG	-	expression tag	UNP P20285
R	214	TRP	-	expression tag	UNP P20285
R	215	GLY	-	expression tag	UNP P20285
R	216	SER	-	expression tag	UNP P20285
R	217	LEU	-	expression tag	UNP P20285
R	218	VAL	-	expression tag	UNP P20285
R	219	PRO	-	expression tag	UNP P20285
R	220	ARG	-	expression tag	UNP P20285
R	221	GLY	-	expression tag	UNP P20285
R	222	SER	-	expression tag	UNP P20285
R	223	HIS	-	expression tag	UNP P20285
R	224	MET	-	expression tag	UNP P20285
R	225	ALA	-	expression tag	UNP P20285
R	226	ALA	-	expression tag	UNP P20285
S	181	MET	-	initiating methionine	UNP P20285
S	182	ARG	-	expression tag	UNP P20285
S	183	GLY	-	expression tag	UNP P20285
S	184	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
S	185	HIS	-	expression tag	UNP P20285
S	186	HIS	-	expression tag	UNP P20285
S	187	HIS	-	expression tag	UNP P20285
S	188	HIS	-	expression tag	UNP P20285
S	189	HIS	-	expression tag	UNP P20285
S	190	HIS	-	expression tag	UNP P20285
S	191	GLY	-	expression tag	UNP P20285
S	192	MET	-	expression tag	UNP P20285
S	193	ALA	-	expression tag	UNP P20285
S	194	SER	-	expression tag	UNP P20285
S	195	MET	-	expression tag	UNP P20285
S	196	THR	-	expression tag	UNP P20285
S	197	GLY	-	expression tag	UNP P20285
S	198	GLY	-	expression tag	UNP P20285
S	199	GLN	-	expression tag	UNP P20285
S	200	GLN	-	expression tag	UNP P20285
S	201	MET	-	expression tag	UNP P20285
S	202	GLY	-	expression tag	UNP P20285
S	203	ARG	-	expression tag	UNP P20285
S	204	ASP	-	expression tag	UNP P20285
S	205	LEU	-	expression tag	UNP P20285
S	206	TYR	-	expression tag	UNP P20285
S	207	ASP	-	expression tag	UNP P20285
S	208	ASP	-	expression tag	UNP P20285
S	209	ASP	-	expression tag	UNP P20285
S	210	ASP	-	expression tag	UNP P20285
S	211	LYS	-	expression tag	UNP P20285
S	212	ASP	-	expression tag	UNP P20285
S	213	ARG	-	expression tag	UNP P20285
S	214	TRP	-	expression tag	UNP P20285
S	215	GLY	-	expression tag	UNP P20285
S	216	SER	-	expression tag	UNP P20285
S	217	LEU	-	expression tag	UNP P20285
S	218	VAL	-	expression tag	UNP P20285
S	219	PRO	-	expression tag	UNP P20285
S	220	ARG	-	expression tag	UNP P20285
S	221	GLY	-	expression tag	UNP P20285
S	222	SER	-	expression tag	UNP P20285
S	223	HIS	-	expression tag	UNP P20285
S	224	MET	-	expression tag	UNP P20285
S	225	ALA	-	expression tag	UNP P20285
S	226	ALA	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
T	181	MET	-	initiating methionine	UNP P20285
T	182	ARG	-	expression tag	UNP P20285
T	183	GLY	-	expression tag	UNP P20285
T	184	SER	-	expression tag	UNP P20285
T	185	HIS	-	expression tag	UNP P20285
T	186	HIS	-	expression tag	UNP P20285
T	187	HIS	-	expression tag	UNP P20285
T	188	HIS	-	expression tag	UNP P20285
T	189	HIS	-	expression tag	UNP P20285
T	190	HIS	-	expression tag	UNP P20285
T	191	GLY	-	expression tag	UNP P20285
T	192	MET	-	expression tag	UNP P20285
T	193	ALA	-	expression tag	UNP P20285
T	194	SER	-	expression tag	UNP P20285
T	195	MET	-	expression tag	UNP P20285
T	196	THR	-	expression tag	UNP P20285
T	197	GLY	-	expression tag	UNP P20285
T	198	GLY	-	expression tag	UNP P20285
T	199	GLN	-	expression tag	UNP P20285
T	200	GLN	-	expression tag	UNP P20285
T	201	MET	-	expression tag	UNP P20285
T	202	GLY	-	expression tag	UNP P20285
T	203	ARG	-	expression tag	UNP P20285
T	204	ASP	-	expression tag	UNP P20285
T	205	LEU	-	expression tag	UNP P20285
T	206	TYR	-	expression tag	UNP P20285
T	207	ASP	-	expression tag	UNP P20285
T	208	ASP	-	expression tag	UNP P20285
T	209	ASP	-	expression tag	UNP P20285
T	210	ASP	-	expression tag	UNP P20285
T	211	LYS	-	expression tag	UNP P20285
T	212	ASP	-	expression tag	UNP P20285
T	213	ARG	-	expression tag	UNP P20285
T	214	TRP	-	expression tag	UNP P20285
T	215	GLY	-	expression tag	UNP P20285
T	216	SER	-	expression tag	UNP P20285
T	217	LEU	-	expression tag	UNP P20285
T	218	VAL	-	expression tag	UNP P20285
T	219	PRO	-	expression tag	UNP P20285
T	220	ARG	-	expression tag	UNP P20285
T	221	GLY	-	expression tag	UNP P20285
T	222	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
T	223	HIS	-	expression tag	UNP P20285
T	224	MET	-	expression tag	UNP P20285
T	225	ALA	-	expression tag	UNP P20285
T	226	ALA	-	expression tag	UNP P20285
V	181	MET	-	initiating methionine	UNP P20285
V	182	ARG	-	expression tag	UNP P20285
V	183	GLY	-	expression tag	UNP P20285
V	184	SER	-	expression tag	UNP P20285
V	185	HIS	-	expression tag	UNP P20285
V	186	HIS	-	expression tag	UNP P20285
V	187	HIS	-	expression tag	UNP P20285
V	188	HIS	-	expression tag	UNP P20285
V	189	HIS	-	expression tag	UNP P20285
V	190	HIS	-	expression tag	UNP P20285
V	191	GLY	-	expression tag	UNP P20285
V	192	MET	-	expression tag	UNP P20285
V	193	ALA	-	expression tag	UNP P20285
V	194	SER	-	expression tag	UNP P20285
V	195	MET	-	expression tag	UNP P20285
V	196	THR	-	expression tag	UNP P20285
V	197	GLY	-	expression tag	UNP P20285
V	198	GLY	-	expression tag	UNP P20285
V	199	GLN	-	expression tag	UNP P20285
V	200	GLN	-	expression tag	UNP P20285
V	201	MET	-	expression tag	UNP P20285
V	202	GLY	-	expression tag	UNP P20285
V	203	ARG	-	expression tag	UNP P20285
V	204	ASP	-	expression tag	UNP P20285
V	205	LEU	-	expression tag	UNP P20285
V	206	TYR	-	expression tag	UNP P20285
V	207	ASP	-	expression tag	UNP P20285
V	208	ASP	-	expression tag	UNP P20285
V	209	ASP	-	expression tag	UNP P20285
V	210	ASP	-	expression tag	UNP P20285
V	211	LYS	-	expression tag	UNP P20285
V	212	ASP	-	expression tag	UNP P20285
V	213	ARG	-	expression tag	UNP P20285
V	214	TRP	-	expression tag	UNP P20285
V	215	GLY	-	expression tag	UNP P20285
V	216	SER	-	expression tag	UNP P20285
V	217	LEU	-	expression tag	UNP P20285
V	218	VAL	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
V	219	PRO	-	expression tag	UNP P20285
V	220	ARG	-	expression tag	UNP P20285
V	221	GLY	-	expression tag	UNP P20285
V	222	SER	-	expression tag	UNP P20285
V	223	HIS	-	expression tag	UNP P20285
V	224	MET	-	expression tag	UNP P20285
V	225	ALA	-	expression tag	UNP P20285
V	226	ALA	-	expression tag	UNP P20285
W	181	MET	-	initiating methionine	UNP P20285
W	182	ARG	-	expression tag	UNP P20285
W	183	GLY	-	expression tag	UNP P20285
W	184	SER	-	expression tag	UNP P20285
W	185	HIS	-	expression tag	UNP P20285
W	186	HIS	-	expression tag	UNP P20285
W	187	HIS	-	expression tag	UNP P20285
W	188	HIS	-	expression tag	UNP P20285
W	189	HIS	-	expression tag	UNP P20285
W	190	HIS	-	expression tag	UNP P20285
W	191	GLY	-	expression tag	UNP P20285
W	192	MET	-	expression tag	UNP P20285
W	193	ALA	-	expression tag	UNP P20285
W	194	SER	-	expression tag	UNP P20285
W	195	MET	-	expression tag	UNP P20285
W	196	THR	-	expression tag	UNP P20285
W	197	GLY	-	expression tag	UNP P20285
W	198	GLY	-	expression tag	UNP P20285
W	199	GLN	-	expression tag	UNP P20285
W	200	GLN	-	expression tag	UNP P20285
W	201	MET	-	expression tag	UNP P20285
W	202	GLY	-	expression tag	UNP P20285
W	203	ARG	-	expression tag	UNP P20285
W	204	ASP	-	expression tag	UNP P20285
W	205	LEU	-	expression tag	UNP P20285
W	206	TYR	-	expression tag	UNP P20285
W	207	ASP	-	expression tag	UNP P20285
W	208	ASP	-	expression tag	UNP P20285
W	209	ASP	-	expression tag	UNP P20285
W	210	ASP	-	expression tag	UNP P20285
W	211	LYS	-	expression tag	UNP P20285
W	212	ASP	-	expression tag	UNP P20285
W	213	ARG	-	expression tag	UNP P20285
W	214	TRP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
W	215	GLY	-	expression tag	UNP P20285
W	216	SER	-	expression tag	UNP P20285
W	217	LEU	-	expression tag	UNP P20285
W	218	VAL	-	expression tag	UNP P20285
W	219	PRO	-	expression tag	UNP P20285
W	220	ARG	-	expression tag	UNP P20285
W	221	GLY	-	expression tag	UNP P20285
W	222	SER	-	expression tag	UNP P20285
W	223	HIS	-	expression tag	UNP P20285
W	224	MET	-	expression tag	UNP P20285
W	225	ALA	-	expression tag	UNP P20285
W	226	ALA	-	expression tag	UNP P20285
X	181	MET	-	initiating methionine	UNP P20285
X	182	ARG	-	expression tag	UNP P20285
X	183	GLY	-	expression tag	UNP P20285
X	184	SER	-	expression tag	UNP P20285
X	185	HIS	-	expression tag	UNP P20285
X	186	HIS	-	expression tag	UNP P20285
X	187	HIS	-	expression tag	UNP P20285
X	188	HIS	-	expression tag	UNP P20285
X	189	HIS	-	expression tag	UNP P20285
X	190	HIS	-	expression tag	UNP P20285
X	191	GLY	-	expression tag	UNP P20285
X	192	MET	-	expression tag	UNP P20285
X	193	ALA	-	expression tag	UNP P20285
X	194	SER	-	expression tag	UNP P20285
X	195	MET	-	expression tag	UNP P20285
X	196	THR	-	expression tag	UNP P20285
X	197	GLY	-	expression tag	UNP P20285
X	198	GLY	-	expression tag	UNP P20285
X	199	GLN	-	expression tag	UNP P20285
X	200	GLN	-	expression tag	UNP P20285
X	201	MET	-	expression tag	UNP P20285
X	202	GLY	-	expression tag	UNP P20285
X	203	ARG	-	expression tag	UNP P20285
X	204	ASP	-	expression tag	UNP P20285
X	205	LEU	-	expression tag	UNP P20285
X	206	TYR	-	expression tag	UNP P20285
X	207	ASP	-	expression tag	UNP P20285
X	208	ASP	-	expression tag	UNP P20285
X	209	ASP	-	expression tag	UNP P20285
X	210	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
X	211	LYS	-	expression tag	UNP P20285
X	212	ASP	-	expression tag	UNP P20285
X	213	ARG	-	expression tag	UNP P20285
X	214	TRP	-	expression tag	UNP P20285
X	215	GLY	-	expression tag	UNP P20285
X	216	SER	-	expression tag	UNP P20285
X	217	LEU	-	expression tag	UNP P20285
X	218	VAL	-	expression tag	UNP P20285
X	219	PRO	-	expression tag	UNP P20285
X	220	ARG	-	expression tag	UNP P20285
X	221	GLY	-	expression tag	UNP P20285
X	222	SER	-	expression tag	UNP P20285
X	223	HIS	-	expression tag	UNP P20285
X	224	MET	-	expression tag	UNP P20285
X	225	ALA	-	expression tag	UNP P20285
X	226	ALA	-	expression tag	UNP P20285
Y	181	MET	-	initiating methionine	UNP P20285
Y	182	ARG	-	expression tag	UNP P20285
Y	183	GLY	-	expression tag	UNP P20285
Y	184	SER	-	expression tag	UNP P20285
Y	185	HIS	-	expression tag	UNP P20285
Y	186	HIS	-	expression tag	UNP P20285
Y	187	HIS	-	expression tag	UNP P20285
Y	188	HIS	-	expression tag	UNP P20285
Y	189	HIS	-	expression tag	UNP P20285
Y	190	HIS	-	expression tag	UNP P20285
Y	191	GLY	-	expression tag	UNP P20285
Y	192	MET	-	expression tag	UNP P20285
Y	193	ALA	-	expression tag	UNP P20285
Y	194	SER	-	expression tag	UNP P20285
Y	195	MET	-	expression tag	UNP P20285
Y	196	THR	-	expression tag	UNP P20285
Y	197	GLY	-	expression tag	UNP P20285
Y	198	GLY	-	expression tag	UNP P20285
Y	199	GLN	-	expression tag	UNP P20285
Y	200	GLN	-	expression tag	UNP P20285
Y	201	MET	-	expression tag	UNP P20285
Y	202	GLY	-	expression tag	UNP P20285
Y	203	ARG	-	expression tag	UNP P20285
Y	204	ASP	-	expression tag	UNP P20285
Y	205	LEU	-	expression tag	UNP P20285
Y	206	TYR	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	207	ASP	-	expression tag	UNP P20285
Y	208	ASP	-	expression tag	UNP P20285
Y	209	ASP	-	expression tag	UNP P20285
Y	210	ASP	-	expression tag	UNP P20285
Y	211	LYS	-	expression tag	UNP P20285
Y	212	ASP	-	expression tag	UNP P20285
Y	213	ARG	-	expression tag	UNP P20285
Y	214	TRP	-	expression tag	UNP P20285
Y	215	GLY	-	expression tag	UNP P20285
Y	216	SER	-	expression tag	UNP P20285
Y	217	LEU	-	expression tag	UNP P20285
Y	218	VAL	-	expression tag	UNP P20285
Y	219	PRO	-	expression tag	UNP P20285
Y	220	ARG	-	expression tag	UNP P20285
Y	221	GLY	-	expression tag	UNP P20285
Y	222	SER	-	expression tag	UNP P20285
Y	223	HIS	-	expression tag	UNP P20285
Y	224	MET	-	expression tag	UNP P20285
Y	225	ALA	-	expression tag	UNP P20285
Y	226	ALA	-	expression tag	UNP P20285
Z	181	MET	-	initiating methionine	UNP P20285
Z	182	ARG	-	expression tag	UNP P20285
Z	183	GLY	-	expression tag	UNP P20285
Z	184	SER	-	expression tag	UNP P20285
Z	185	HIS	-	expression tag	UNP P20285
Z	186	HIS	-	expression tag	UNP P20285
Z	187	HIS	-	expression tag	UNP P20285
Z	188	HIS	-	expression tag	UNP P20285
Z	189	HIS	-	expression tag	UNP P20285
Z	190	HIS	-	expression tag	UNP P20285
Z	191	GLY	-	expression tag	UNP P20285
Z	192	MET	-	expression tag	UNP P20285
Z	193	ALA	-	expression tag	UNP P20285
Z	194	SER	-	expression tag	UNP P20285
Z	195	MET	-	expression tag	UNP P20285
Z	196	THR	-	expression tag	UNP P20285
Z	197	GLY	-	expression tag	UNP P20285
Z	198	GLY	-	expression tag	UNP P20285
Z	199	GLN	-	expression tag	UNP P20285
Z	200	GLN	-	expression tag	UNP P20285
Z	201	MET	-	expression tag	UNP P20285
Z	202	GLY	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	203	ARG	-	expression tag	UNP P20285
Z	204	ASP	-	expression tag	UNP P20285
Z	205	LEU	-	expression tag	UNP P20285
Z	206	TYR	-	expression tag	UNP P20285
Z	207	ASP	-	expression tag	UNP P20285
Z	208	ASP	-	expression tag	UNP P20285
Z	209	ASP	-	expression tag	UNP P20285
Z	210	ASP	-	expression tag	UNP P20285
Z	211	LYS	-	expression tag	UNP P20285
Z	212	ASP	-	expression tag	UNP P20285
Z	213	ARG	-	expression tag	UNP P20285
Z	214	TRP	-	expression tag	UNP P20285
Z	215	GLY	-	expression tag	UNP P20285
Z	216	SER	-	expression tag	UNP P20285
Z	217	LEU	-	expression tag	UNP P20285
Z	218	VAL	-	expression tag	UNP P20285
Z	219	PRO	-	expression tag	UNP P20285
Z	220	ARG	-	expression tag	UNP P20285
Z	221	GLY	-	expression tag	UNP P20285
Z	222	SER	-	expression tag	UNP P20285
Z	223	HIS	-	expression tag	UNP P20285
Z	224	MET	-	expression tag	UNP P20285
Z	225	ALA	-	expression tag	UNP P20285
Z	226	ALA	-	expression tag	UNP P20285
AA	181	MET	-	initiating methionine	UNP P20285
AA	182	ARG	-	expression tag	UNP P20285
AA	183	GLY	-	expression tag	UNP P20285
AA	184	SER	-	expression tag	UNP P20285
AA	185	HIS	-	expression tag	UNP P20285
AA	186	HIS	-	expression tag	UNP P20285
AA	187	HIS	-	expression tag	UNP P20285
AA	188	HIS	-	expression tag	UNP P20285
AA	189	HIS	-	expression tag	UNP P20285
AA	190	HIS	-	expression tag	UNP P20285
AA	191	GLY	-	expression tag	UNP P20285
AA	192	MET	-	expression tag	UNP P20285
AA	193	ALA	-	expression tag	UNP P20285
AA	194	SER	-	expression tag	UNP P20285
AA	195	MET	-	expression tag	UNP P20285
AA	196	THR	-	expression tag	UNP P20285
AA	197	GLY	-	expression tag	UNP P20285
AA	198	GLY	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
AA	199	GLN	-	expression tag	UNP P20285
AA	200	GLN	-	expression tag	UNP P20285
AA	201	MET	-	expression tag	UNP P20285
AA	202	GLY	-	expression tag	UNP P20285
AA	203	ARG	-	expression tag	UNP P20285
AA	204	ASP	-	expression tag	UNP P20285
AA	205	LEU	-	expression tag	UNP P20285
AA	206	TYR	-	expression tag	UNP P20285
AA	207	ASP	-	expression tag	UNP P20285
AA	208	ASP	-	expression tag	UNP P20285
AA	209	ASP	-	expression tag	UNP P20285
AA	210	ASP	-	expression tag	UNP P20285
AA	211	LYS	-	expression tag	UNP P20285
AA	212	ASP	-	expression tag	UNP P20285
AA	213	ARG	-	expression tag	UNP P20285
AA	214	TRP	-	expression tag	UNP P20285
AA	215	GLY	-	expression tag	UNP P20285
AA	216	SER	-	expression tag	UNP P20285
AA	217	LEU	-	expression tag	UNP P20285
AA	218	VAL	-	expression tag	UNP P20285
AA	219	PRO	-	expression tag	UNP P20285
AA	220	ARG	-	expression tag	UNP P20285
AA	221	GLY	-	expression tag	UNP P20285
AA	222	SER	-	expression tag	UNP P20285
AA	223	HIS	-	expression tag	UNP P20285
AA	224	MET	-	expression tag	UNP P20285
AA	225	ALA	-	expression tag	UNP P20285
AA	226	ALA	-	expression tag	UNP P20285
BA	181	MET	-	initiating methionine	UNP P20285
BA	182	ARG	-	expression tag	UNP P20285
BA	183	GLY	-	expression tag	UNP P20285
BA	184	SER	-	expression tag	UNP P20285
BA	185	HIS	-	expression tag	UNP P20285
BA	186	HIS	-	expression tag	UNP P20285
BA	187	HIS	-	expression tag	UNP P20285
BA	188	HIS	-	expression tag	UNP P20285
BA	189	HIS	-	expression tag	UNP P20285
BA	190	HIS	-	expression tag	UNP P20285
BA	191	GLY	-	expression tag	UNP P20285
BA	192	MET	-	expression tag	UNP P20285
BA	193	ALA	-	expression tag	UNP P20285
BA	194	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	195	MET	-	expression tag	UNP P20285
BA	196	THR	-	expression tag	UNP P20285
BA	197	GLY	-	expression tag	UNP P20285
BA	198	GLY	-	expression tag	UNP P20285
BA	199	GLN	-	expression tag	UNP P20285
BA	200	GLN	-	expression tag	UNP P20285
BA	201	MET	-	expression tag	UNP P20285
BA	202	GLY	-	expression tag	UNP P20285
BA	203	ARG	-	expression tag	UNP P20285
BA	204	ASP	-	expression tag	UNP P20285
BA	205	LEU	-	expression tag	UNP P20285
BA	206	TYR	-	expression tag	UNP P20285
BA	207	ASP	-	expression tag	UNP P20285
BA	208	ASP	-	expression tag	UNP P20285
BA	209	ASP	-	expression tag	UNP P20285
BA	210	ASP	-	expression tag	UNP P20285
BA	211	LYS	-	expression tag	UNP P20285
BA	212	ASP	-	expression tag	UNP P20285
BA	213	ARG	-	expression tag	UNP P20285
BA	214	TRP	-	expression tag	UNP P20285
BA	215	GLY	-	expression tag	UNP P20285
BA	216	SER	-	expression tag	UNP P20285
BA	217	LEU	-	expression tag	UNP P20285
BA	218	VAL	-	expression tag	UNP P20285
BA	219	PRO	-	expression tag	UNP P20285
BA	220	ARG	-	expression tag	UNP P20285
BA	221	GLY	-	expression tag	UNP P20285
BA	222	SER	-	expression tag	UNP P20285
BA	223	HIS	-	expression tag	UNP P20285
BA	224	MET	-	expression tag	UNP P20285
BA	225	ALA	-	expression tag	UNP P20285
BA	226	ALA	-	expression tag	UNP P20285
CA	181	MET	-	initiating methionine	UNP P20285
CA	182	ARG	-	expression tag	UNP P20285
CA	183	GLY	-	expression tag	UNP P20285
CA	184	SER	-	expression tag	UNP P20285
CA	185	HIS	-	expression tag	UNP P20285
CA	186	HIS	-	expression tag	UNP P20285
CA	187	HIS	-	expression tag	UNP P20285
CA	188	HIS	-	expression tag	UNP P20285
CA	189	HIS	-	expression tag	UNP P20285
CA	190	HIS	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
CA	191	GLY	-	expression tag	UNP P20285
CA	192	MET	-	expression tag	UNP P20285
CA	193	ALA	-	expression tag	UNP P20285
CA	194	SER	-	expression tag	UNP P20285
CA	195	MET	-	expression tag	UNP P20285
CA	196	THR	-	expression tag	UNP P20285
CA	197	GLY	-	expression tag	UNP P20285
CA	198	GLY	-	expression tag	UNP P20285
CA	199	GLN	-	expression tag	UNP P20285
CA	200	GLN	-	expression tag	UNP P20285
CA	201	MET	-	expression tag	UNP P20285
CA	202	GLY	-	expression tag	UNP P20285
CA	203	ARG	-	expression tag	UNP P20285
CA	204	ASP	-	expression tag	UNP P20285
CA	205	LEU	-	expression tag	UNP P20285
CA	206	TYR	-	expression tag	UNP P20285
CA	207	ASP	-	expression tag	UNP P20285
CA	208	ASP	-	expression tag	UNP P20285
CA	209	ASP	-	expression tag	UNP P20285
CA	210	ASP	-	expression tag	UNP P20285
CA	211	LYS	-	expression tag	UNP P20285
CA	212	ASP	-	expression tag	UNP P20285
CA	213	ARG	-	expression tag	UNP P20285
CA	214	TRP	-	expression tag	UNP P20285
CA	215	GLY	-	expression tag	UNP P20285
CA	216	SER	-	expression tag	UNP P20285
CA	217	LEU	-	expression tag	UNP P20285
CA	218	VAL	-	expression tag	UNP P20285
CA	219	PRO	-	expression tag	UNP P20285
CA	220	ARG	-	expression tag	UNP P20285
CA	221	GLY	-	expression tag	UNP P20285
CA	222	SER	-	expression tag	UNP P20285
CA	223	HIS	-	expression tag	UNP P20285
CA	224	MET	-	expression tag	UNP P20285
CA	225	ALA	-	expression tag	UNP P20285
CA	226	ALA	-	expression tag	UNP P20285
DA	181	MET	-	initiating methionine	UNP P20285
DA	182	ARG	-	expression tag	UNP P20285
DA	183	GLY	-	expression tag	UNP P20285
DA	184	SER	-	expression tag	UNP P20285
DA	185	HIS	-	expression tag	UNP P20285
DA	186	HIS	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	187	HIS	-	expression tag	UNP P20285
DA	188	HIS	-	expression tag	UNP P20285
DA	189	HIS	-	expression tag	UNP P20285
DA	190	HIS	-	expression tag	UNP P20285
DA	191	GLY	-	expression tag	UNP P20285
DA	192	MET	-	expression tag	UNP P20285
DA	193	ALA	-	expression tag	UNP P20285
DA	194	SER	-	expression tag	UNP P20285
DA	195	MET	-	expression tag	UNP P20285
DA	196	THR	-	expression tag	UNP P20285
DA	197	GLY	-	expression tag	UNP P20285
DA	198	GLY	-	expression tag	UNP P20285
DA	199	GLN	-	expression tag	UNP P20285
DA	200	GLN	-	expression tag	UNP P20285
DA	201	MET	-	expression tag	UNP P20285
DA	202	GLY	-	expression tag	UNP P20285
DA	203	ARG	-	expression tag	UNP P20285
DA	204	ASP	-	expression tag	UNP P20285
DA	205	LEU	-	expression tag	UNP P20285
DA	206	TYR	-	expression tag	UNP P20285
DA	207	ASP	-	expression tag	UNP P20285
DA	208	ASP	-	expression tag	UNP P20285
DA	209	ASP	-	expression tag	UNP P20285
DA	210	ASP	-	expression tag	UNP P20285
DA	211	LYS	-	expression tag	UNP P20285
DA	212	ASP	-	expression tag	UNP P20285
DA	213	ARG	-	expression tag	UNP P20285
DA	214	TRP	-	expression tag	UNP P20285
DA	215	GLY	-	expression tag	UNP P20285
DA	216	SER	-	expression tag	UNP P20285
DA	217	LEU	-	expression tag	UNP P20285
DA	218	VAL	-	expression tag	UNP P20285
DA	219	PRO	-	expression tag	UNP P20285
DA	220	ARG	-	expression tag	UNP P20285
DA	221	GLY	-	expression tag	UNP P20285
DA	222	SER	-	expression tag	UNP P20285
DA	223	HIS	-	expression tag	UNP P20285
DA	224	MET	-	expression tag	UNP P20285
DA	225	ALA	-	expression tag	UNP P20285
DA	226	ALA	-	expression tag	UNP P20285
EA	181	MET	-	initiating methionine	UNP P20285
EA	182	ARG	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
EA	183	GLY	-	expression tag	UNP P20285
EA	184	SER	-	expression tag	UNP P20285
EA	185	HIS	-	expression tag	UNP P20285
EA	186	HIS	-	expression tag	UNP P20285
EA	187	HIS	-	expression tag	UNP P20285
EA	188	HIS	-	expression tag	UNP P20285
EA	189	HIS	-	expression tag	UNP P20285
EA	190	HIS	-	expression tag	UNP P20285
EA	191	GLY	-	expression tag	UNP P20285
EA	192	MET	-	expression tag	UNP P20285
EA	193	ALA	-	expression tag	UNP P20285
EA	194	SER	-	expression tag	UNP P20285
EA	195	MET	-	expression tag	UNP P20285
EA	196	THR	-	expression tag	UNP P20285
EA	197	GLY	-	expression tag	UNP P20285
EA	198	GLY	-	expression tag	UNP P20285
EA	199	GLN	-	expression tag	UNP P20285
EA	200	GLN	-	expression tag	UNP P20285
EA	201	MET	-	expression tag	UNP P20285
EA	202	GLY	-	expression tag	UNP P20285
EA	203	ARG	-	expression tag	UNP P20285
EA	204	ASP	-	expression tag	UNP P20285
EA	205	LEU	-	expression tag	UNP P20285
EA	206	TYR	-	expression tag	UNP P20285
EA	207	ASP	-	expression tag	UNP P20285
EA	208	ASP	-	expression tag	UNP P20285
EA	209	ASP	-	expression tag	UNP P20285
EA	210	ASP	-	expression tag	UNP P20285
EA	211	LYS	-	expression tag	UNP P20285
EA	212	ASP	-	expression tag	UNP P20285
EA	213	ARG	-	expression tag	UNP P20285
EA	214	TRP	-	expression tag	UNP P20285
EA	215	GLY	-	expression tag	UNP P20285
EA	216	SER	-	expression tag	UNP P20285
EA	217	LEU	-	expression tag	UNP P20285
EA	218	VAL	-	expression tag	UNP P20285
EA	219	PRO	-	expression tag	UNP P20285
EA	220	ARG	-	expression tag	UNP P20285
EA	221	GLY	-	expression tag	UNP P20285
EA	222	SER	-	expression tag	UNP P20285
EA	223	HIS	-	expression tag	UNP P20285
EA	224	MET	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
EA	225	ALA	-	expression tag	UNP P20285
EA	226	ALA	-	expression tag	UNP P20285
FA	181	MET	-	initiating methionine	UNP P20285
FA	182	ARG	-	expression tag	UNP P20285
FA	183	GLY	-	expression tag	UNP P20285
FA	184	SER	-	expression tag	UNP P20285
FA	185	HIS	-	expression tag	UNP P20285
FA	186	HIS	-	expression tag	UNP P20285
FA	187	HIS	-	expression tag	UNP P20285
FA	188	HIS	-	expression tag	UNP P20285
FA	189	HIS	-	expression tag	UNP P20285
FA	190	HIS	-	expression tag	UNP P20285
FA	191	GLY	-	expression tag	UNP P20285
FA	192	MET	-	expression tag	UNP P20285
FA	193	ALA	-	expression tag	UNP P20285
FA	194	SER	-	expression tag	UNP P20285
FA	195	MET	-	expression tag	UNP P20285
FA	196	THR	-	expression tag	UNP P20285
FA	197	GLY	-	expression tag	UNP P20285
FA	198	GLY	-	expression tag	UNP P20285
FA	199	GLN	-	expression tag	UNP P20285
FA	200	GLN	-	expression tag	UNP P20285
FA	201	MET	-	expression tag	UNP P20285
FA	202	GLY	-	expression tag	UNP P20285
FA	203	ARG	-	expression tag	UNP P20285
FA	204	ASP	-	expression tag	UNP P20285
FA	205	LEU	-	expression tag	UNP P20285
FA	206	TYR	-	expression tag	UNP P20285
FA	207	ASP	-	expression tag	UNP P20285
FA	208	ASP	-	expression tag	UNP P20285
FA	209	ASP	-	expression tag	UNP P20285
FA	210	ASP	-	expression tag	UNP P20285
FA	211	LYS	-	expression tag	UNP P20285
FA	212	ASP	-	expression tag	UNP P20285
FA	213	ARG	-	expression tag	UNP P20285
FA	214	TRP	-	expression tag	UNP P20285
FA	215	GLY	-	expression tag	UNP P20285
FA	216	SER	-	expression tag	UNP P20285
FA	217	LEU	-	expression tag	UNP P20285
FA	218	VAL	-	expression tag	UNP P20285
FA	219	PRO	-	expression tag	UNP P20285
FA	220	ARG	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
FA	221	GLY	-	expression tag	UNP P20285
FA	222	SER	-	expression tag	UNP P20285
FA	223	HIS	-	expression tag	UNP P20285
FA	224	MET	-	expression tag	UNP P20285
FA	225	ALA	-	expression tag	UNP P20285
FA	226	ALA	-	expression tag	UNP P20285
GA	181	MET	-	initiating methionine	UNP P20285
GA	182	ARG	-	expression tag	UNP P20285
GA	183	GLY	-	expression tag	UNP P20285
GA	184	SER	-	expression tag	UNP P20285
GA	185	HIS	-	expression tag	UNP P20285
GA	186	HIS	-	expression tag	UNP P20285
GA	187	HIS	-	expression tag	UNP P20285
GA	188	HIS	-	expression tag	UNP P20285
GA	189	HIS	-	expression tag	UNP P20285
GA	190	HIS	-	expression tag	UNP P20285
GA	191	GLY	-	expression tag	UNP P20285
GA	192	MET	-	expression tag	UNP P20285
GA	193	ALA	-	expression tag	UNP P20285
GA	194	SER	-	expression tag	UNP P20285
GA	195	MET	-	expression tag	UNP P20285
GA	196	THR	-	expression tag	UNP P20285
GA	197	GLY	-	expression tag	UNP P20285
GA	198	GLY	-	expression tag	UNP P20285
GA	199	GLN	-	expression tag	UNP P20285
GA	200	GLN	-	expression tag	UNP P20285
GA	201	MET	-	expression tag	UNP P20285
GA	202	GLY	-	expression tag	UNP P20285
GA	203	ARG	-	expression tag	UNP P20285
GA	204	ASP	-	expression tag	UNP P20285
GA	205	LEU	-	expression tag	UNP P20285
GA	206	TYR	-	expression tag	UNP P20285
GA	207	ASP	-	expression tag	UNP P20285
GA	208	ASP	-	expression tag	UNP P20285
GA	209	ASP	-	expression tag	UNP P20285
GA	210	ASP	-	expression tag	UNP P20285
GA	211	LYS	-	expression tag	UNP P20285
GA	212	ASP	-	expression tag	UNP P20285
GA	213	ARG	-	expression tag	UNP P20285
GA	214	TRP	-	expression tag	UNP P20285
GA	215	GLY	-	expression tag	UNP P20285
GA	216	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
GA	217	LEU	-	expression tag	UNP P20285
GA	218	VAL	-	expression tag	UNP P20285
GA	219	PRO	-	expression tag	UNP P20285
GA	220	ARG	-	expression tag	UNP P20285
GA	221	GLY	-	expression tag	UNP P20285
GA	222	SER	-	expression tag	UNP P20285
GA	223	HIS	-	expression tag	UNP P20285
GA	224	MET	-	expression tag	UNP P20285
GA	225	ALA	-	expression tag	UNP P20285
GA	226	ALA	-	expression tag	UNP P20285
HA	181	MET	-	initiating methionine	UNP P20285
HA	182	ARG	-	expression tag	UNP P20285
HA	183	GLY	-	expression tag	UNP P20285
HA	184	SER	-	expression tag	UNP P20285
HA	185	HIS	-	expression tag	UNP P20285
HA	186	HIS	-	expression tag	UNP P20285
HA	187	HIS	-	expression tag	UNP P20285
HA	188	HIS	-	expression tag	UNP P20285
HA	189	HIS	-	expression tag	UNP P20285
HA	190	HIS	-	expression tag	UNP P20285
HA	191	GLY	-	expression tag	UNP P20285
HA	192	MET	-	expression tag	UNP P20285
HA	193	ALA	-	expression tag	UNP P20285
HA	194	SER	-	expression tag	UNP P20285
HA	195	MET	-	expression tag	UNP P20285
HA	196	THR	-	expression tag	UNP P20285
HA	197	GLY	-	expression tag	UNP P20285
HA	198	GLY	-	expression tag	UNP P20285
HA	199	GLN	-	expression tag	UNP P20285
HA	200	GLN	-	expression tag	UNP P20285
HA	201	MET	-	expression tag	UNP P20285
HA	202	GLY	-	expression tag	UNP P20285
HA	203	ARG	-	expression tag	UNP P20285
HA	204	ASP	-	expression tag	UNP P20285
HA	205	LEU	-	expression tag	UNP P20285
HA	206	TYR	-	expression tag	UNP P20285
HA	207	ASP	-	expression tag	UNP P20285
HA	208	ASP	-	expression tag	UNP P20285
HA	209	ASP	-	expression tag	UNP P20285
HA	210	ASP	-	expression tag	UNP P20285
HA	211	LYS	-	expression tag	UNP P20285
HA	212	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
HA	213	ARG	-	expression tag	UNP P20285
HA	214	TRP	-	expression tag	UNP P20285
HA	215	GLY	-	expression tag	UNP P20285
HA	216	SER	-	expression tag	UNP P20285
HA	217	LEU	-	expression tag	UNP P20285
HA	218	VAL	-	expression tag	UNP P20285
HA	219	PRO	-	expression tag	UNP P20285
HA	220	ARG	-	expression tag	UNP P20285
HA	221	GLY	-	expression tag	UNP P20285
HA	222	SER	-	expression tag	UNP P20285
HA	223	HIS	-	expression tag	UNP P20285
HA	224	MET	-	expression tag	UNP P20285
HA	225	ALA	-	expression tag	UNP P20285
HA	226	ALA	-	expression tag	UNP P20285
IA	181	MET	-	initiating methionine	UNP P20285
IA	182	ARG	-	expression tag	UNP P20285
IA	183	GLY	-	expression tag	UNP P20285
IA	184	SER	-	expression tag	UNP P20285
IA	185	HIS	-	expression tag	UNP P20285
IA	186	HIS	-	expression tag	UNP P20285
IA	187	HIS	-	expression tag	UNP P20285
IA	188	HIS	-	expression tag	UNP P20285
IA	189	HIS	-	expression tag	UNP P20285
IA	190	HIS	-	expression tag	UNP P20285
IA	191	GLY	-	expression tag	UNP P20285
IA	192	MET	-	expression tag	UNP P20285
IA	193	ALA	-	expression tag	UNP P20285
IA	194	SER	-	expression tag	UNP P20285
IA	195	MET	-	expression tag	UNP P20285
IA	196	THR	-	expression tag	UNP P20285
IA	197	GLY	-	expression tag	UNP P20285
IA	198	GLY	-	expression tag	UNP P20285
IA	199	GLN	-	expression tag	UNP P20285
IA	200	GLN	-	expression tag	UNP P20285
IA	201	MET	-	expression tag	UNP P20285
IA	202	GLY	-	expression tag	UNP P20285
IA	203	ARG	-	expression tag	UNP P20285
IA	204	ASP	-	expression tag	UNP P20285
IA	205	LEU	-	expression tag	UNP P20285
IA	206	TYR	-	expression tag	UNP P20285
IA	207	ASP	-	expression tag	UNP P20285
IA	208	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
IA	209	ASP	-	expression tag	UNP P20285
IA	210	ASP	-	expression tag	UNP P20285
IA	211	LYS	-	expression tag	UNP P20285
IA	212	ASP	-	expression tag	UNP P20285
IA	213	ARG	-	expression tag	UNP P20285
IA	214	TRP	-	expression tag	UNP P20285
IA	215	GLY	-	expression tag	UNP P20285
IA	216	SER	-	expression tag	UNP P20285
IA	217	LEU	-	expression tag	UNP P20285
IA	218	VAL	-	expression tag	UNP P20285
IA	219	PRO	-	expression tag	UNP P20285
IA	220	ARG	-	expression tag	UNP P20285
IA	221	GLY	-	expression tag	UNP P20285
IA	222	SER	-	expression tag	UNP P20285
IA	223	HIS	-	expression tag	UNP P20285
IA	224	MET	-	expression tag	UNP P20285
IA	225	ALA	-	expression tag	UNP P20285
IA	226	ALA	-	expression tag	UNP P20285
JA	181	MET	-	initiating methionine	UNP P20285
JA	182	ARG	-	expression tag	UNP P20285
JA	183	GLY	-	expression tag	UNP P20285
JA	184	SER	-	expression tag	UNP P20285
JA	185	HIS	-	expression tag	UNP P20285
JA	186	HIS	-	expression tag	UNP P20285
JA	187	HIS	-	expression tag	UNP P20285
JA	188	HIS	-	expression tag	UNP P20285
JA	189	HIS	-	expression tag	UNP P20285
JA	190	HIS	-	expression tag	UNP P20285
JA	191	GLY	-	expression tag	UNP P20285
JA	192	MET	-	expression tag	UNP P20285
JA	193	ALA	-	expression tag	UNP P20285
JA	194	SER	-	expression tag	UNP P20285
JA	195	MET	-	expression tag	UNP P20285
JA	196	THR	-	expression tag	UNP P20285
JA	197	GLY	-	expression tag	UNP P20285
JA	198	GLY	-	expression tag	UNP P20285
JA	199	GLN	-	expression tag	UNP P20285
JA	200	GLN	-	expression tag	UNP P20285
JA	201	MET	-	expression tag	UNP P20285
JA	202	GLY	-	expression tag	UNP P20285
JA	203	ARG	-	expression tag	UNP P20285
JA	204	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
JA	205	LEU	-	expression tag	UNP P20285
JA	206	TYR	-	expression tag	UNP P20285
JA	207	ASP	-	expression tag	UNP P20285
JA	208	ASP	-	expression tag	UNP P20285
JA	209	ASP	-	expression tag	UNP P20285
JA	210	ASP	-	expression tag	UNP P20285
JA	211	LYS	-	expression tag	UNP P20285
JA	212	ASP	-	expression tag	UNP P20285
JA	213	ARG	-	expression tag	UNP P20285
JA	214	TRP	-	expression tag	UNP P20285
JA	215	GLY	-	expression tag	UNP P20285
JA	216	SER	-	expression tag	UNP P20285
JA	217	LEU	-	expression tag	UNP P20285
JA	218	VAL	-	expression tag	UNP P20285
JA	219	PRO	-	expression tag	UNP P20285
JA	220	ARG	-	expression tag	UNP P20285
JA	221	GLY	-	expression tag	UNP P20285
JA	222	SER	-	expression tag	UNP P20285
JA	223	HIS	-	expression tag	UNP P20285
JA	224	MET	-	expression tag	UNP P20285
JA	225	ALA	-	expression tag	UNP P20285
JA	226	ALA	-	expression tag	UNP P20285
KA	181	MET	-	initiating methionine	UNP P20285
KA	182	ARG	-	expression tag	UNP P20285
KA	183	GLY	-	expression tag	UNP P20285
KA	184	SER	-	expression tag	UNP P20285
KA	185	HIS	-	expression tag	UNP P20285
KA	186	HIS	-	expression tag	UNP P20285
KA	187	HIS	-	expression tag	UNP P20285
KA	188	HIS	-	expression tag	UNP P20285
KA	189	HIS	-	expression tag	UNP P20285
KA	190	HIS	-	expression tag	UNP P20285
KA	191	GLY	-	expression tag	UNP P20285
KA	192	MET	-	expression tag	UNP P20285
KA	193	ALA	-	expression tag	UNP P20285
KA	194	SER	-	expression tag	UNP P20285
KA	195	MET	-	expression tag	UNP P20285
KA	196	THR	-	expression tag	UNP P20285
KA	197	GLY	-	expression tag	UNP P20285
KA	198	GLY	-	expression tag	UNP P20285
KA	199	GLN	-	expression tag	UNP P20285
KA	200	GLN	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
KA	201	MET	-	expression tag	UNP P20285
KA	202	GLY	-	expression tag	UNP P20285
KA	203	ARG	-	expression tag	UNP P20285
KA	204	ASP	-	expression tag	UNP P20285
KA	205	LEU	-	expression tag	UNP P20285
KA	206	TYR	-	expression tag	UNP P20285
KA	207	ASP	-	expression tag	UNP P20285
KA	208	ASP	-	expression tag	UNP P20285
KA	209	ASP	-	expression tag	UNP P20285
KA	210	ASP	-	expression tag	UNP P20285
KA	211	LYS	-	expression tag	UNP P20285
KA	212	ASP	-	expression tag	UNP P20285
KA	213	ARG	-	expression tag	UNP P20285
KA	214	TRP	-	expression tag	UNP P20285
KA	215	GLY	-	expression tag	UNP P20285
KA	216	SER	-	expression tag	UNP P20285
KA	217	LEU	-	expression tag	UNP P20285
KA	218	VAL	-	expression tag	UNP P20285
KA	219	PRO	-	expression tag	UNP P20285
KA	220	ARG	-	expression tag	UNP P20285
KA	221	GLY	-	expression tag	UNP P20285
KA	222	SER	-	expression tag	UNP P20285
KA	223	HIS	-	expression tag	UNP P20285
KA	224	MET	-	expression tag	UNP P20285
KA	225	ALA	-	expression tag	UNP P20285
KA	226	ALA	-	expression tag	UNP P20285
LA	181	MET	-	initiating methionine	UNP P20285
LA	182	ARG	-	expression tag	UNP P20285
LA	183	GLY	-	expression tag	UNP P20285
LA	184	SER	-	expression tag	UNP P20285
LA	185	HIS	-	expression tag	UNP P20285
LA	186	HIS	-	expression tag	UNP P20285
LA	187	HIS	-	expression tag	UNP P20285
LA	188	HIS	-	expression tag	UNP P20285
LA	189	HIS	-	expression tag	UNP P20285
LA	190	HIS	-	expression tag	UNP P20285
LA	191	GLY	-	expression tag	UNP P20285
LA	192	MET	-	expression tag	UNP P20285
LA	193	ALA	-	expression tag	UNP P20285
LA	194	SER	-	expression tag	UNP P20285
LA	195	MET	-	expression tag	UNP P20285
LA	196	THR	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
LA	197	GLY	-	expression tag	UNP P20285
LA	198	GLY	-	expression tag	UNP P20285
LA	199	GLN	-	expression tag	UNP P20285
LA	200	GLN	-	expression tag	UNP P20285
LA	201	MET	-	expression tag	UNP P20285
LA	202	GLY	-	expression tag	UNP P20285
LA	203	ARG	-	expression tag	UNP P20285
LA	204	ASP	-	expression tag	UNP P20285
LA	205	LEU	-	expression tag	UNP P20285
LA	206	TYR	-	expression tag	UNP P20285
LA	207	ASP	-	expression tag	UNP P20285
LA	208	ASP	-	expression tag	UNP P20285
LA	209	ASP	-	expression tag	UNP P20285
LA	210	ASP	-	expression tag	UNP P20285
LA	211	LYS	-	expression tag	UNP P20285
LA	212	ASP	-	expression tag	UNP P20285
LA	213	ARG	-	expression tag	UNP P20285
LA	214	TRP	-	expression tag	UNP P20285
LA	215	GLY	-	expression tag	UNP P20285
LA	216	SER	-	expression tag	UNP P20285
LA	217	LEU	-	expression tag	UNP P20285
LA	218	VAL	-	expression tag	UNP P20285
LA	219	PRO	-	expression tag	UNP P20285
LA	220	ARG	-	expression tag	UNP P20285
LA	221	GLY	-	expression tag	UNP P20285
LA	222	SER	-	expression tag	UNP P20285
LA	223	HIS	-	expression tag	UNP P20285
LA	224	MET	-	expression tag	UNP P20285
LA	225	ALA	-	expression tag	UNP P20285
LA	226	ALA	-	expression tag	UNP P20285
MA	181	MET	-	initiating methionine	UNP P20285
MA	182	ARG	-	expression tag	UNP P20285
MA	183	GLY	-	expression tag	UNP P20285
MA	184	SER	-	expression tag	UNP P20285
MA	185	HIS	-	expression tag	UNP P20285
MA	186	HIS	-	expression tag	UNP P20285
MA	187	HIS	-	expression tag	UNP P20285
MA	188	HIS	-	expression tag	UNP P20285
MA	189	HIS	-	expression tag	UNP P20285
MA	190	HIS	-	expression tag	UNP P20285
MA	191	GLY	-	expression tag	UNP P20285
MA	192	MET	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
MA	193	ALA	-	expression tag	UNP P20285
MA	194	SER	-	expression tag	UNP P20285
MA	195	MET	-	expression tag	UNP P20285
MA	196	THR	-	expression tag	UNP P20285
MA	197	GLY	-	expression tag	UNP P20285
MA	198	GLY	-	expression tag	UNP P20285
MA	199	GLN	-	expression tag	UNP P20285
MA	200	GLN	-	expression tag	UNP P20285
MA	201	MET	-	expression tag	UNP P20285
MA	202	GLY	-	expression tag	UNP P20285
MA	203	ARG	-	expression tag	UNP P20285
MA	204	ASP	-	expression tag	UNP P20285
MA	205	LEU	-	expression tag	UNP P20285
MA	206	TYR	-	expression tag	UNP P20285
MA	207	ASP	-	expression tag	UNP P20285
MA	208	ASP	-	expression tag	UNP P20285
MA	209	ASP	-	expression tag	UNP P20285
MA	210	ASP	-	expression tag	UNP P20285
MA	211	LYS	-	expression tag	UNP P20285
MA	212	ASP	-	expression tag	UNP P20285
MA	213	ARG	-	expression tag	UNP P20285
MA	214	TRP	-	expression tag	UNP P20285
MA	215	GLY	-	expression tag	UNP P20285
MA	216	SER	-	expression tag	UNP P20285
MA	217	LEU	-	expression tag	UNP P20285
MA	218	VAL	-	expression tag	UNP P20285
MA	219	PRO	-	expression tag	UNP P20285
MA	220	ARG	-	expression tag	UNP P20285
MA	221	GLY	-	expression tag	UNP P20285
MA	222	SER	-	expression tag	UNP P20285
MA	223	HIS	-	expression tag	UNP P20285
MA	224	MET	-	expression tag	UNP P20285
MA	225	ALA	-	expression tag	UNP P20285
MA	226	ALA	-	expression tag	UNP P20285
NA	181	MET	-	initiating methionine	UNP P20285
NA	182	ARG	-	expression tag	UNP P20285
NA	183	GLY	-	expression tag	UNP P20285
NA	184	SER	-	expression tag	UNP P20285
NA	185	HIS	-	expression tag	UNP P20285
NA	186	HIS	-	expression tag	UNP P20285
NA	187	HIS	-	expression tag	UNP P20285
NA	188	HIS	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
NA	189	HIS	-	expression tag	UNP P20285
NA	190	HIS	-	expression tag	UNP P20285
NA	191	GLY	-	expression tag	UNP P20285
NA	192	MET	-	expression tag	UNP P20285
NA	193	ALA	-	expression tag	UNP P20285
NA	194	SER	-	expression tag	UNP P20285
NA	195	MET	-	expression tag	UNP P20285
NA	196	THR	-	expression tag	UNP P20285
NA	197	GLY	-	expression tag	UNP P20285
NA	198	GLY	-	expression tag	UNP P20285
NA	199	GLN	-	expression tag	UNP P20285
NA	200	GLN	-	expression tag	UNP P20285
NA	201	MET	-	expression tag	UNP P20285
NA	202	GLY	-	expression tag	UNP P20285
NA	203	ARG	-	expression tag	UNP P20285
NA	204	ASP	-	expression tag	UNP P20285
NA	205	LEU	-	expression tag	UNP P20285
NA	206	TYR	-	expression tag	UNP P20285
NA	207	ASP	-	expression tag	UNP P20285
NA	208	ASP	-	expression tag	UNP P20285
NA	209	ASP	-	expression tag	UNP P20285
NA	210	ASP	-	expression tag	UNP P20285
NA	211	LYS	-	expression tag	UNP P20285
NA	212	ASP	-	expression tag	UNP P20285
NA	213	ARG	-	expression tag	UNP P20285
NA	214	TRP	-	expression tag	UNP P20285
NA	215	GLY	-	expression tag	UNP P20285
NA	216	SER	-	expression tag	UNP P20285
NA	217	LEU	-	expression tag	UNP P20285
NA	218	VAL	-	expression tag	UNP P20285
NA	219	PRO	-	expression tag	UNP P20285
NA	220	ARG	-	expression tag	UNP P20285
NA	221	GLY	-	expression tag	UNP P20285
NA	222	SER	-	expression tag	UNP P20285
NA	223	HIS	-	expression tag	UNP P20285
NA	224	MET	-	expression tag	UNP P20285
NA	225	ALA	-	expression tag	UNP P20285
NA	226	ALA	-	expression tag	UNP P20285
OA	181	MET	-	initiating methionine	UNP P20285
OA	182	ARG	-	expression tag	UNP P20285
OA	183	GLY	-	expression tag	UNP P20285
OA	184	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
OA	185	HIS	-	expression tag	UNP P20285
OA	186	HIS	-	expression tag	UNP P20285
OA	187	HIS	-	expression tag	UNP P20285
OA	188	HIS	-	expression tag	UNP P20285
OA	189	HIS	-	expression tag	UNP P20285
OA	190	HIS	-	expression tag	UNP P20285
OA	191	GLY	-	expression tag	UNP P20285
OA	192	MET	-	expression tag	UNP P20285
OA	193	ALA	-	expression tag	UNP P20285
OA	194	SER	-	expression tag	UNP P20285
OA	195	MET	-	expression tag	UNP P20285
OA	196	THR	-	expression tag	UNP P20285
OA	197	GLY	-	expression tag	UNP P20285
OA	198	GLY	-	expression tag	UNP P20285
OA	199	GLN	-	expression tag	UNP P20285
OA	200	GLN	-	expression tag	UNP P20285
OA	201	MET	-	expression tag	UNP P20285
OA	202	GLY	-	expression tag	UNP P20285
OA	203	ARG	-	expression tag	UNP P20285
OA	204	ASP	-	expression tag	UNP P20285
OA	205	LEU	-	expression tag	UNP P20285
OA	206	TYR	-	expression tag	UNP P20285
OA	207	ASP	-	expression tag	UNP P20285
OA	208	ASP	-	expression tag	UNP P20285
OA	209	ASP	-	expression tag	UNP P20285
OA	210	ASP	-	expression tag	UNP P20285
OA	211	LYS	-	expression tag	UNP P20285
OA	212	ASP	-	expression tag	UNP P20285
OA	213	ARG	-	expression tag	UNP P20285
OA	214	TRP	-	expression tag	UNP P20285
OA	215	GLY	-	expression tag	UNP P20285
OA	216	SER	-	expression tag	UNP P20285
OA	217	LEU	-	expression tag	UNP P20285
OA	218	VAL	-	expression tag	UNP P20285
OA	219	PRO	-	expression tag	UNP P20285
OA	220	ARG	-	expression tag	UNP P20285
OA	221	GLY	-	expression tag	UNP P20285
OA	222	SER	-	expression tag	UNP P20285
OA	223	HIS	-	expression tag	UNP P20285
OA	224	MET	-	expression tag	UNP P20285
OA	225	ALA	-	expression tag	UNP P20285
OA	226	ALA	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
PA	181	MET	-	initiating methionine	UNP P20285
PA	182	ARG	-	expression tag	UNP P20285
PA	183	GLY	-	expression tag	UNP P20285
PA	184	SER	-	expression tag	UNP P20285
PA	185	HIS	-	expression tag	UNP P20285
PA	186	HIS	-	expression tag	UNP P20285
PA	187	HIS	-	expression tag	UNP P20285
PA	188	HIS	-	expression tag	UNP P20285
PA	189	HIS	-	expression tag	UNP P20285
PA	190	HIS	-	expression tag	UNP P20285
PA	191	GLY	-	expression tag	UNP P20285
PA	192	MET	-	expression tag	UNP P20285
PA	193	ALA	-	expression tag	UNP P20285
PA	194	SER	-	expression tag	UNP P20285
PA	195	MET	-	expression tag	UNP P20285
PA	196	THR	-	expression tag	UNP P20285
PA	197	GLY	-	expression tag	UNP P20285
PA	198	GLY	-	expression tag	UNP P20285
PA	199	GLN	-	expression tag	UNP P20285
PA	200	GLN	-	expression tag	UNP P20285
PA	201	MET	-	expression tag	UNP P20285
PA	202	GLY	-	expression tag	UNP P20285
PA	203	ARG	-	expression tag	UNP P20285
PA	204	ASP	-	expression tag	UNP P20285
PA	205	LEU	-	expression tag	UNP P20285
PA	206	TYR	-	expression tag	UNP P20285
PA	207	ASP	-	expression tag	UNP P20285
PA	208	ASP	-	expression tag	UNP P20285
PA	209	ASP	-	expression tag	UNP P20285
PA	210	ASP	-	expression tag	UNP P20285
PA	211	LYS	-	expression tag	UNP P20285
PA	212	ASP	-	expression tag	UNP P20285
PA	213	ARG	-	expression tag	UNP P20285
PA	214	TRP	-	expression tag	UNP P20285
PA	215	GLY	-	expression tag	UNP P20285
PA	216	SER	-	expression tag	UNP P20285
PA	217	LEU	-	expression tag	UNP P20285
PA	218	VAL	-	expression tag	UNP P20285
PA	219	PRO	-	expression tag	UNP P20285
PA	220	ARG	-	expression tag	UNP P20285
PA	221	GLY	-	expression tag	UNP P20285
PA	222	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
PA	223	HIS	-	expression tag	UNP P20285
PA	224	MET	-	expression tag	UNP P20285
PA	225	ALA	-	expression tag	UNP P20285
PA	226	ALA	-	expression tag	UNP P20285
QA	181	MET	-	initiating methionine	UNP P20285
QA	182	ARG	-	expression tag	UNP P20285
QA	183	GLY	-	expression tag	UNP P20285
QA	184	SER	-	expression tag	UNP P20285
QA	185	HIS	-	expression tag	UNP P20285
QA	186	HIS	-	expression tag	UNP P20285
QA	187	HIS	-	expression tag	UNP P20285
QA	188	HIS	-	expression tag	UNP P20285
QA	189	HIS	-	expression tag	UNP P20285
QA	190	HIS	-	expression tag	UNP P20285
QA	191	GLY	-	expression tag	UNP P20285
QA	192	MET	-	expression tag	UNP P20285
QA	193	ALA	-	expression tag	UNP P20285
QA	194	SER	-	expression tag	UNP P20285
QA	195	MET	-	expression tag	UNP P20285
QA	196	THR	-	expression tag	UNP P20285
QA	197	GLY	-	expression tag	UNP P20285
QA	198	GLY	-	expression tag	UNP P20285
QA	199	GLN	-	expression tag	UNP P20285
QA	200	GLN	-	expression tag	UNP P20285
QA	201	MET	-	expression tag	UNP P20285
QA	202	GLY	-	expression tag	UNP P20285
QA	203	ARG	-	expression tag	UNP P20285
QA	204	ASP	-	expression tag	UNP P20285
QA	205	LEU	-	expression tag	UNP P20285
QA	206	TYR	-	expression tag	UNP P20285
QA	207	ASP	-	expression tag	UNP P20285
QA	208	ASP	-	expression tag	UNP P20285
QA	209	ASP	-	expression tag	UNP P20285
QA	210	ASP	-	expression tag	UNP P20285
QA	211	LYS	-	expression tag	UNP P20285
QA	212	ASP	-	expression tag	UNP P20285
QA	213	ARG	-	expression tag	UNP P20285
QA	214	TRP	-	expression tag	UNP P20285
QA	215	GLY	-	expression tag	UNP P20285
QA	216	SER	-	expression tag	UNP P20285
QA	217	LEU	-	expression tag	UNP P20285
QA	218	VAL	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
QA	219	PRO	-	expression tag	UNP P20285
QA	220	ARG	-	expression tag	UNP P20285
QA	221	GLY	-	expression tag	UNP P20285
QA	222	SER	-	expression tag	UNP P20285
QA	223	HIS	-	expression tag	UNP P20285
QA	224	MET	-	expression tag	UNP P20285
QA	225	ALA	-	expression tag	UNP P20285
QA	226	ALA	-	expression tag	UNP P20285
RA	181	MET	-	initiating methionine	UNP P20285
RA	182	ARG	-	expression tag	UNP P20285
RA	183	GLY	-	expression tag	UNP P20285
RA	184	SER	-	expression tag	UNP P20285
RA	185	HIS	-	expression tag	UNP P20285
RA	186	HIS	-	expression tag	UNP P20285
RA	187	HIS	-	expression tag	UNP P20285
RA	188	HIS	-	expression tag	UNP P20285
RA	189	HIS	-	expression tag	UNP P20285
RA	190	HIS	-	expression tag	UNP P20285
RA	191	GLY	-	expression tag	UNP P20285
RA	192	MET	-	expression tag	UNP P20285
RA	193	ALA	-	expression tag	UNP P20285
RA	194	SER	-	expression tag	UNP P20285
RA	195	MET	-	expression tag	UNP P20285
RA	196	THR	-	expression tag	UNP P20285
RA	197	GLY	-	expression tag	UNP P20285
RA	198	GLY	-	expression tag	UNP P20285
RA	199	GLN	-	expression tag	UNP P20285
RA	200	GLN	-	expression tag	UNP P20285
RA	201	MET	-	expression tag	UNP P20285
RA	202	GLY	-	expression tag	UNP P20285
RA	203	ARG	-	expression tag	UNP P20285
RA	204	ASP	-	expression tag	UNP P20285
RA	205	LEU	-	expression tag	UNP P20285
RA	206	TYR	-	expression tag	UNP P20285
RA	207	ASP	-	expression tag	UNP P20285
RA	208	ASP	-	expression tag	UNP P20285
RA	209	ASP	-	expression tag	UNP P20285
RA	210	ASP	-	expression tag	UNP P20285
RA	211	LYS	-	expression tag	UNP P20285
RA	212	ASP	-	expression tag	UNP P20285
RA	213	ARG	-	expression tag	UNP P20285
RA	214	TRP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
RA	215	GLY	-	expression tag	UNP P20285
RA	216	SER	-	expression tag	UNP P20285
RA	217	LEU	-	expression tag	UNP P20285
RA	218	VAL	-	expression tag	UNP P20285
RA	219	PRO	-	expression tag	UNP P20285
RA	220	ARG	-	expression tag	UNP P20285
RA	221	GLY	-	expression tag	UNP P20285
RA	222	SER	-	expression tag	UNP P20285
RA	223	HIS	-	expression tag	UNP P20285
RA	224	MET	-	expression tag	UNP P20285
RA	225	ALA	-	expression tag	UNP P20285
RA	226	ALA	-	expression tag	UNP P20285
SA	181	MET	-	initiating methionine	UNP P20285
SA	182	ARG	-	expression tag	UNP P20285
SA	183	GLY	-	expression tag	UNP P20285
SA	184	SER	-	expression tag	UNP P20285
SA	185	HIS	-	expression tag	UNP P20285
SA	186	HIS	-	expression tag	UNP P20285
SA	187	HIS	-	expression tag	UNP P20285
SA	188	HIS	-	expression tag	UNP P20285
SA	189	HIS	-	expression tag	UNP P20285
SA	190	HIS	-	expression tag	UNP P20285
SA	191	GLY	-	expression tag	UNP P20285
SA	192	MET	-	expression tag	UNP P20285
SA	193	ALA	-	expression tag	UNP P20285
SA	194	SER	-	expression tag	UNP P20285
SA	195	MET	-	expression tag	UNP P20285
SA	196	THR	-	expression tag	UNP P20285
SA	197	GLY	-	expression tag	UNP P20285
SA	198	GLY	-	expression tag	UNP P20285
SA	199	GLN	-	expression tag	UNP P20285
SA	200	GLN	-	expression tag	UNP P20285
SA	201	MET	-	expression tag	UNP P20285
SA	202	GLY	-	expression tag	UNP P20285
SA	203	ARG	-	expression tag	UNP P20285
SA	204	ASP	-	expression tag	UNP P20285
SA	205	LEU	-	expression tag	UNP P20285
SA	206	TYR	-	expression tag	UNP P20285
SA	207	ASP	-	expression tag	UNP P20285
SA	208	ASP	-	expression tag	UNP P20285
SA	209	ASP	-	expression tag	UNP P20285
SA	210	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
SA	211	LYS	-	expression tag	UNP P20285
SA	212	ASP	-	expression tag	UNP P20285
SA	213	ARG	-	expression tag	UNP P20285
SA	214	TRP	-	expression tag	UNP P20285
SA	215	GLY	-	expression tag	UNP P20285
SA	216	SER	-	expression tag	UNP P20285
SA	217	LEU	-	expression tag	UNP P20285
SA	218	VAL	-	expression tag	UNP P20285
SA	219	PRO	-	expression tag	UNP P20285
SA	220	ARG	-	expression tag	UNP P20285
SA	221	GLY	-	expression tag	UNP P20285
SA	222	SER	-	expression tag	UNP P20285
SA	223	HIS	-	expression tag	UNP P20285
SA	224	MET	-	expression tag	UNP P20285
SA	225	ALA	-	expression tag	UNP P20285
SA	226	ALA	-	expression tag	UNP P20285
TA	181	MET	-	initiating methionine	UNP P20285
TA	182	ARG	-	expression tag	UNP P20285
TA	183	GLY	-	expression tag	UNP P20285
TA	184	SER	-	expression tag	UNP P20285
TA	185	HIS	-	expression tag	UNP P20285
TA	186	HIS	-	expression tag	UNP P20285
TA	187	HIS	-	expression tag	UNP P20285
TA	188	HIS	-	expression tag	UNP P20285
TA	189	HIS	-	expression tag	UNP P20285
TA	190	HIS	-	expression tag	UNP P20285
TA	191	GLY	-	expression tag	UNP P20285
TA	192	MET	-	expression tag	UNP P20285
TA	193	ALA	-	expression tag	UNP P20285
TA	194	SER	-	expression tag	UNP P20285
TA	195	MET	-	expression tag	UNP P20285
TA	196	THR	-	expression tag	UNP P20285
TA	197	GLY	-	expression tag	UNP P20285
TA	198	GLY	-	expression tag	UNP P20285
TA	199	GLN	-	expression tag	UNP P20285
TA	200	GLN	-	expression tag	UNP P20285
TA	201	MET	-	expression tag	UNP P20285
TA	202	GLY	-	expression tag	UNP P20285
TA	203	ARG	-	expression tag	UNP P20285
TA	204	ASP	-	expression tag	UNP P20285
TA	205	LEU	-	expression tag	UNP P20285
TA	206	TYR	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
TA	207	ASP	-	expression tag	UNP P20285
TA	208	ASP	-	expression tag	UNP P20285
TA	209	ASP	-	expression tag	UNP P20285
TA	210	ASP	-	expression tag	UNP P20285
TA	211	LYS	-	expression tag	UNP P20285
TA	212	ASP	-	expression tag	UNP P20285
TA	213	ARG	-	expression tag	UNP P20285
TA	214	TRP	-	expression tag	UNP P20285
TA	215	GLY	-	expression tag	UNP P20285
TA	216	SER	-	expression tag	UNP P20285
TA	217	LEU	-	expression tag	UNP P20285
TA	218	VAL	-	expression tag	UNP P20285
TA	219	PRO	-	expression tag	UNP P20285
TA	220	ARG	-	expression tag	UNP P20285
TA	221	GLY	-	expression tag	UNP P20285
TA	222	SER	-	expression tag	UNP P20285
TA	223	HIS	-	expression tag	UNP P20285
TA	224	MET	-	expression tag	UNP P20285
TA	225	ALA	-	expression tag	UNP P20285
TA	226	ALA	-	expression tag	UNP P20285
UA	181	MET	-	initiating methionine	UNP P20285
UA	182	ARG	-	expression tag	UNP P20285
UA	183	GLY	-	expression tag	UNP P20285
UA	184	SER	-	expression tag	UNP P20285
UA	185	HIS	-	expression tag	UNP P20285
UA	186	HIS	-	expression tag	UNP P20285
UA	187	HIS	-	expression tag	UNP P20285
UA	188	HIS	-	expression tag	UNP P20285
UA	189	HIS	-	expression tag	UNP P20285
UA	190	HIS	-	expression tag	UNP P20285
UA	191	GLY	-	expression tag	UNP P20285
UA	192	MET	-	expression tag	UNP P20285
UA	193	ALA	-	expression tag	UNP P20285
UA	194	SER	-	expression tag	UNP P20285
UA	195	MET	-	expression tag	UNP P20285
UA	196	THR	-	expression tag	UNP P20285
UA	197	GLY	-	expression tag	UNP P20285
UA	198	GLY	-	expression tag	UNP P20285
UA	199	GLN	-	expression tag	UNP P20285
UA	200	GLN	-	expression tag	UNP P20285
UA	201	MET	-	expression tag	UNP P20285
UA	202	GLY	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
UA	203	ARG	-	expression tag	UNP P20285
UA	204	ASP	-	expression tag	UNP P20285
UA	205	LEU	-	expression tag	UNP P20285
UA	206	TYR	-	expression tag	UNP P20285
UA	207	ASP	-	expression tag	UNP P20285
UA	208	ASP	-	expression tag	UNP P20285
UA	209	ASP	-	expression tag	UNP P20285
UA	210	ASP	-	expression tag	UNP P20285
UA	211	LYS	-	expression tag	UNP P20285
UA	212	ASP	-	expression tag	UNP P20285
UA	213	ARG	-	expression tag	UNP P20285
UA	214	TRP	-	expression tag	UNP P20285
UA	215	GLY	-	expression tag	UNP P20285
UA	216	SER	-	expression tag	UNP P20285
UA	217	LEU	-	expression tag	UNP P20285
UA	218	VAL	-	expression tag	UNP P20285
UA	219	PRO	-	expression tag	UNP P20285
UA	220	ARG	-	expression tag	UNP P20285
UA	221	GLY	-	expression tag	UNP P20285
UA	222	SER	-	expression tag	UNP P20285
UA	223	HIS	-	expression tag	UNP P20285
UA	224	MET	-	expression tag	UNP P20285
UA	225	ALA	-	expression tag	UNP P20285
UA	226	ALA	-	expression tag	UNP P20285
VA	181	MET	-	initiating methionine	UNP P20285
VA	182	ARG	-	expression tag	UNP P20285
VA	183	GLY	-	expression tag	UNP P20285
VA	184	SER	-	expression tag	UNP P20285
VA	185	HIS	-	expression tag	UNP P20285
VA	186	HIS	-	expression tag	UNP P20285
VA	187	HIS	-	expression tag	UNP P20285
VA	188	HIS	-	expression tag	UNP P20285
VA	189	HIS	-	expression tag	UNP P20285
VA	190	HIS	-	expression tag	UNP P20285
VA	191	GLY	-	expression tag	UNP P20285
VA	192	MET	-	expression tag	UNP P20285
VA	193	ALA	-	expression tag	UNP P20285
VA	194	SER	-	expression tag	UNP P20285
VA	195	MET	-	expression tag	UNP P20285
VA	196	THR	-	expression tag	UNP P20285
VA	197	GLY	-	expression tag	UNP P20285
VA	198	GLY	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
VA	199	GLN	-	expression tag	UNP P20285
VA	200	GLN	-	expression tag	UNP P20285
VA	201	MET	-	expression tag	UNP P20285
VA	202	GLY	-	expression tag	UNP P20285
VA	203	ARG	-	expression tag	UNP P20285
VA	204	ASP	-	expression tag	UNP P20285
VA	205	LEU	-	expression tag	UNP P20285
VA	206	TYR	-	expression tag	UNP P20285
VA	207	ASP	-	expression tag	UNP P20285
VA	208	ASP	-	expression tag	UNP P20285
VA	209	ASP	-	expression tag	UNP P20285
VA	210	ASP	-	expression tag	UNP P20285
VA	211	LYS	-	expression tag	UNP P20285
VA	212	ASP	-	expression tag	UNP P20285
VA	213	ARG	-	expression tag	UNP P20285
VA	214	TRP	-	expression tag	UNP P20285
VA	215	GLY	-	expression tag	UNP P20285
VA	216	SER	-	expression tag	UNP P20285
VA	217	LEU	-	expression tag	UNP P20285
VA	218	VAL	-	expression tag	UNP P20285
VA	219	PRO	-	expression tag	UNP P20285
VA	220	ARG	-	expression tag	UNP P20285
VA	221	GLY	-	expression tag	UNP P20285
VA	222	SER	-	expression tag	UNP P20285
VA	223	HIS	-	expression tag	UNP P20285
VA	224	MET	-	expression tag	UNP P20285
VA	225	ALA	-	expression tag	UNP P20285
VA	226	ALA	-	expression tag	UNP P20285
WA	181	MET	-	initiating methionine	UNP P20285
WA	182	ARG	-	expression tag	UNP P20285
WA	183	GLY	-	expression tag	UNP P20285
WA	184	SER	-	expression tag	UNP P20285
WA	185	HIS	-	expression tag	UNP P20285
WA	186	HIS	-	expression tag	UNP P20285
WA	187	HIS	-	expression tag	UNP P20285
WA	188	HIS	-	expression tag	UNP P20285
WA	189	HIS	-	expression tag	UNP P20285
WA	190	HIS	-	expression tag	UNP P20285
WA	191	GLY	-	expression tag	UNP P20285
WA	192	MET	-	expression tag	UNP P20285
WA	193	ALA	-	expression tag	UNP P20285
WA	194	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
WA	195	MET	-	expression tag	UNP P20285
WA	196	THR	-	expression tag	UNP P20285
WA	197	GLY	-	expression tag	UNP P20285
WA	198	GLY	-	expression tag	UNP P20285
WA	199	GLN	-	expression tag	UNP P20285
WA	200	GLN	-	expression tag	UNP P20285
WA	201	MET	-	expression tag	UNP P20285
WA	202	GLY	-	expression tag	UNP P20285
WA	203	ARG	-	expression tag	UNP P20285
WA	204	ASP	-	expression tag	UNP P20285
WA	205	LEU	-	expression tag	UNP P20285
WA	206	TYR	-	expression tag	UNP P20285
WA	207	ASP	-	expression tag	UNP P20285
WA	208	ASP	-	expression tag	UNP P20285
WA	209	ASP	-	expression tag	UNP P20285
WA	210	ASP	-	expression tag	UNP P20285
WA	211	LYS	-	expression tag	UNP P20285
WA	212	ASP	-	expression tag	UNP P20285
WA	213	ARG	-	expression tag	UNP P20285
WA	214	TRP	-	expression tag	UNP P20285
WA	215	GLY	-	expression tag	UNP P20285
WA	216	SER	-	expression tag	UNP P20285
WA	217	LEU	-	expression tag	UNP P20285
WA	218	VAL	-	expression tag	UNP P20285
WA	219	PRO	-	expression tag	UNP P20285
WA	220	ARG	-	expression tag	UNP P20285
WA	221	GLY	-	expression tag	UNP P20285
WA	222	SER	-	expression tag	UNP P20285
WA	223	HIS	-	expression tag	UNP P20285
WA	224	MET	-	expression tag	UNP P20285
WA	225	ALA	-	expression tag	UNP P20285
WA	226	ALA	-	expression tag	UNP P20285
XA	181	MET	-	initiating methionine	UNP P20285
XA	182	ARG	-	expression tag	UNP P20285
XA	183	GLY	-	expression tag	UNP P20285
XA	184	SER	-	expression tag	UNP P20285
XA	185	HIS	-	expression tag	UNP P20285
XA	186	HIS	-	expression tag	UNP P20285
XA	187	HIS	-	expression tag	UNP P20285
XA	188	HIS	-	expression tag	UNP P20285
XA	189	HIS	-	expression tag	UNP P20285
XA	190	HIS	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
XA	191	GLY	-	expression tag	UNP P20285
XA	192	MET	-	expression tag	UNP P20285
XA	193	ALA	-	expression tag	UNP P20285
XA	194	SER	-	expression tag	UNP P20285
XA	195	MET	-	expression tag	UNP P20285
XA	196	THR	-	expression tag	UNP P20285
XA	197	GLY	-	expression tag	UNP P20285
XA	198	GLY	-	expression tag	UNP P20285
XA	199	GLN	-	expression tag	UNP P20285
XA	200	GLN	-	expression tag	UNP P20285
XA	201	MET	-	expression tag	UNP P20285
XA	202	GLY	-	expression tag	UNP P20285
XA	203	ARG	-	expression tag	UNP P20285
XA	204	ASP	-	expression tag	UNP P20285
XA	205	LEU	-	expression tag	UNP P20285
XA	206	TYR	-	expression tag	UNP P20285
XA	207	ASP	-	expression tag	UNP P20285
XA	208	ASP	-	expression tag	UNP P20285
XA	209	ASP	-	expression tag	UNP P20285
XA	210	ASP	-	expression tag	UNP P20285
XA	211	LYS	-	expression tag	UNP P20285
XA	212	ASP	-	expression tag	UNP P20285
XA	213	ARG	-	expression tag	UNP P20285
XA	214	TRP	-	expression tag	UNP P20285
XA	215	GLY	-	expression tag	UNP P20285
XA	216	SER	-	expression tag	UNP P20285
XA	217	LEU	-	expression tag	UNP P20285
XA	218	VAL	-	expression tag	UNP P20285
XA	219	PRO	-	expression tag	UNP P20285
XA	220	ARG	-	expression tag	UNP P20285
XA	221	GLY	-	expression tag	UNP P20285
XA	222	SER	-	expression tag	UNP P20285
XA	223	HIS	-	expression tag	UNP P20285
XA	224	MET	-	expression tag	UNP P20285
XA	225	ALA	-	expression tag	UNP P20285
XA	226	ALA	-	expression tag	UNP P20285
YA	181	MET	-	initiating methionine	UNP P20285
YA	182	ARG	-	expression tag	UNP P20285
YA	183	GLY	-	expression tag	UNP P20285
YA	184	SER	-	expression tag	UNP P20285
YA	185	HIS	-	expression tag	UNP P20285
YA	186	HIS	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
YA	187	HIS	-	expression tag	UNP P20285
YA	188	HIS	-	expression tag	UNP P20285
YA	189	HIS	-	expression tag	UNP P20285
YA	190	HIS	-	expression tag	UNP P20285
YA	191	GLY	-	expression tag	UNP P20285
YA	192	MET	-	expression tag	UNP P20285
YA	193	ALA	-	expression tag	UNP P20285
YA	194	SER	-	expression tag	UNP P20285
YA	195	MET	-	expression tag	UNP P20285
YA	196	THR	-	expression tag	UNP P20285
YA	197	GLY	-	expression tag	UNP P20285
YA	198	GLY	-	expression tag	UNP P20285
YA	199	GLN	-	expression tag	UNP P20285
YA	200	GLN	-	expression tag	UNP P20285
YA	201	MET	-	expression tag	UNP P20285
YA	202	GLY	-	expression tag	UNP P20285
YA	203	ARG	-	expression tag	UNP P20285
YA	204	ASP	-	expression tag	UNP P20285
YA	205	LEU	-	expression tag	UNP P20285
YA	206	TYR	-	expression tag	UNP P20285
YA	207	ASP	-	expression tag	UNP P20285
YA	208	ASP	-	expression tag	UNP P20285
YA	209	ASP	-	expression tag	UNP P20285
YA	210	ASP	-	expression tag	UNP P20285
YA	211	LYS	-	expression tag	UNP P20285
YA	212	ASP	-	expression tag	UNP P20285
YA	213	ARG	-	expression tag	UNP P20285
YA	214	TRP	-	expression tag	UNP P20285
YA	215	GLY	-	expression tag	UNP P20285
YA	216	SER	-	expression tag	UNP P20285
YA	217	LEU	-	expression tag	UNP P20285
YA	218	VAL	-	expression tag	UNP P20285
YA	219	PRO	-	expression tag	UNP P20285
YA	220	ARG	-	expression tag	UNP P20285
YA	221	GLY	-	expression tag	UNP P20285
YA	222	SER	-	expression tag	UNP P20285
YA	223	HIS	-	expression tag	UNP P20285
YA	224	MET	-	expression tag	UNP P20285
YA	225	ALA	-	expression tag	UNP P20285
YA	226	ALA	-	expression tag	UNP P20285
ZA	181	MET	-	initiating methionine	UNP P20285
ZA	182	ARG	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
ZA	183	GLY	-	expression tag	UNP P20285
ZA	184	SER	-	expression tag	UNP P20285
ZA	185	HIS	-	expression tag	UNP P20285
ZA	186	HIS	-	expression tag	UNP P20285
ZA	187	HIS	-	expression tag	UNP P20285
ZA	188	HIS	-	expression tag	UNP P20285
ZA	189	HIS	-	expression tag	UNP P20285
ZA	190	HIS	-	expression tag	UNP P20285
ZA	191	GLY	-	expression tag	UNP P20285
ZA	192	MET	-	expression tag	UNP P20285
ZA	193	ALA	-	expression tag	UNP P20285
ZA	194	SER	-	expression tag	UNP P20285
ZA	195	MET	-	expression tag	UNP P20285
ZA	196	THR	-	expression tag	UNP P20285
ZA	197	GLY	-	expression tag	UNP P20285
ZA	198	GLY	-	expression tag	UNP P20285
ZA	199	GLN	-	expression tag	UNP P20285
ZA	200	GLN	-	expression tag	UNP P20285
ZA	201	MET	-	expression tag	UNP P20285
ZA	202	GLY	-	expression tag	UNP P20285
ZA	203	ARG	-	expression tag	UNP P20285
ZA	204	ASP	-	expression tag	UNP P20285
ZA	205	LEU	-	expression tag	UNP P20285
ZA	206	TYR	-	expression tag	UNP P20285
ZA	207	ASP	-	expression tag	UNP P20285
ZA	208	ASP	-	expression tag	UNP P20285
ZA	209	ASP	-	expression tag	UNP P20285
ZA	210	ASP	-	expression tag	UNP P20285
ZA	211	LYS	-	expression tag	UNP P20285
ZA	212	ASP	-	expression tag	UNP P20285
ZA	213	ARG	-	expression tag	UNP P20285
ZA	214	TRP	-	expression tag	UNP P20285
ZA	215	GLY	-	expression tag	UNP P20285
ZA	216	SER	-	expression tag	UNP P20285
ZA	217	LEU	-	expression tag	UNP P20285
ZA	218	VAL	-	expression tag	UNP P20285
ZA	219	PRO	-	expression tag	UNP P20285
ZA	220	ARG	-	expression tag	UNP P20285
ZA	221	GLY	-	expression tag	UNP P20285
ZA	222	SER	-	expression tag	UNP P20285
ZA	223	HIS	-	expression tag	UNP P20285
ZA	224	MET	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
ZA	225	ALA	-	expression tag	UNP P20285
ZA	226	ALA	-	expression tag	UNP P20285
AB	181	MET	-	initiating methionine	UNP P20285
AB	182	ARG	-	expression tag	UNP P20285
AB	183	GLY	-	expression tag	UNP P20285
AB	184	SER	-	expression tag	UNP P20285
AB	185	HIS	-	expression tag	UNP P20285
AB	186	HIS	-	expression tag	UNP P20285
AB	187	HIS	-	expression tag	UNP P20285
AB	188	HIS	-	expression tag	UNP P20285
AB	189	HIS	-	expression tag	UNP P20285
AB	190	HIS	-	expression tag	UNP P20285
AB	191	GLY	-	expression tag	UNP P20285
AB	192	MET	-	expression tag	UNP P20285
AB	193	ALA	-	expression tag	UNP P20285
AB	194	SER	-	expression tag	UNP P20285
AB	195	MET	-	expression tag	UNP P20285
AB	196	THR	-	expression tag	UNP P20285
AB	197	GLY	-	expression tag	UNP P20285
AB	198	GLY	-	expression tag	UNP P20285
AB	199	GLN	-	expression tag	UNP P20285
AB	200	GLN	-	expression tag	UNP P20285
AB	201	MET	-	expression tag	UNP P20285
AB	202	GLY	-	expression tag	UNP P20285
AB	203	ARG	-	expression tag	UNP P20285
AB	204	ASP	-	expression tag	UNP P20285
AB	205	LEU	-	expression tag	UNP P20285
AB	206	TYR	-	expression tag	UNP P20285
AB	207	ASP	-	expression tag	UNP P20285
AB	208	ASP	-	expression tag	UNP P20285
AB	209	ASP	-	expression tag	UNP P20285
AB	210	ASP	-	expression tag	UNP P20285
AB	211	LYS	-	expression tag	UNP P20285
AB	212	ASP	-	expression tag	UNP P20285
AB	213	ARG	-	expression tag	UNP P20285
AB	214	TRP	-	expression tag	UNP P20285
AB	215	GLY	-	expression tag	UNP P20285
AB	216	SER	-	expression tag	UNP P20285
AB	217	LEU	-	expression tag	UNP P20285
AB	218	VAL	-	expression tag	UNP P20285
AB	219	PRO	-	expression tag	UNP P20285
AB	220	ARG	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
AB	221	GLY	-	expression tag	UNP P20285
AB	222	SER	-	expression tag	UNP P20285
AB	223	HIS	-	expression tag	UNP P20285
AB	224	MET	-	expression tag	UNP P20285
AB	225	ALA	-	expression tag	UNP P20285
AB	226	ALA	-	expression tag	UNP P20285
BB	181	MET	-	initiating methionine	UNP P20285
BB	182	ARG	-	expression tag	UNP P20285
BB	183	GLY	-	expression tag	UNP P20285
BB	184	SER	-	expression tag	UNP P20285
BB	185	HIS	-	expression tag	UNP P20285
BB	186	HIS	-	expression tag	UNP P20285
BB	187	HIS	-	expression tag	UNP P20285
BB	188	HIS	-	expression tag	UNP P20285
BB	189	HIS	-	expression tag	UNP P20285
BB	190	HIS	-	expression tag	UNP P20285
BB	191	GLY	-	expression tag	UNP P20285
BB	192	MET	-	expression tag	UNP P20285
BB	193	ALA	-	expression tag	UNP P20285
BB	194	SER	-	expression tag	UNP P20285
BB	195	MET	-	expression tag	UNP P20285
BB	196	THR	-	expression tag	UNP P20285
BB	197	GLY	-	expression tag	UNP P20285
BB	198	GLY	-	expression tag	UNP P20285
BB	199	GLN	-	expression tag	UNP P20285
BB	200	GLN	-	expression tag	UNP P20285
BB	201	MET	-	expression tag	UNP P20285
BB	202	GLY	-	expression tag	UNP P20285
BB	203	ARG	-	expression tag	UNP P20285
BB	204	ASP	-	expression tag	UNP P20285
BB	205	LEU	-	expression tag	UNP P20285
BB	206	TYR	-	expression tag	UNP P20285
BB	207	ASP	-	expression tag	UNP P20285
BB	208	ASP	-	expression tag	UNP P20285
BB	209	ASP	-	expression tag	UNP P20285
BB	210	ASP	-	expression tag	UNP P20285
BB	211	LYS	-	expression tag	UNP P20285
BB	212	ASP	-	expression tag	UNP P20285
BB	213	ARG	-	expression tag	UNP P20285
BB	214	TRP	-	expression tag	UNP P20285
BB	215	GLY	-	expression tag	UNP P20285
BB	216	SER	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
BB	217	LEU	-	expression tag	UNP P20285
BB	218	VAL	-	expression tag	UNP P20285
BB	219	PRO	-	expression tag	UNP P20285
BB	220	ARG	-	expression tag	UNP P20285
BB	221	GLY	-	expression tag	UNP P20285
BB	222	SER	-	expression tag	UNP P20285
BB	223	HIS	-	expression tag	UNP P20285
BB	224	MET	-	expression tag	UNP P20285
BB	225	ALA	-	expression tag	UNP P20285
BB	226	ALA	-	expression tag	UNP P20285
CB	181	MET	-	initiating methionine	UNP P20285
CB	182	ARG	-	expression tag	UNP P20285
CB	183	GLY	-	expression tag	UNP P20285
CB	184	SER	-	expression tag	UNP P20285
CB	185	HIS	-	expression tag	UNP P20285
CB	186	HIS	-	expression tag	UNP P20285
CB	187	HIS	-	expression tag	UNP P20285
CB	188	HIS	-	expression tag	UNP P20285
CB	189	HIS	-	expression tag	UNP P20285
CB	190	HIS	-	expression tag	UNP P20285
CB	191	GLY	-	expression tag	UNP P20285
CB	192	MET	-	expression tag	UNP P20285
CB	193	ALA	-	expression tag	UNP P20285
CB	194	SER	-	expression tag	UNP P20285
CB	195	MET	-	expression tag	UNP P20285
CB	196	THR	-	expression tag	UNP P20285
CB	197	GLY	-	expression tag	UNP P20285
CB	198	GLY	-	expression tag	UNP P20285
CB	199	GLN	-	expression tag	UNP P20285
CB	200	GLN	-	expression tag	UNP P20285
CB	201	MET	-	expression tag	UNP P20285
CB	202	GLY	-	expression tag	UNP P20285
CB	203	ARG	-	expression tag	UNP P20285
CB	204	ASP	-	expression tag	UNP P20285
CB	205	LEU	-	expression tag	UNP P20285
CB	206	TYR	-	expression tag	UNP P20285
CB	207	ASP	-	expression tag	UNP P20285
CB	208	ASP	-	expression tag	UNP P20285
CB	209	ASP	-	expression tag	UNP P20285
CB	210	ASP	-	expression tag	UNP P20285
CB	211	LYS	-	expression tag	UNP P20285
CB	212	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
CB	213	ARG	-	expression tag	UNP P20285
CB	214	TRP	-	expression tag	UNP P20285
CB	215	GLY	-	expression tag	UNP P20285
CB	216	SER	-	expression tag	UNP P20285
CB	217	LEU	-	expression tag	UNP P20285
CB	218	VAL	-	expression tag	UNP P20285
CB	219	PRO	-	expression tag	UNP P20285
CB	220	ARG	-	expression tag	UNP P20285
CB	221	GLY	-	expression tag	UNP P20285
CB	222	SER	-	expression tag	UNP P20285
CB	223	HIS	-	expression tag	UNP P20285
CB	224	MET	-	expression tag	UNP P20285
CB	225	ALA	-	expression tag	UNP P20285
CB	226	ALA	-	expression tag	UNP P20285
DB	181	MET	-	initiating methionine	UNP P20285
DB	182	ARG	-	expression tag	UNP P20285
DB	183	GLY	-	expression tag	UNP P20285
DB	184	SER	-	expression tag	UNP P20285
DB	185	HIS	-	expression tag	UNP P20285
DB	186	HIS	-	expression tag	UNP P20285
DB	187	HIS	-	expression tag	UNP P20285
DB	188	HIS	-	expression tag	UNP P20285
DB	189	HIS	-	expression tag	UNP P20285
DB	190	HIS	-	expression tag	UNP P20285
DB	191	GLY	-	expression tag	UNP P20285
DB	192	MET	-	expression tag	UNP P20285
DB	193	ALA	-	expression tag	UNP P20285
DB	194	SER	-	expression tag	UNP P20285
DB	195	MET	-	expression tag	UNP P20285
DB	196	THR	-	expression tag	UNP P20285
DB	197	GLY	-	expression tag	UNP P20285
DB	198	GLY	-	expression tag	UNP P20285
DB	199	GLN	-	expression tag	UNP P20285
DB	200	GLN	-	expression tag	UNP P20285
DB	201	MET	-	expression tag	UNP P20285
DB	202	GLY	-	expression tag	UNP P20285
DB	203	ARG	-	expression tag	UNP P20285
DB	204	ASP	-	expression tag	UNP P20285
DB	205	LEU	-	expression tag	UNP P20285
DB	206	TYR	-	expression tag	UNP P20285
DB	207	ASP	-	expression tag	UNP P20285
DB	208	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	209	ASP	-	expression tag	UNP P20285
DB	210	ASP	-	expression tag	UNP P20285
DB	211	LYS	-	expression tag	UNP P20285
DB	212	ASP	-	expression tag	UNP P20285
DB	213	ARG	-	expression tag	UNP P20285
DB	214	TRP	-	expression tag	UNP P20285
DB	215	GLY	-	expression tag	UNP P20285
DB	216	SER	-	expression tag	UNP P20285
DB	217	LEU	-	expression tag	UNP P20285
DB	218	VAL	-	expression tag	UNP P20285
DB	219	PRO	-	expression tag	UNP P20285
DB	220	ARG	-	expression tag	UNP P20285
DB	221	GLY	-	expression tag	UNP P20285
DB	222	SER	-	expression tag	UNP P20285
DB	223	HIS	-	expression tag	UNP P20285
DB	224	MET	-	expression tag	UNP P20285
DB	225	ALA	-	expression tag	UNP P20285
DB	226	ALA	-	expression tag	UNP P20285
EB	181	MET	-	initiating methionine	UNP P20285
EB	182	ARG	-	expression tag	UNP P20285
EB	183	GLY	-	expression tag	UNP P20285
EB	184	SER	-	expression tag	UNP P20285
EB	185	HIS	-	expression tag	UNP P20285
EB	186	HIS	-	expression tag	UNP P20285
EB	187	HIS	-	expression tag	UNP P20285
EB	188	HIS	-	expression tag	UNP P20285
EB	189	HIS	-	expression tag	UNP P20285
EB	190	HIS	-	expression tag	UNP P20285
EB	191	GLY	-	expression tag	UNP P20285
EB	192	MET	-	expression tag	UNP P20285
EB	193	ALA	-	expression tag	UNP P20285
EB	194	SER	-	expression tag	UNP P20285
EB	195	MET	-	expression tag	UNP P20285
EB	196	THR	-	expression tag	UNP P20285
EB	197	GLY	-	expression tag	UNP P20285
EB	198	GLY	-	expression tag	UNP P20285
EB	199	GLN	-	expression tag	UNP P20285
EB	200	GLN	-	expression tag	UNP P20285
EB	201	MET	-	expression tag	UNP P20285
EB	202	GLY	-	expression tag	UNP P20285
EB	203	ARG	-	expression tag	UNP P20285
EB	204	ASP	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
EB	205	LEU	-	expression tag	UNP P20285
EB	206	TYR	-	expression tag	UNP P20285
EB	207	ASP	-	expression tag	UNP P20285
EB	208	ASP	-	expression tag	UNP P20285
EB	209	ASP	-	expression tag	UNP P20285
EB	210	ASP	-	expression tag	UNP P20285
EB	211	LYS	-	expression tag	UNP P20285
EB	212	ASP	-	expression tag	UNP P20285
EB	213	ARG	-	expression tag	UNP P20285
EB	214	TRP	-	expression tag	UNP P20285
EB	215	GLY	-	expression tag	UNP P20285
EB	216	SER	-	expression tag	UNP P20285
EB	217	LEU	-	expression tag	UNP P20285
EB	218	VAL	-	expression tag	UNP P20285
EB	219	PRO	-	expression tag	UNP P20285
EB	220	ARG	-	expression tag	UNP P20285
EB	221	GLY	-	expression tag	UNP P20285
EB	222	SER	-	expression tag	UNP P20285
EB	223	HIS	-	expression tag	UNP P20285
EB	224	MET	-	expression tag	UNP P20285
EB	225	ALA	-	expression tag	UNP P20285
EB	226	ALA	-	expression tag	UNP P20285
FB	181	MET	-	initiating methionine	UNP P20285
FB	182	ARG	-	expression tag	UNP P20285
FB	183	GLY	-	expression tag	UNP P20285
FB	184	SER	-	expression tag	UNP P20285
FB	185	HIS	-	expression tag	UNP P20285
FB	186	HIS	-	expression tag	UNP P20285
FB	187	HIS	-	expression tag	UNP P20285
FB	188	HIS	-	expression tag	UNP P20285
FB	189	HIS	-	expression tag	UNP P20285
FB	190	HIS	-	expression tag	UNP P20285
FB	191	GLY	-	expression tag	UNP P20285
FB	192	MET	-	expression tag	UNP P20285
FB	193	ALA	-	expression tag	UNP P20285
FB	194	SER	-	expression tag	UNP P20285
FB	195	MET	-	expression tag	UNP P20285
FB	196	THR	-	expression tag	UNP P20285
FB	197	GLY	-	expression tag	UNP P20285
FB	198	GLY	-	expression tag	UNP P20285
FB	199	GLN	-	expression tag	UNP P20285
FB	200	GLN	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
FB	201	MET	-	expression tag	UNP P20285
FB	202	GLY	-	expression tag	UNP P20285
FB	203	ARG	-	expression tag	UNP P20285
FB	204	ASP	-	expression tag	UNP P20285
FB	205	LEU	-	expression tag	UNP P20285
FB	206	TYR	-	expression tag	UNP P20285
FB	207	ASP	-	expression tag	UNP P20285
FB	208	ASP	-	expression tag	UNP P20285
FB	209	ASP	-	expression tag	UNP P20285
FB	210	ASP	-	expression tag	UNP P20285
FB	211	LYS	-	expression tag	UNP P20285
FB	212	ASP	-	expression tag	UNP P20285
FB	213	ARG	-	expression tag	UNP P20285
FB	214	TRP	-	expression tag	UNP P20285
FB	215	GLY	-	expression tag	UNP P20285
FB	216	SER	-	expression tag	UNP P20285
FB	217	LEU	-	expression tag	UNP P20285
FB	218	VAL	-	expression tag	UNP P20285
FB	219	PRO	-	expression tag	UNP P20285
FB	220	ARG	-	expression tag	UNP P20285
FB	221	GLY	-	expression tag	UNP P20285
FB	222	SER	-	expression tag	UNP P20285
FB	223	HIS	-	expression tag	UNP P20285
FB	224	MET	-	expression tag	UNP P20285
FB	225	ALA	-	expression tag	UNP P20285
FB	226	ALA	-	expression tag	UNP P20285
GB	181	MET	-	initiating methionine	UNP P20285
GB	182	ARG	-	expression tag	UNP P20285
GB	183	GLY	-	expression tag	UNP P20285
GB	184	SER	-	expression tag	UNP P20285
GB	185	HIS	-	expression tag	UNP P20285
GB	186	HIS	-	expression tag	UNP P20285
GB	187	HIS	-	expression tag	UNP P20285
GB	188	HIS	-	expression tag	UNP P20285
GB	189	HIS	-	expression tag	UNP P20285
GB	190	HIS	-	expression tag	UNP P20285
GB	191	GLY	-	expression tag	UNP P20285
GB	192	MET	-	expression tag	UNP P20285
GB	193	ALA	-	expression tag	UNP P20285
GB	194	SER	-	expression tag	UNP P20285
GB	195	MET	-	expression tag	UNP P20285
GB	196	THR	-	expression tag	UNP P20285

