



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:25 AM GMT

PDB ID : 2GLJ  
Title : crystal structure of aminopeptidase I from Clostridium acetobutylicum  
Authors : Min, T.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2006-04-04  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

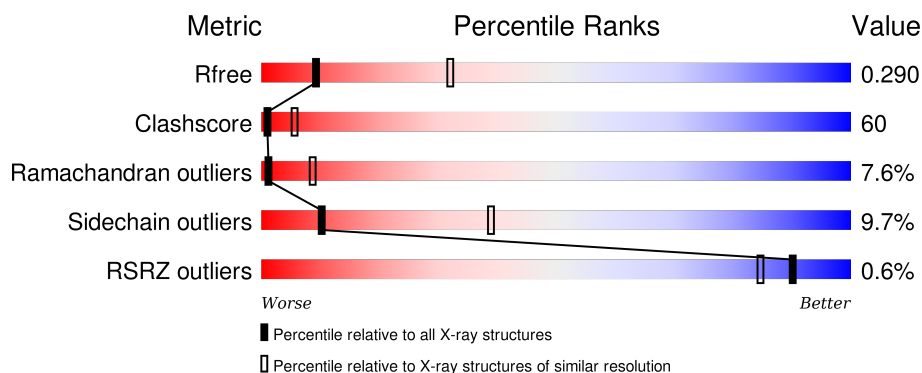
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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







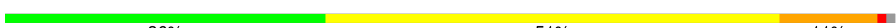
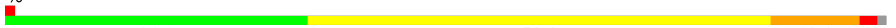







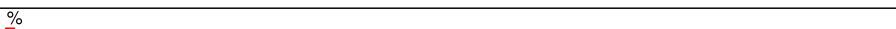





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	<div> <div>%</div> <div> <div></div> <div>39%</div> <div>48%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	461	<div> <div>41%</div> <div>47%</div> <div>10%</div> <div>..</div> </div>
1	C	461	<div> <div>36%</div> <div>51%</div> <div>10%</div> <div>..</div> </div>
1	D	461	<div> <div>37%</div> <div>49%</div> <div>11%</div> <div>..</div> </div>
1	E	461	<div> <div>%</div> <div>37%</div> <div>49%</div> <div>12%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	461	
1	G	461	
1	H	461	% 
1	I	461	% 
1	J	461	
1	K	461	% 
1	L	461	% 
1	M	461	% 
1	N	461	% 
1	O	461	
1	P	461	
1	Q	461	
1	R	461	% 
1	S	461	% 
1	T	461	% 
1	U	461	
1	V	461	
1	W	461	% 
1	X	461	% 

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 91225 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Probable M18-family aminopeptidase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	B	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	C	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	D	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	E	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	F	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	G	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	H	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	I	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	J	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	K	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	L	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	M	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	N	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	O	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	P	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	R	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	S	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	T	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	U	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	V	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	W	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			
1	X	456	Total	C	N	O	S	Se	0	0	0
			3581	2268	592	701	19	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
B	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
C	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
D	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
E	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
F	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
G	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
H	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
I	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
J	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
K	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
L	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
M	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
N	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
O	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
P	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
Q	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
R	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
S	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
T	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
U	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
V	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30
W	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30

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Chain	Residue	Modelled	Actual	Comment	Reference
X	440	MSE	MET	MODIFIED RESIDUE	UNP Q97K30

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total 2	Mn 2	0	0
2	K	2	Total 2	Mn 2	0	0
2	B	2	Total 2	Mn 2	0	0
2	W	2	Total 2	Mn 2	0	0
2	N	2	Total 2	Mn 2	0	0
2	X	2	Total 2	Mn 2	0	0
2	S	2	Total 2	Mn 2	0	0
2	J	2	Total 2	Mn 2	0	0
2	E	2	Total 2	Mn 2	0	0
2	V	2	Total 2	Mn 2	0	0
2	A	2	Total 2	Mn 2	0	0
2	R	2	Total 2	Mn 2	0	0
2	M	2	Total 2	Mn 2	0	0
2	D	2	Total 2	Mn 2	0	0
2	I	2	Total 2	Mn 2	0	0
2	U	2	Total 2	Mn 2	0	0
2	L	2	Total 2	Mn 2	0	0
2	G	2	Total 2	Mn 2	0	0
2	Q	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	2	Total 2	Mn 2	0	0
2	C	2	Total 2	Mn 2	0	0
2	T	2	Total 2	Mn 2	0	0
2	O	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	206	Total 206	O 206	0	0
3	B	187	Total 187	O 187	0	0
3	C	239	Total 239	O 239	0	0
3	D	238	Total 238	O 238	0	0
3	E	210	Total 210	O 210	0	0
3	F	219	Total 219	O 219	0	0
3	G	231	Total 231	O 231	0	0
3	H	215	Total 215	O 215	0	0
3	I	233	Total 233	O 233	0	0
3	J	237	Total 237	O 237	0	0
3	K	219	Total 219	O 219	0	0
3	L	222	Total 222	O 222	0	0
3	M	227	Total 227	O 227	0	0
3	N	246	Total 246	O 246	0	0

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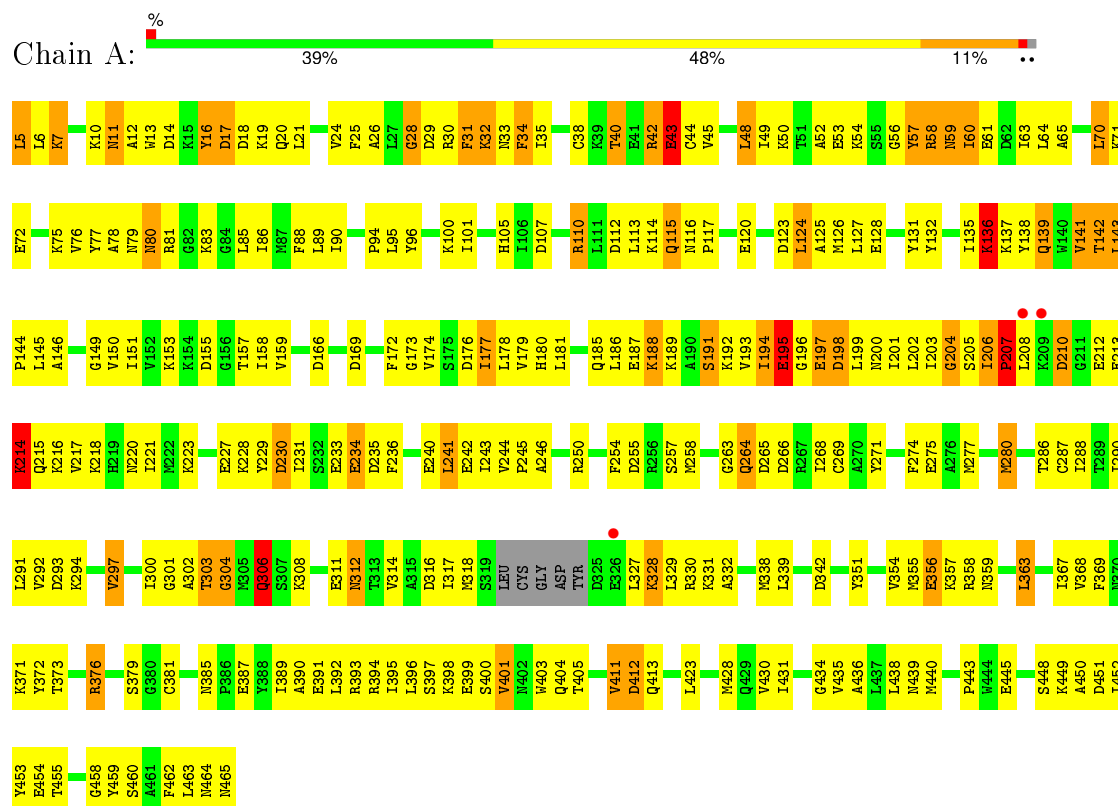
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	205	Total 205	O 205	0	0
3	P	208	Total 208	O 208	0	0
3	Q	211	Total 211	O 211	0	0
3	R	200	Total 200	O 200	0	0
3	S	205	Total 205	O 205	0	0
3	T	226	Total 226	O 226	0	0
3	U	214	Total 214	O 214	0	0
3	V	225	Total 225	O 225	0	0
3	W	217	Total 217	O 217	0	0
3	X	193	Total 193	O 193	0	0



