



Full wwPDB NMR Structure Validation 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 Full wwPDB NMR Structure 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/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

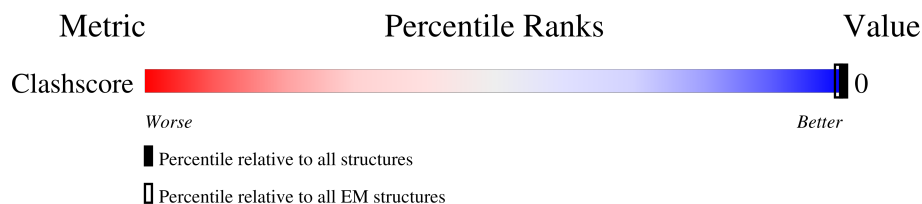
The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY, SOLUTION NMR

The reported resolution of this entry is 4.10 Å.

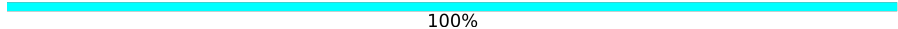
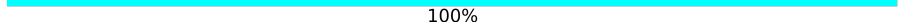
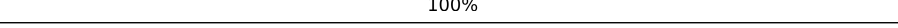
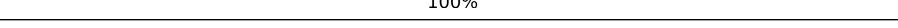
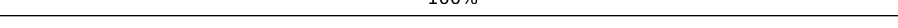
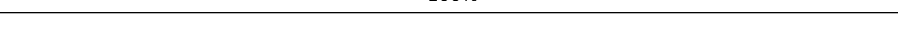
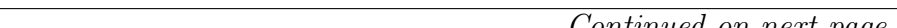
The overall completeness of chemical shifts assignment is 3%.

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.



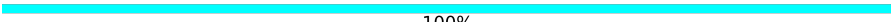
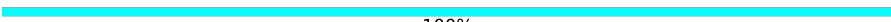
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	4297

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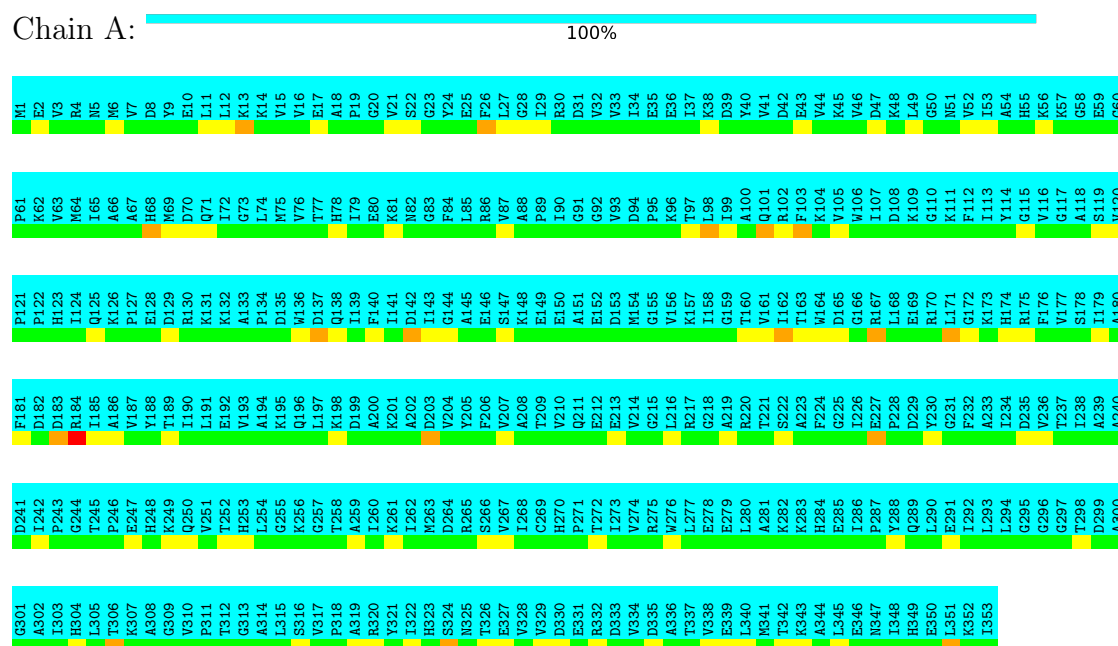
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Mol	Chain	Residues	Atoms		AltConf
2	D	2	Total 2	Zn 2	
2	E	2	Total 2	Zn 2	
2	F	2	Total 2	Zn 2	
2	G	2	Total 2	Zn 2	
2	H	2	Total 2	Zn 2	
2	I	2	Total 2	Zn 2	
2	J	2	Total 2	Zn 2	
2	K	2	Total 2	Zn 2	
2	L	2	Total 2	Zn 2	