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Chain	Residue	Modelled	Actual	Comment	Reference
GB	197	GLY	-	expression tag	UNP P20285
GB	198	GLY	-	expression tag	UNP P20285
GB	199	GLN	-	expression tag	UNP P20285
GB	200	GLN	-	expression tag	UNP P20285
GB	201	MET	-	expression tag	UNP P20285
GB	202	GLY	-	expression tag	UNP P20285
GB	203	ARG	-	expression tag	UNP P20285
GB	204	ASP	-	expression tag	UNP P20285
GB	205	LEU	-	expression tag	UNP P20285
GB	206	TYR	-	expression tag	UNP P20285
GB	207	ASP	-	expression tag	UNP P20285
GB	208	ASP	-	expression tag	UNP P20285
GB	209	ASP	-	expression tag	UNP P20285
GB	210	ASP	-	expression tag	UNP P20285
GB	211	LYS	-	expression tag	UNP P20285
GB	212	ASP	-	expression tag	UNP P20285
GB	213	ARG	-	expression tag	UNP P20285
GB	214	TRP	-	expression tag	UNP P20285
GB	215	GLY	-	expression tag	UNP P20285
GB	216	SER	-	expression tag	UNP P20285
GB	217	LEU	-	expression tag	UNP P20285
GB	218	VAL	-	expression tag	UNP P20285
GB	219	PRO	-	expression tag	UNP P20285
GB	220	ARG	-	expression tag	UNP P20285
GB	221	GLY	-	expression tag	UNP P20285
GB	222	SER	-	expression tag	UNP P20285
GB	223	HIS	-	expression tag	UNP P20285
GB	224	MET	-	expression tag	UNP P20285
GB	225	ALA	-	expression tag	UNP P20285
GB	226	ALA	-	expression tag	UNP P20285
HB	181	MET	-	initiating methionine	UNP P20285
HB	182	ARG	-	expression tag	UNP P20285
HB	183	GLY	-	expression tag	UNP P20285
HB	184	SER	-	expression tag	UNP P20285
HB	185	HIS	-	expression tag	UNP P20285
HB	186	HIS	-	expression tag	UNP P20285
HB	187	HIS	-	expression tag	UNP P20285
HB	188	HIS	-	expression tag	UNP P20285
HB	189	HIS	-	expression tag	UNP P20285
HB	190	HIS	-	expression tag	UNP P20285
HB	191	GLY	-	expression tag	UNP P20285
HB	192	MET	-	expression tag	UNP P20285