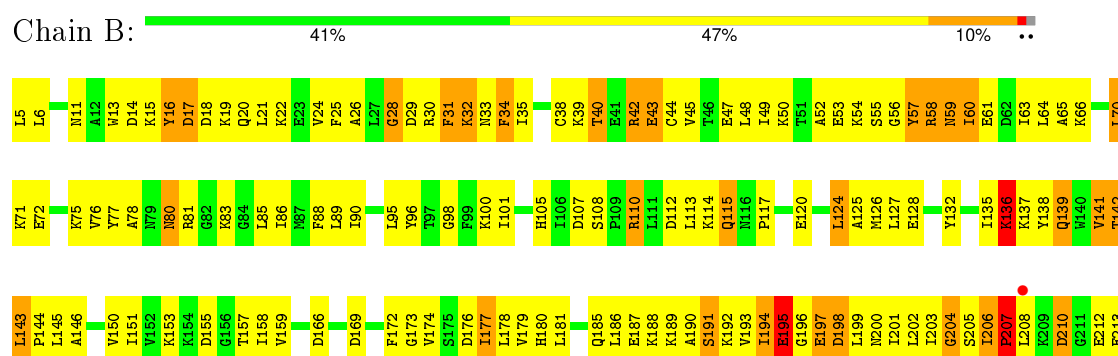
### 3 Residue-property plots

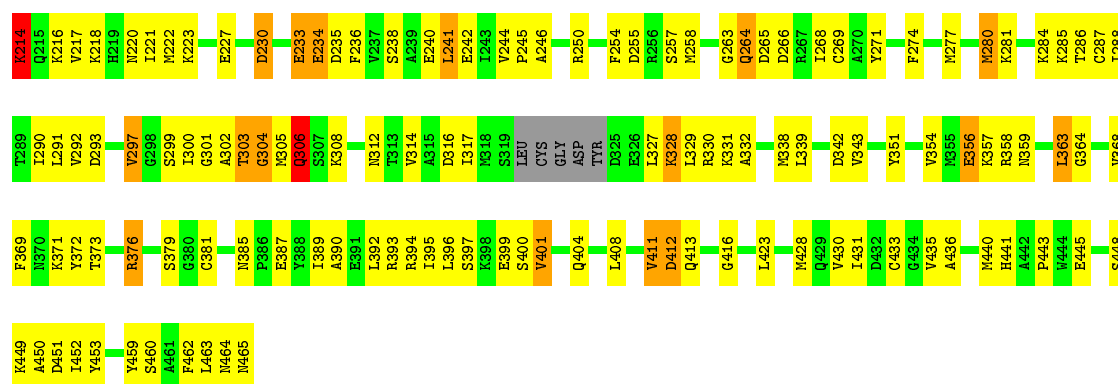
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Probable M18-family aminopeptidase 1



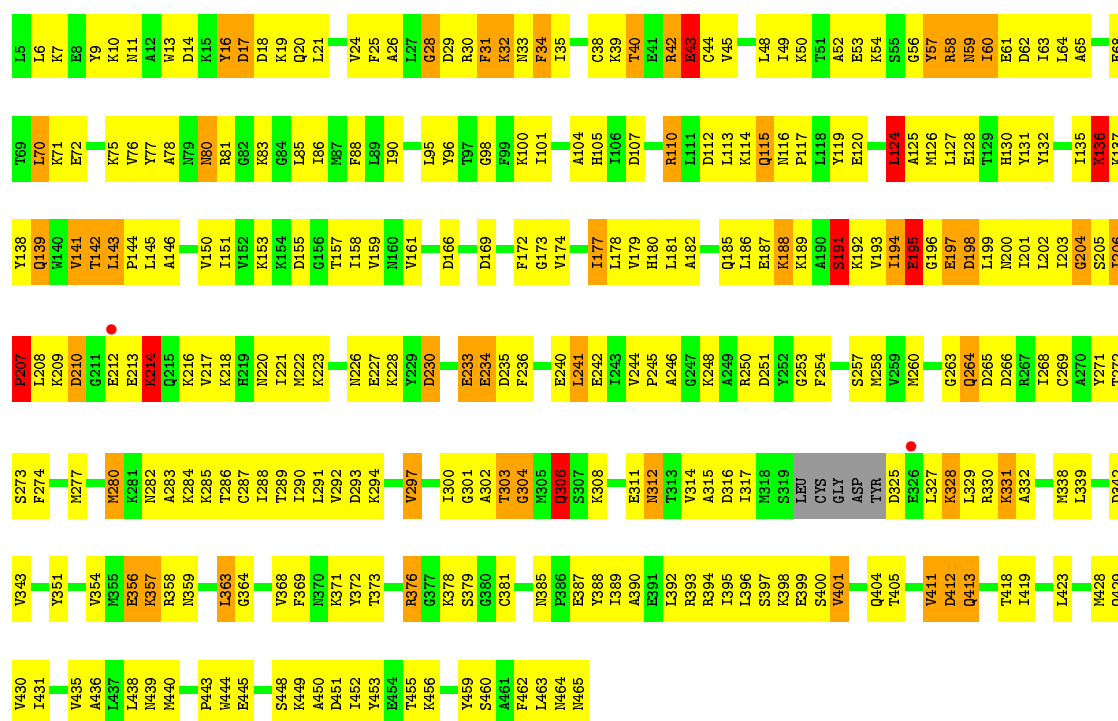
#### • Molecule 1: Probable M18-family aminopeptidase 1





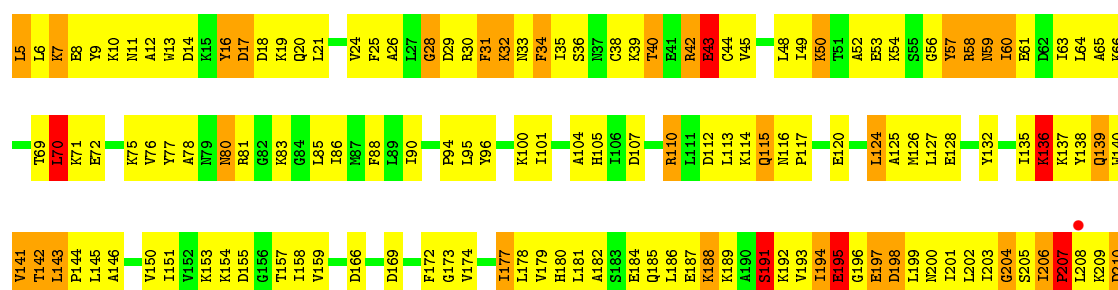
• Molecule 1: Probable M18-family aminopeptidase 1

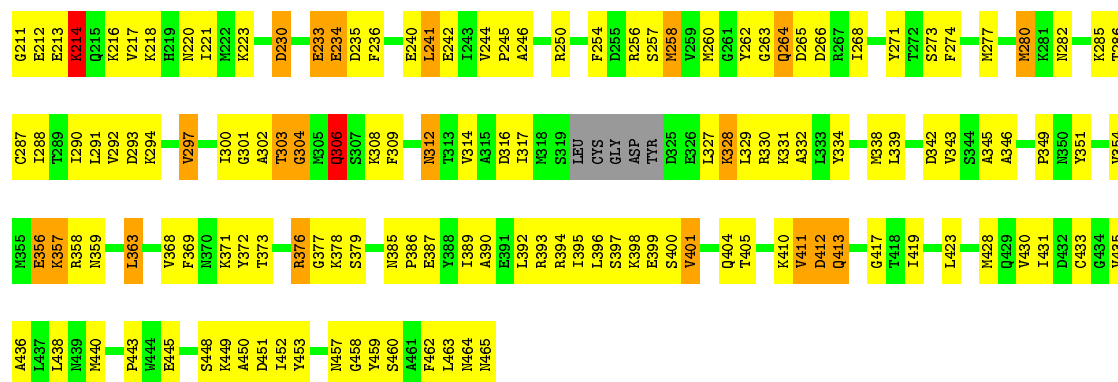
Chain C: 36% 51% 10% ..



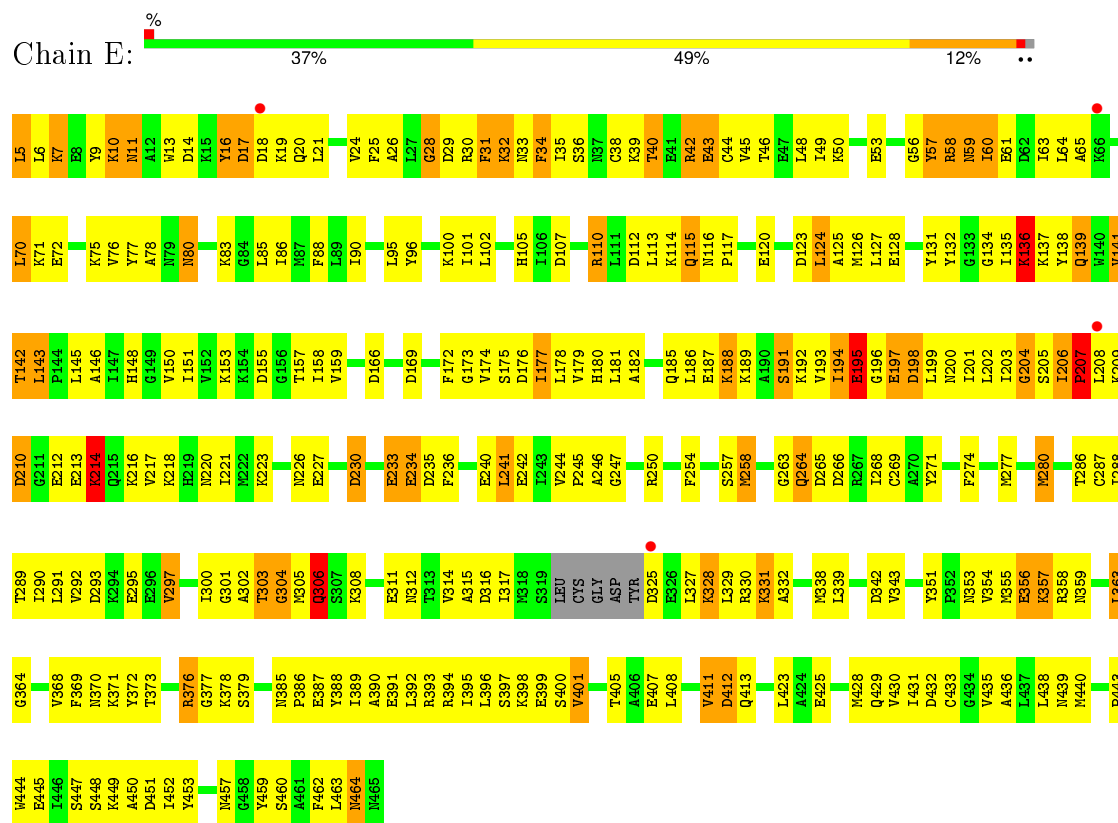
• Molecule 1: Probable M18-family aminopeptidase 1

Chain D: 37% 49% 11% ..