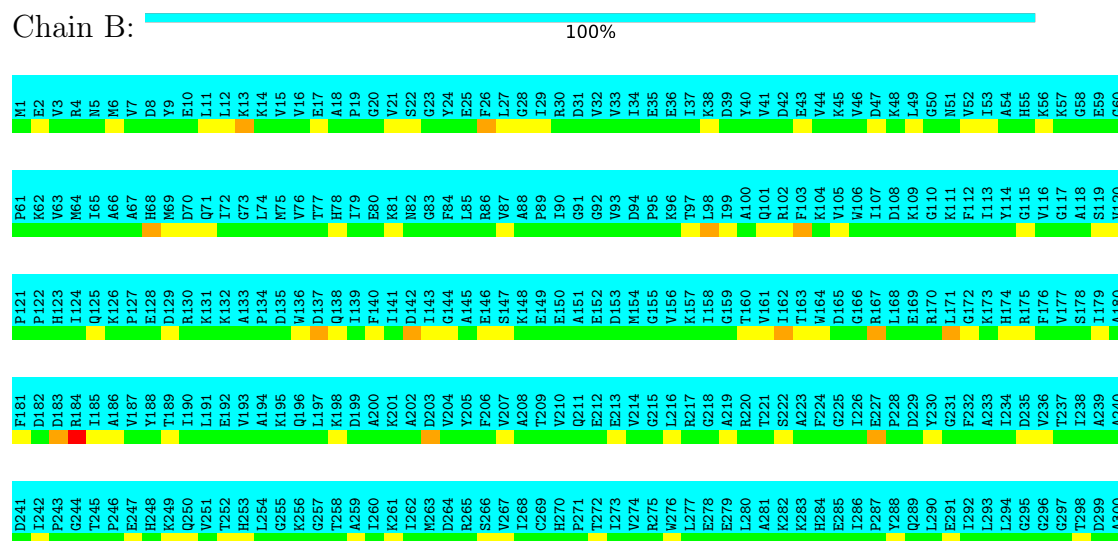
4 Residue-property plots

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.

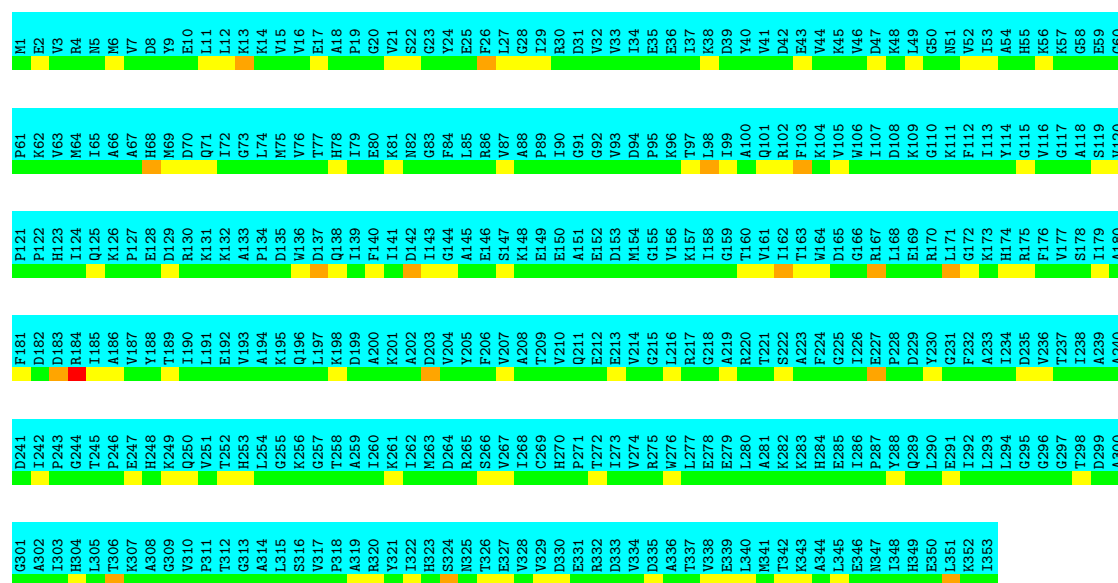
• Molecule 1: Tetrahedral aminopeptidase