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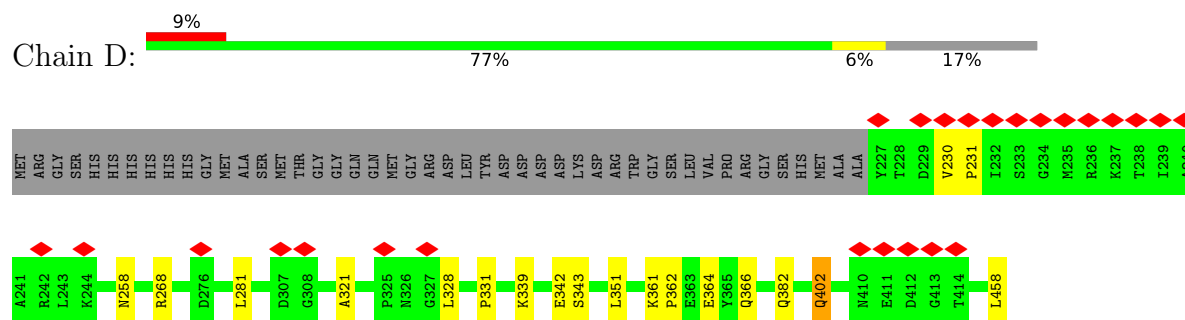
Chain	Residue	Modelled	Actual	Comment	Reference
HB	193	ALA	-	expression tag	UNP P20285
HB	194	SER	-	expression tag	UNP P20285
HB	195	MET	-	expression tag	UNP P20285
HB	196	THR	-	expression tag	UNP P20285
HB	197	GLY	-	expression tag	UNP P20285
HB	198	GLY	-	expression tag	UNP P20285
HB	199	GLN	-	expression tag	UNP P20285
HB	200	GLN	-	expression tag	UNP P20285
HB	201	MET	-	expression tag	UNP P20285
HB	202	GLY	-	expression tag	UNP P20285
HB	203	ARG	-	expression tag	UNP P20285
HB	204	ASP	-	expression tag	UNP P20285
HB	205	LEU	-	expression tag	UNP P20285
HB	206	TYR	-	expression tag	UNP P20285
HB	207	ASP	-	expression tag	UNP P20285
HB	208	ASP	-	expression tag	UNP P20285
HB	209	ASP	-	expression tag	UNP P20285
HB	210	ASP	-	expression tag	UNP P20285
HB	211	LYS	-	expression tag	UNP P20285
HB	212	ASP	-	expression tag	UNP P20285
HB	213	ARG	-	expression tag	UNP P20285
HB	214	TRP	-	expression tag	UNP P20285
HB	215	GLY	-	expression tag	UNP P20285
HB	216	SER	-	expression tag	UNP P20285
HB	217	LEU	-	expression tag	UNP P20285
HB	218	VAL	-	expression tag	UNP P20285
HB	219	PRO	-	expression tag	UNP P20285
HB	220	ARG	-	expression tag	UNP P20285
HB	221	GLY	-	expression tag	UNP P20285
HB	222	SER	-	expression tag	UNP P20285
HB	223	HIS	-	expression tag	UNP P20285
HB	224	MET	-	expression tag	UNP P20285
HB	225	ALA	-	expression tag	UNP P20285
HB	226	ALA	-	expression tag	UNP P20285
IB	181	MET	-	initiating methionine	UNP P20285
IB	182	ARG	-	expression tag	UNP P20285
IB	183	GLY	-	expression tag	UNP P20285
IB	184	SER	-	expression tag	UNP P20285
IB	185	HIS	-	expression tag	UNP P20285
IB	186	HIS	-	expression tag	UNP P20285
IB	187	HIS	-	expression tag	UNP P20285
IB	188	HIS	-	expression tag	UNP P20285