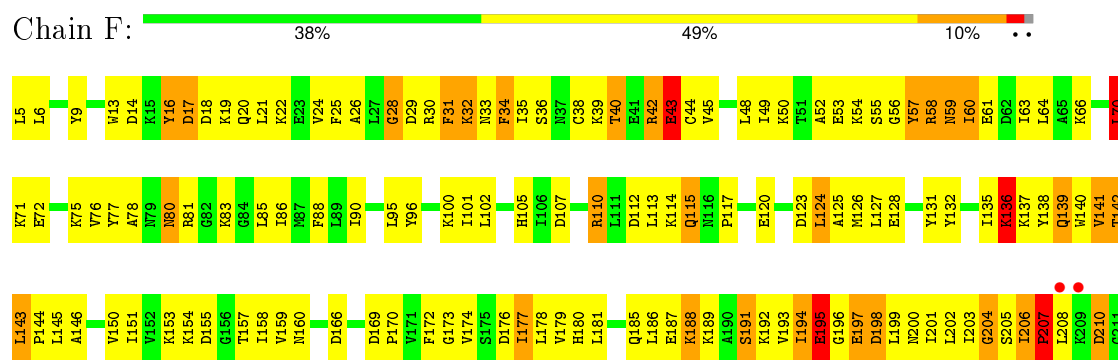




• Molecule 1: Probable M18-family aminopeptidase 1

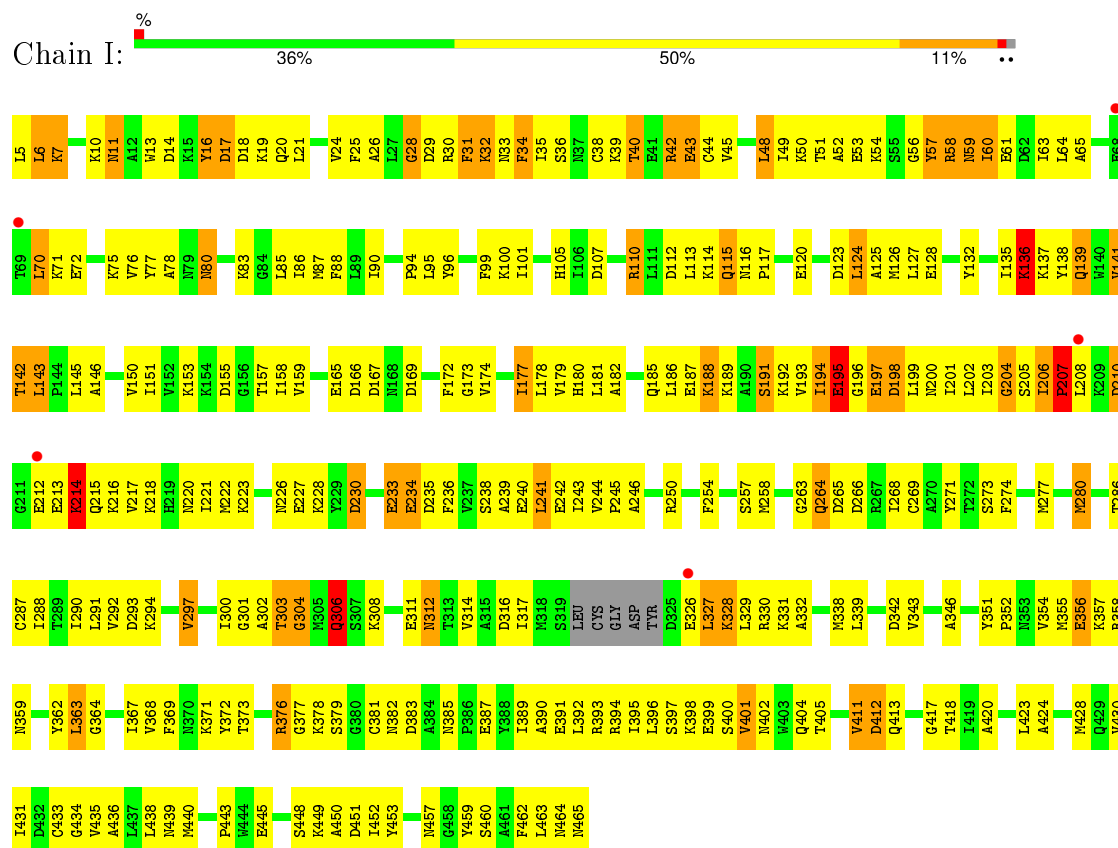


• Molecule 1: Probable M18-family aminopeptidase 1

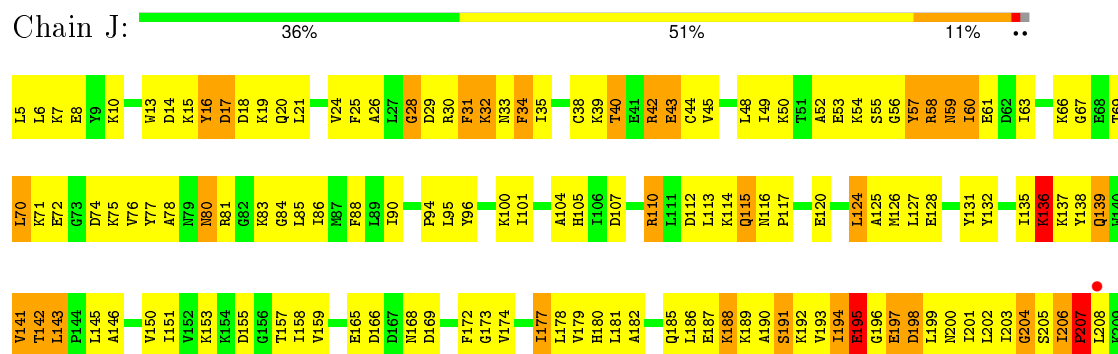




- Molecule 1: Probable M18-family aminopeptidase 1



- Molecule 1: Probable M18-family aminopeptidase 1

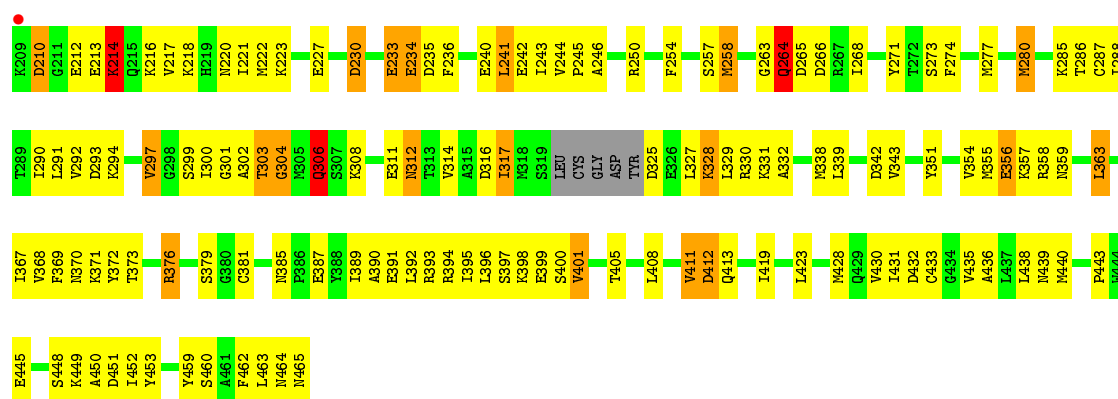


- Molecule 1: Probable M18-family aminopeptidase 1

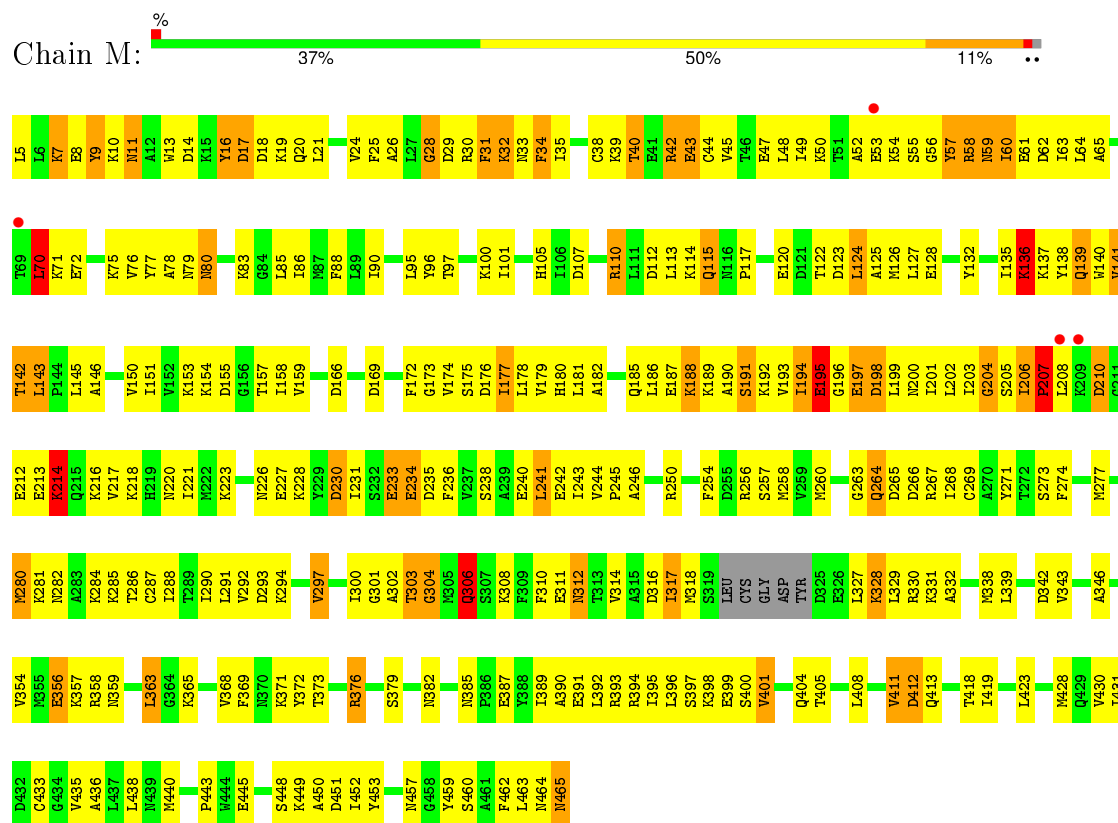


- Molecule 1: Probable M18-family aminopeptidase 1

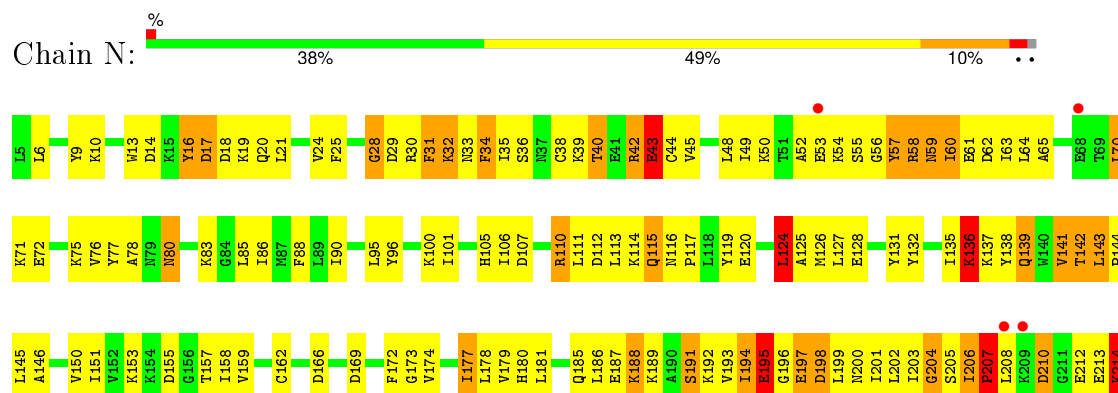


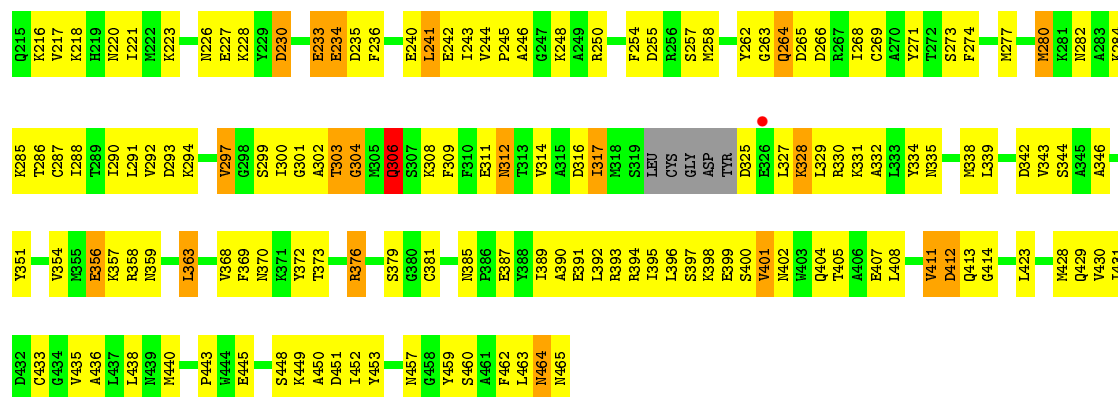


● Molecule 1: Probable M18-family aminopeptidase 1



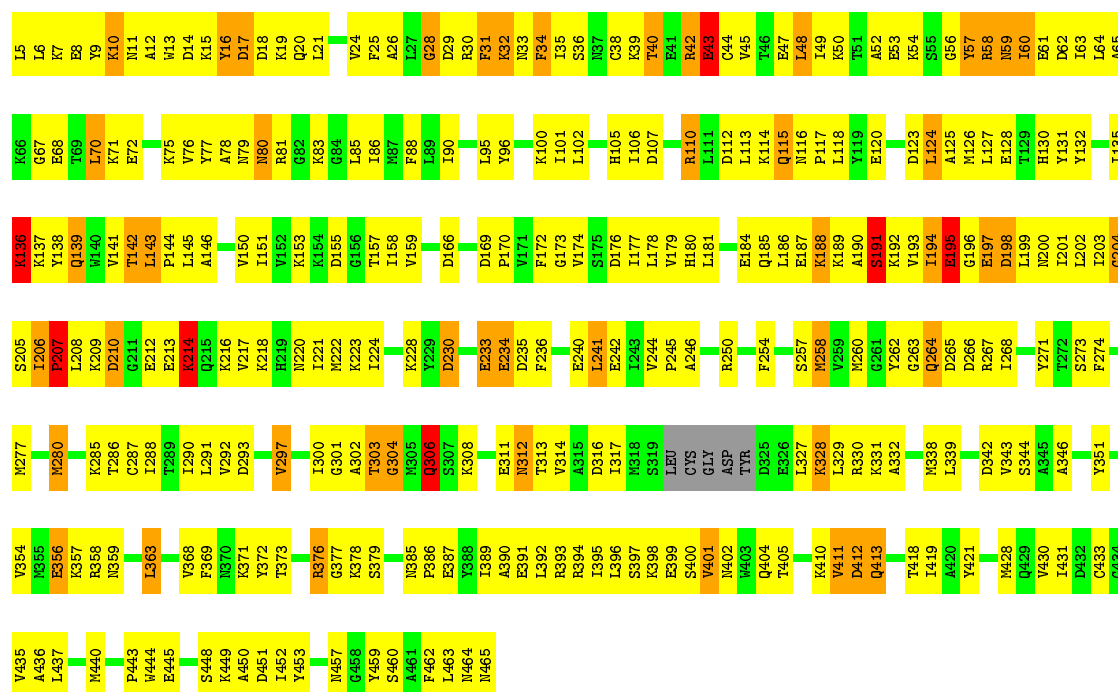
● Molecule 1: Probable M18-family aminopeptidase 1





• Molecule 1: Probable M18-family aminopeptidase 1

Chain O: 35% 52% 10% ..