• Molecule 1: Tetrahedral aminopeptidase



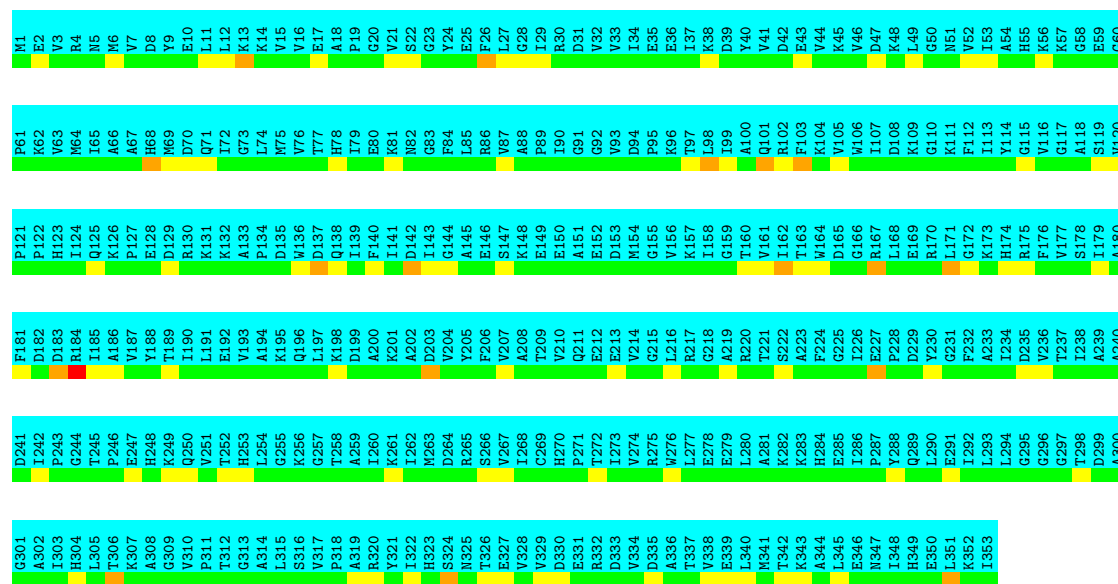




• Molecule 1: Tetrahedral aminopeptidase

Chain F:

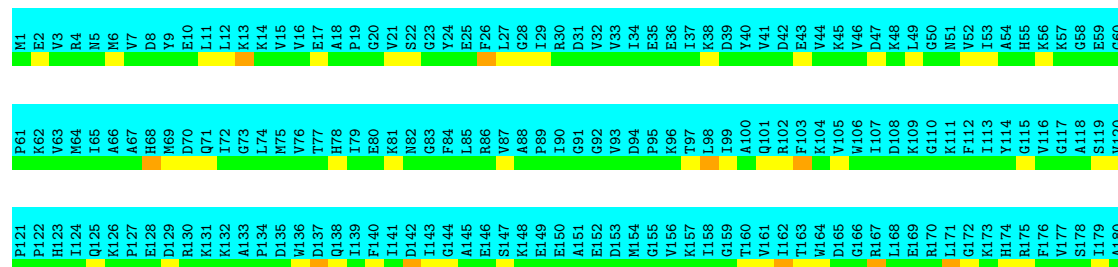
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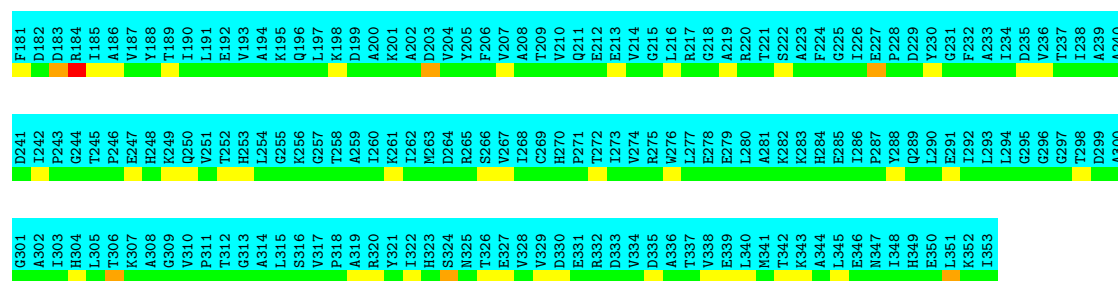