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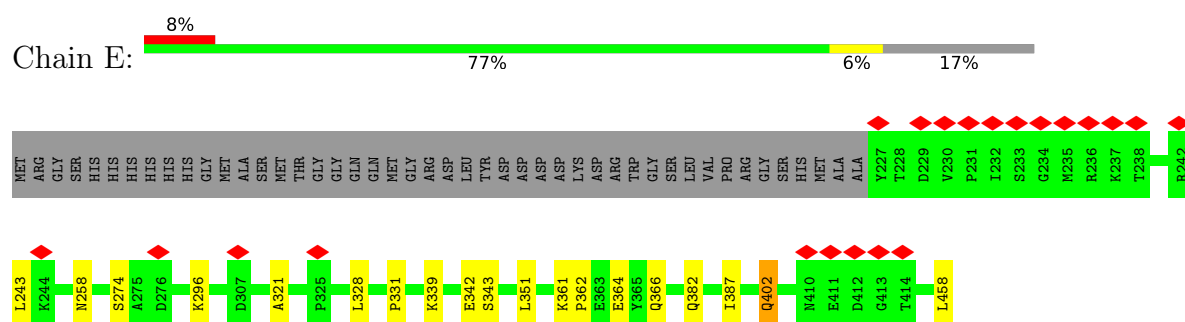
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Chain	Residue	Modelled	Actual	Comment	Reference
IB	189	HIS	-	expression tag	UNP P20285
IB	190	HIS	-	expression tag	UNP P20285
IB	191	GLY	-	expression tag	UNP P20285
IB	192	MET	-	expression tag	UNP P20285
IB	193	ALA	-	expression tag	UNP P20285
IB	194	SER	-	expression tag	UNP P20285
IB	195	MET	-	expression tag	UNP P20285
IB	196	THR	-	expression tag	UNP P20285
IB	197	GLY	-	expression tag	UNP P20285
IB	198	GLY	-	expression tag	UNP P20285
IB	199	GLN	-	expression tag	UNP P20285
IB	200	GLN	-	expression tag	UNP P20285
IB	201	MET	-	expression tag	UNP P20285
IB	202	GLY	-	expression tag	UNP P20285
IB	203	ARG	-	expression tag	UNP P20285
IB	204	ASP	-	expression tag	UNP P20285
IB	205	LEU	-	expression tag	UNP P20285
IB	206	TYR	-	expression tag	UNP P20285
IB	207	ASP	-	expression tag	UNP P20285
IB	208	ASP	-	expression tag	UNP P20285
IB	209	ASP	-	expression tag	UNP P20285
IB	210	ASP	-	expression tag	UNP P20285
IB	211	LYS	-	expression tag	UNP P20285
IB	212	ASP	-	expression tag	UNP P20285
IB	213	ARG	-	expression tag	UNP P20285
IB	214	TRP	-	expression tag	UNP P20285
IB	215	GLY	-	expression tag	UNP P20285
IB	216	SER	-	expression tag	UNP P20285
IB	217	LEU	-	expression tag	UNP P20285
IB	218	VAL	-	expression tag	UNP P20285
IB	219	PRO	-	expression tag	UNP P20285
IB	220	ARG	-	expression tag	UNP P20285
IB	221	GLY	-	expression tag	UNP P20285
IB	222	SER	-	expression tag	UNP P20285
IB	223	HIS	-	expression tag	UNP P20285
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IB	225	ALA	-	expression tag	UNP P20285
IB	226	ALA	-	expression tag	UNP P20285

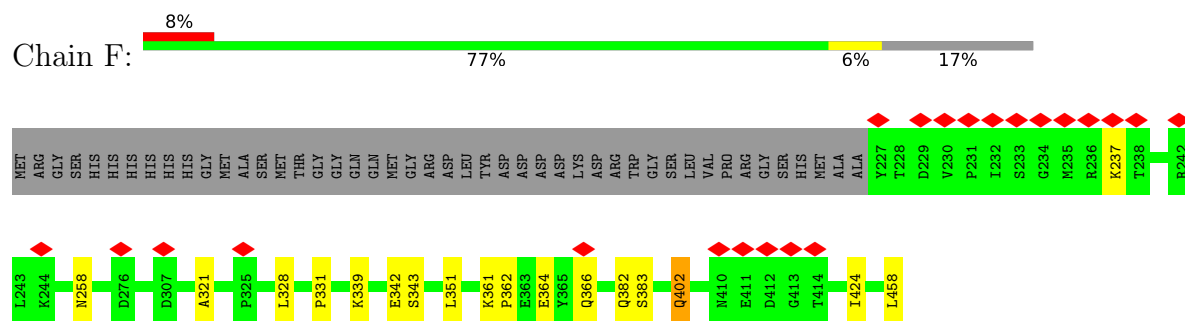
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



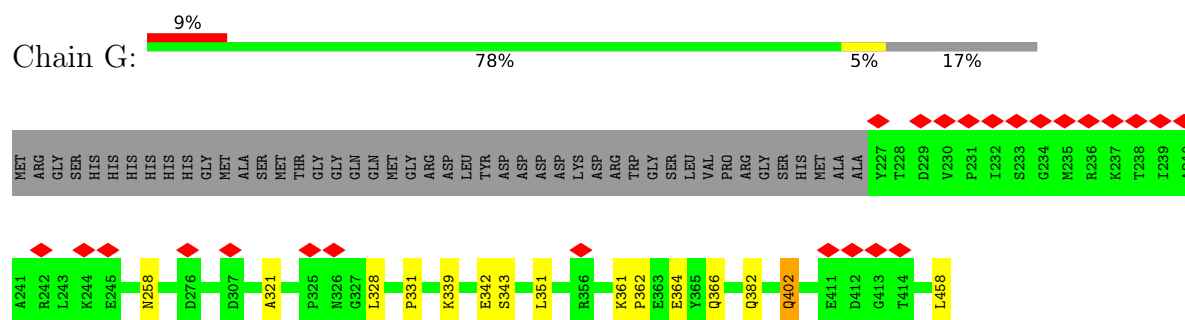
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



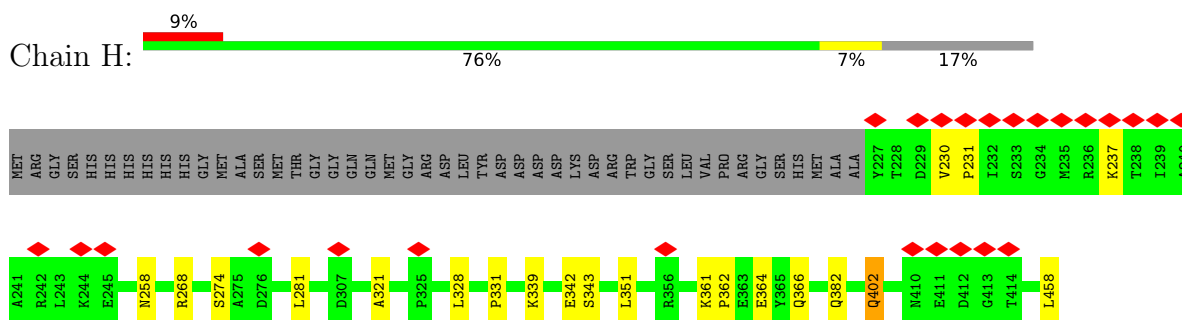
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



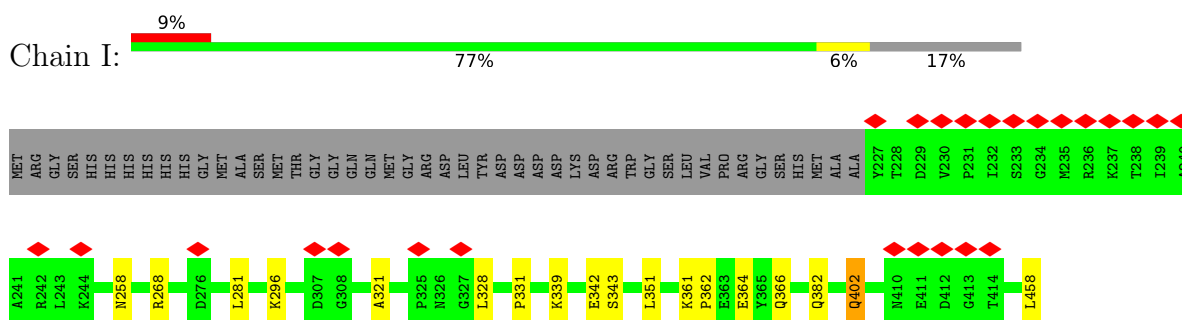
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



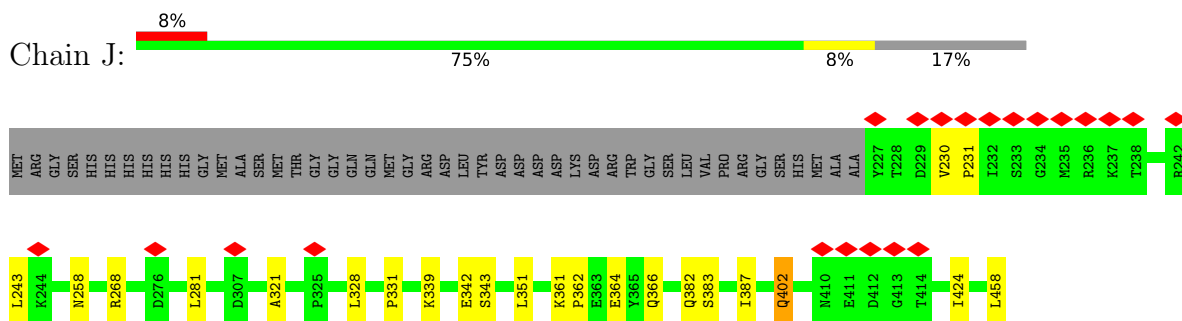
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



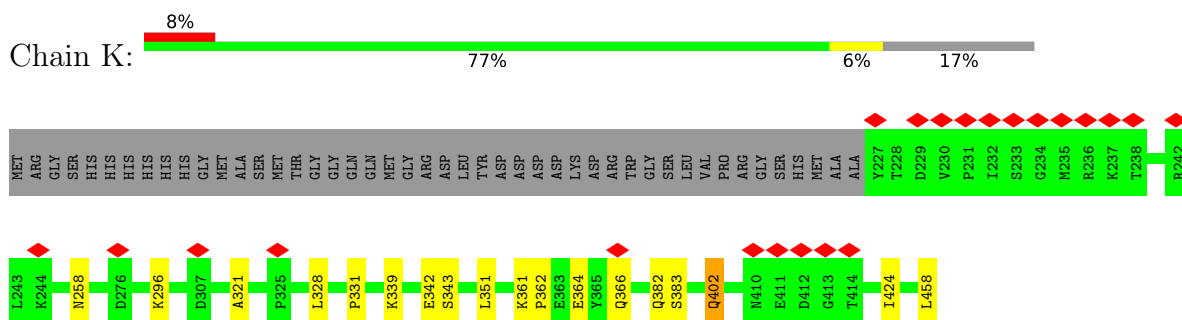
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



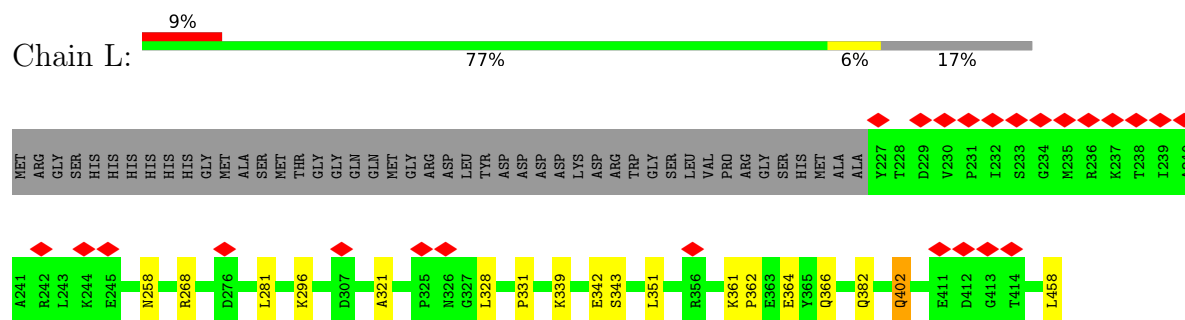
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



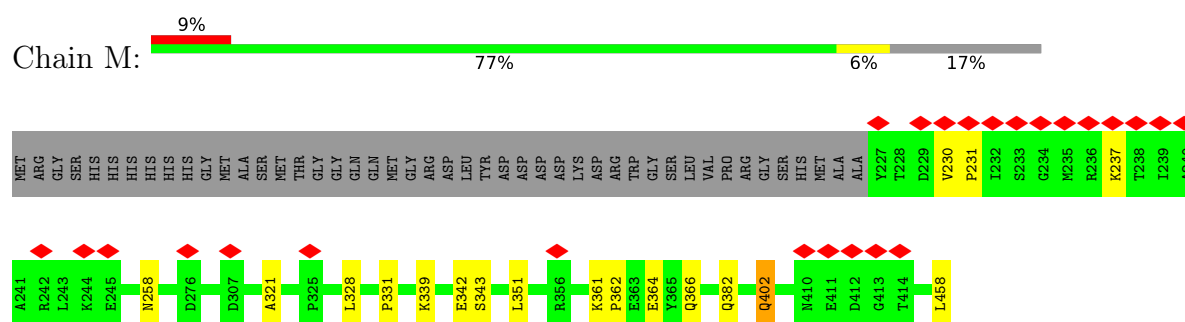
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



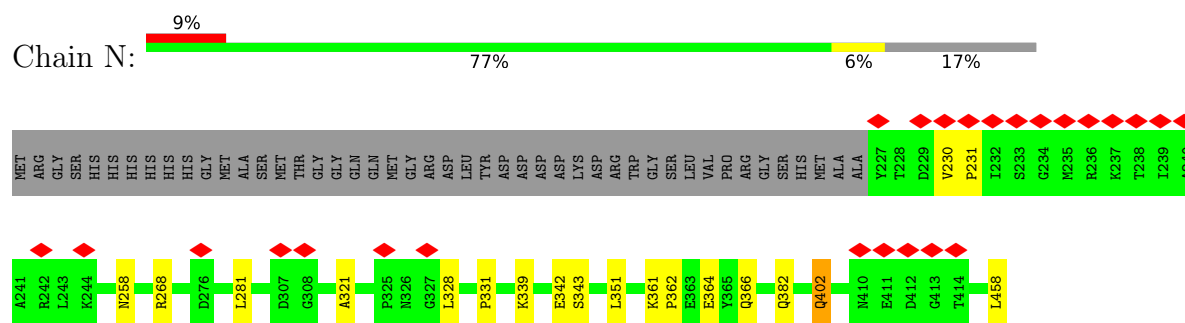
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



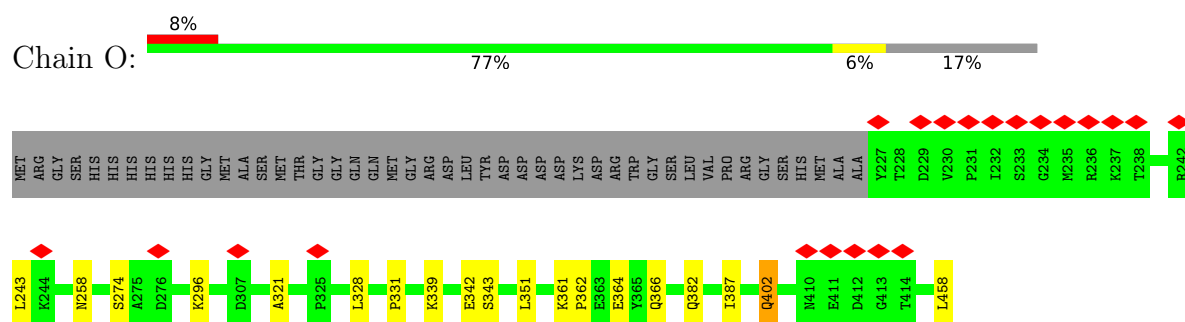
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



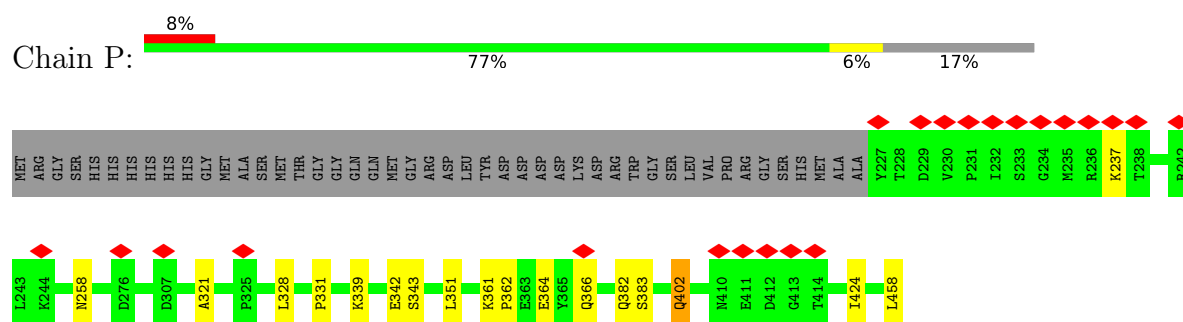
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



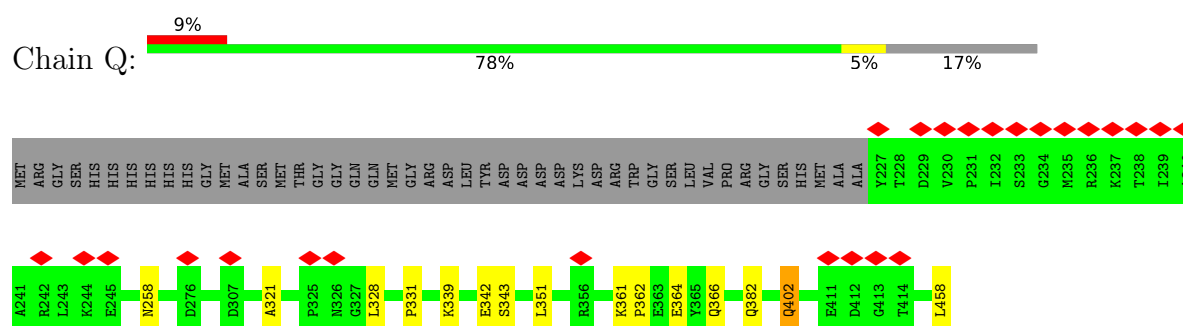
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



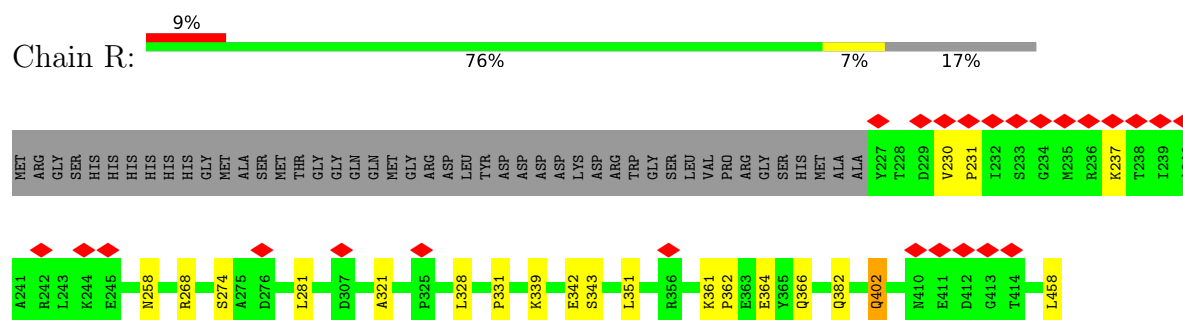
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



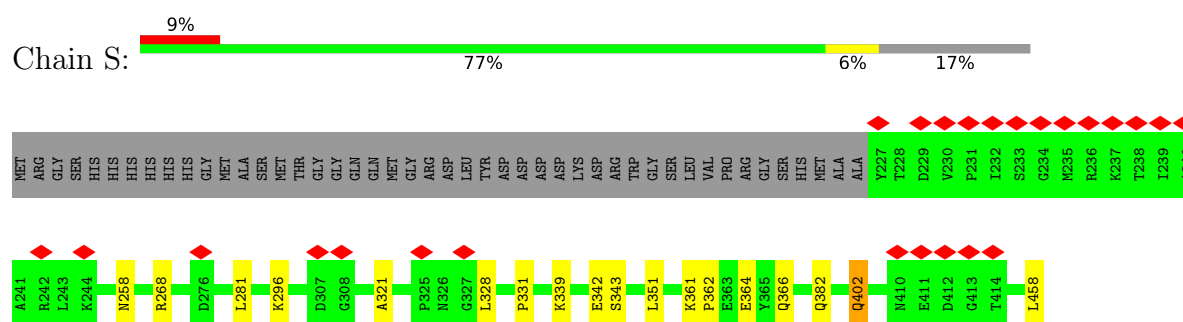
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



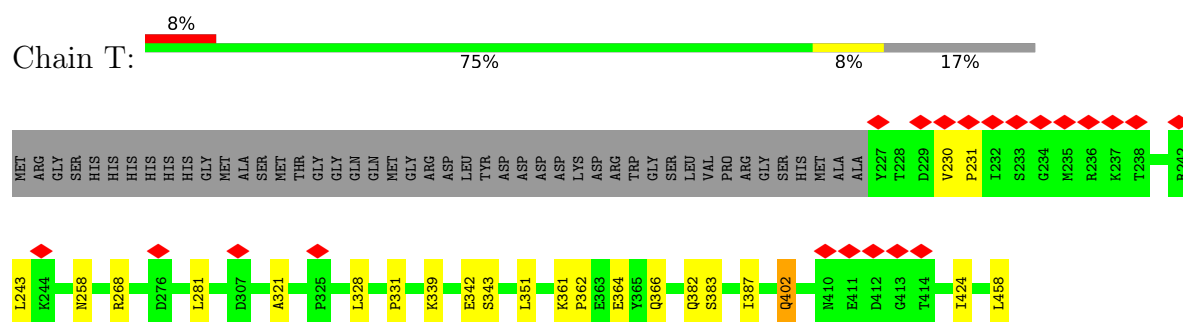
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



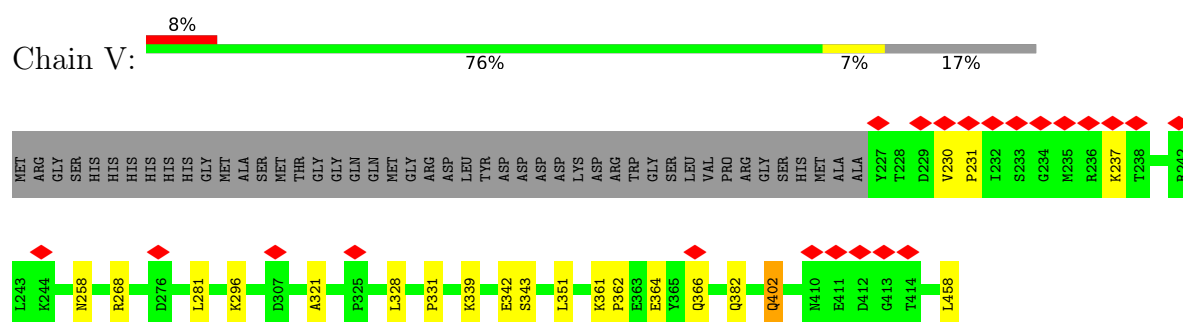
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



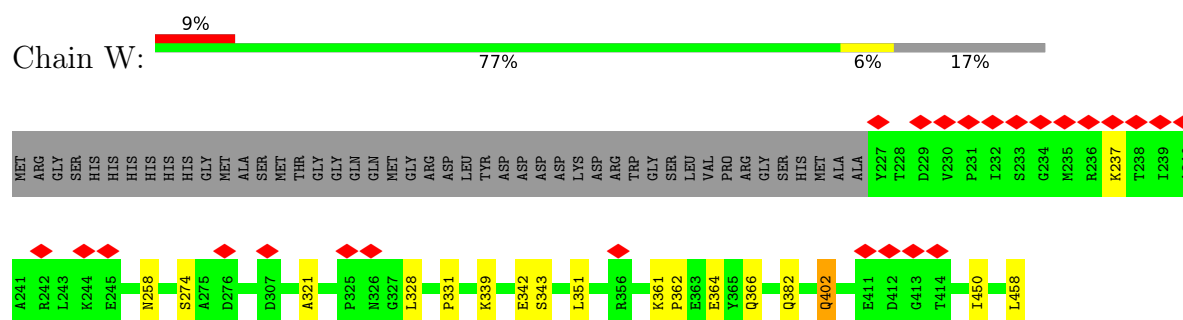
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



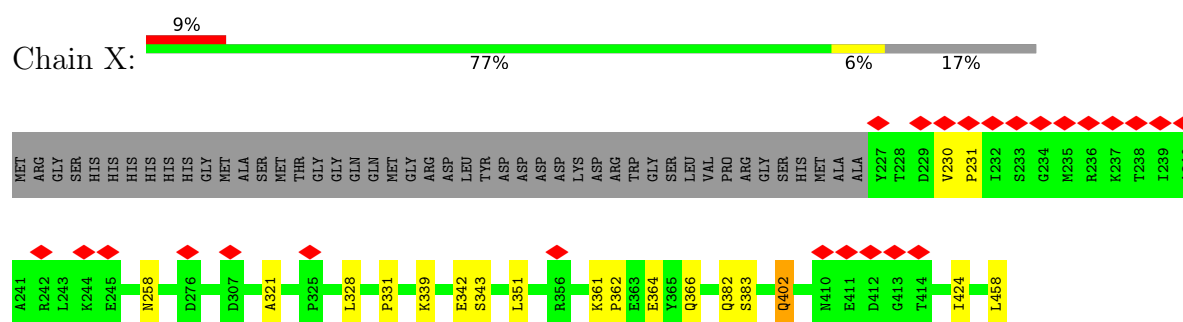
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



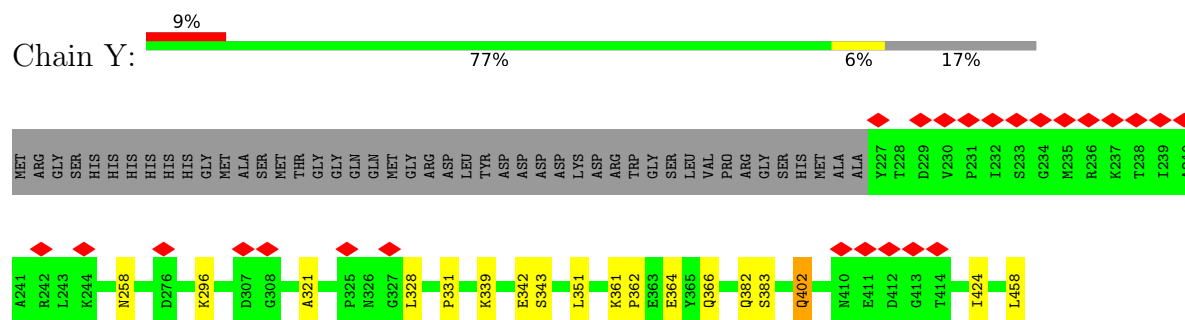
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



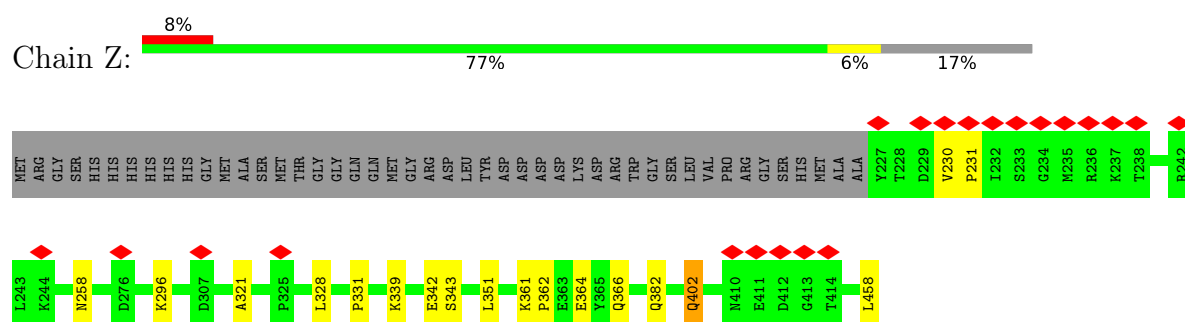
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



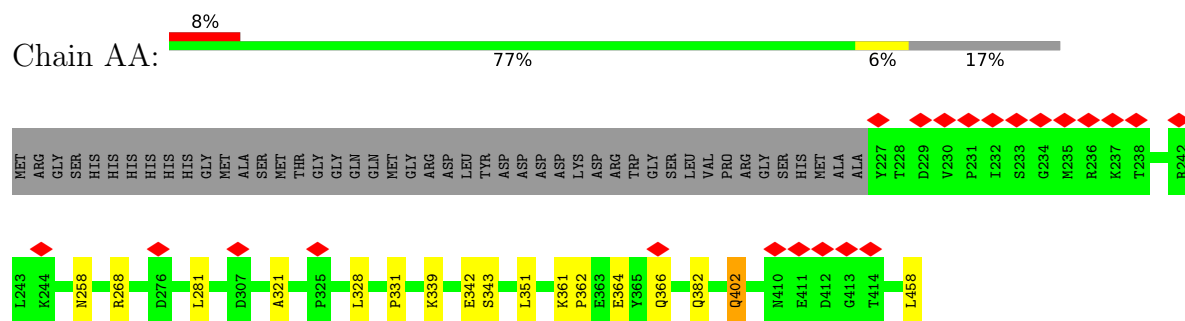
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



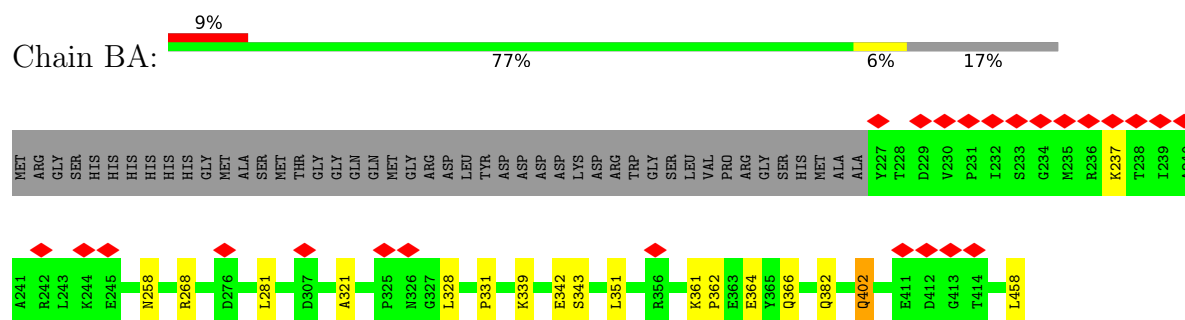
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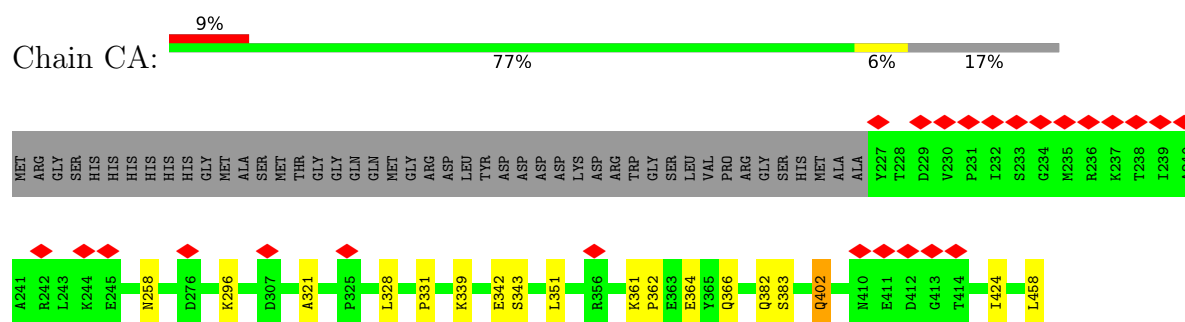
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



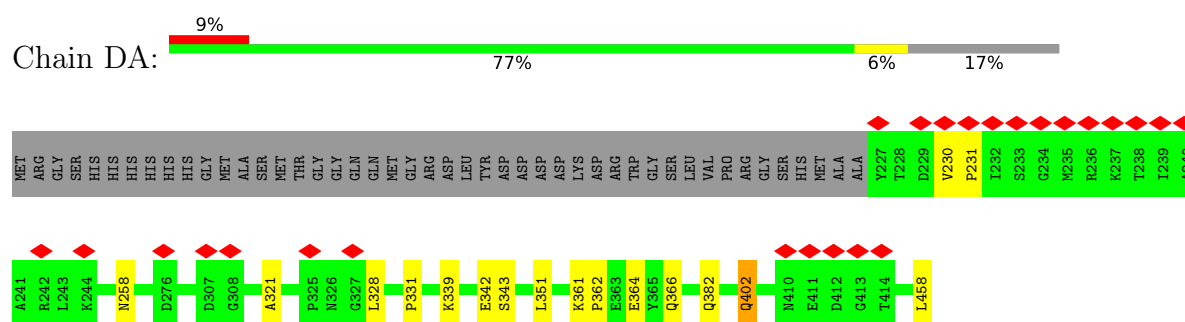
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