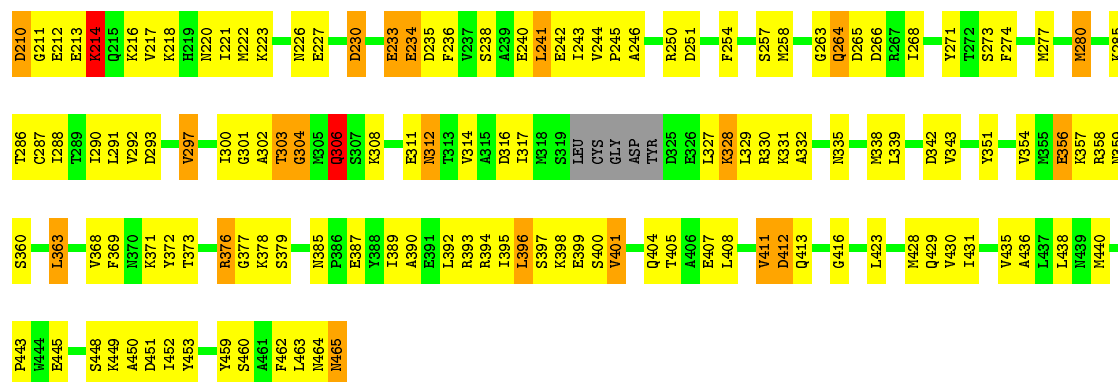


• Molecule 1: Probable M18-family aminopeptidase 1

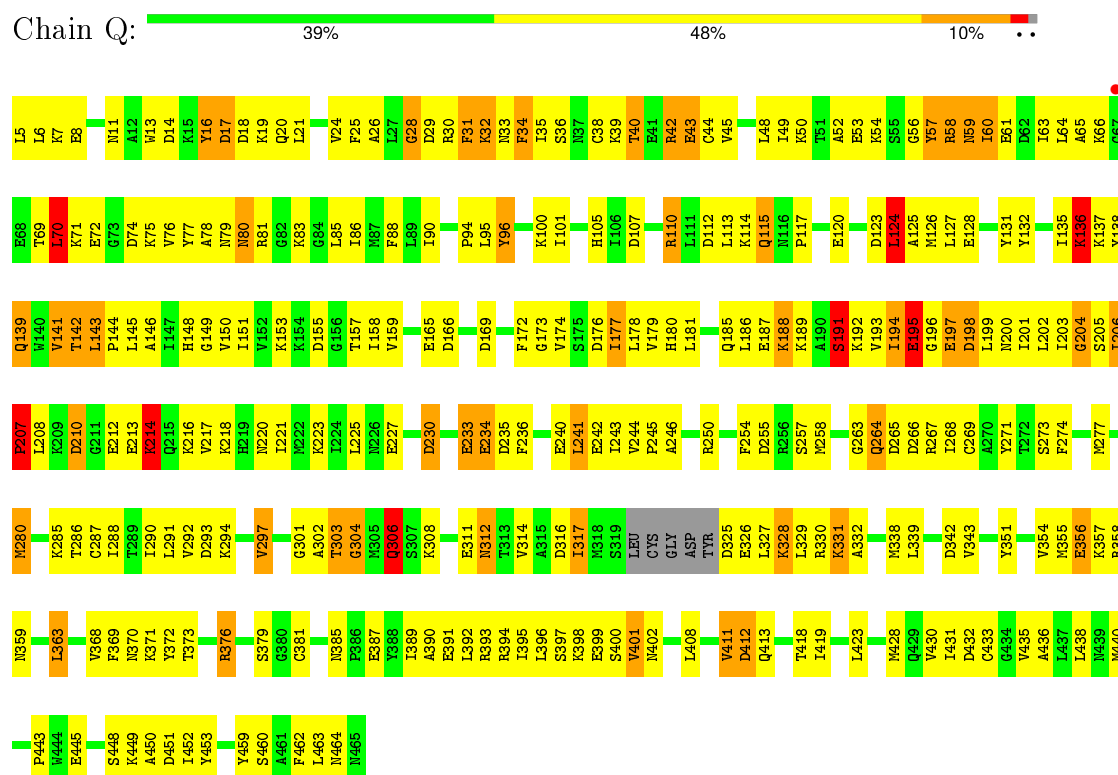
Chain P: 39% 48% 11% ..



