



wwPDB NMR Structure Validation Summary Report ⓘ

Nov 20, 2022 – 11:37 am GMT

PDB ID : 6R8N
EMDB ID : EMD-4179
BMRB ID : 27211
Title : STRUCTURE DETERMINATION OF THE TETRAHEDRAL AMINOPEPTIDASE TET2 FROM P. HORIKOSHII BY USE OF COMBINED SOLID-STATE NMR, SOLUTION-STATE NMR AND EM DATA 4.1 Å, FOLLOWED BY REAL_SPACE_REFINEMENT AT 4.1 Å
Authors : Colletier, J.-P.; Gauto, D.; Estrozi, L.; Favier, A.; Effantin, G.; Schoehn, G.; Boisbouvier, J.; Schanda, P.
Deposited on : 2019-04-02

This is a wwPDB NMR Structure Validation Summary 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/NMRValidationReportHelp>

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 : **NOT EXECUTED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

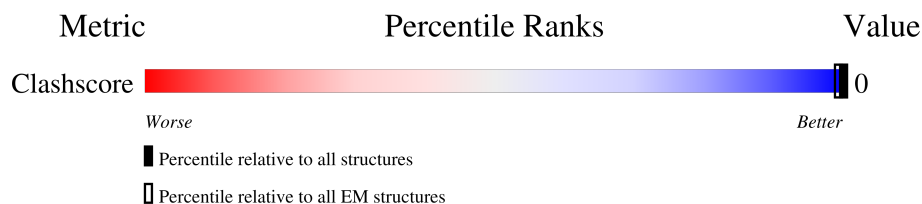
The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY, SOLUTION NMR

The reported resolution of this entry is 4.10 Å.

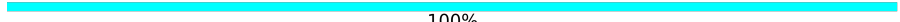

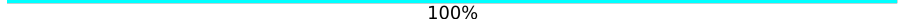
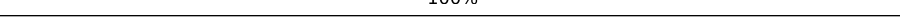

The overall completeness of chemical shifts assignment is 3%.

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.



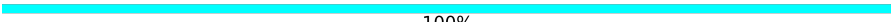
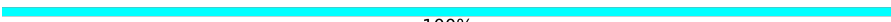
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	4297

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

Mol	Chain	Length	Quality of chain
1	A	353	 100%
1	B	353	 100%
1	C	353	 100%
1	D	353	 100%
1	E	353	 100%
1	F	353	 100%
1	G	353	 100%
1	H	353	 100%
1	I	353	 100%
1	J	353	 100%

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Mol	Chain	Length	Quality of chain
1	K	353	 100%
1	L	353	 100%

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 66528 atoms, of which 33516 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 Tetrahedral aminopeptidase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	B	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	C	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	D	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	E	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	F	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	G	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	H	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	I	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	J	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	K	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		
1	L	353	Total	C	H	N	O	S	0	
			5542	1759	2793	469	512	9		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Zn	
			2	2	
2	B	2	Total	Zn	
			2	2	
2	C	2	Total	Zn	
			2	2	