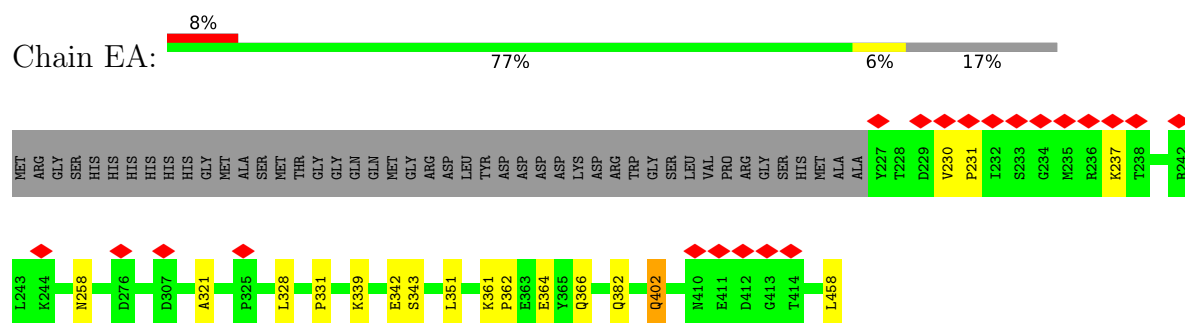
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



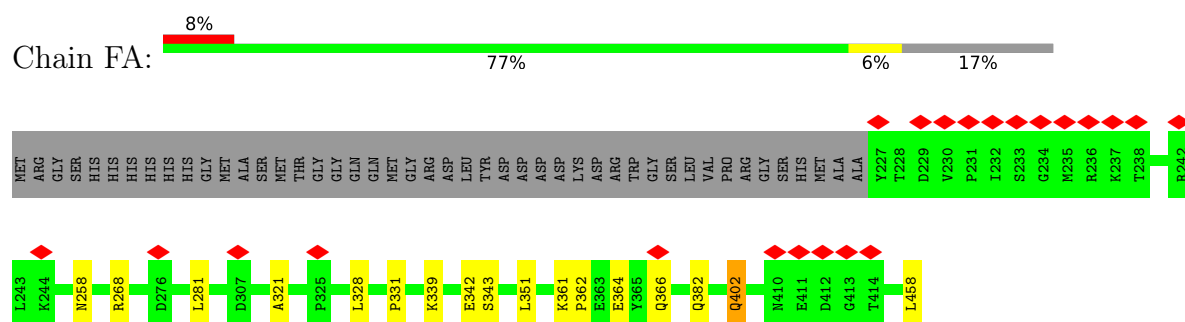
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



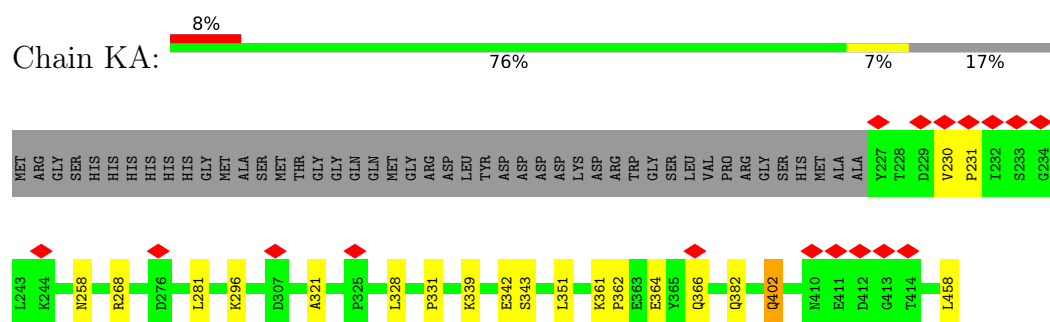
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



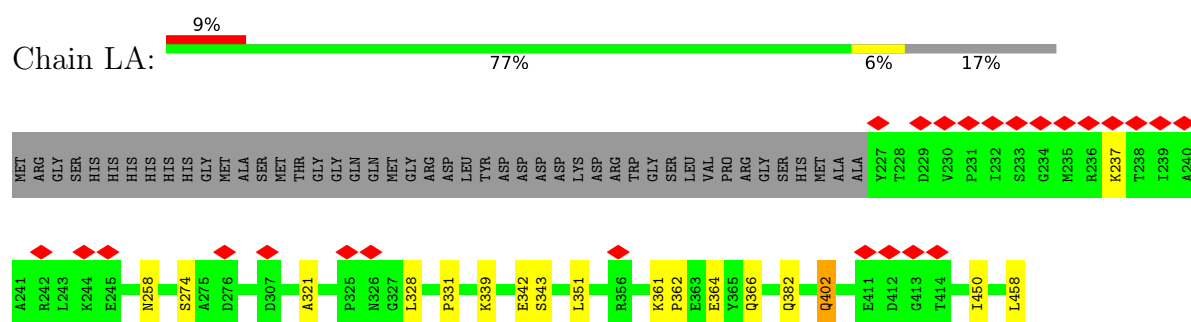
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



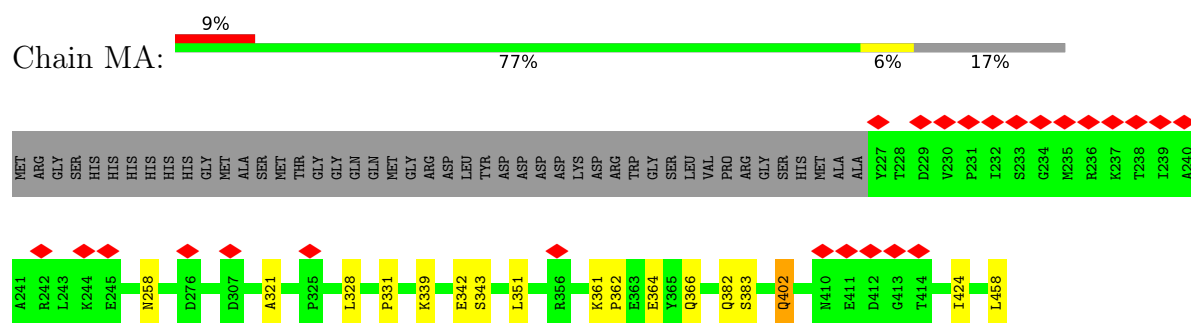
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



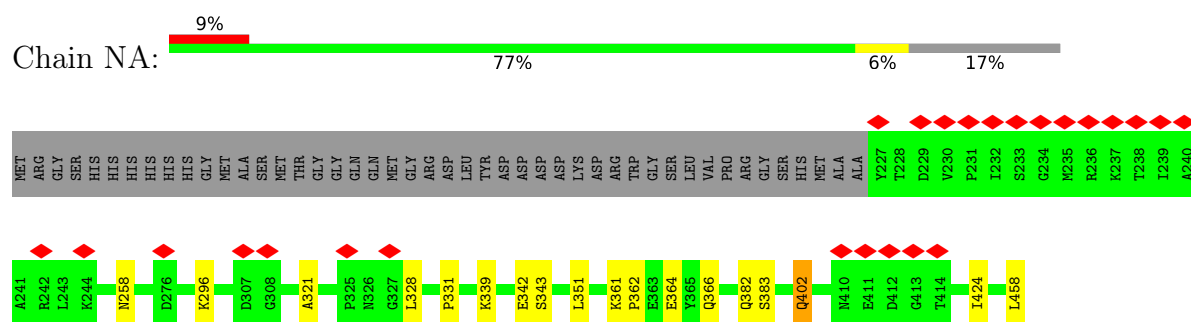
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



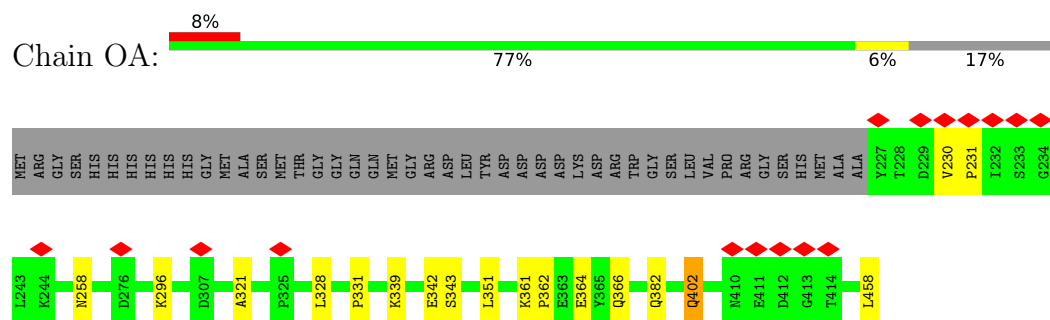
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



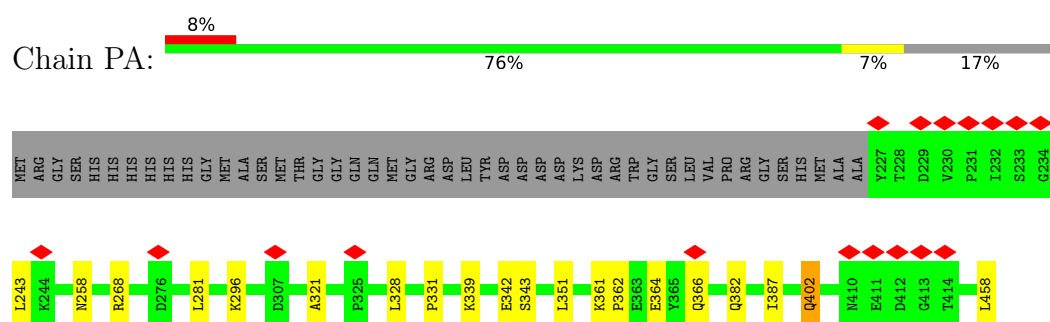
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



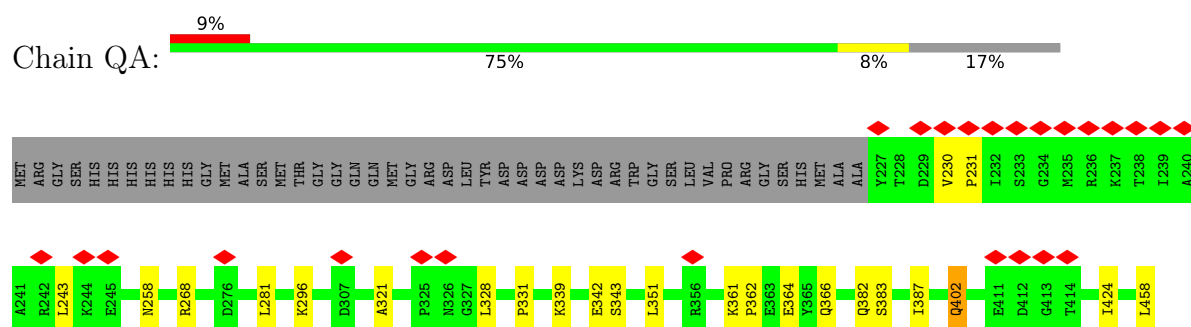
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



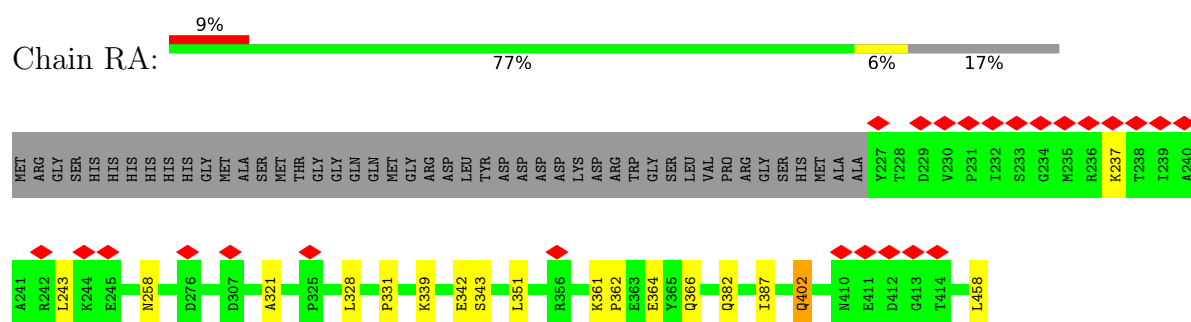
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



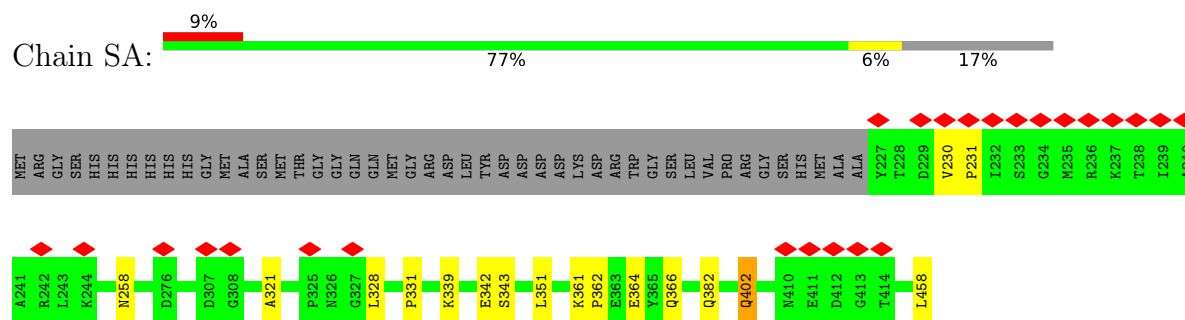
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



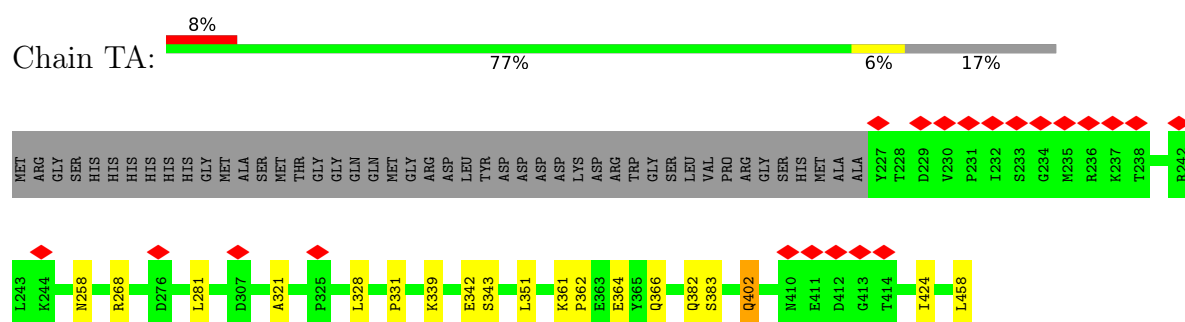
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



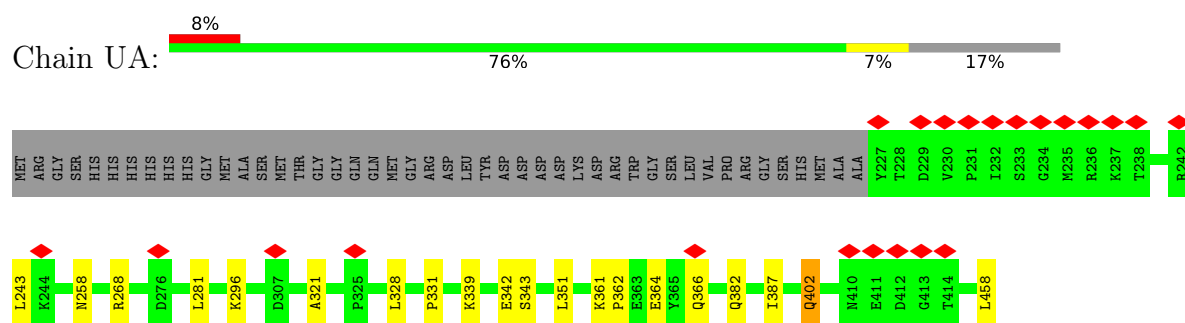
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



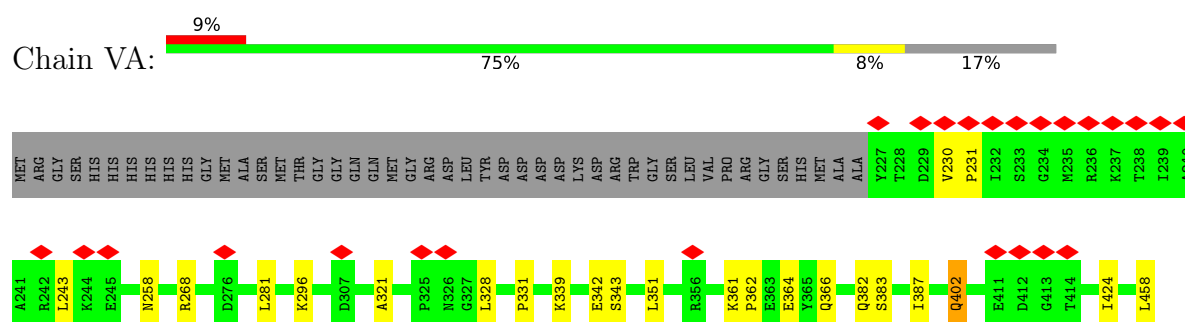
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



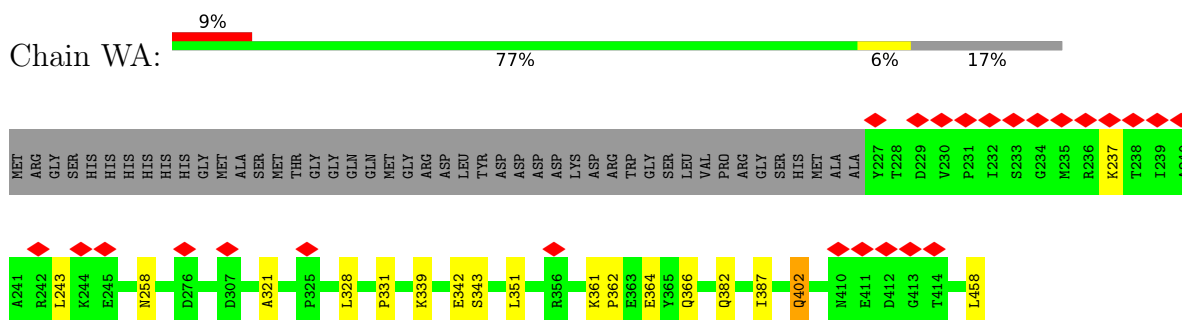
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



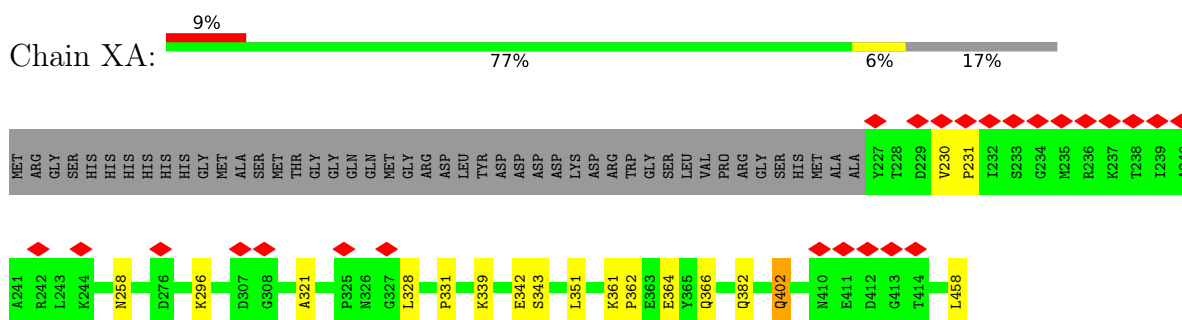
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



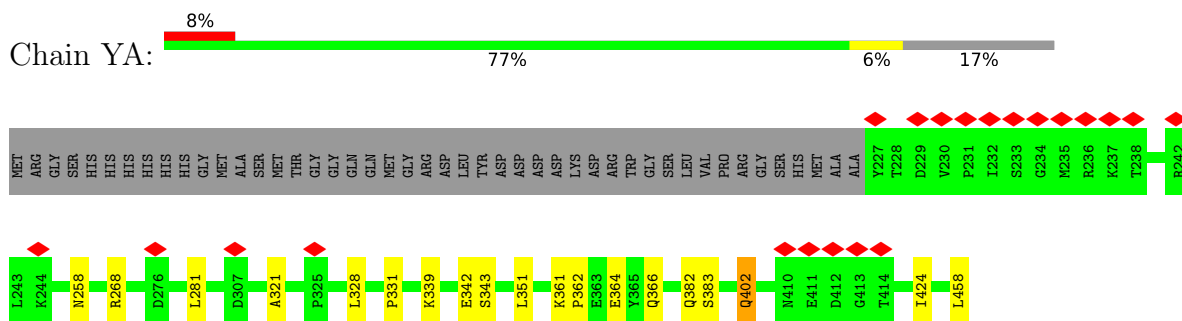
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



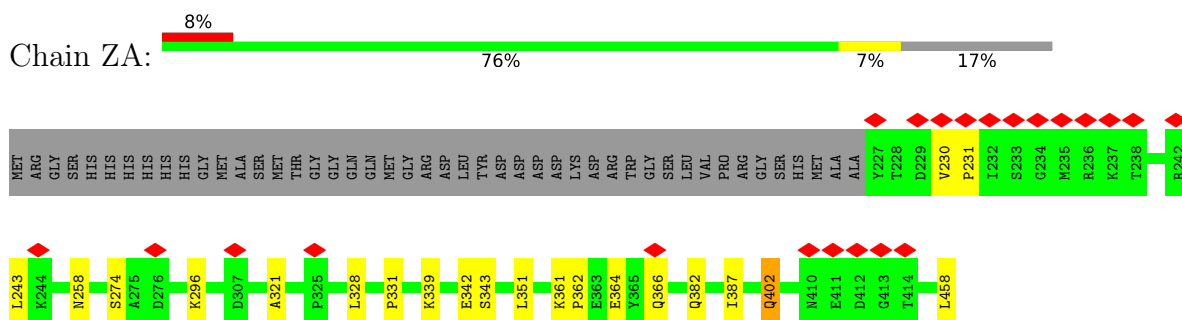
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



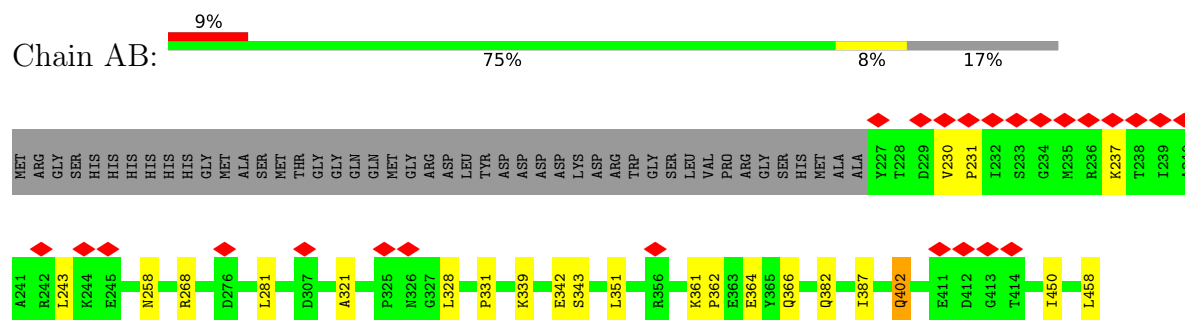
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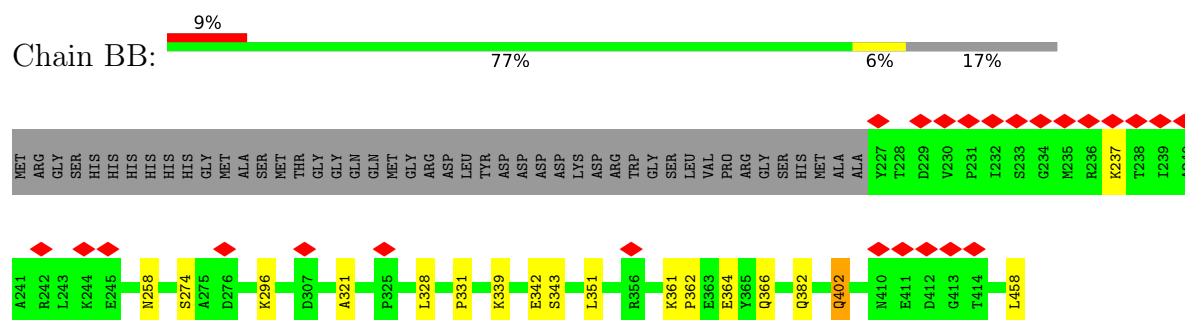
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



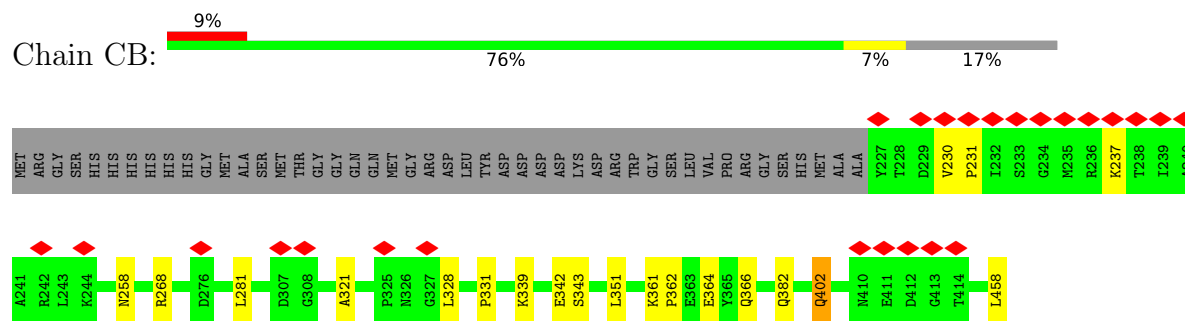
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



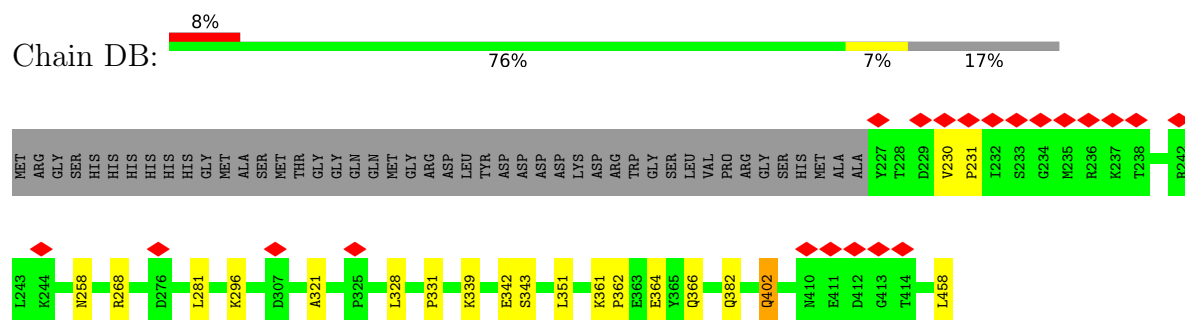
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



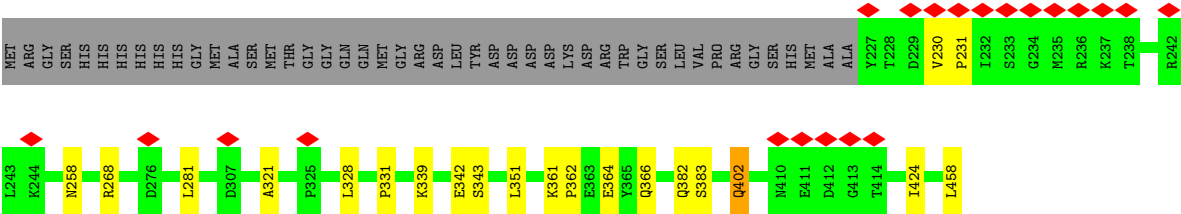
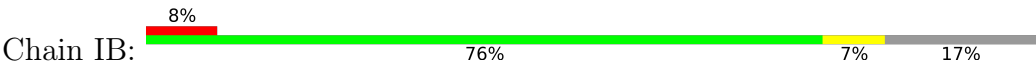
- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



- Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



● Molecule 1: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	129588	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 ($e^-/\text{\AA}^2$)	27.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.193	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0235	Depositor
Map size (Å)	430.08002, 430.08002, 430.08002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/1779	0.44	0/2413
1	AA	0.18	0/1779	0.44	0/2413
1	AB	0.19	0/1779	0.45	0/2413
1	B	0.19	0/1779	0.45	0/2413
1	BA	0.19	0/1779	0.45	0/2413
1	BB	0.19	0/1779	0.45	0/2413
1	C	0.19	0/1779	0.45	0/2413
1	CA	0.19	0/1779	0.45	0/2413
1	CB	0.19	0/1779	0.45	0/2413
1	D	0.19	0/1779	0.45	0/2413
1	DA	0.19	0/1779	0.45	0/2413
1	DB	0.19	0/1779	0.44	0/2413
1	E	0.19	0/1779	0.44	0/2413
1	EA	0.19	0/1779	0.44	0/2413
1	EB	0.18	0/1779	0.44	0/2413
1	F	0.18	0/1779	0.44	0/2413
1	FA	0.18	0/1779	0.44	0/2413
1	FB	0.19	0/1779	0.45	0/2413
1	G	0.19	0/1779	0.45	0/2413
1	GA	0.19	0/1779	0.45	0/2413
1	GB	0.19	0/1779	0.45	0/2413
1	H	0.19	0/1779	0.45	0/2413
1	HA	0.19	0/1779	0.44	0/2413
1	HB	0.19	0/1779	0.45	0/2413
1	I	0.19	0/1779	0.45	0/2413
1	IA	0.19	0/1779	0.45	0/2413
1	IB	0.19	0/1779	0.44	0/2413
1	J	0.19	0/1779	0.44	0/2413
1	JA	0.19	0/1779	0.44	0/2413
1	K	0.18	0/1779	0.44	0/2413
1	KA	0.18	0/1779	0.44	0/2413
1	L	0.19	0/1779	0.45	0/2413
1	LA	0.19	0/1779	0.45	0/2413
1	M	0.19	0/1779	0.45	0/2413

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	MA	0.19	0/1779	0.45	0/2413
1	N	0.19	0/1779	0.45	0/2413
1	NA	0.19	0/1779	0.45	0/2413
1	O	0.19	0/1779	0.44	0/2413
1	OA	0.19	0/1779	0.44	0/2413
1	P	0.18	0/1779	0.44	0/2413
1	PA	0.18	0/1779	0.44	0/2413
1	Q	0.19	0/1779	0.45	0/2413
1	QA	0.19	0/1779	0.45	0/2413
1	R	0.19	0/1779	0.44	0/2413
1	RA	0.19	0/1779	0.44	0/2413
1	S	0.19	0/1779	0.45	0/2413
1	SA	0.19	0/1779	0.45	0/2413
1	T	0.19	0/1779	0.44	0/2413
1	TA	0.19	0/1779	0.44	0/2413
1	UA	0.18	0/1779	0.44	0/2413
1	V	0.18	0/1779	0.44	0/2413
1	VA	0.19	0/1779	0.45	0/2413
1	W	0.19	0/1779	0.45	0/2413
1	WA	0.19	0/1779	0.45	0/2413
1	X	0.19	0/1779	0.45	0/2413
1	XA	0.19	0/1779	0.45	0/2413
1	Y	0.19	0/1779	0.45	0/2413
1	YA	0.19	0/1779	0.44	0/2413
1	Z	0.19	0/1779	0.44	0/2413
1	ZA	0.18	0/1779	0.44	0/2413
All	All	0.19	0/106740	0.45	0/144780

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1751	0	1811	11	0
1	AA	1751	0	1811	10	0
1	AB	1751	0	1811	14	0
1	B	1751	0	1811	11	0
1	BA	1751	0	1811	11	0
1	BB	1751	0	1811	12	0
1	C	1751	0	1811	10	0
1	CA	1751	0	1811	11	0
1	CB	1751	0	1811	12	0
1	D	1751	0	1811	11	0
1	DA	1751	0	1811	10	0
1	DB	1751	0	1811	12	0
1	E	1751	0	1811	12	0
1	EA	1751	0	1811	11	0
1	EB	1751	0	1811	13	0
1	F	1751	0	1811	11	0
1	FA	1751	0	1811	10	0
1	FB	1751	0	1811	12	0
1	G	1751	0	1811	9	0
1	GA	1751	0	1811	11	0
1	GB	1751	0	1811	10	0
1	H	1751	0	1811	13	0
1	HA	1751	0	1811	11	0
1	HB	1751	0	1811	12	0
1	I	1751	0	1811	11	0
1	IA	1751	0	1811	10	0
1	IB	1751	0	1811	12	0
1	J	1751	0	1811	13	0
1	JA	1751	0	1811	12	0
1	K	1751	0	1811	11	0
1	KA	1751	0	1811	13	0
1	L	1751	0	1811	11	0
1	LA	1751	0	1811	12	0
1	M	1751	0	1811	11	0
1	MA	1751	0	1811	10	0
1	N	1751	0	1811	11	0
1	NA	1751	0	1811	11	0
1	O	1751	0	1811	12	0
1	OA	1751	0	1811	11	0
1	P	1751	0	1811	11	0
1	PA	1751	0	1811	12	0
1	Q	1751	0	1811	9	0
1	QA	1751	0	1811	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1751	0	1811	13	0
1	RA	1751	0	1811	11	0
1	S	1751	0	1811	11	0
1	SA	1751	0	1811	10	0
1	T	1751	0	1811	13	0
1	TA	1751	0	1811	11	0
1	UA	1751	0	1811	12	0
1	V	1751	0	1811	13	0
1	VA	1751	0	1811	14	0
1	W	1751	0	1811	12	0
1	WA	1751	0	1811	11	0
1	X	1751	0	1811	11	0
1	XA	1751	0	1811	11	0
1	Y	1751	0	1811	11	0
1	YA	1751	0	1811	11	0
1	Z	1751	0	1811	11	0
1	ZA	1751	0	1811	13	0
All	All	105060	0	108660	626	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 3.