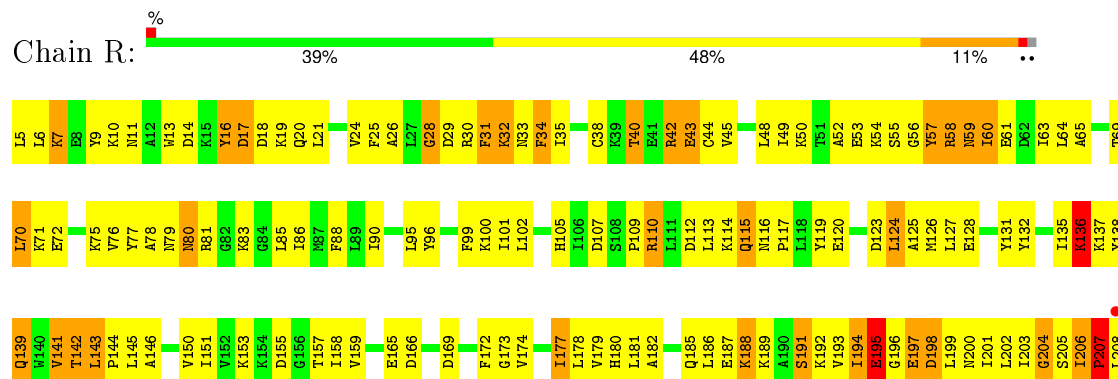


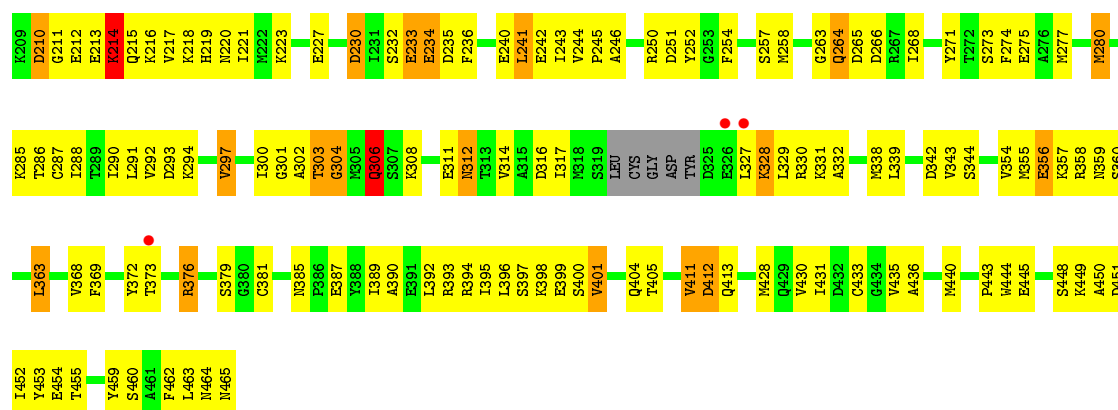


• Molecule 1: Probable M18-family aminopeptidase 1

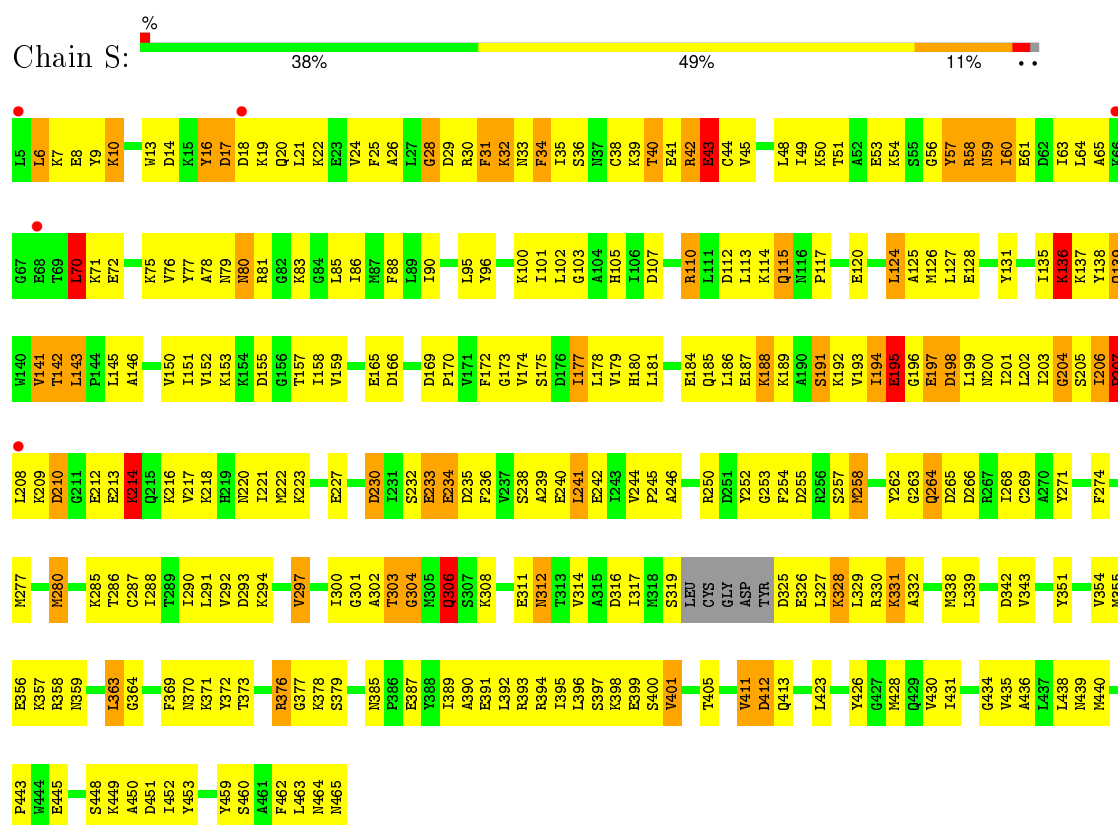


• Molecule 1: Probable M18-family aminopeptidase 1

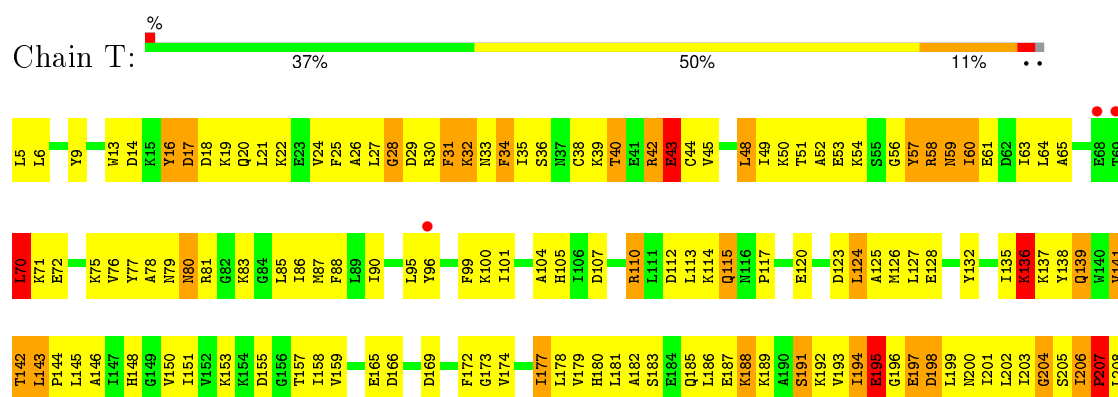


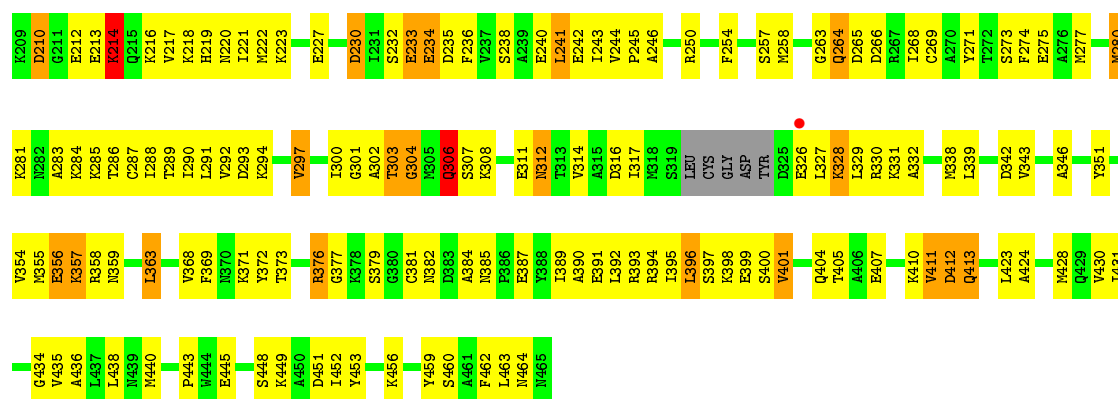


● Molecule 1: Probable M18-family aminopeptidase 1