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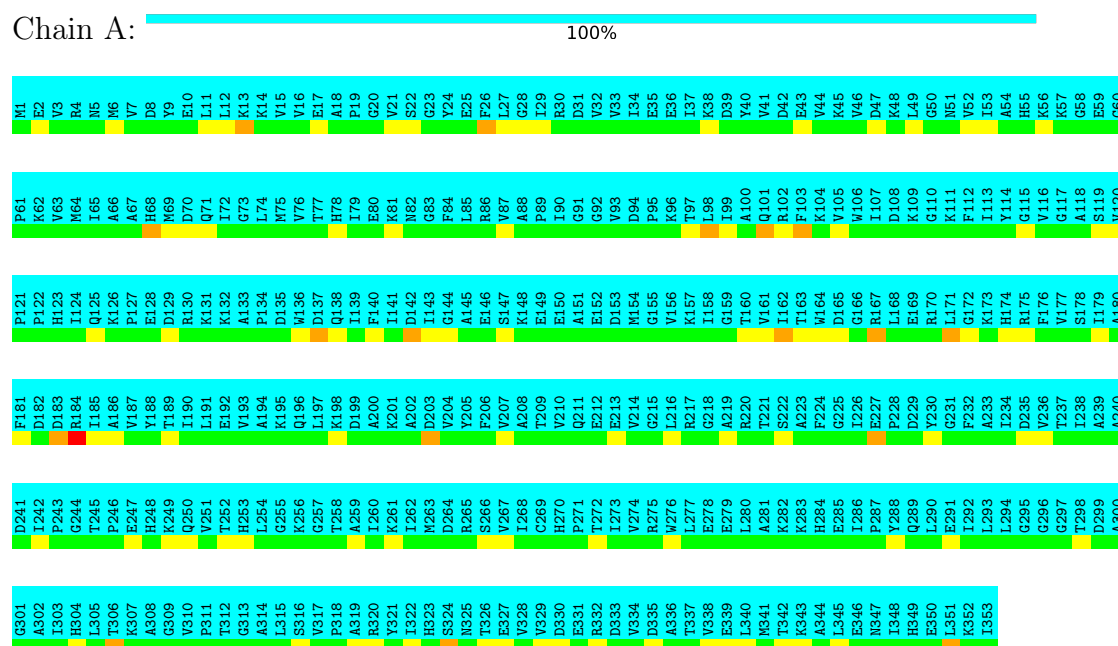
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Mol	Chain	Residues	Atoms		AltConf
2	D	2	Total 2	Zn 2	
2	E	2	Total 2	Zn 2	
2	F	2	Total 2	Zn 2	
2	G	2	Total 2	Zn 2	
2	H	2	Total 2	Zn 2	
2	I	2	Total 2	Zn 2	
2	J	2	Total 2	Zn 2	
2	K	2	Total 2	Zn 2	
2	L	2	Total 2	Zn 2	

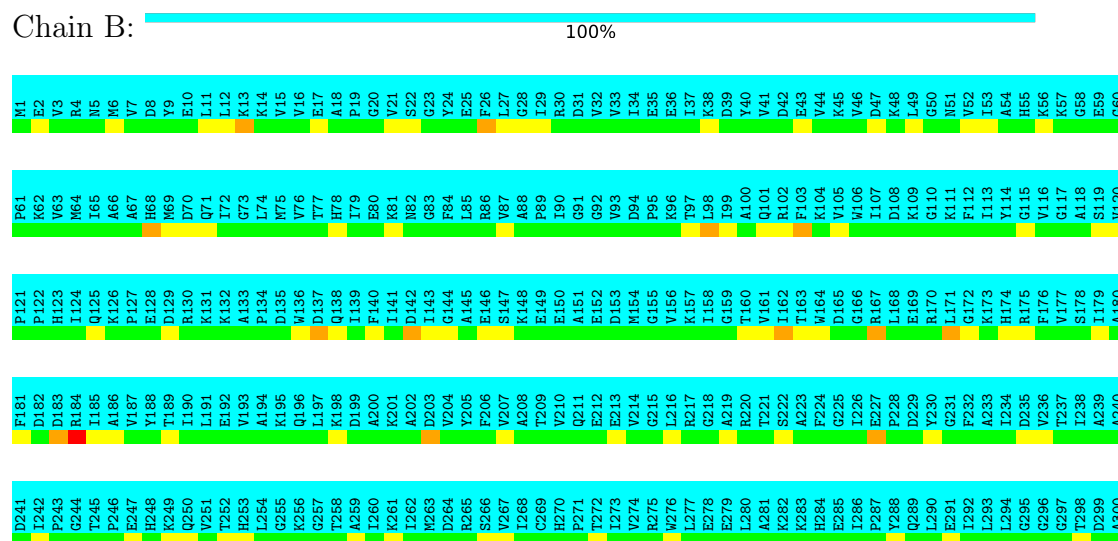
4 Residue-property plots

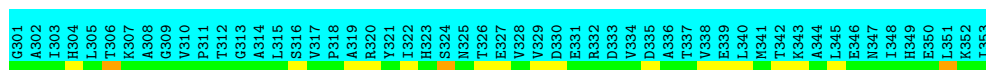
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Tetrahedral aminopeptidase