All (626) 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:GA:458:LEU:HD23	1:GB:342:GLU:HB2	1.78	0.66
1:BA:458:LEU:HD23	1:BB:342:GLU:HB2	1.78	0.66
1:T:342:GLU:HB2	1:NA:458:LEU:HD23	1.78	0.66
1:Z:342:GLU:HB2	1:CB:458:LEU:HD23	1.78	0.66
1:OA:342:GLU:HB2	1:HB:458:LEU:HD23	1.78	0.66
1:B:458:LEU:HD23	1:X:342:GLU:HB2	1.78	0.66
1:E:458:LEU:HD23	1:IA:342:GLU:HB2	1.78	0.66
1:J:342:GLU:HB2	1:Y:458:LEU:HD23	1.78	0.66
1:L:458:LEU:HD23	1:MA:342:GLU:HB2	1.78	0.66
1:I:458:LEU:HD23	1:DB:342:GLU:HB2	1.78	0.66
1:O:458:LEU:HD23	1:DA:342:GLU:HB2	1.78	0.66
1:W:342:GLU:HB2	1:RA:458:LEU:HD23	1.78	0.66
1:D:458:LEU:HD23	1:YA:342:GLU:HB2	1.78	0.66
1:N:458:LEU:HD23	1:TA:342:GLU:HB2	1.78	0.66
1:S:458:LEU:HD23	1:IB:342:GLU:HB2	1.78	0.66
1:LA:342:GLU:HB2	1:WA:458:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:342:GLU:HB2	1:EB:458:LEU:HD23	1.78	0.66
1:N:342:GLU:HB2	1:TA:458:LEU:HD23	1.78	0.66
1:ZA:458:LEU:HD23	1:EB:342:GLU:HB2	1.78	0.66
1:A:342:GLU:HB2	1:F:458:LEU:HD23	1.78	0.66
1:D:342:GLU:HB2	1:YA:458:LEU:HD23	1.78	0.66
1:W:458:LEU:HD23	1:RA:342:GLU:HB2	1.78	0.66
1:LA:458:LEU:HD23	1:WA:342:GLU:HB2	1.78	0.66
1:PA:458:LEU:HD23	1:UA:342:GLU:HB2	1.78	0.66
1:K:342:GLU:HB2	1:P:458:LEU:HD23	1.78	0.66
1:PA:342:GLU:HB2	1:UA:458:LEU:HD23	1.78	0.66
1:A:458:LEU:HD23	1:F:342:GLU:HB2	1.78	0.65
1:C:342:GLU:HB2	1:QA:458:LEU:HD23	1.78	0.65
1:C:458:LEU:HD23	1:QA:342:GLU:HB2	1.78	0.65
1:H:342:GLU:HB2	1:FB:458:LEU:HD23	1.78	0.65
1:Q:458:LEU:HD23	1:CA:342:GLU:HB2	1.78	0.65
1:JA:458:LEU:HD23	1:XA:342:GLU:HB2	1.78	0.65
1:G:458:LEU:HD23	1:HA:342:GLU:HB2	1.78	0.65
1:K:458:LEU:HD23	1:P:342:GLU:HB2	1.78	0.65
1:M:342:GLU:HB2	1:VA:458:LEU:HD23	1.78	0.65
1:M:458:LEU:HD23	1:VA:342:GLU:HB2	1.78	0.65
1:V:458:LEU:HD23	1:AA:342:GLU:HB2	1.78	0.65
1:EA:458:LEU:HD23	1:SA:342:GLU:HB2	1.78	0.65
1:B:342:GLU:HB2	1:X:458:LEU:HD23	1.78	0.65
1:R:342:GLU:HB2	1:AB:458:LEU:HD23	1.78	0.65
1:T:458:LEU:HD23	1:NA:342:GLU:HB2	1.78	0.65
1:EA:342:GLU:HB2	1:SA:458:LEU:HD23	1.78	0.65
1:FA:342:GLU:HB2	1:KA:458:LEU:HD23	1.78	0.65
1:JA:342:GLU:HB2	1:XA:458:LEU:HD23	1.78	0.65
1:L:342:GLU:HB2	1:MA:458:LEU:HD23	1.78	0.65
1:J:458:LEU:HD23	1:Y:342:GLU:HB2	1.78	0.65
1:O:342:GLU:HB2	1:DA:458:LEU:HD23	1.78	0.65
1:BA:342:GLU:HB2	1:BB:458:LEU:HD23	1.78	0.65
1:GA:342:GLU:HB2	1:GB:458:LEU:HD23	1.78	0.65
1:E:342:GLU:HB2	1:IA:458:LEU:HD23	1.78	0.65
1:G:342:GLU:HB2	1:HA:458:LEU:HD23	1.78	0.65
1:I:342:GLU:HB2	1:DB:458:LEU:HD23	1.78	0.64
1:Q:342:GLU:HB2	1:CA:458:LEU:HD23	1.78	0.64
1:S:342:GLU:HB2	1:IB:458:LEU:HD23	1.78	0.64
1:H:458:LEU:HD23	1:FB:342:GLU:HB2	1.78	0.64
1:FA:458:LEU:HD23	1:KA:342:GLU:HB2	1.78	0.64
1:R:458:LEU:HD23	1:AB:342:GLU:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:342:GLU:HB2	1:AA:458:LEU:HD23	1.78	0.64
1:OA:458:LEU:HD23	1:HB:342:GLU:HB2	1.78	0.64
1:Z:458:LEU:HD23	1:CB:342:GLU:HB2	1.78	0.64
1:FB:382:GLN:HG3	1:FB:402:GLN:OE1	2.07	0.55
1:D:382:GLN:HG3	1:D:402:GLN:OE1	2.07	0.55
1:G:382:GLN:HG3	1:G:402:GLN:OE1	2.07	0.55
1:J:382:GLN:HG3	1:J:402:GLN:OE1	2.07	0.55
1:N:382:GLN:HG3	1:N:402:GLN:OE1	2.07	0.55
1:Q:382:GLN:HG3	1:Q:402:GLN:OE1	2.07	0.55
1:T:382:GLN:HG3	1:T:402:GLN:OE1	2.07	0.55
1:EA:382:GLN:HG3	1:EA:402:GLN:OE1	2.07	0.55
1:JA:382:GLN:HG3	1:JA:402:GLN:OE1	2.07	0.55
1:AB:382:GLN:HG3	1:AB:402:GLN:OE1	2.07	0.55
1:IA:382:GLN:HG3	1:IA:402:GLN:OE1	2.07	0.55
1:DB:382:GLN:HG3	1:DB:402:GLN:OE1	2.07	0.55
1:A:382:GLN:HG3	1:A:402:GLN:OE1	2.07	0.55
1:K:382:GLN:HG3	1:K:402:GLN:OE1	2.07	0.55
1:DA:382:GLN:HG3	1:DA:402:GLN:OE1	2.07	0.55
1:QA:382:GLN:HG3	1:QA:402:GLN:OE1	2.07	0.55
1:ZA:382:GLN:HG3	1:ZA:402:GLN:OE1	2.07	0.55
1:IB:382:GLN:HG3	1:IB:402:GLN:OE1	2.07	0.55
1:L:382:GLN:HG3	1:L:402:GLN:OE1	2.07	0.55
1:P:382:GLN:HG3	1:P:402:GLN:OE1	2.07	0.55
1:HA:382:GLN:HG3	1:HA:402:GLN:OE1	2.07	0.55
1:VA:382:GLN:HG3	1:VA:402:GLN:OE1	2.07	0.55
1:EB:382:GLN:HG3	1:EB:402:GLN:OE1	2.07	0.55
1:HB:382:GLN:HG3	1:HB:402:GLN:OE1	2.07	0.55
1:B:382:GLN:HG3	1:B:402:GLN:OE1	2.07	0.54
1:F:382:GLN:HG3	1:F:402:GLN:OE1	2.07	0.54
1:M:382:GLN:HG3	1:M:402:GLN:OE1	2.07	0.54
1:Y:382:GLN:HG3	1:Y:402:GLN:OE1	2.07	0.54
1:Z:382:GLN:HG3	1:Z:402:GLN:OE1	2.07	0.54
1:CA:382:GLN:HG3	1:CA:402:GLN:OE1	2.07	0.54
1:LA:382:GLN:HG3	1:LA:402:GLN:OE1	2.07	0.54
1:OA:382:GLN:HG3	1:OA:402:GLN:OE1	2.07	0.54
1:CB:382:GLN:HG3	1:CB:402:GLN:OE1	2.07	0.54
1:C:382:GLN:HG3	1:C:402:GLN:OE1	2.07	0.54
1:W:382:GLN:HG3	1:W:402:GLN:OE1	2.07	0.54
1:AA:382:GLN:HG3	1:AA:402:GLN:OE1	2.07	0.54
1:E:382:GLN:HG3	1:E:402:GLN:OE1	2.07	0.54
1:H:382:GLN:HG3	1:H:402:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:382:GLN:HG3	1:O:402:GLN:OE1	2.07	0.54
1:FA:382:GLN:HG3	1:FA:402:GLN:OE1	2.07	0.54
1:NA:382:GLN:HG3	1:NA:402:GLN:OE1	2.07	0.54
1:BB:382:GLN:HG3	1:BB:402:GLN:OE1	2.07	0.54
1:R:382:GLN:HG3	1:R:402:GLN:OE1	2.07	0.54
1:GB:382:GLN:HG3	1:GB:402:GLN:OE1	2.07	0.54
1:X:382:GLN:HG3	1:X:402:GLN:OE1	2.07	0.54
1:GA:382:GLN:HG3	1:GA:402:GLN:OE1	2.07	0.54
1:BA:382:GLN:HG3	1:BA:402:GLN:OE1	2.07	0.54
1:SA:382:GLN:HG3	1:SA:402:GLN:OE1	2.07	0.54
1:UA:382:GLN:HG3	1:UA:402:GLN:OE1	2.07	0.54
1:MA:382:GLN:HG3	1:MA:402:GLN:OE1	2.07	0.54
1:XA:382:GLN:HG3	1:XA:402:GLN:OE1	2.07	0.54
1:OA:362:PRO:O	1:OA:366:GLN:HB2	2.09	0.54
1:PA:382:GLN:HG3	1:PA:402:GLN:OE1	2.07	0.54
1:RA:382:GLN:HG3	1:RA:402:GLN:OE1	2.07	0.54
1:LA:362:PRO:O	1:LA:366:GLN:HB2	2.09	0.53
1:WA:382:GLN:HG3	1:WA:402:GLN:OE1	2.07	0.53
1:T:362:PRO:O	1:T:366:GLN:HB2	2.09	0.53
1:W:362:PRO:O	1:W:366:GLN:HB2	2.09	0.53
1:Z:362:PRO:O	1:Z:366:GLN:HB2	2.09	0.53
1:EA:362:PRO:O	1:EA:366:GLN:HB2	2.09	0.53
1:ZA:362:PRO:O	1:ZA:366:GLN:HB2	2.09	0.53
1:DB:362:PRO:O	1:DB:366:GLN:HB2	2.09	0.53
1:EB:362:PRO:O	1:EB:366:GLN:HB2	2.09	0.53
1:IB:362:PRO:O	1:IB:366:GLN:HB2	2.09	0.53
1:J:362:PRO:O	1:J:366:GLN:HB2	2.09	0.53
1:DA:362:PRO:O	1:DA:366:GLN:HB2	2.09	0.53
1:IA:362:PRO:O	1:IA:366:GLN:HB2	2.09	0.53
1:YA:382:GLN:HG3	1:YA:402:GLN:OE1	2.07	0.53
1:B:362:PRO:O	1:B:366:GLN:HB2	2.09	0.53
1:JA:362:PRO:O	1:JA:366:GLN:HB2	2.09	0.53
1:TA:382:GLN:HG3	1:TA:402:GLN:OE1	2.07	0.53
1:FB:362:PRO:O	1:FB:366:GLN:HB2	2.09	0.53
1:A:362:PRO:O	1:A:366:GLN:HB2	2.09	0.53
1:I:362:PRO:O	1:I:366:GLN:HB2	2.09	0.53
1:L:362:PRO:O	1:L:366:GLN:HB2	2.09	0.53
1:AB:362:PRO:O	1:AB:366:GLN:HB2	2.09	0.53
1:K:362:PRO:O	1:K:366:GLN:HB2	2.09	0.53
1:R:362:PRO:O	1:R:366:GLN:HB2	2.09	0.53
1:S:362:PRO:O	1:S:366:GLN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:382:GLN:HG3	1:S:402:GLN:OE1	2.07	0.53
1:KA:382:GLN:HG3	1:KA:402:GLN:OE1	2.07	0.53
1:OA:361:LYS:HB2	1:OA:364:GLU:HG3	1.91	0.53
1:H:362:PRO:O	1:H:366:GLN:HB2	2.09	0.53
1:W:361:LYS:HB2	1:W:364:GLU:HG3	1.91	0.53
1:Z:361:LYS:HB2	1:Z:364:GLU:HG3	1.91	0.53
1:CA:362:PRO:O	1:CA:366:GLN:HB2	2.09	0.53
1:SA:362:PRO:O	1:SA:366:GLN:HB2	2.09	0.53
1:I:382:GLN:HG3	1:I:402:GLN:OE1	2.07	0.53
1:V:382:GLN:HG3	1:V:402:GLN:OE1	2.07	0.53
1:GA:362:PRO:O	1:GA:366:GLN:HB2	2.09	0.53
1:HA:362:PRO:O	1:HA:366:GLN:HB2	2.09	0.53
1:LA:361:LYS:HB2	1:LA:364:GLU:HG3	1.91	0.53
1:XA:362:PRO:O	1:XA:366:GLN:HB2	2.09	0.53
1:BB:362:PRO:O	1:BB:366:GLN:HB2	2.09	0.53
1:X:361:LYS:HB2	1:X:364:GLU:HG3	1.91	0.53
1:BA:362:PRO:O	1:BA:366:GLN:HB2	2.09	0.53
1:KA:361:LYS:HB2	1:KA:364:GLU:HG3	1.91	0.53
1:MA:361:LYS:HB2	1:MA:364:GLU:HG3	1.91	0.53
1:DB:361:LYS:HB2	1:DB:364:GLU:HG3	1.91	0.53
1:GB:362:PRO:O	1:GB:366:GLN:HB2	2.09	0.53
1:C:362:PRO:O	1:C:366:GLN:HB2	2.09	0.53
1:F:361:LYS:HB2	1:F:364:GLU:HG3	1.91	0.53
1:P:361:LYS:HB2	1:P:364:GLU:HG3	1.91	0.53
1:V:361:LYS:HB2	1:V:364:GLU:HG3	1.91	0.53
1:AA:362:PRO:O	1:AA:366:GLN:HB2	2.09	0.53
1:FA:362:PRO:O	1:FA:366:GLN:HB2	2.09	0.53
1:HA:361:LYS:HB2	1:HA:364:GLU:HG3	1.91	0.53
1:RA:361:LYS:HB2	1:RA:364:GLU:HG3	1.91	0.53
1:IB:361:LYS:HB2	1:IB:364:GLU:HG3	1.91	0.53
1:B:361:LYS:HB2	1:B:364:GLU:HG3	1.91	0.52
1:L:361:LYS:HB2	1:L:364:GLU:HG3	1.91	0.52
1:M:362:PRO:O	1:M:366:GLN:HB2	2.09	0.52
1:CA:361:LYS:HB2	1:CA:364:GLU:HG3	1.91	0.52
1:DA:361:LYS:HB2	1:DA:364:GLU:HG3	1.91	0.52
1:WA:361:LYS:HB2	1:WA:364:GLU:HG3	1.91	0.52
1:K:361:LYS:HB2	1:K:364:GLU:HG3	1.91	0.52
1:O:362:PRO:O	1:O:366:GLN:HB2	2.09	0.52
1:Q:361:LYS:HB2	1:Q:364:GLU:HG3	1.91	0.52
1:IA:361:LYS:HB2	1:IA:364:GLU:HG3	1.91	0.52
1:NA:362:PRO:O	1:NA:366:GLN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:VA:361:LYS:HB2	1:VA:364:GLU:HG3	1.91	0.52
1:A:361:LYS:HB2	1:A:364:GLU:HG3	1.91	0.52
1:G:361:LYS:HB2	1:G:364:GLU:HG3	1.91	0.52
1:X:362:PRO:O	1:X:366:GLN:HB2	2.09	0.52
1:Y:362:PRO:O	1:Y:366:GLN:HB2	2.09	0.52
1:NA:361:LYS:HB2	1:NA:364:GLU:HG3	1.91	0.52
1:QA:361:LYS:HB2	1:QA:364:GLU:HG3	1.91	0.52
1:Y:361:LYS:HB2	1:Y:364:GLU:HG3	1.91	0.52
1:VA:362:PRO:O	1:VA:366:GLN:HB2	2.09	0.52
1:WA:362:PRO:O	1:WA:366:GLN:HB2	2.09	0.52
1:YA:362:PRO:O	1:YA:366:GLN:HB2	2.09	0.52
1:E:361:LYS:HB2	1:E:364:GLU:HG3	1.91	0.52
1:E:362:PRO:O	1:E:366:GLN:HB2	2.09	0.52
1:G:362:PRO:O	1:G:366:GLN:HB2	2.09	0.52
1:J:361:LYS:HB2	1:J:364:GLU:HG3	1.91	0.52
1:O:361:LYS:HB2	1:O:364:GLU:HG3	1.91	0.52
1:P:362:PRO:O	1:P:366:GLN:HB2	2.09	0.52
1:T:361:LYS:HB2	1:T:364:GLU:HG3	1.91	0.52
1:EA:361:LYS:HB2	1:EA:364:GLU:HG3	1.91	0.52
1:JA:361:LYS:HB2	1:JA:364:GLU:HG3	1.91	0.52
1:MA:362:PRO:O	1:MA:366:GLN:HB2	2.09	0.52
1:RA:362:PRO:O	1:RA:366:GLN:HB2	2.09	0.52
1:CB:361:LYS:HB2	1:CB:364:GLU:HG3	1.91	0.52
1:CB:362:PRO:O	1:CB:366:GLN:HB2	2.09	0.52
1:F:362:PRO:O	1:F:366:GLN:HB2	2.09	0.52
1:Q:362:PRO:O	1:Q:366:GLN:HB2	2.09	0.52
1:V:362:PRO:O	1:V:366:GLN:HB2	2.09	0.52
1:QA:362:PRO:O	1:QA:366:GLN:HB2	2.09	0.52
1:TA:362:PRO:O	1:TA:366:GLN:HB2	2.09	0.52
1:HB:361:LYS:HB2	1:HB:364:GLU:HG3	1.91	0.52
1:PA:362:PRO:O	1:PA:366:GLN:HB2	2.09	0.52
1:ZA:361:LYS:HB2	1:ZA:364:GLU:HG3	1.91	0.52
1:HB:362:PRO:O	1:HB:366:GLN:HB2	2.09	0.52
1:N:362:PRO:O	1:N:366:GLN:HB2	2.09	0.52
1:KA:362:PRO:O	1:KA:366:GLN:HB2	2.09	0.52
1:EB:361:LYS:HB2	1:EB:364:GLU:HG3	1.91	0.52
1:D:362:PRO:O	1:D:366:GLN:HB2	2.09	0.52
1:UA:362:PRO:O	1:UA:366:GLN:HB2	2.09	0.52
1:C:361:LYS:HB2	1:C:364:GLU:HG3	1.91	0.52
1:TA:361:LYS:HB2	1:TA:364:GLU:HG3	1.91	0.52
1:H:361:LYS:HB2	1:H:364:GLU:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:361:LYS:HB2	1:M:364:GLU:HG3	1.91	0.51
1:R:361:LYS:HB2	1:R:364:GLU:HG3	1.91	0.51
1:BA:361:LYS:HB2	1:BA:364:GLU:HG3	1.91	0.51
1:GA:361:LYS:HB2	1:GA:364:GLU:HG3	1.91	0.51
1:SA:361:LYS:HB2	1:SA:364:GLU:HG3	1.91	0.51
1:XA:361:LYS:HB2	1:XA:364:GLU:HG3	1.91	0.51
1:YA:361:LYS:HB2	1:YA:364:GLU:HG3	1.91	0.51
1:GB:361:LYS:HB2	1:GB:364:GLU:HG3	1.91	0.51
1:BB:361:LYS:HB2	1:BB:364:GLU:HG3	1.91	0.51
1:I:361:LYS:HB2	1:I:364:GLU:HG3	1.91	0.51
1:UA:361:LYS:HB2	1:UA:364:GLU:HG3	1.91	0.51
1:PA:361:LYS:HB2	1:PA:364:GLU:HG3	1.91	0.51
1:AB:361:LYS:HB2	1:AB:364:GLU:HG3	1.91	0.51
1:S:361:LYS:HB2	1:S:364:GLU:HG3	1.91	0.51
1:FB:361:LYS:HB2	1:FB:364:GLU:HG3	1.91	0.51
1:N:361:LYS:HB2	1:N:364:GLU:HG3	1.91	0.51
1:AA:361:LYS:HB2	1:AA:364:GLU:HG3	1.91	0.51
1:D:361:LYS:HB2	1:D:364:GLU:HG3	1.91	0.51
1:FA:361:LYS:HB2	1:FA:364:GLU:HG3	1.91	0.51
1:X:331:PRO:HB2	1:X:351:LEU:HD13	1.93	0.51
1:CA:331:PRO:HB2	1:CA:351:LEU:HD13	1.93	0.51
1:HA:331:PRO:HB2	1:HA:351:LEU:HD13	1.93	0.51
1:MA:331:PRO:HB2	1:MA:351:LEU:HD13	1.93	0.51
1:H:331:PRO:HB2	1:H:351:LEU:HD13	1.93	0.50
1:R:331:PRO:HB2	1:R:351:LEU:HD13	1.93	0.50
1:ZA:331:PRO:HB2	1:ZA:351:LEU:HD13	1.93	0.50
1:AB:331:PRO:HB2	1:AB:351:LEU:HD13	1.94	0.50
1:EB:331:PRO:HB2	1:EB:351:LEU:HD13	1.93	0.50
1:A:331:PRO:HB2	1:A:351:LEU:HD13	1.93	0.50
1:K:331:PRO:HB2	1:K:351:LEU:HD13	1.93	0.50
1:W:331:PRO:HB2	1:W:351:LEU:HD13	1.94	0.50
1:EA:331:PRO:HB2	1:EA:351:LEU:HD13	1.93	0.50
1:TA:331:PRO:HB2	1:TA:351:LEU:HD13	1.94	0.50
1:YA:331:PRO:HB2	1:YA:351:LEU:HD13	1.94	0.50
1:FB:331:PRO:HB2	1:FB:351:LEU:HD13	1.94	0.50
1:IB:331:PRO:HB2	1:IB:351:LEU:HD13	1.93	0.50
1:M:331:PRO:HB2	1:M:351:LEU:HD13	1.93	0.50
1:V:331:PRO:HB2	1:V:351:LEU:HD13	1.93	0.50
1:Z:331:PRO:HB2	1:Z:351:LEU:HD13	1.94	0.50
1:JA:331:PRO:HB2	1:JA:351:LEU:HD13	1.94	0.50
1:KA:331:PRO:HB2	1:KA:351:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:331:PRO:HB2	1:LA:351:LEU:HD13	1.94	0.50
1:DB:331:PRO:HB2	1:DB:351:LEU:HD13	1.94	0.50
1:C:331:PRO:HB2	1:C:351:LEU:HD13	1.93	0.50
1:O:331:PRO:HB2	1:O:351:LEU:HD13	1.94	0.50
1:GA:331:PRO:HB2	1:GA:351:LEU:HD13	1.94	0.50
1:OA:331:PRO:HB2	1:OA:351:LEU:HD13	1.94	0.50
1:PA:331:PRO:HB2	1:PA:351:LEU:HD13	1.93	0.50
1:UA:331:PRO:HB2	1:UA:351:LEU:HD13	1.93	0.50
1:E:331:PRO:HB2	1:E:351:LEU:HD13	1.94	0.50
1:BA:331:PRO:HB2	1:BA:351:LEU:HD13	1.94	0.50
1:BB:331:PRO:HB2	1:BB:351:LEU:HD13	1.93	0.50
1:CB:331:PRO:HB2	1:CB:351:LEU:HD13	1.94	0.50
1:GB:331:PRO:HB2	1:GB:351:LEU:HD13	1.93	0.50
1:HB:331:PRO:HB2	1:HB:351:LEU:HD13	1.94	0.50
1:N:331:PRO:HB2	1:N:351:LEU:HD13	1.94	0.50
1:FA:331:PRO:HB2	1:FA:351:LEU:HD13	1.93	0.50
1:AA:331:PRO:HB2	1:AA:351:LEU:HD13	1.93	0.49
1:QA:331:PRO:HB2	1:QA:351:LEU:HD13	1.94	0.49
1:VA:331:PRO:HB2	1:VA:351:LEU:HD13	1.94	0.49
1:D:331:PRO:HB2	1:D:351:LEU:HD13	1.94	0.49
1:Y:331:PRO:HB2	1:Y:351:LEU:HD13	1.94	0.49
1:NA:331:PRO:HB2	1:NA:351:LEU:HD13	1.94	0.49
1:G:331:PRO:HB2	1:G:351:LEU:HD13	1.94	0.49
1:Q:331:PRO:HB2	1:Q:351:LEU:HD13	1.94	0.49
1:DA:331:PRO:HB2	1:DA:351:LEU:HD13	1.94	0.49
1:B:331:PRO:HB2	1:B:351:LEU:HD13	1.94	0.49
1:IA:331:PRO:HB2	1:IA:351:LEU:HD13	1.94	0.49
1:L:331:PRO:HB2	1:L:351:LEU:HD13	1.94	0.49
1:P:331:PRO:HB2	1:P:351:LEU:HD13	1.93	0.49
1:SA:331:PRO:HB2	1:SA:351:LEU:HD13	1.94	0.49
1:XA:331:PRO:HB2	1:XA:351:LEU:HD13	1.94	0.49
1:F:331:PRO:HB2	1:F:351:LEU:HD13	1.93	0.49
1:S:331:PRO:HB2	1:S:351:LEU:HD13	1.94	0.49
1:I:331:PRO:HB2	1:I:351:LEU:HD13	1.94	0.49
1:J:331:PRO:HB2	1:J:351:LEU:HD13	1.94	0.49
1:T:331:PRO:HB2	1:T:351:LEU:HD13	1.94	0.49
1:RA:331:PRO:HB2	1:RA:351:LEU:HD13	1.93	0.48
1:WA:331:PRO:HB2	1:WA:351:LEU:HD13	1.93	0.48
1:DB:339:LYS:HG2	1:DB:343:SER:OG	2.14	0.48
1:G:339:LYS:HG2	1:G:343:SER:OG	2.14	0.48
1:Q:339:LYS:HG2	1:Q:343:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:339:LYS:HG2	1:JA:343:SER:OG	2.14	0.48
1:IB:339:LYS:HG2	1:IB:343:SER:OG	2.14	0.48
1:V:339:LYS:HG2	1:V:343:SER:OG	2.14	0.48
1:EA:339:LYS:HG2	1:EA:343:SER:OG	2.14	0.48
1:KA:339:LYS:HG2	1:KA:343:SER:OG	2.14	0.48
1:TA:339:LYS:HG2	1:TA:343:SER:OG	2.14	0.48
1:YA:339:LYS:HG2	1:YA:343:SER:OG	2.14	0.48
1:ZA:339:LYS:HG2	1:ZA:343:SER:OG	2.14	0.48
1:EB:339:LYS:HG2	1:EB:343:SER:OG	2.14	0.48
1:BB:339:LYS:HG2	1:BB:343:SER:OG	2.14	0.47
1:GB:339:LYS:HG2	1:GB:343:SER:OG	2.14	0.47
1:Y:339:LYS:HG2	1:Y:343:SER:OG	2.14	0.47
1:AA:339:LYS:HG2	1:AA:343:SER:OG	2.14	0.47
1:BA:339:LYS:HG2	1:BA:343:SER:OG	2.14	0.47
1:FA:339:LYS:HG2	1:FA:343:SER:OG	2.14	0.47
1:A:339:LYS:HG2	1:A:343:SER:OG	2.14	0.47
1:D:339:LYS:HG2	1:D:343:SER:OG	2.14	0.47
1:N:339:LYS:HG2	1:N:343:SER:OG	2.14	0.47
1:GA:339:LYS:HG2	1:GA:343:SER:OG	2.14	0.47
1:NA:339:LYS:HG2	1:NA:343:SER:OG	2.14	0.47
1:XA:339:LYS:HG2	1:XA:343:SER:OG	2.14	0.47
1:K:339:LYS:HG2	1:K:343:SER:OG	2.14	0.47
1:QA:339:LYS:HG2	1:QA:343:SER:OG	2.14	0.47
1:SA:339:LYS:HG2	1:SA:343:SER:OG	2.14	0.47
1:E:339:LYS:HG2	1:E:343:SER:OG	2.14	0.47
1:O:339:LYS:HG2	1:O:343:SER:OG	2.14	0.47
1:CA:339:LYS:HG2	1:CA:343:SER:OG	2.14	0.47
1:QA:321:ALA:HB1	1:QA:328:LEU:HD11	1.97	0.47
1:VA:339:LYS:HG2	1:VA:343:SER:OG	2.14	0.47
1:HB:339:LYS:HG2	1:HB:343:SER:OG	2.14	0.47
1:C:339:LYS:HG2	1:C:343:SER:OG	2.14	0.47
1:F:339:LYS:HG2	1:F:343:SER:OG	2.14	0.47
1:I:339:LYS:HG2	1:I:343:SER:OG	2.14	0.47
1:J:339:LYS:HG2	1:J:343:SER:OG	2.14	0.47
1:M:339:LYS:HG2	1:M:343:SER:OG	2.14	0.47
1:S:339:LYS:HG2	1:S:343:SER:OG	2.14	0.47
1:T:339:LYS:HG2	1:T:343:SER:OG	2.14	0.47
1:W:339:LYS:HG2	1:W:343:SER:OG	2.14	0.47
1:Z:321:ALA:HB1	1:Z:328:LEU:HD11	1.97	0.47
1:Z:339:LYS:HG2	1:Z:343:SER:OG	2.14	0.47
1:EA:321:ALA:HB1	1:EA:328:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:339:LYS:HG2	1:HA:343:SER:OG	2.14	0.47
1:LA:339:LYS:HG2	1:LA:343:SER:OG	2.14	0.47
1:OA:321:ALA:HB1	1:OA:328:LEU:HD11	1.97	0.47
1:OA:339:LYS:HG2	1:OA:343:SER:OG	2.14	0.47
1:UA:339:LYS:HG2	1:UA:343:SER:OG	2.14	0.47
1:VA:321:ALA:HB1	1:VA:328:LEU:HD11	1.97	0.47
1:CB:339:LYS:HG2	1:CB:343:SER:OG	2.14	0.47
1:C:321:ALA:HB1	1:C:328:LEU:HD11	1.97	0.47
1:D:321:ALA:HB1	1:D:328:LEU:HD11	1.97	0.47
1:H:321:ALA:HB1	1:H:328:LEU:HD11	1.97	0.47
1:I:321:ALA:HB1	1:I:328:LEU:HD11	1.97	0.47
1:L:339:LYS:HG2	1:L:343:SER:OG	2.14	0.47
1:M:321:ALA:HB1	1:M:328:LEU:HD11	1.97	0.47
1:N:321:ALA:HB1	1:N:328:LEU:HD11	1.97	0.47
1:R:321:ALA:HB1	1:R:328:LEU:HD11	1.97	0.47
1:R:339:LYS:HG2	1:R:343:SER:OG	2.14	0.47
1:FA:258:ASN:OD1	1:FA:258:ASN:N	2.48	0.47
1:JA:321:ALA:HB1	1:JA:328:LEU:HD11	1.97	0.47
1:PA:339:LYS:HG2	1:PA:343:SER:OG	2.14	0.47
1:WA:339:LYS:HG2	1:WA:343:SER:OG	2.14	0.47
1:ZA:321:ALA:HB1	1:ZA:328:LEU:HD11	1.97	0.47
1:EB:321:ALA:HB1	1:EB:328:LEU:HD11	1.97	0.47
1:B:339:LYS:HG2	1:B:343:SER:OG	2.14	0.47
1:H:339:LYS:HG2	1:H:343:SER:OG	2.14	0.47
1:P:339:LYS:HG2	1:P:343:SER:OG	2.14	0.47
1:Q:321:ALA:HB1	1:Q:328:LEU:HD11	1.97	0.47
1:S:321:ALA:HB1	1:S:328:LEU:HD11	1.97	0.47
1:T:321:ALA:HB1	1:T:328:LEU:HD11	1.97	0.47
1:AA:258:ASN:OD1	1:AA:258:ASN:N	2.48	0.47
1:QA:258:ASN:OD1	1:QA:258:ASN:N	2.48	0.47
1:RA:339:LYS:HG2	1:RA:343:SER:OG	2.14	0.47
1:HB:258:ASN:OD1	1:HB:258:ASN:N	2.48	0.47
1:Y:258:ASN:OD1	1:Y:258:ASN:N	2.48	0.47
1:VA:258:ASN:OD1	1:VA:258:ASN:N	2.48	0.47
1:BB:321:ALA:HB1	1:BB:328:LEU:HD11	1.97	0.47
1:CB:258:ASN:OD1	1:CB:258:ASN:N	2.48	0.47
1:G:321:ALA:HB1	1:G:328:LEU:HD11	1.97	0.46
1:J:321:ALA:HB1	1:J:328:LEU:HD11	1.97	0.46
1:S:258:ASN:OD1	1:S:258:ASN:N	2.48	0.46
1:DA:321:ALA:HB1	1:DA:328:LEU:HD11	1.97	0.46
1:DA:339:LYS:HG2	1:DA:343:SER:OG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:339:LYS:HG2	1:IA:343:SER:OG	2.14	0.46
1:KA:321:ALA:HB1	1:KA:328:LEU:HD11	1.97	0.46
1:NA:258:ASN:OD1	1:NA:258:ASN:N	2.48	0.46
1:SA:258:ASN:OD1	1:SA:258:ASN:N	2.48	0.46
1:FB:321:ALA:HB1	1:FB:328:LEU:HD11	1.97	0.46
1:GB:321:ALA:HB1	1:GB:328:LEU:HD11	1.97	0.46
1:HB:321:ALA:HB1	1:HB:328:LEU:HD11	1.97	0.46
1:B:258:ASN:OD1	1:B:258:ASN:N	2.48	0.46
1:B:321:ALA:HB1	1:B:328:LEU:HD11	1.97	0.46
1:I:258:ASN:OD1	1:I:258:ASN:N	2.48	0.46
1:L:258:ASN:OD1	1:L:258:ASN:N	2.48	0.46
1:L:321:ALA:HB1	1:L:328:LEU:HD11	1.97	0.46
1:V:321:ALA:HB1	1:V:328:LEU:HD11	1.97	0.46
1:IA:321:ALA:HB1	1:IA:328:LEU:HD11	1.97	0.46
1:XA:258:ASN:OD1	1:XA:258:ASN:N	2.48	0.46
1:AB:321:ALA:HB1	1:AB:328:LEU:HD11	1.97	0.46
1:CB:321:ALA:HB1	1:CB:328:LEU:HD11	1.97	0.46
1:AA:321:ALA:HB1	1:AA:328:LEU:HD11	1.97	0.46
1:FA:321:ALA:HB1	1:FA:328:LEU:HD11	1.97	0.46
1:PA:321:ALA:HB1	1:PA:328:LEU:HD11	1.97	0.46
1:J:258:ASN:OD1	1:J:258:ASN:N	2.48	0.46
1:T:258:ASN:OD1	1:T:258:ASN:N	2.48	0.46
1:MA:258:ASN:OD1	1:MA:258:ASN:N	2.48	0.46
1:MA:339:LYS:HG2	1:MA:343:SER:OG	2.14	0.46
1:UA:258:ASN:OD1	1:UA:258:ASN:N	2.48	0.46
1:UA:321:ALA:HB1	1:UA:328:LEU:HD11	1.97	0.46
1:AB:339:LYS:HG2	1:AB:343:SER:OG	2.14	0.46
1:A:258:ASN:OD1	1:A:258:ASN:N	2.48	0.46
1:K:258:ASN:OD1	1:K:258:ASN:N	2.48	0.46
1:O:321:ALA:HB1	1:O:328:LEU:HD11	1.97	0.46
1:P:321:ALA:HB1	1:P:328:LEU:HD11	1.97	0.46
1:W:321:ALA:HB1	1:W:328:LEU:HD11	1.97	0.46
1:X:258:ASN:OD1	1:X:258:ASN:N	2.48	0.46
1:PA:258:ASN:OD1	1:PA:258:ASN:N	2.48	0.46
1:XA:321:ALA:HB1	1:XA:328:LEU:HD11	1.97	0.46
1:DB:258:ASN:OD1	1:DB:258:ASN:N	2.48	0.46
1:DB:321:ALA:HB1	1:DB:328:LEU:HD11	1.97	0.46
1:IB:321:ALA:HB1	1:IB:328:LEU:HD11	1.97	0.46
1:F:321:ALA:HB1	1:F:328:LEU:HD11	1.97	0.46
1:X:339:LYS:HG2	1:X:343:SER:OG	2.14	0.46
1:LA:321:ALA:HB1	1:LA:328:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:321:ALA:HB1	1:SA:328:LEU:HD11	1.97	0.46
1:FB:339:LYS:HG2	1:FB:343:SER:OG	2.14	0.46
1:IB:258:ASN:OD1	1:IB:258:ASN:N	2.48	0.46
1:A:321:ALA:HB1	1:A:328:LEU:HD11	1.97	0.46
1:E:321:ALA:HB1	1:E:328:LEU:HD11	1.97	0.46
1:K:321:ALA:HB1	1:K:328:LEU:HD11	1.97	0.46
1:GA:321:ALA:HB1	1:GA:328:LEU:HD11	1.97	0.46
1:Y:321:ALA:HB1	1:Y:328:LEU:HD11	1.97	0.46
1:BA:258:ASN:OD1	1:BA:258:ASN:N	2.48	0.46
1:BA:321:ALA:HB1	1:BA:328:LEU:HD11	1.97	0.46
1:CA:321:ALA:HB1	1:CA:328:LEU:HD11	1.97	0.46
1:GA:258:ASN:OD1	1:GA:258:ASN:N	2.48	0.46
1:HA:321:ALA:HB1	1:HA:328:LEU:HD11	1.97	0.46
1:NA:321:ALA:HB1	1:NA:328:LEU:HD11	1.97	0.46
1:C:258:ASN:OD1	1:C:258:ASN:N	2.48	0.45
1:H:258:ASN:OD1	1:H:258:ASN:N	2.48	0.45
1:M:258:ASN:OD1	1:M:258:ASN:N	2.48	0.45
1:R:258:ASN:OD1	1:R:258:ASN:N	2.48	0.45
1:JA:258:ASN:OD1	1:JA:258:ASN:N	2.48	0.45
1:ZA:258:ASN:OD1	1:ZA:258:ASN:N	2.48	0.45
1:YA:258:ASN:OD1	1:YA:258:ASN:N	2.48	0.45
1:EB:258:ASN:OD1	1:EB:258:ASN:N	2.48	0.45
1:O:258:ASN:OD1	1:O:258:ASN:N	2.48	0.45
1:DA:258:ASN:OD1	1:DA:258:ASN:N	2.48	0.45
1:TA:258:ASN:OD1	1:TA:258:ASN:N	2.48	0.45
1:TA:321:ALA:HB1	1:TA:328:LEU:HD11	1.97	0.45
1:YA:321:ALA:HB1	1:YA:328:LEU:HD11	1.97	0.45
1:F:258:ASN:OD1	1:F:258:ASN:N	2.48	0.45
1:X:321:ALA:HB1	1:X:328:LEU:HD11	1.97	0.45
1:KA:237:LYS:HE3	1:KA:237:LYS:HB3	1.85	0.45
1:MA:321:ALA:HB1	1:MA:328:LEU:HD11	1.97	0.45
1:RA:321:ALA:HB1	1:RA:328:LEU:HD11	1.97	0.45
1:E:258:ASN:OD1	1:E:258:ASN:N	2.48	0.45
1:IA:258:ASN:OD1	1:IA:258:ASN:N	2.48	0.45
1:WA:321:ALA:HB1	1:WA:328:LEU:HD11	1.97	0.45
1:N:258:ASN:OD1	1:N:258:ASN:N	2.48	0.45
1:P:258:ASN:OD1	1:P:258:ASN:N	2.48	0.45
1:V:237:LYS:HE3	1:V:237:LYS:HB3	1.85	0.45
1:RA:258:ASN:OD1	1:RA:258:ASN:N	2.48	0.45
1:Z:258:ASN:OD1	1:Z:258:ASN:N	2.48	0.45
1:KA:258:ASN:OD1	1:KA:258:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:258:ASN:OD1	1:OA:258:ASN:N	2.48	0.45
1:BB:274:SER:O	1:BB:274:SER:OG	2.35	0.45
1:D:258:ASN:OD1	1:D:258:ASN:N	2.48	0.45
1:G:258:ASN:OD1	1:G:258:ASN:N	2.48	0.45
1:WA:258:ASN:OD1	1:WA:258:ASN:N	2.48	0.45
1:GB:274:SER:O	1:GB:274:SER:OG	2.35	0.45
1:V:258:ASN:OD1	1:V:258:ASN:N	2.48	0.45
1:Q:258:ASN:OD1	1:Q:258:ASN:N	2.48	0.44
1:BA:237:LYS:HE3	1:BA:237:LYS:HB3	1.85	0.44
1:SA:230:VAL:HA	1:SA:231:PRO:HD3	1.88	0.44
1:GA:237:LYS:HE3	1:GA:237:LYS:HB3	1.85	0.44
1:HA:258:ASN:OD1	1:HA:258:ASN:N	2.48	0.44
1:X:230:VAL:HA	1:X:231:PRO:HD3	1.88	0.44
1:CA:258:ASN:OD1	1:CA:258:ASN:N	2.48	0.44
1:GB:258:ASN:OD1	1:GB:258:ASN:N	2.48	0.44
1:C:230:VAL:HA	1:C:231:PRO:HD3	1.88	0.43
1:V:296:LYS:HD2	1:V:296:LYS:HA	1.89	0.43
1:RA:237:LYS:HE3	1:RA:237:LYS:HB3	1.85	0.43
1:BB:258:ASN:OD1	1:BB:258:ASN:N	2.48	0.43
1:M:230:VAL:HA	1:M:231:PRO:HD3	1.88	0.43
1:XA:230:VAL:HA	1:XA:231:PRO:HD3	1.88	0.43
1:EB:296:LYS:HD2	1:EB:296:LYS:HA	1.89	0.43
1:EA:237:LYS:HE3	1:EA:237:LYS:HB3	1.85	0.43
1:WA:237:LYS:HE3	1:WA:237:LYS:HB3	1.85	0.43
1:DB:296:LYS:HD2	1:DB:296:LYS:HA	1.89	0.43
1:JA:237:LYS:HE3	1:JA:237:LYS:HB3	1.85	0.43
1:KA:296:LYS:HD2	1:KA:296:LYS:HA	1.89	0.43
1:Z:230:VAL:HA	1:Z:231:PRO:HD3	1.88	0.43
1:ZA:296:LYS:HD2	1:ZA:296:LYS:HA	1.89	0.43
1:L:268:ARG:NH1	1:L:281:LEU:O	2.50	0.43
1:B:268:ARG:NH1	1:B:281:LEU:O	2.50	0.43
1:ZA:230:VAL:HA	1:ZA:231:PRO:HD3	1.88	0.43
1:P:237:LYS:HE3	1:P:237:LYS:HB3	1.85	0.43
1:AB:258:ASN:OD1	1:AB:258:ASN:N	2.48	0.42
1:AA:268:ARG:NH1	1:AA:281:LEU:O	2.50	0.42
1:UA:268:ARG:NH1	1:UA:281:LEU:O	2.50	0.42
1:HB:268:ARG:NH1	1:HB:281:LEU:O	2.50	0.42
1:F:237:LYS:HE3	1:F:237:LYS:HB3	1.85	0.42
1:PA:268:ARG:NH1	1:PA:281:LEU:O	2.50	0.42
1:QA:268:ARG:NH1	1:QA:281:LEU:O	2.50	0.42
1:ZA:274:SER:O	1:ZA:274:SER:OG	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:274:SER:O	1:EB:274:SER:OG	2.35	0.42
1:FB:258:ASN:OD1	1:FB:258:ASN:N	2.48	0.42
1:FA:268:ARG:NH1	1:FA:281:LEU:O	2.50	0.42
1:OA:230:VAL:HA	1:OA:231:PRO:HD3	1.89	0.42
1:VA:268:ARG:NH1	1:VA:281:LEU:O	2.50	0.42
1:CB:268:ARG:NH1	1:CB:281:LEU:O	2.50	0.42
1:EB:230:VAL:HA	1:EB:231:PRO:HD3	1.88	0.42
1:IA:230:VAL:HA	1:IA:231:PRO:HD3	1.88	0.42
1:PA:296:LYS:HD2	1:PA:296:LYS:HA	1.89	0.42
1:LA:274:SER:O	1:LA:274:SER:OG	2.35	0.42
1:BB:237:LYS:HE3	1:BB:237:LYS:HB3	1.85	0.42
1:W:274:SER:O	1:W:274:SER:OG	2.35	0.42
1:LA:237:LYS:HE3	1:LA:237:LYS:HB3	1.85	0.42
1:V:230:VAL:HA	1:V:231:PRO:HD3	1.88	0.42
1:JA:230:VAL:HA	1:JA:231:PRO:HD3	1.88	0.42
1:W:258:ASN:OD1	1:W:258:ASN:N	2.48	0.42
1:DA:230:VAL:HA	1:DA:231:PRO:HD3	1.88	0.42
1:KA:230:VAL:HA	1:KA:231:PRO:HD3	1.88	0.42
1:I:296:LYS:HD2	1:I:296:LYS:HA	1.89	0.42
1:UA:296:LYS:HD2	1:UA:296:LYS:HA	1.89	0.42
1:O:274:SER:O	1:O:274:SER:OG	2.35	0.41
1:AB:268:ARG:NH1	1:AB:281:LEU:O	2.50	0.41
1:T:268:ARG:NH1	1:T:281:LEU:O	2.50	0.41
1:EA:230:VAL:HA	1:EA:231:PRO:HD3	1.88	0.41
1:QA:296:LYS:HA	1:QA:296:LYS:HD2	1.89	0.41
1:AB:237:LYS:HE3	1:AB:237:LYS:HB3	1.85	0.41
1:FB:268:ARG:NH1	1:FB:281:LEU:O	2.50	0.41
1:E:274:SER:O	1:E:274:SER:OG	2.35	0.41
1:J:268:ARG:NH1	1:J:281:LEU:O	2.50	0.41
1:R:268:ARG:NH1	1:R:281:LEU:O	2.50	0.41
1:W:237:LYS:HE3	1:W:237:LYS:HB3	1.85	0.41
1:B:296:LYS:HD2	1:B:296:LYS:HA	1.89	0.41
1:H:268:ARG:NH1	1:H:281:LEU:O	2.50	0.41
1:L:296:LYS:HD2	1:L:296:LYS:HA	1.89	0.41
1:S:268:ARG:NH1	1:S:281:LEU:O	2.50	0.41
1:S:296:LYS:HD2	1:S:296:LYS:HA	1.89	0.41
1:VA:296:LYS:HA	1:VA:296:LYS:HD2	1.89	0.41
1:BB:296:LYS:HA	1:BB:296:LYS:HD2	1.89	0.41
1:FB:237:LYS:HE3	1:FB:237:LYS:HB3	1.85	0.41
1:K:296:LYS:HD2	1:K:296:LYS:HA	1.89	0.41
1:R:237:LYS:HE3	1:R:237:LYS:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:268:ARG:NH1	1:KA:281:LEU:O	2.50	0.41
1:A:296:LYS:HD2	1:A:296:LYS:HA	1.89	0.41
1:I:268:ARG:NH1	1:I:281:LEU:O	2.50	0.41
1:O:296:LYS:HA	1:O:296:LYS:HD2	1.89	0.41
1:V:268:ARG:NH1	1:V:281:LEU:O	2.50	0.41
1:Y:296:LYS:HA	1:Y:296:LYS:HD2	1.89	0.41
1:QA:230:VAL:HA	1:QA:231:PRO:HD3	1.88	0.41
1:CB:237:LYS:HE3	1:CB:237:LYS:HB3	1.85	0.41
1:N:268:ARG:NH1	1:N:281:LEU:O	2.50	0.41
1:Z:296:LYS:HD2	1:Z:296:LYS:HA	1.89	0.41
1:BA:268:ARG:NH1	1:BA:281:LEU:O	2.50	0.41
1:HB:237:LYS:HE3	1:HB:237:LYS:HB3	1.85	0.41
1:E:296:LYS:HA	1:E:296:LYS:HD2	1.89	0.41
1:H:230:VAL:HA	1:H:231:PRO:HD3	1.88	0.41
1:N:230:VAL:HA	1:N:231:PRO:HD3	1.88	0.41
1:R:230:VAL:HA	1:R:231:PRO:HD3	1.88	0.41
1:EA:258:ASN:OD1	1:EA:258:ASN:N	2.48	0.41
1:GA:268:ARG:NH1	1:GA:281:LEU:O	2.50	0.41
1:LA:258:ASN:OD1	1:LA:258:ASN:N	2.48	0.41
1:OA:296:LYS:HD2	1:OA:296:LYS:HA	1.89	0.41
1:VA:230:VAL:HA	1:VA:231:PRO:HD3	1.88	0.41
1:AB:450:ILE:HD13	1:AB:450:ILE:HA	1.98	0.41
1:DB:230:VAL:HA	1:DB:231:PRO:HD3	1.88	0.41
1:HB:230:VAL:HA	1:HB:231:PRO:HD3	1.88	0.41
1:D:268:ARG:NH1	1:D:281:LEU:O	2.50	0.41
1:H:237:LYS:HE3	1:H:237:LYS:HB3	1.85	0.40
1:M:237:LYS:HE3	1:M:237:LYS:HB3	1.85	0.40
1:T:230:VAL:HA	1:T:231:PRO:HD3	1.89	0.40
1:NA:296:LYS:HA	1:NA:296:LYS:HD2	1.89	0.40
1:YA:268:ARG:NH1	1:YA:281:LEU:O	2.50	0.40
1:F:383:SER:HB2	1:F:424:ILE:HG21	2.04	0.40
1:P:383:SER:HB2	1:P:424:ILE:HG21	2.04	0.40
1:CA:296:LYS:HD2	1:CA:296:LYS:HA	1.89	0.40
1:QA:243:LEU:HD22	1:QA:387:ILE:HD12	2.04	0.40
1:CB:230:VAL:HA	1:CB:231:PRO:HD3	1.88	0.40
1:DB:268:ARG:NH1	1:DB:281:LEU:O	2.50	0.40
1:J:230:VAL:HA	1:J:231:PRO:HD3	1.88	0.40
1:J:243:LEU:HD22	1:J:387:ILE:HD12	2.04	0.40
1:Y:383:SER:HB2	1:Y:424:ILE:HG21	2.04	0.40
1:HA:296:LYS:HD2	1:HA:296:LYS:HA	1.89	0.40
1:LA:450:ILE:HD13	1:LA:450:ILE:HA	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:383:SER:HB2	1:NA:424:ILE:HG21	2.04	0.40
1:TA:268:ARG:NH1	1:TA:281:LEU:O	2.50	0.40
1:TA:383:SER:HB2	1:TA:424:ILE:HG21	2.04	0.40
1:VA:243:LEU:HD22	1:VA:387:ILE:HD12	2.04	0.40
1:VA:383:SER:HB2	1:VA:424:ILE:HG21	2.04	0.40
1:YA:383:SER:HB2	1:YA:424:ILE:HG21	2.04	0.40
1:ZA:243:LEU:HD22	1:ZA:387:ILE:HD12	2.04	0.40
1:EB:243:LEU:HD22	1:EB:387:ILE:HD12	2.04	0.40
1:FB:243:LEU:HD22	1:FB:387:ILE:HD12	2.04	0.40
1:D:230:VAL:HA	1:D:231:PRO:HD3	1.88	0.40
1:H:274:SER:O	1:H:274:SER:OG	2.35	0.40
1:J:383:SER:HB2	1:J:424:ILE:HG21	2.04	0.40
1:R:274:SER:O	1:R:274:SER:OG	2.35	0.40
1:T:243:LEU:HD22	1:T:387:ILE:HD12	2.04	0.40
1:T:383:SER:HB2	1:T:424:ILE:HG21	2.04	0.40
1:X:383:SER:HB2	1:X:424:ILE:HG21	2.04	0.40
1:MA:383:SER:HB2	1:MA:424:ILE:HG21	2.04	0.40
1:PA:243:LEU:HD22	1:PA:387:ILE:HD12	2.04	0.40
1:QA:383:SER:HB2	1:QA:424:ILE:HG21	2.04	0.40
1:AB:243:LEU:HD22	1:AB:387:ILE:HD12	2.04	0.40
1:IB:230:VAL:HA	1:IB:231:PRO:HD3	1.88	0.40
1:A:383:SER:HB2	1:A:424:ILE:HG21	2.04	0.40
1:E:243:LEU:HD22	1:E:387:ILE:HD12	2.04	0.40
1:K:383:SER:HB2	1:K:424:ILE:HG21	2.04	0.40
1:O:243:LEU:HD22	1:O:387:ILE:HD12	2.04	0.40
1:W:450:ILE:HD13	1:W:450:ILE:HA	1.98	0.40
1:CA:383:SER:HB2	1:CA:424:ILE:HG21	2.04	0.40
1:HA:383:SER:HB2	1:HA:424:ILE:HG21	2.04	0.40
1:JA:274:SER:O	1:JA:274:SER:OG	2.35	0.40
1:RA:243:LEU:HD22	1:RA:387:ILE:HD12	2.04	0.40
1:UA:243:LEU:HD22	1:UA:387:ILE:HD12	2.04	0.40
1:WA:243:LEU:HD22	1:WA:387:ILE:HD12	2.04	0.40
1:XA:296:LYS:HD2	1:XA:296:LYS:HA	1.89	0.40
1:AB:230:VAL:HA	1:AB:231:PRO:HD3	1.88	0.40
1:IB:268:ARG:NH1	1:IB:281:LEU:O	2.50	0.40
1:IB:383:SER:HB2	1:IB:424:ILE:HG21	2.04	0.40