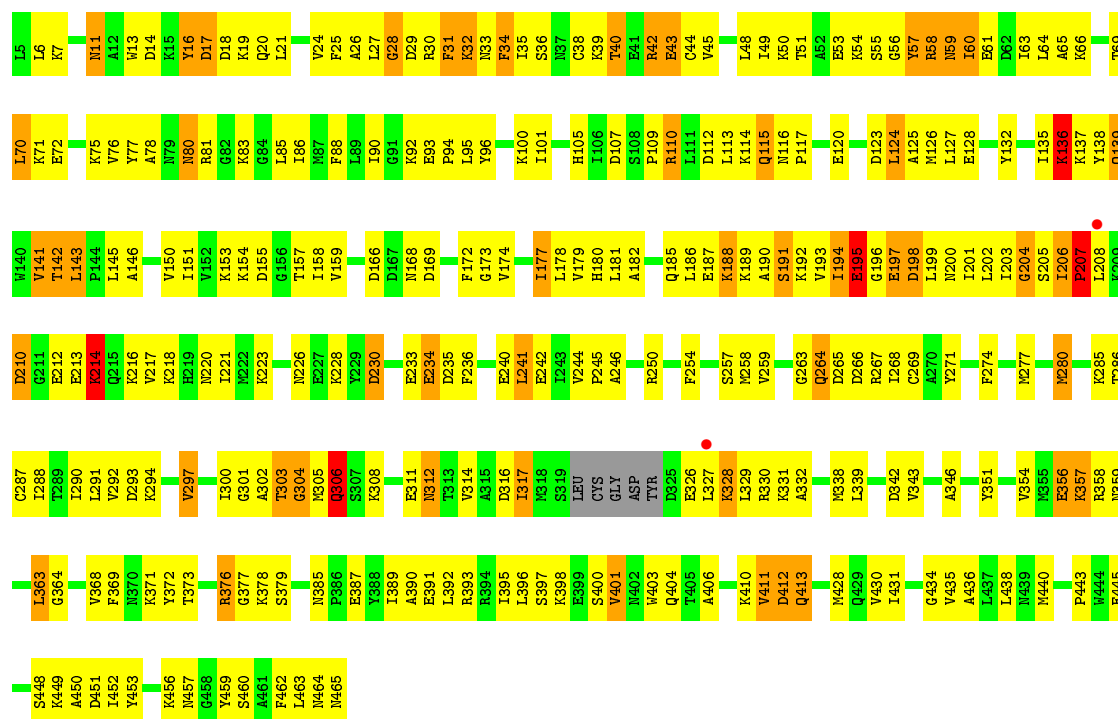
● Molecule 1: Probable M18-family aminopeptidase 1





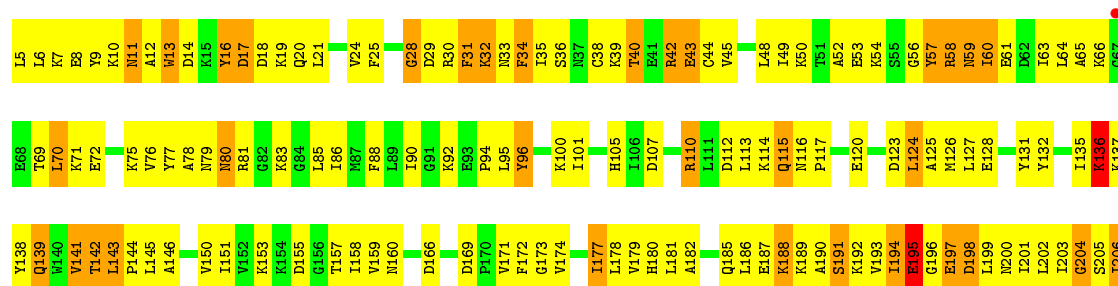
• Molecule 1: Probable M18-family aminopeptidase 1

Chain U: 39% 48% 11% ..

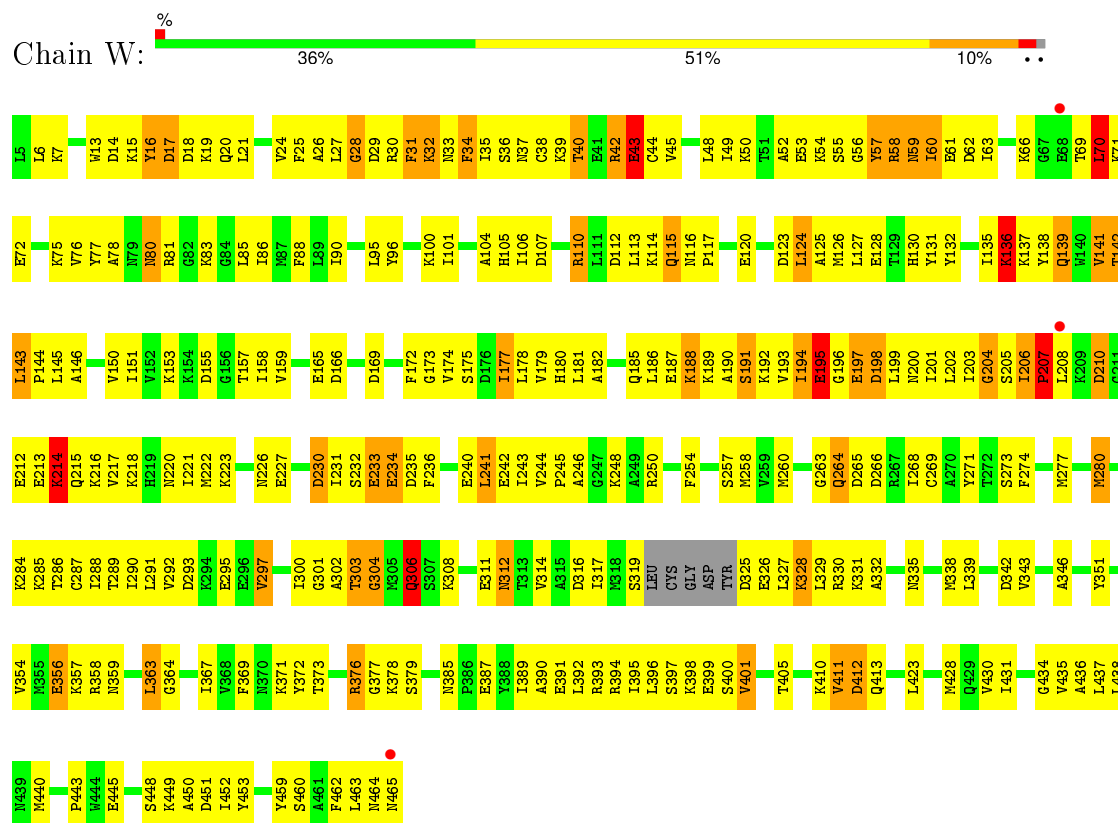


• Molecule 1: Probable M18-family aminopeptidase 1

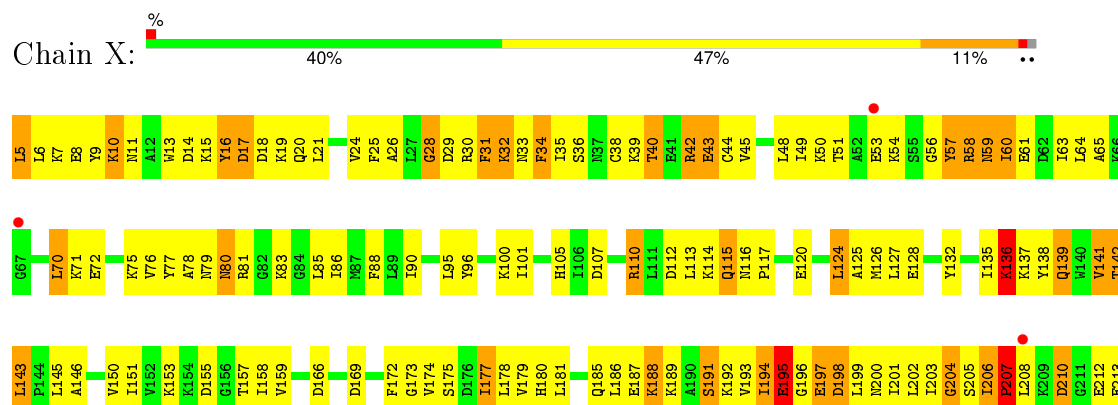
Chain V: 37% 49% 11% ..