• Molecule 1: Tetrahedral aminopeptidase

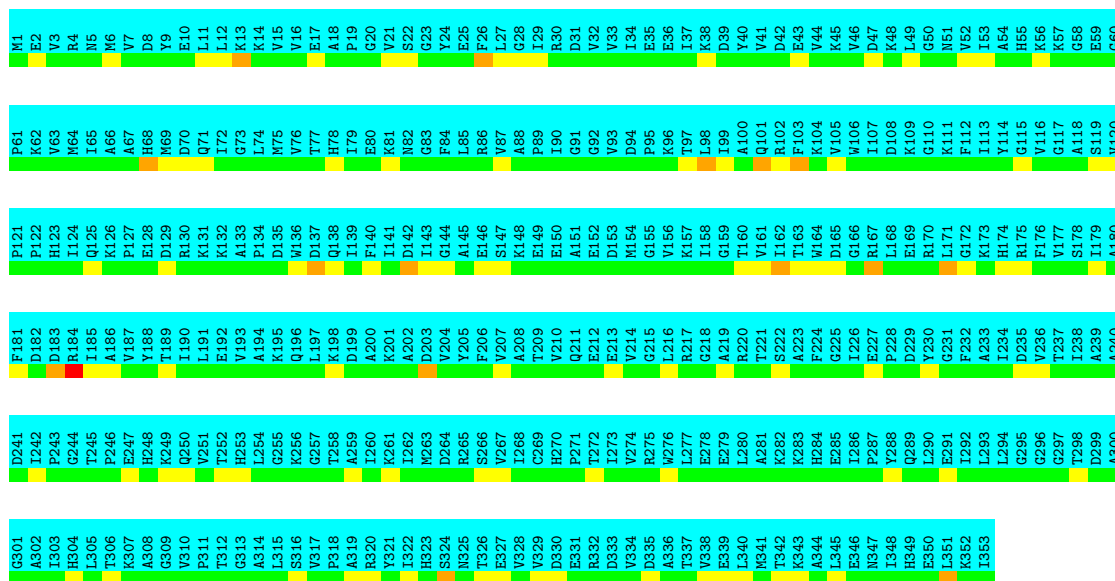




• Molecule 1: Tetrahedral aminopeptidase

Chain C:

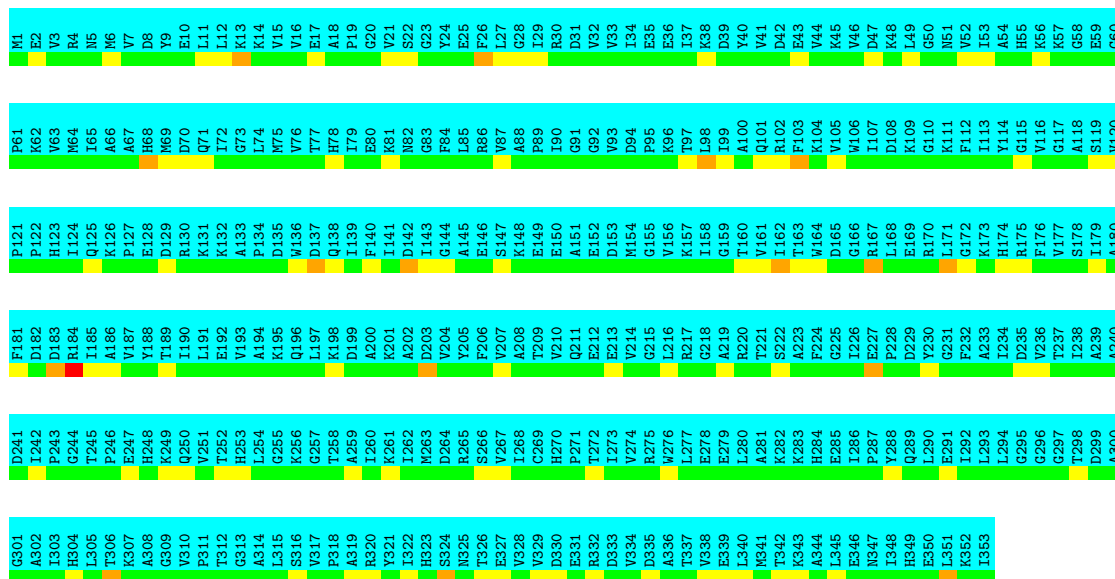
100%



• Molecule 1: Tetrahedral aminopeptidase

Chain D:

100%

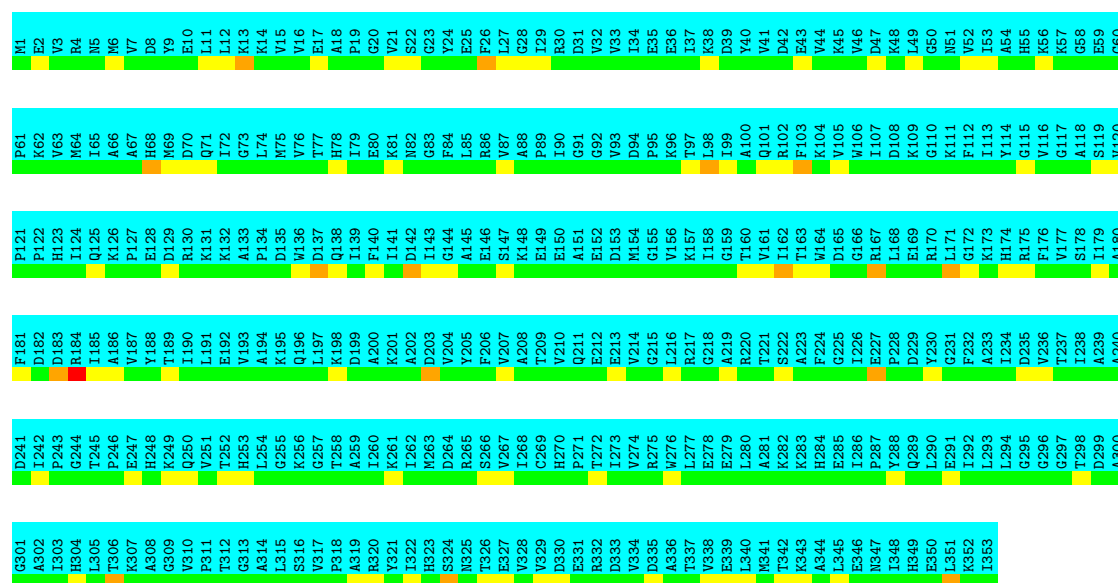


• Molecule 1: Tetrahedral aminopeptidase

Chain E:

100%

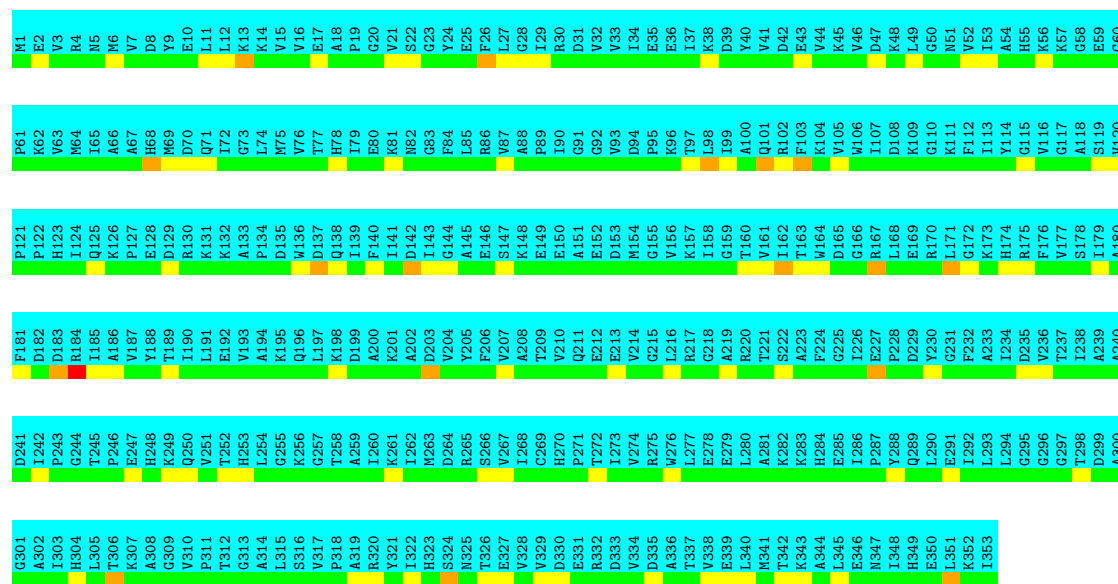




• Molecule 1: Tetrahedral aminopeptidase

Chain F:

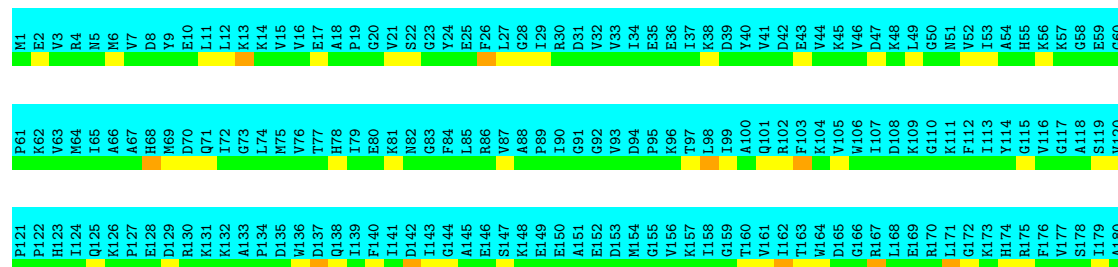
100%

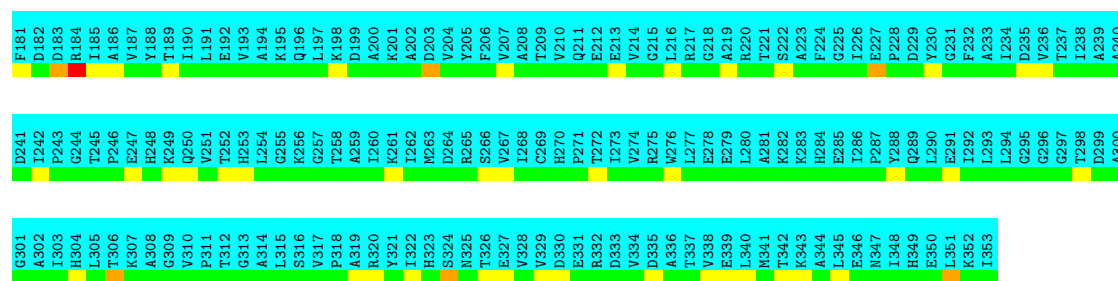


• Molecule 1: Tetrahedral aminopeptidase

Chain G:

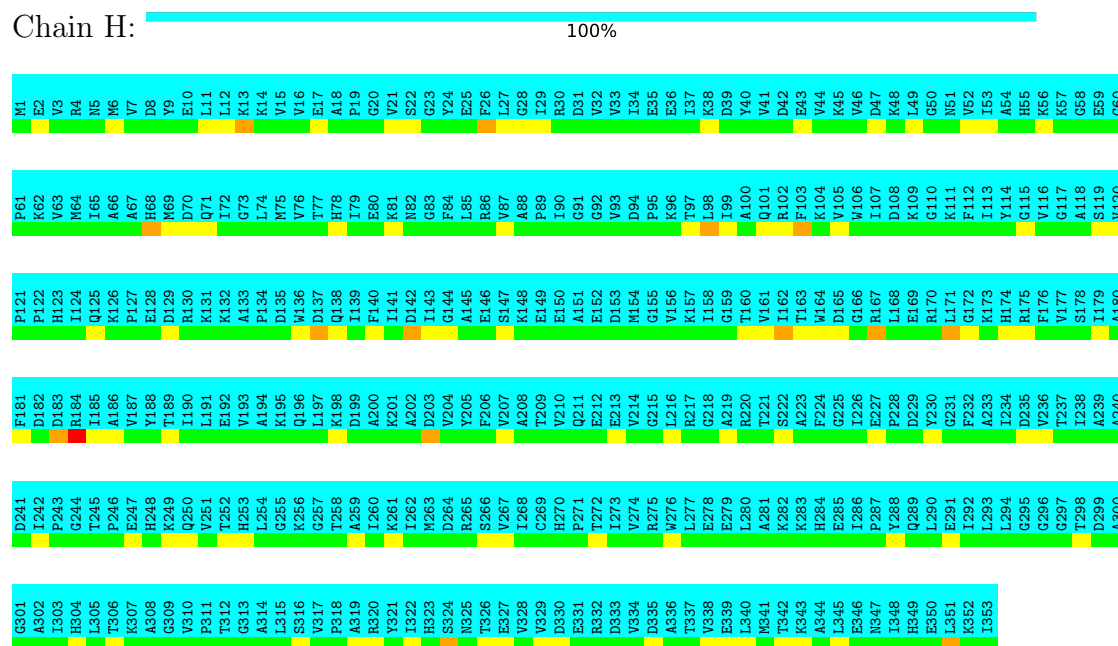
100%





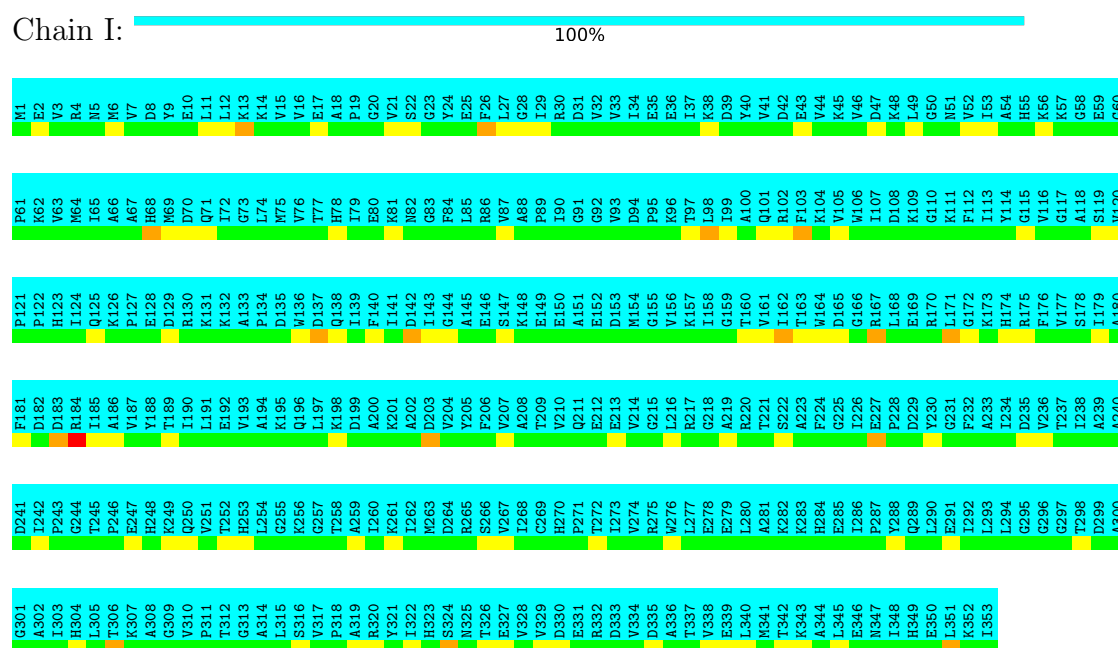
• Molecule 1: Tetrahedral aminopeptidase

Chain H:



• Molecule 1: Tetrahedral aminopeptidase

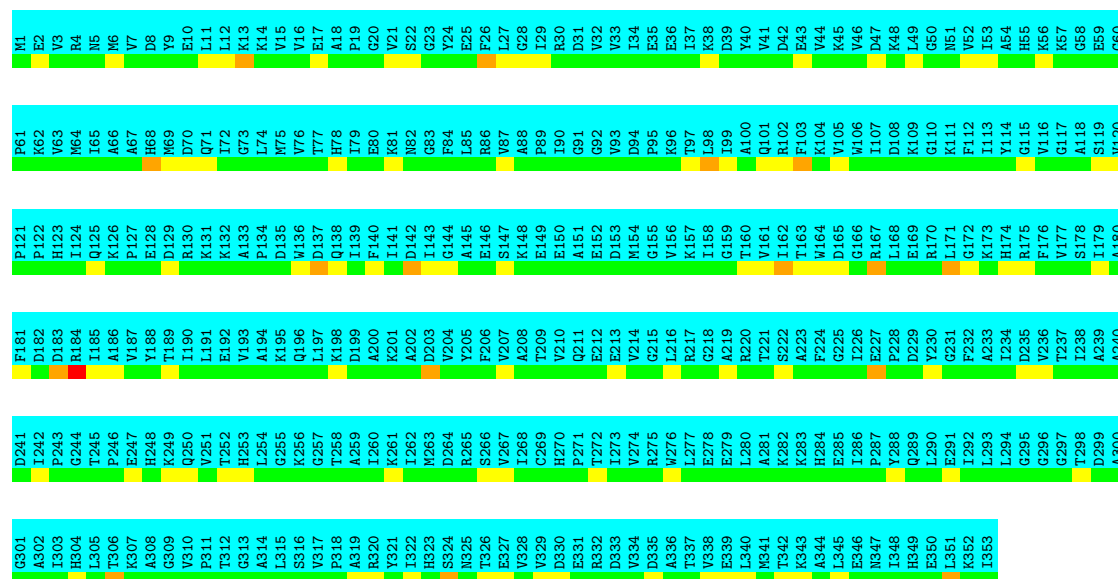
Chain I:



- Molecule 1: Tetrahedral aminopeptidase

Chain J:

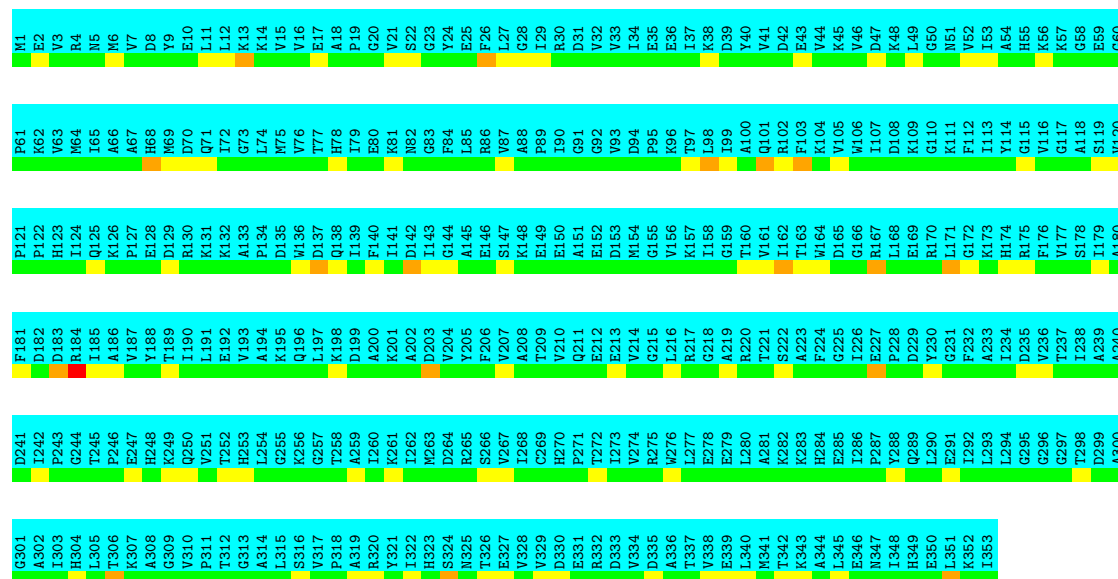
100%



- Molecule 1: Tetrahedral aminopeptidase

Chain K:

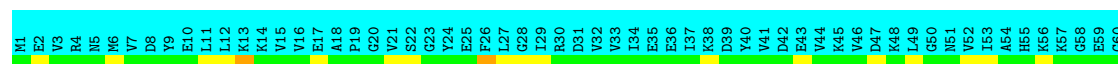
100%

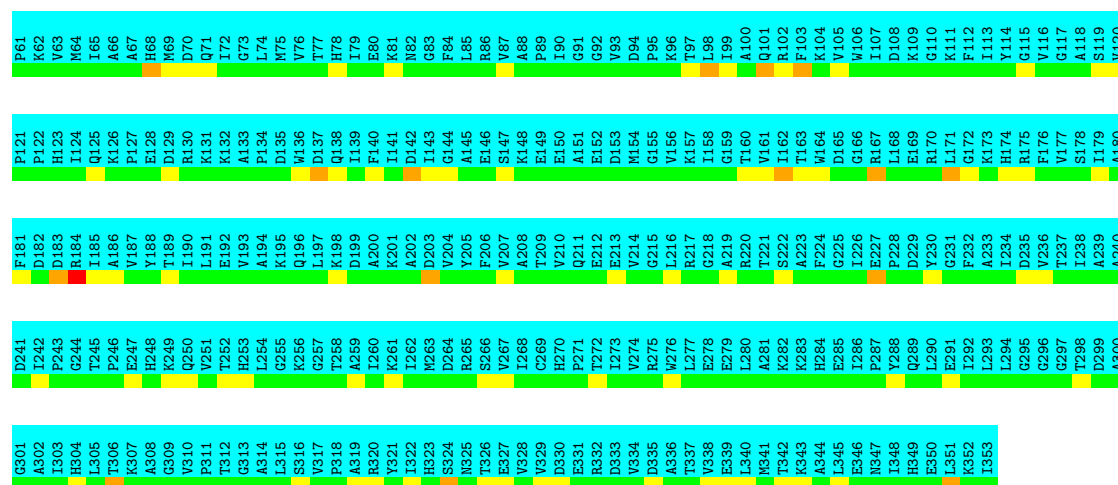


- Molecule 1: Tetrahedral aminopeptidase

Chain L:

100%





5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 1 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	3.97
Xplor-NIH	structure calculation	2.44.8

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	3036
Number of shifts mapped to atoms	3036
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	0	0	0	0
1	B	0	0	0	0
1	C	0	0	0	0
1	D	0	0	0	0
1	E	0	0	0	0
1	F	0	0	0	0
1	G	0	0	0	0
1	H	0	0	0	0
1	I	0	0	0	0
1	J	0	0	0	0
1	K	0	0	0	0
1	L	0	0	0	0
All	All	24	0	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 -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR 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	0	-	-	-	-
1	B	0	-	-	-	-
1	C	0	-	-	-	-
1	D	0	-	-	-	-
1	E	0	-	-	-	-
1	F	0	-	-	-	-
1	G	0	-	-	-	-
1	H	0	-	-	-	-
1	I	0	-	-	-	-
1	J	0	-	-	-	-
1	K	0	-	-	-	-
1	L	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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 NMR 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	0	-	-	-
1	B	0	-	-	-
1	C	0	-	-	-
1	D	0	-	-	-
1	E	0	-	-	-
1	F	0	-	-	-
1	G	0	-	-	-
1	H	0	-	-	-
1	I	0	-	-	-
1	J	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	0	-	-	-
1	L	0	-	-	-
All	All	0	-	-	-

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

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *27211.txt_assigned_chem_shift_list*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1518
Number of shifts mapped to atoms	1518
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	283	0.12 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	241	0.06 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	282	0.16 ± 0.11	None needed (< 0.5 ppm)
^{15}N	289	1.25 ± 0.16	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 1483 atoms were assigned a chemical shift out of a possible 51564. 6 out of 720 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	982/20820 (5%)	140/8292 (2%)	565/8472 (7%)	277/4056 (7%)
Sidechain	501/27360 (2%)	3/15852 (0%)	498/10452 (5%)	0/1056 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/3384 (0%)	0/1896 (0%)	0/1440 (0%)	0/48 (0%)
Overall	1483/51564 (3%)	143/26040 (1%)	1063/20364 (5%)	277/5160 (5%)

7.1.4 Statistically unusual chemical shifts [i](#)

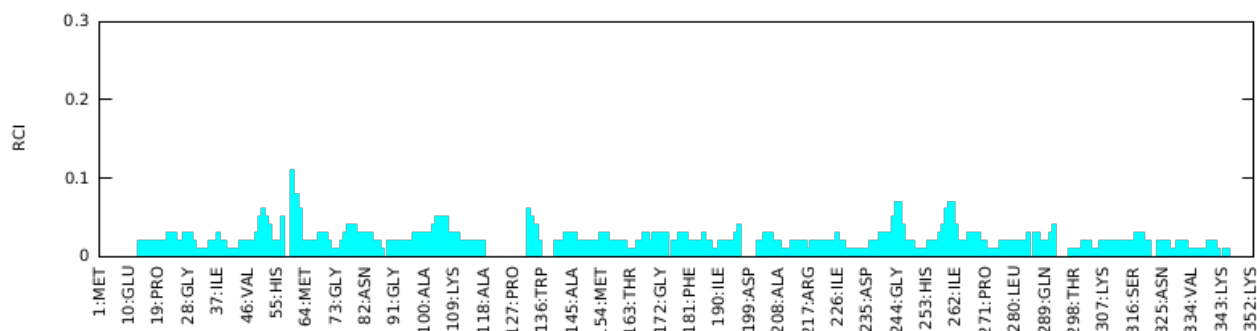
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	255	GLY	H	12.12	11.63 – 5.03	5.7

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.2.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1518
Number of shifts mapped to atoms	1518
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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^{15}N	289	1.24 ± 0.40	Should be applied

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 1483 atoms were assigned a chemical shift out of a possible 51564. 6 out of 720 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	982/20820 (5%)	140/8292 (2%)	565/8472 (7%)	277/4056 (7%)
Sidechain	501/27360 (2%)	3/15852 (0%)	498/10452 (5%)	0/1056 (0%)
Aromatic	0/3384 (0%)	0/1896 (0%)	0/1440 (0%)	0/48 (0%)
Overall	1483/51564 (3%)	143/26040 (1%)	1063/20364 (5%)	277/5160 (5%)

7.2.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	255	GLY	H	12.12	11.63 – 5.03	5.7

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