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	A	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	AA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	AB	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	B	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	BA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	BB	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	C	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	CA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	CB	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	D	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	DA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	DB	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	E	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	EA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	EB	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	F	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	FA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	FB	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	G	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	GA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	GB	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	H	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	HA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	HB	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	I	230/278 (83%)	224 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	IB	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	J	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	JA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	K	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	KA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	L	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	LA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	M	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	MA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	N	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	NA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	O	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	OA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	P	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	PA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	Q	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	QA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	R	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	RA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	S	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	SA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	T	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	TA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	UA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	V	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	VA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	W	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	WA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	X	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	XA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	YA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	Z	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
1	ZA	230/278 (83%)	224 (97%)	6 (3%)	0	100	100
All	All	13800/16680 (83%)	13440 (97%)	360 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	AA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	AB	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	B	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	BA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	BB	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	C	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	CA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	CB	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	D	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	DA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	DB	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	E	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	EA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	EB	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	F	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	FA	193/229 (84%)	192 (100%)	1 (0%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FB	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	G	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	GA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	GB	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	H	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	HA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	HB	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	I	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	IA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	IB	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	J	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	JA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	K	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	KA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	L	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	LA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	M	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	MA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	N	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	NA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	O	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	OA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	P	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	PA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	Q	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	QA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	R	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	RA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	S	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	SA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	T	193/229 (84%)	192 (100%)	1 (0%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	TA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	UA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	V	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	VA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	W	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	WA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	X	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	XA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	Y	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	YA	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	Z	193/229 (84%)	192 (100%)	1 (0%)	81	93
1	ZA	193/229 (84%)	192 (100%)	1 (0%)	81	93
All	All	11580/13740 (84%)	11520 (100%)	60 (0%)	78	93

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	GLN
1	B	402	GLN
1	C	402	GLN
1	D	402	GLN
1	E	402	GLN
1	F	402	GLN
1	G	402	GLN
1	H	402	GLN
1	I	402	GLN
1	J	402	GLN
1	K	402	GLN
1	L	402	GLN
1	M	402	GLN
1	N	402	GLN
1	O	402	GLN
1	P	402	GLN
1	Q	402	GLN
1	R	402	GLN
1	S	402	GLN
1	T	402	GLN
1	V	402	GLN

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Mol	Chain	Res	Type
1	W	402	GLN
1	X	402	GLN
1	Y	402	GLN
1	Z	402	GLN
1	AA	402	GLN
1	BA	402	GLN
1	CA	402	GLN
1	DA	402	GLN
1	EA	402	GLN
1	FA	402	GLN
1	GA	402	GLN
1	HA	402	GLN
1	IA	402	GLN
1	JA	402	GLN
1	KA	402	GLN
1	LA	402	GLN
1	MA	402	GLN
1	NA	402	GLN
1	OA	402	GLN
1	PA	402	GLN
1	QA	402	GLN
1	RA	402	GLN
1	SA	402	GLN
1	TA	402	GLN
1	UA	402	GLN
1	VA	402	GLN
1	WA	402	GLN
1	XA	402	GLN
1	YA	402	GLN
1	ZA	402	GLN
1	AB	402	GLN
1	BB	402	GLN
1	CB	402	GLN
1	DB	402	GLN
1	EB	402	GLN
1	FB	402	GLN
1	GB	402	GLN
1	HB	402	GLN
1	IB	402	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	GLN
1	A	452	ASN
1	B	382	GLN
1	B	452	ASN
1	C	382	GLN
1	C	452	ASN
1	D	382	GLN
1	D	452	ASN
1	E	382	GLN
1	E	452	ASN
1	F	382	GLN
1	F	452	ASN
1	G	382	GLN
1	G	452	ASN
1	H	382	GLN
1	H	452	ASN
1	I	382	GLN
1	I	452	ASN
1	J	382	GLN
1	J	452	ASN
1	K	382	GLN
1	K	452	ASN
1	L	382	GLN
1	L	452	ASN
1	M	382	GLN
1	M	452	ASN
1	N	382	GLN
1	N	452	ASN
1	O	382	GLN
1	O	452	ASN
1	P	382	GLN
1	P	452	ASN
1	Q	382	GLN
1	Q	452	ASN
1	R	382	GLN
1	R	452	ASN
1	S	382	GLN
1	S	452	ASN
1	T	382	GLN
1	T	452	ASN
1	V	382	GLN
1	V	452	ASN
1	W	382	GLN

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Mol	Chain	Res	Type
1	W	452	ASN
1	X	382	GLN
1	X	452	ASN
1	Y	382	GLN
1	Y	452	ASN
1	Z	382	GLN
1	Z	452	ASN
1	AA	382	GLN
1	AA	452	ASN
1	BA	382	GLN
1	BA	452	ASN
1	CA	382	GLN
1	CA	452	ASN
1	DA	382	GLN
1	DA	452	ASN
1	EA	382	GLN
1	EA	452	ASN
1	FA	382	GLN
1	FA	452	ASN
1	GA	382	GLN
1	GA	452	ASN
1	HA	382	GLN
1	HA	452	ASN
1	IA	382	GLN
1	IA	452	ASN
1	JA	382	GLN
1	JA	452	ASN
1	KA	382	GLN
1	KA	452	ASN
1	LA	382	GLN
1	LA	392	GLN
1	LA	452	ASN
1	MA	382	GLN
1	MA	452	ASN
1	NA	382	GLN
1	NA	452	ASN
1	OA	382	GLN
1	OA	452	ASN
1	PA	382	GLN
1	PA	452	ASN
1	QA	382	GLN
1	QA	452	ASN

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Mol	Chain	Res	Type
1	RA	382	GLN
1	RA	452	ASN
1	SA	382	GLN
1	SA	452	ASN
1	TA	382	GLN
1	TA	452	ASN
1	UA	382	GLN
1	UA	452	ASN
1	VA	382	GLN
1	VA	452	ASN
1	WA	382	GLN
1	WA	452	ASN
1	XA	382	GLN
1	XA	452	ASN
1	YA	382	GLN
1	YA	452	ASN
1	ZA	382	GLN
1	ZA	452	ASN
1	AB	382	GLN
1	AB	452	ASN
1	BB	382	GLN
1	BB	452	ASN
1	CB	382	GLN
1	CB	452	ASN
1	DB	382	GLN
1	DB	452	ASN
1	EB	382	GLN
1	EB	452	ASN
1	FB	382	GLN
1	FB	452	ASN
1	GB	382	GLN
1	GB	452	ASN
1	HB	382	GLN
1	HB	452	ASN
1	IB	382	GLN
1	IB	452	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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.

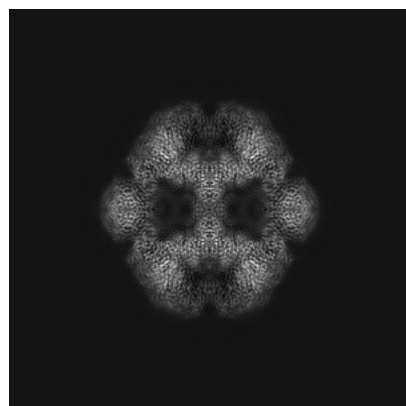
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11270. These allow visual inspection of the internal detail of the map and identification of artifacts.

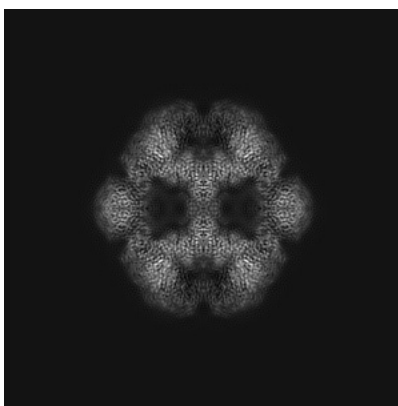
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

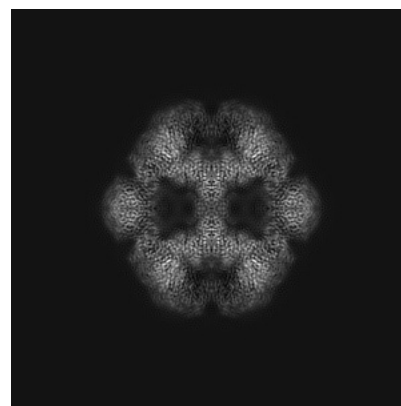
6.1.1 Primary map



X

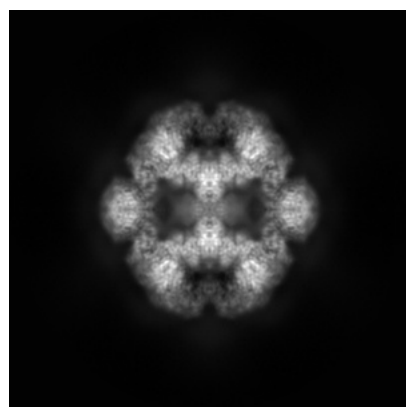


Y

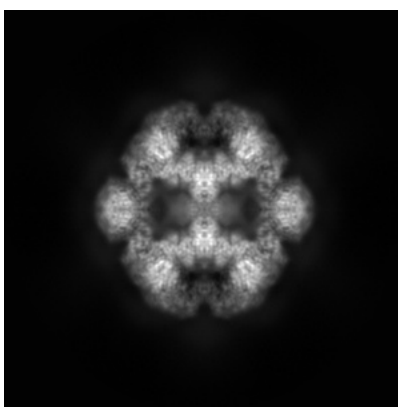


Z

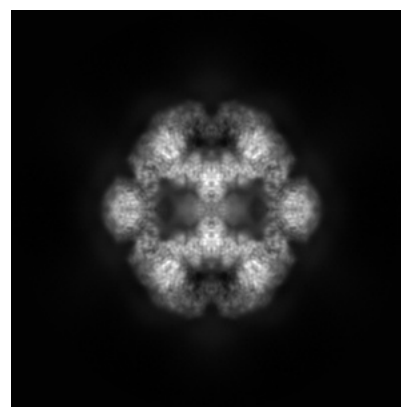
6.1.2 Raw map



X



Y

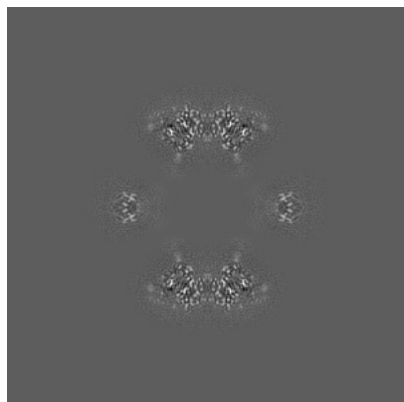


Z

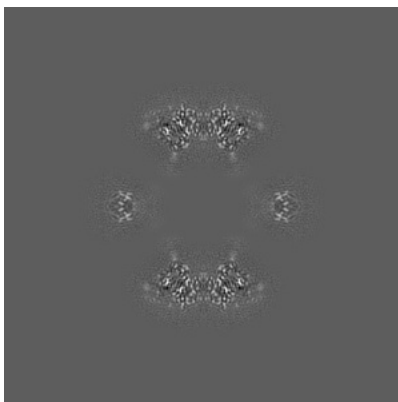
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

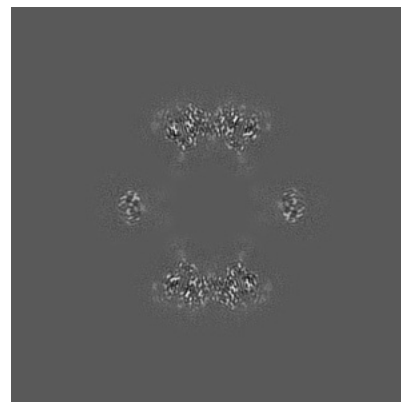
6.2.1 Primary map



X Index: 192

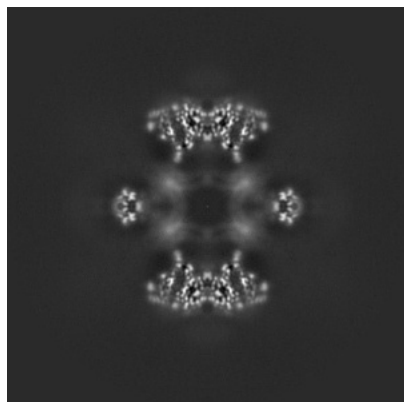


Y Index: 192

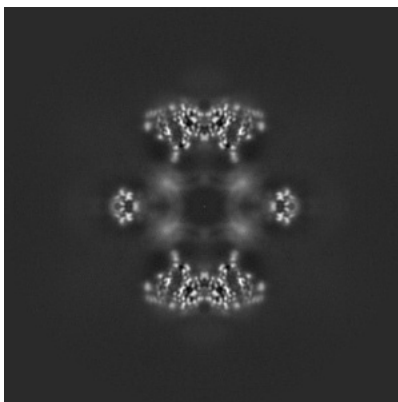


Z Index: 192

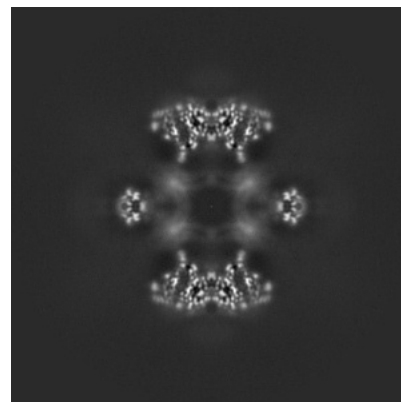
6.2.2 Raw map



X Index: 192



Y Index: 192

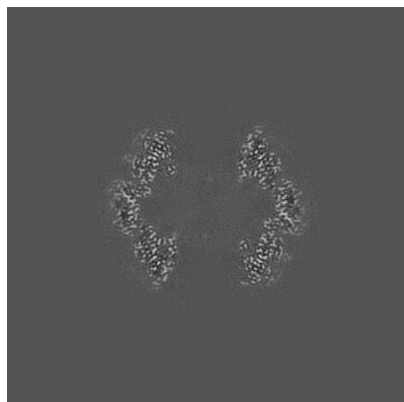


Z Index: 192

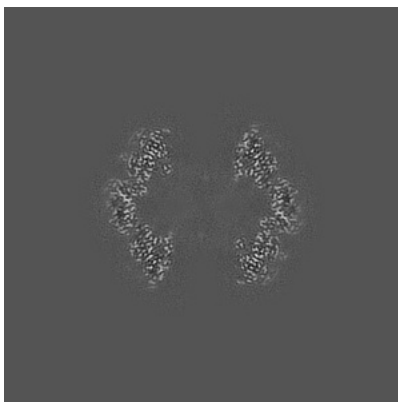
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