- Molecule 1: Probable M18-family aminopeptidase 1



- Molecule 1: Probable M18-family aminopeptidase 1



E445	L363	L288	K214
S448	Y368	T289	Q215
K449	F369	I290	K216
A450	N370	L291	V217
D451	K371	V292	K218
I452	Y372	D293	D219
Y453	T373	K294	V220
		V297	I221
			N222
		I300	K223
	R376	G301	E227
	G377	A302	V228
	K378	T303	Y229
	S379	G304	D230
	G380	M305	
	C381	Q306	E233
		P386	E234
	N385	S307	D235
	P386	K308	F236
	E387		
	N388	E311	
	I389	E240	E241
	A390	N312	L241
	E391	T313	
	L392	V314	E242
	R393	A315	T243
	R394	D316	V244
	I395	I317	P245
	L396	M318	A246
	S397	S319	
	K398	LEU	K250
	E399	CYS	
	S400	GLY	F254
	V401	ASP	D255
		TYR	R256
	Q404	D325	S257
	T405	E326	N258
		L327	
	V411	K328	Y262
	D412	L329	G263
	Q413	R330	Q264
		K331	D265
	T418	A332	D266
			R267
	L423	M338	I268
		L339	C269
	N428		A270
	Q429	D342	Y271
	V430	V343	
	I431		F274
	D432	A346	
	C433		N277
	G434	Y351	
	V435		M280
	A436	V354	K281
		M355	N282
	M439	E356	A283
	N440	K357	K284
		R358	K285
		N359	T286
	P443		C287
	N444		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.71Å 129.68Å 222.73Å 89.88° 90.00° 116.68°	Depositor
Resolution (Å)	19.95 – 3.20 19.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	60.1 (19.95-3.20) 93.0 (19.95-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.250 , 0.297 0.249 , 0.290	Depositor DCC
$R_{free}$ test set	6234 reflections (3.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 21.2	EDS
Estimated twinning fraction	0.012 for h,-h-k,-l 0.357 for -h,-k,l 0.008 for -h,h+k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 311235 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	91225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.44	0/3639	0.63	0/4893
1	B	0.43	0/3639	0.63	0/4893
1	C	0.43	0/3639	0.63	0/4893
1	D	0.44	0/3639	0.64	0/4893
1	E	0.44	0/3639	0.63	0/4893
1	F	0.45	0/3639	0.63	0/4893
1	G	0.44	0/3639	0.63	0/4893
1	H	0.46	0/3639	0.64	0/4893
1	I	0.44	0/3639	0.63	0/4893
1	J	0.44	0/3639	0.64	0/4893
1	K	0.45	0/3639	0.64	0/4893
1	L	0.43	0/3639	0.63	0/4893
1	M	0.45	0/3639	0.63	0/4893
1	N	0.43	0/3639	0.63	0/4893
1	O	0.45	0/3639	0.64	0/4893
1	P	0.44	0/3639	0.64	0/4893
1	Q	0.44	0/3639	0.63	0/4893
1	R	0.44	0/3639	0.63	0/4893
1	S	0.44	0/3639	0.63	0/4893
1	T	0.44	0/3639	0.63	0/4893
1	U	0.44	0/3639	0.64	0/4893
1	V	0.44	0/3639	0.64	0/4893
1	W	0.43	0/3639	0.64	0/4893
1	X	0.45	0/3639	0.64	0/4893
All	All	0.44	0/87336	0.63	0/117432

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	9	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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	3581	0	3567	469	0
1	B	3581	0	3567	454	0
1	C	3581	0	3567	501	0
1	D	3581	0	3567	477	1
1	E	3581	0	3567	480	1
1	F	3581	0	3567	481	0
1	G	3581	0	3567	464	0
1	H	3581	0	3567	467	0
1	I	3581	0	3567	497	0
1	J	3581	0	3567	482	0
1	K	3581	0	3567	496	1
1	L	3581	0	3567	482	0
1	M	3581	0	3567	491	0
1	N	3581	0	3567	504	0
1	O	3581	0	3567	503	0
1	P	3581	0	3567	473	0
1	Q	3581	0	3567	476	0
1	R	3581	0	3567	497	0
1	S	3581	0	3567	490	0
1	T	3581	0	3567	499	0
1	U	3581	0	3567	468	0
1	V	3581	0	3567	483	0
1	W	3581	0	3567	482	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	3581	0	3567	440	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	X	2	0	0	0	0
3	A	206	0	0	50	0
3	B	187	0	0	41	0
3	C	239	0	0	87	0
3	D	238	0	0	67	0
3	E	210	0	0	72	0
3	F	219	0	0	74	0
3	G	231	0	0	65	0
3	H	215	0	0	63	0
3	I	233	0	0	80	0
3	J	237	0	0	77	0
3	K	219	0	0	69	0
3	L	222	0	0	60	0
3	M	227	0	0	64	0
3	N	246	0	0	88	0
3	O	205	0	0	68	0
3	P	208	0	0	53	0
3	Q	211	0	0	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	200	0	0	63	0
3	S	205	0	0	71	0
3	T	226	0	0	77	0
3	U	214	0	0	68	0
3	V	225	0	0	65	0
3	W	217	0	0	73	0
3	X	193	0	0	42	0
All	All	91225	0	85608	10349	2

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 60.

The worst 5 of 10349 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:M:317:ILE:HD13	3:M:6168:HOH:O	1.38	1.20
1:T:87:MET:HB2	3:T:6087:HOH:O	1.52	1.08
1:F:54:LYS:HA	3:F:6039:HOH:O	1.52	1.07
1:R:235:ASP:HA	1:S:393:ARG:HH12	1.19	1.07
1:S:179:VAL:HG12	1:V:137:LYS:HG3	1.33	1.06

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LYS:NZ	1:W:284:LYS:NZ[1_654]	2.11	0.09
1:E:400:SER:OG	1:K:325:ASP:OD1[1_665]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	452/461 (98%)	316 (70%)	103 (23%)	33 (7%)	1	9
1	B	452/461 (98%)	314 (70%)	106 (24%)	32 (7%)	1	10
1	C	452/461 (98%)	315 (70%)	102 (23%)	35 (8%)	1	8
1	D	452/461 (98%)	312 (69%)	105 (23%)	35 (8%)	1	8
1	E	452/461 (98%)	312 (69%)	105 (23%)	35 (8%)	1	8
1	F	452/461 (98%)	317 (70%)	102 (23%)	33 (7%)	1	9
1	G	452/461 (98%)	319 (71%)	100 (22%)	33 (7%)	1	9
1	H	452/461 (98%)	316 (70%)	101 (22%)	35 (8%)	1	8
1	I	452/461 (98%)	315 (70%)	103 (23%)	34 (8%)	1	9
1	J	452/461 (98%)	316 (70%)	101 (22%)	35 (8%)	1	8
1	K	452/461 (98%)	316 (70%)	101 (22%)	35 (8%)	1	8
1	L	452/461 (98%)	314 (70%)	102 (23%)	36 (8%)	1	7
1	M	452/461 (98%)	314 (70%)	103 (23%)	35 (8%)	1	8
1	N	452/461 (98%)	315 (70%)	102 (23%)	35 (8%)	1	8
1	O	452/461 (98%)	316 (70%)	102 (23%)	34 (8%)	1	9
1	P	452/461 (98%)	314 (70%)	103 (23%)	35 (8%)	1	8
1	Q	452/461 (98%)	316 (70%)	102 (23%)	34 (8%)	1	9
1	R	452/461 (98%)	317 (70%)	101 (22%)	34 (8%)	1	9
1	S	452/461 (98%)	319 (71%)	100 (22%)	33 (7%)	1	9
1	T	452/461 (98%)	317 (70%)	100 (22%)	35 (8%)	1	8
1	U	452/461 (98%)	313 (69%)	105 (23%)	34 (8%)	1	9
1	V	452/461 (98%)	315 (70%)	102 (23%)	35 (8%)	1	8
1	W	452/461 (98%)	316 (70%)	103 (23%)	33 (7%)	1	9
1	X	452/461 (98%)	316 (70%)	102 (23%)	34 (8%)	1	9
All	All	10848/11064 (98%)	7570 (70%)	2456 (23%)	822 (8%)	1	9