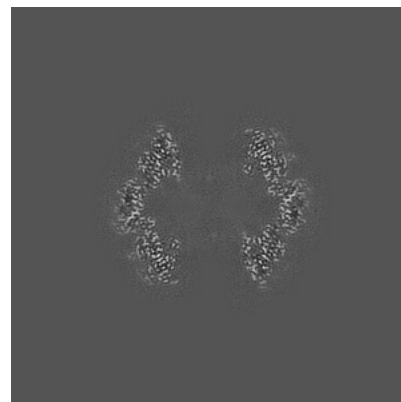
6.3.1 Primary map



X Index: 234

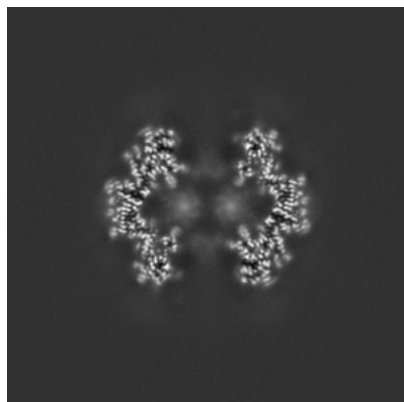


Y Index: 234

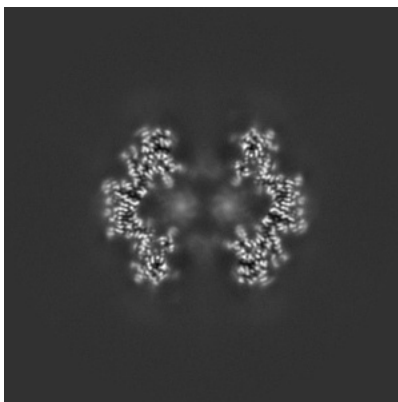


Z Index: 149

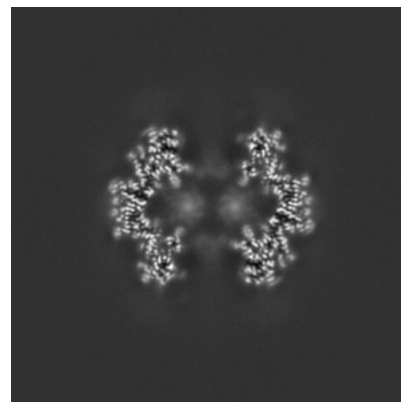
6.3.2 Raw map



X Index: 155



Y Index: 155

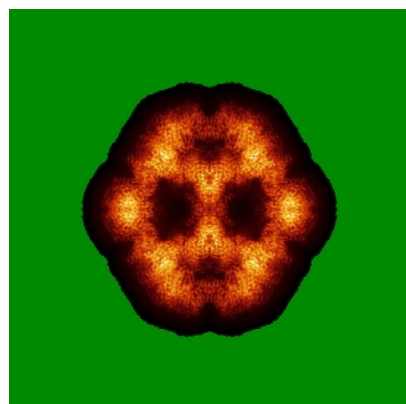


Z Index: 155

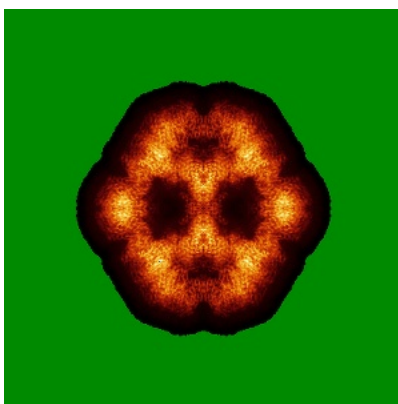
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

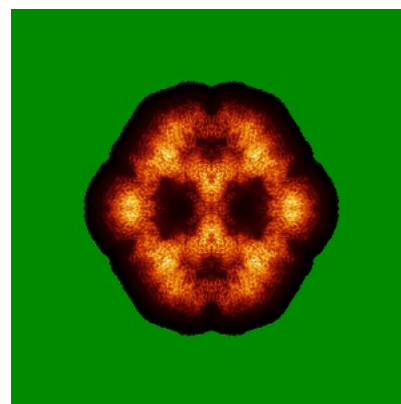
6.4.1 Primary map



X

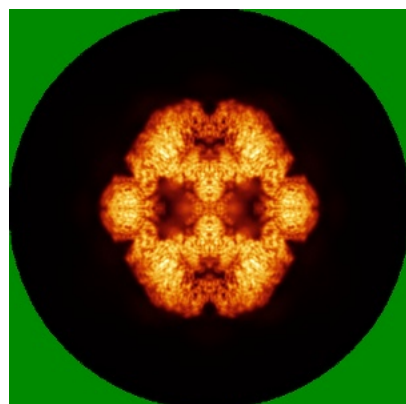


Y

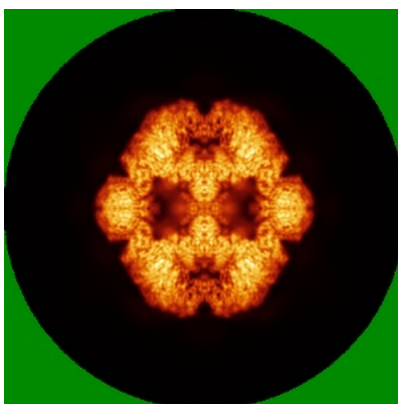


Z

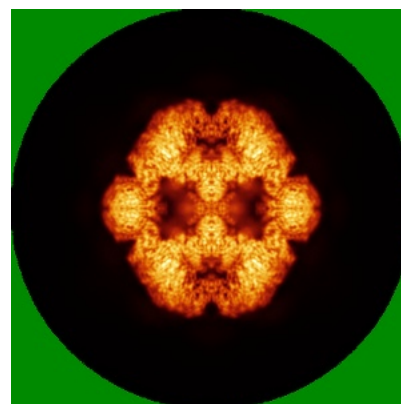
6.4.2 Raw map



X



Y

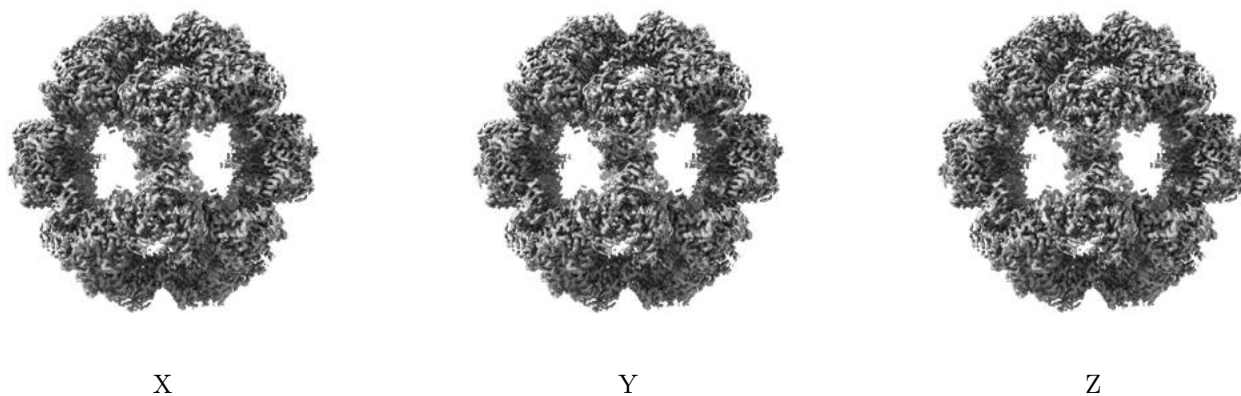


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

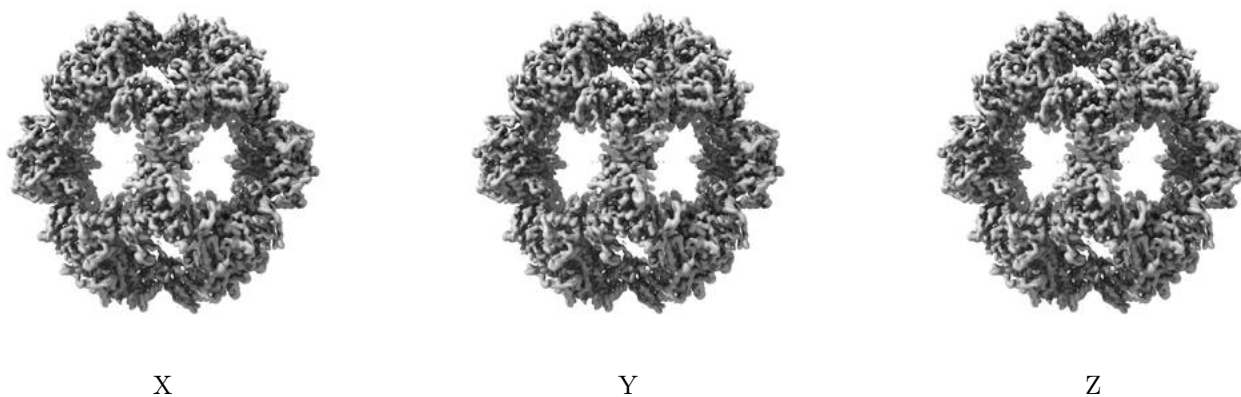
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0235. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

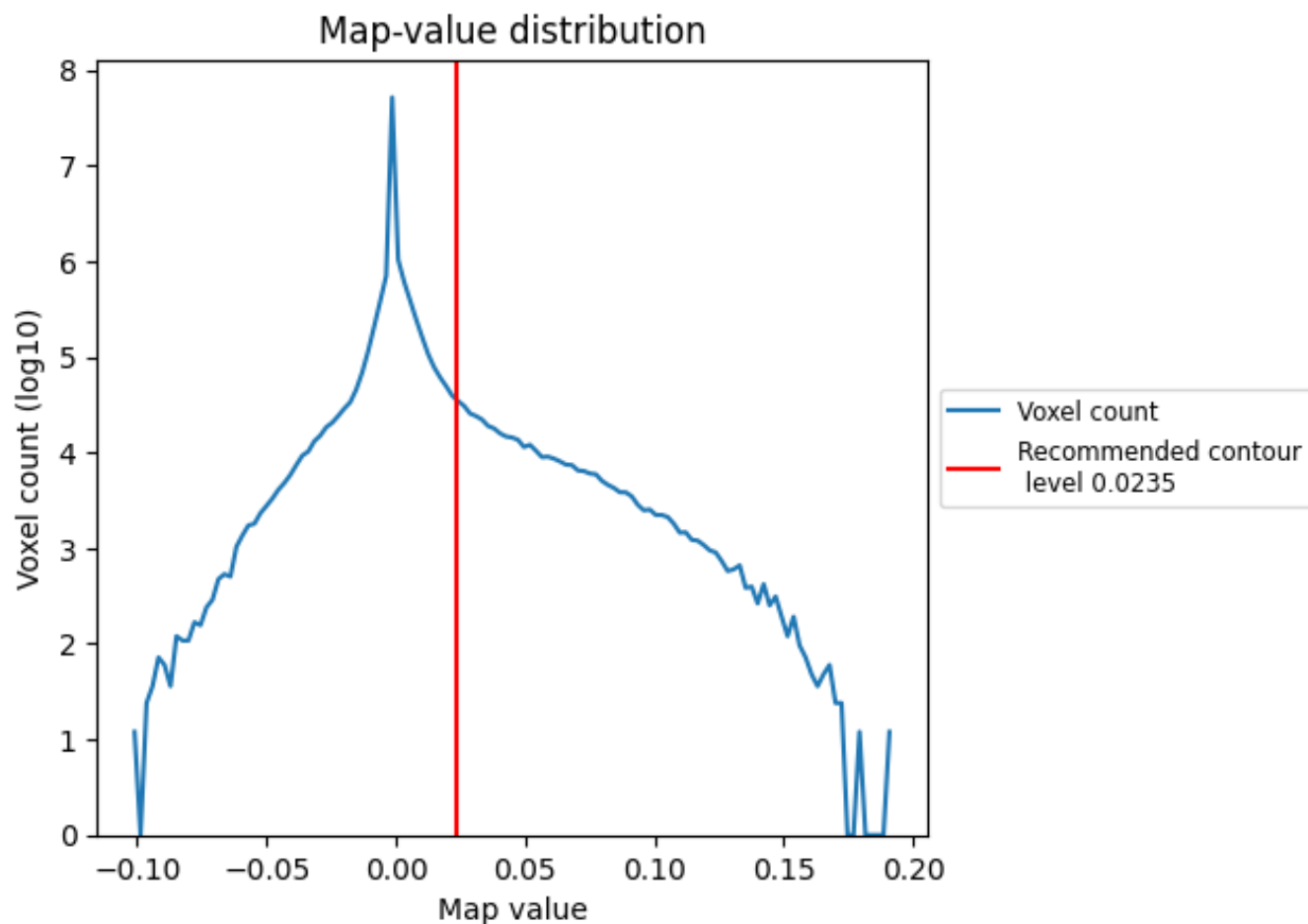
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

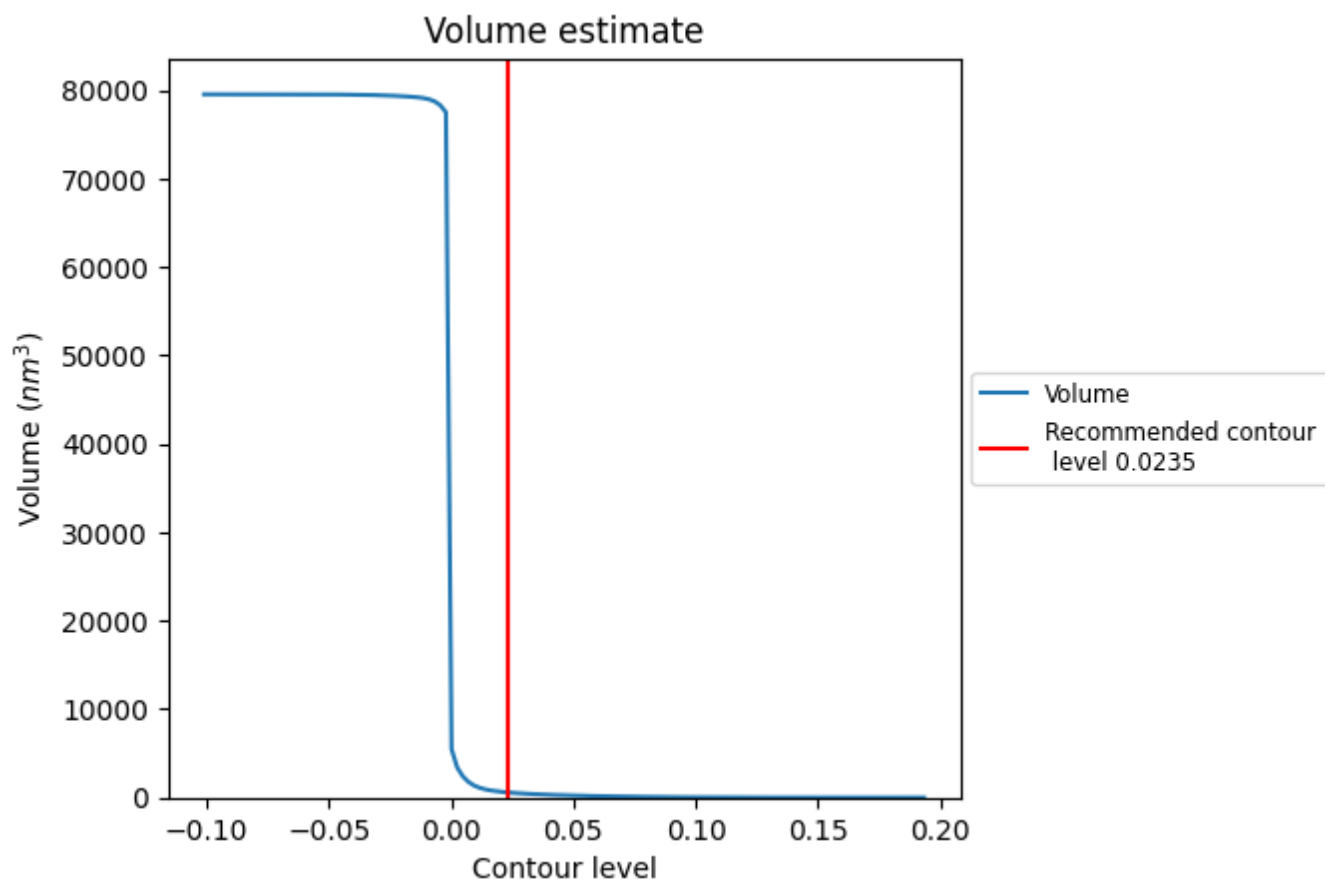
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

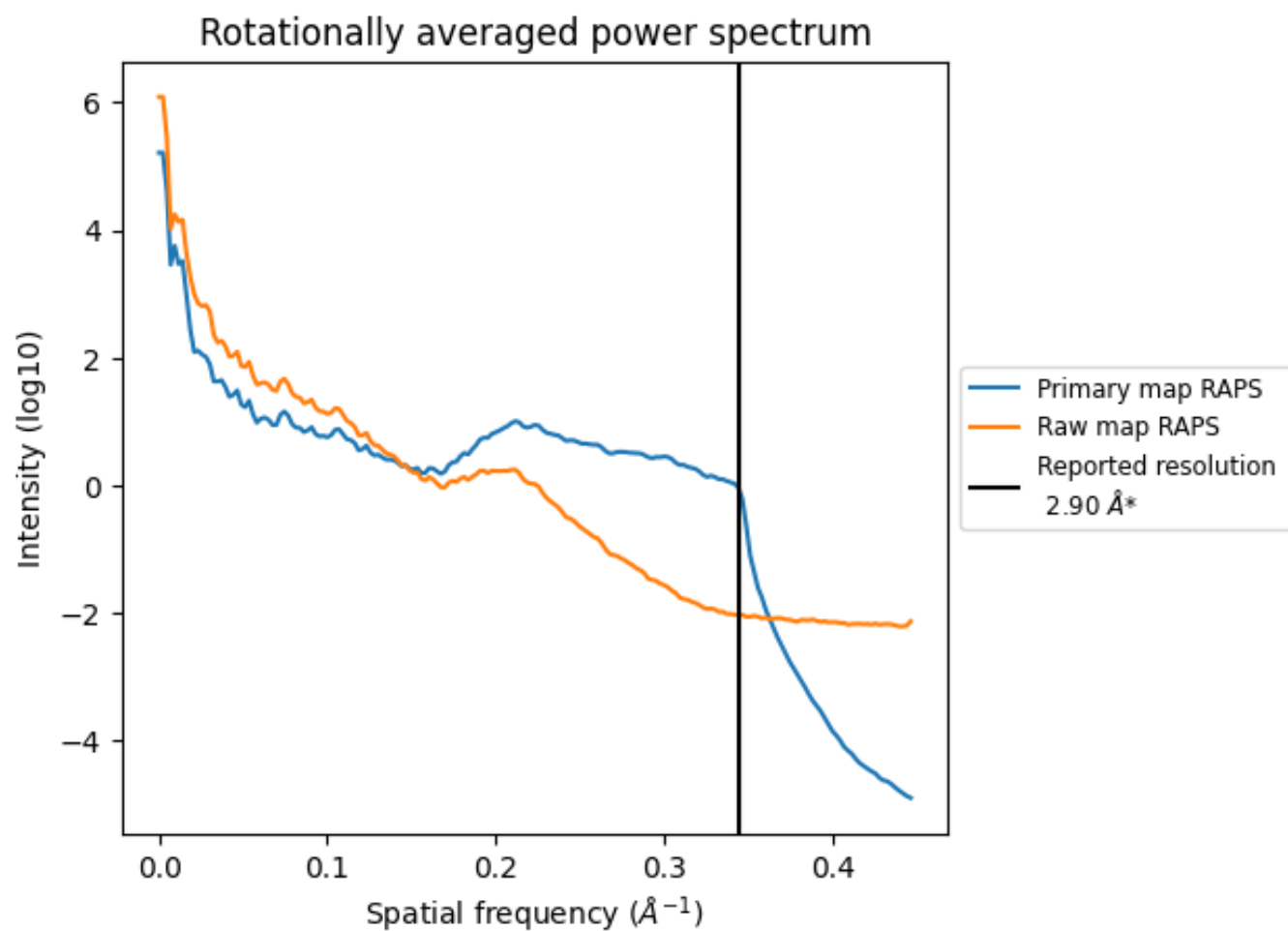
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 569 nm³; this corresponds to an approximate mass of 514 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

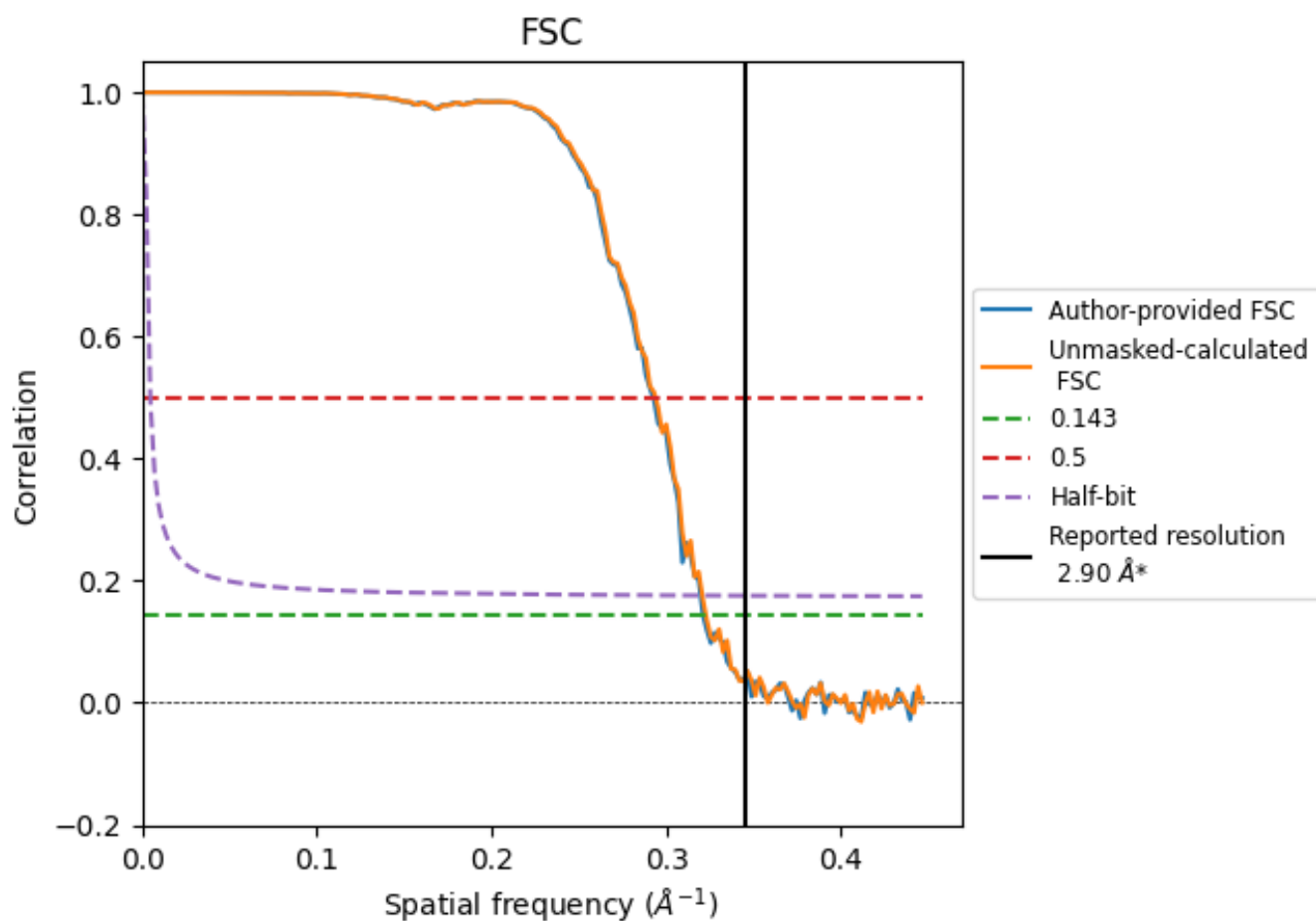


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

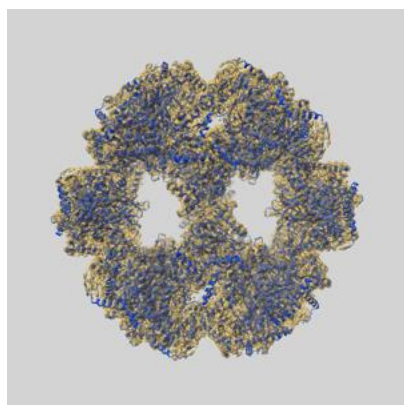
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	3.12	3.42	3.13
Unmasked-calculated*	3.10	3.40	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

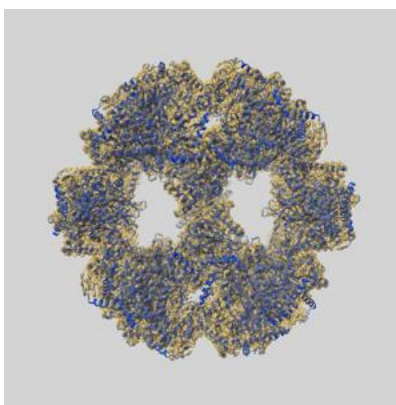
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11270 and PDB model 6ZLO. Per-residue inclusion information can be found in section [3](#) on page [75](#).

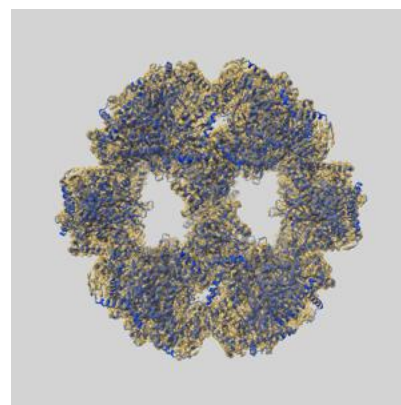
9.1 Map-model overlay [i](#)



X



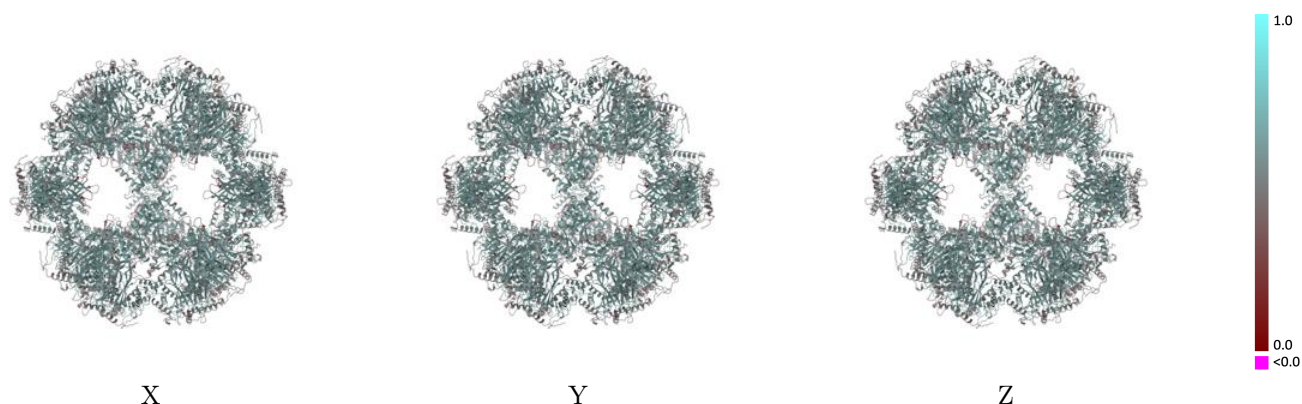
Y



Z

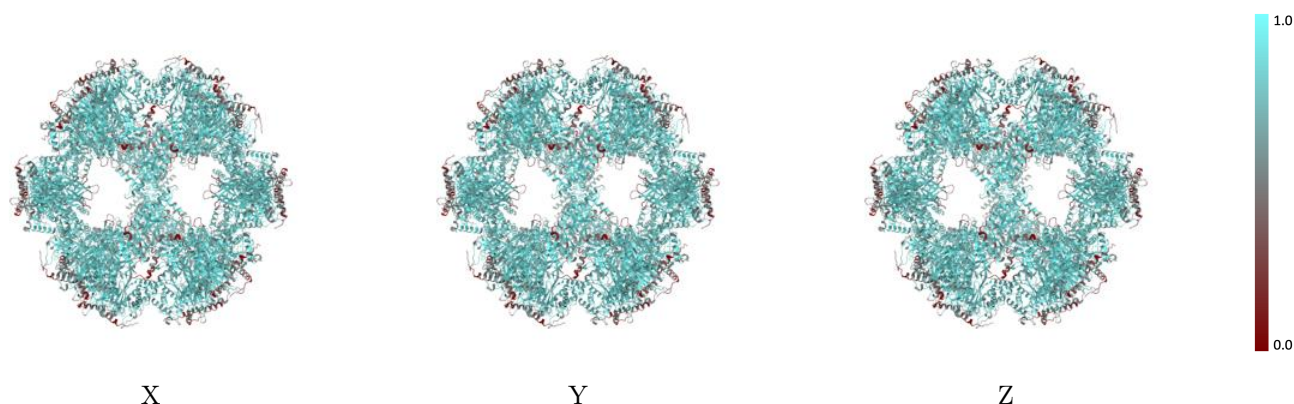
The images above show the 3D surface view of the map at the recommended contour level 0.0235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



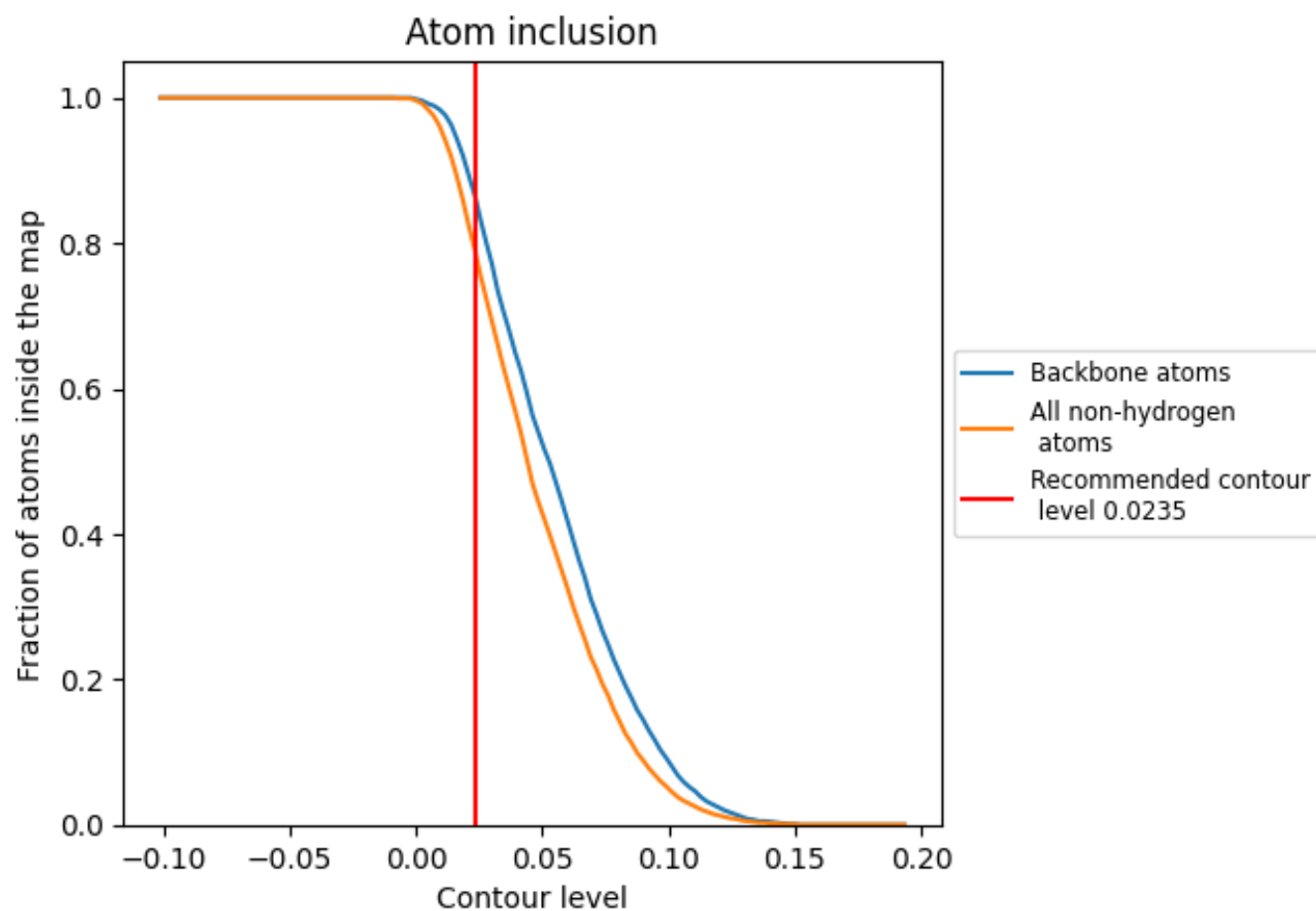
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0235).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.5570
A	 0.7870	 0.5560
AA	 0.7870	 0.5570
AB	 0.7870	 0.5570
B	 0.7870	 0.5570
BA	 0.7870	 0.5570
BB	 0.7890	 0.5600
C	 0.7880	 0.5580
CA	 0.7890	 0.5570
CB	 0.7870	 0.5570
D	 0.7870	 0.5570
DA	 0.7870	 0.5550
DB	 0.7890	 0.5570
E	 0.7890	 0.5580
EA	 0.7890	 0.5570
EB	 0.7870	 0.5570
F	 0.7870	 0.5560
FA	 0.7870	 0.5570
FB	 0.7870	 0.5560
G	 0.7870	 0.5570
GA	 0.7870	 0.5560
GB	 0.7880	 0.5580
H	 0.7890	 0.5590
HA	 0.7880	 0.5580
HB	 0.7870	 0.5570
I	 0.7870	 0.5580
IA	 0.7860	 0.5560
IB	 0.7890	 0.5570
J	 0.7890	 0.5550
JA	 0.7890	 0.5590
K	 0.7870	 0.5550
KA	 0.7870	 0.5570
L	 0.7870	 0.5560
LA	 0.7870	 0.5570
M	 0.7880	 0.5590



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Chain	Atom inclusion	Q-score
MA	 0.7890	 0.5570
N	 0.7870	 0.5550
NA	 0.7870	 0.5580
O	 0.7890	 0.5550
OA	 0.7890	 0.5580
P	 0.7870	 0.5550
PA	 0.7870	 0.5590
Q	 0.7870	 0.5580
QA	 0.7870	 0.5560
R	 0.7890	 0.5600
RA	 0.7890	 0.5610
S	 0.7870	 0.5580
SA	 0.7870	 0.5560
T	 0.7890	 0.5560
TA	 0.7890	 0.5580
UA	 0.7870	 0.5580
V	 0.7870	 0.5570
VA	 0.7870	 0.5580
W	 0.7870	 0.5570
WA	 0.7880	 0.5610
X	 0.7880	 0.5570
XA	 0.7870	 0.5560
Y	 0.7870	 0.5570
YA	 0.7890	 0.5580
Z	 0.7890	 0.5580
ZA	 0.7870	 0.5590