5 of 822 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	TYR
1	A	43	GLU
1	A	60	ILE
1	A	136	LYS
1	A	141	VAL

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	387/390 (99%)	347 (90%)	40 (10%)	9	36
1	B	387/390 (99%)	350 (90%)	37 (10%)	10	39
1	C	387/390 (99%)	351 (91%)	36 (9%)	11	41
1	D	387/390 (99%)	348 (90%)	39 (10%)	9	36
1	E	387/390 (99%)	347 (90%)	40 (10%)	9	36
1	F	387/390 (99%)	352 (91%)	35 (9%)	12	43
1	G	387/390 (99%)	350 (90%)	37 (10%)	10	39
1	H	387/390 (99%)	349 (90%)	38 (10%)	10	38
1	I	387/390 (99%)	349 (90%)	38 (10%)	10	38
1	J	387/390 (99%)	351 (91%)	36 (9%)	11	41
1	K	387/390 (99%)	348 (90%)	39 (10%)	9	36
1	L	387/390 (99%)	348 (90%)	39 (10%)	9	36
1	M	387/390 (99%)	348 (90%)	39 (10%)	9	36
1	N	387/390 (99%)	351 (91%)	36 (9%)	11	41
1	O	387/390 (99%)	348 (90%)	39 (10%)	9	36
1	P	387/390 (99%)	348 (90%)	39 (10%)	9	36
1	Q	387/390 (99%)	350 (90%)	37 (10%)	10	39
1	R	387/390 (99%)	351 (91%)	36 (9%)	11	41
1	S	387/390 (99%)	347 (90%)	40 (10%)	9	36
1	T	387/390 (99%)	351 (91%)	36 (9%)	11	41
1	U	387/390 (99%)	351 (91%)	36 (9%)	11	41
1	V	387/390 (99%)	350 (90%)	37 (10%)	10	39
1	W	387/390 (99%)	352 (91%)	35 (9%)	12	43
1	X	387/390 (99%)	349 (90%)	38 (10%)	10	38
All	All	9288/9360 (99%)	8386 (90%)	902 (10%)	10	39

5 of 902 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	297	VAL
1	N	124	LEU
1	W	43	GLU
1	L	42	ARG
1	M	32	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 225 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	465	ASN
1	N	413	GLN
1	W	220	ASN
1	L	116	ASN
1	M	264	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	455/461 (98%)	-0.49	3 (0%) 89 83	4, 27, 72, 106	0
1	B	455/461 (98%)	-0.45	1 (0%) 95 94	3, 27, 73, 106	0
1	C	455/461 (98%)	-0.44	2 (0%) 93 90	3, 27, 73, 105	0
1	D	455/461 (98%)	-0.46	1 (0%) 95 94	4, 26, 72, 107	0
1	E	455/461 (98%)	-0.42	4 (0%) 85 78	3, 26, 72, 104	0
1	F	455/461 (98%)	-0.43	2 (0%) 93 90	4, 27, 72, 105	0
1	G	455/461 (98%)	-0.45	2 (0%) 93 90	3, 26, 73, 105	0
1	H	455/461 (98%)	-0.43	5 (1%) 82 72	3, 26, 72, 106	0
1	I	455/461 (98%)	-0.46	5 (1%) 82 72	3, 27, 72, 108	0
1	J	455/461 (98%)	-0.46	2 (0%) 93 90	3, 26, 72, 103	0
1	K	455/461 (98%)	-0.43	3 (0%) 89 83	3, 26, 72, 105	0
1	L	455/461 (98%)	-0.46	3 (0%) 89 83	4, 26, 72, 101	0
1	M	455/461 (98%)	-0.44	4 (0%) 85 78	4, 26, 74, 106	0
1	N	455/461 (98%)	-0.44	5 (1%) 82 72	4, 27, 74, 106	0
1	O	455/461 (98%)	-0.43	0 100 100	4, 27, 73, 103	0
1	P	455/461 (98%)	-0.48	2 (0%) 93 90	3, 27, 74, 103	0
1	Q	455/461 (98%)	-0.42	1 (0%) 95 94	2, 27, 72, 104	0
1	R	455/461 (98%)	-0.44	4 (0%) 85 78	4, 27, 73, 107	0
1	S	455/461 (98%)	-0.45	5 (1%) 82 72	3, 27, 73, 102	0
1	T	455/461 (98%)	-0.45	4 (0%) 85 78	2, 27, 73, 104	0
1	U	455/461 (98%)	-0.45	2 (0%) 93 90	4, 26, 73, 102	0
1	V	455/461 (98%)	-0.43	2 (0%) 93 90	2, 26, 72, 104	0
1	W	455/461 (98%)	-0.45	3 (0%) 89 83	4, 26, 73, 104	0
1	X	455/461 (98%)	-0.45	3 (0%) 89 83	5, 26, 72, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	10920/11064 (98%)	-0.45	68 (0%) 90 84	2, 27, 73, 108	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	208	LEU	4.3
1	C	326	GLU	4.2
1	K	69	THR	4.1
1	E	18	ASP	4.1
1	I	68	GLU	3.7

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MN	S	6037	1/1	0.95	0.18	1.13	26,26,26,26	0
2	MN	R	6035	1/1	0.90	0.15	1.08	35,35,35,35	0
2	MN	F	6011	1/1	0.94	0.14	-0.10	21,21,21,21	0
2	MN	B	6003	1/1	0.97	0.16	-0.12	31,31,31,31	0
2	MN	E	6009	1/1	0.94	0.13	-0.17	35,35,35,35	0
2	MN	K	6021	1/1	0.98	0.12	-0.75	20,20,20,20	0
2	MN	P	6031	1/1	0.97	0.12	-0.77	33,33,33,33	0
2	MN	Q	6034	1/1	0.99	0.12	-0.87	38,38,38,38	0
2	MN	G	6013	1/1	0.97	0.11	-0.91	40,40,40,40	0
2	MN	O	6030	1/1	0.92	0.12	-1.05	28,28,28,28	0
2	MN	N	6028	1/1	0.99	0.10	-1.25	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	S	6038	1/1	0.97	0.10	-1.33	0,0,0,0	0
2	MN	C	6005	1/1	0.95	0.10	-1.39	44,44,44,44	0
2	MN	M	6025	1/1	0.97	0.11	-1.43	29,29,29,29	0
2	MN	X	6048	1/1	0.99	0.08	-1.51	0,0,0,0	0
2	MN	W	6045	1/1	0.83	0.12	-1.52	31,31,31,31	0
2	MN	E	6010	1/1	0.98	0.10	-1.53	12,12,12,12	0
2	MN	X	6047	1/1	0.98	0.08	-1.56	30,30,30,30	0
2	MN	N	6027	1/1	0.95	0.08	-1.68	39,39,39,39	0
2	MN	D	6008	1/1	0.96	0.09	-1.69	16,16,16,16	0
2	MN	G	6014	1/1	0.99	0.07	-1.70	5,5,5,5	0
2	MN	L	6023	1/1	0.94	0.10	-1.71	25,25,25,25	0
2	MN	T	6039	1/1	0.98	0.06	-1.74	21,21,21,21	0
2	MN	P	6032	1/1	0.96	0.09	-1.77	22,22,22,22	0
2	MN	L	6024	1/1	0.98	0.10	-1.80	34,34,34,34	0
2	MN	J	6020	1/1	0.98	0.11	-1.85	8,8,8,8	0
2	MN	J	6019	1/1	0.99	0.11	-1.87	14,14,14,14	0
2	MN	Q	6033	1/1	0.96	0.09	-1.91	25,25,25,25	0
2	MN	R	6036	1/1	0.98	0.09	-1.95	2,2,2,2	0
2	MN	H	6016	1/1	0.98	0.09	-2.00	4,4,4,4	0
2	MN	B	6004	1/1	0.99	0.08	-2.03	7,7,7,7	0
2	MN	T	6040	1/1	0.96	0.09	-2.07	8,8,8,8	0
2	MN	C	6006	1/1	0.99	0.07	-2.13	6,6,6,6	0
2	MN	A	6002	1/1	0.98	0.04	-2.14	1,1,1,1	0
2	MN	V	6043	1/1	0.97	0.07	-2.27	11,11,11,11	0
2	MN	H	6015	1/1	0.97	0.10	-2.28	16,16,16,16	0
2	MN	I	6018	1/1	0.98	0.07	-2.33	15,15,15,15	0
2	MN	F	6012	1/1	0.98	0.08	-2.34	1,1,1,1	0
2	MN	U	6042	1/1	0.99	0.08	-2.34	9,9,9,9	0
2	MN	A	6001	1/1	0.92	0.08	-2.43	31,31,31,31	0
2	MN	U	6041	1/1	0.95	0.09	-2.58	29,29,29,29	0
2	MN	D	6007	1/1	0.98	0.06	-2.76	0,0,0,0	0
2	MN	W	6046	1/1	0.99	0.07	-2.77	0,0,0,0	0
2	MN	O	6029	1/1	0.99	0.05	-3.05	14,14,14,14	0
2	MN	V	6044	1/1	0.99	0.03	-3.14	0,0,0,0	0
2	MN	M	6026	1/1	0.99	0.05	-3.16	15,15,15,15	0
2	MN	K	6022	1/1	0.97	0.07	-3.60	16,16,16,16	0
2	MN	I	6017	1/1	0.97	0.05	-3.82	43,43,43,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.