• Molecule 1: Tetrahedral aminopeptidase

Chain G:

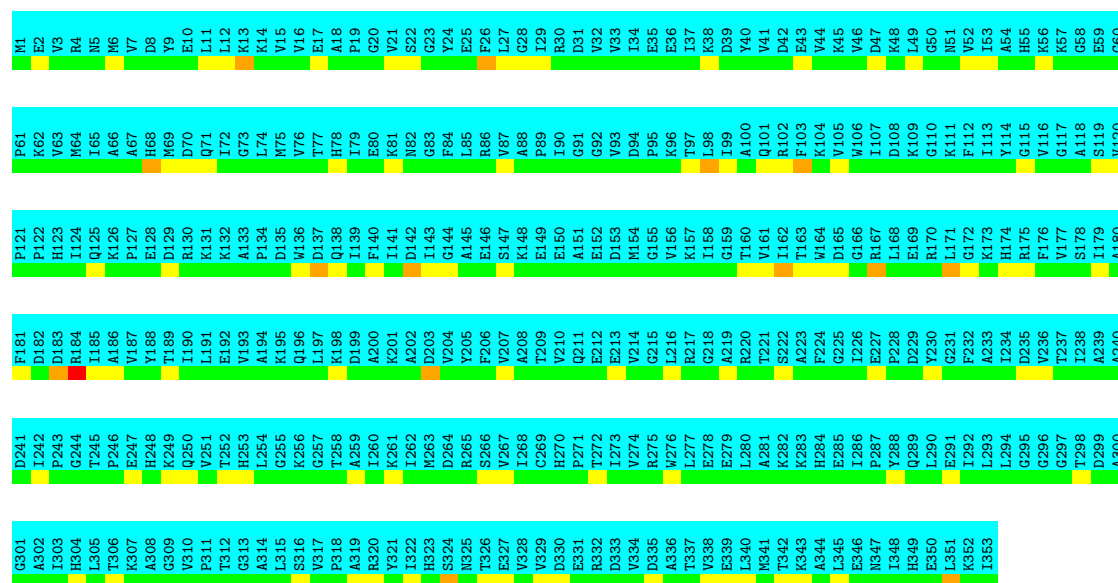
100%





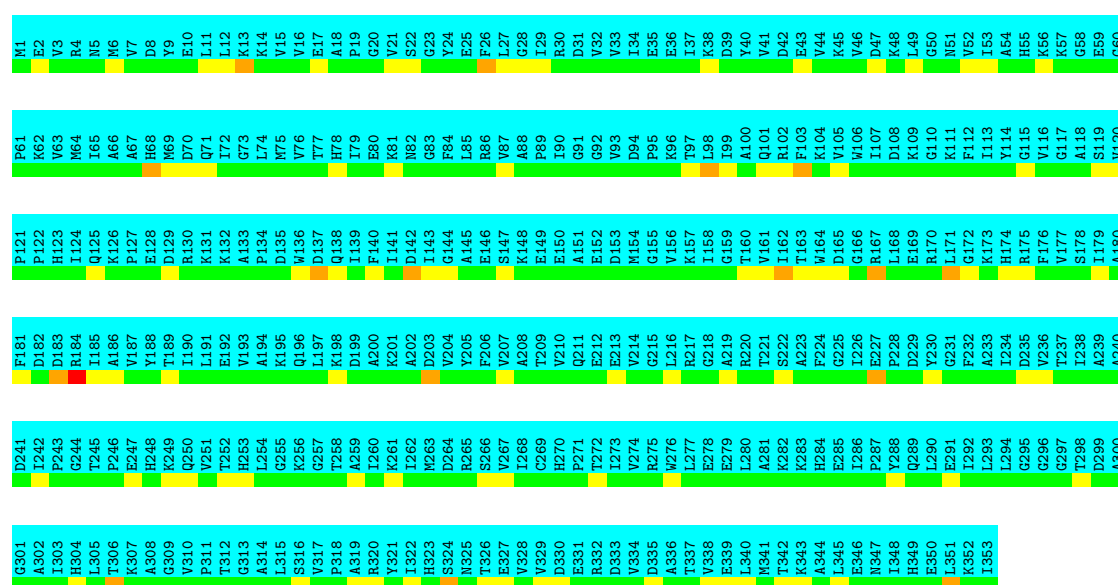
• Molecule 1: Tetrahedral aminopeptidase

Chain H:



• Molecule 1: Tetrahedral aminopeptidase

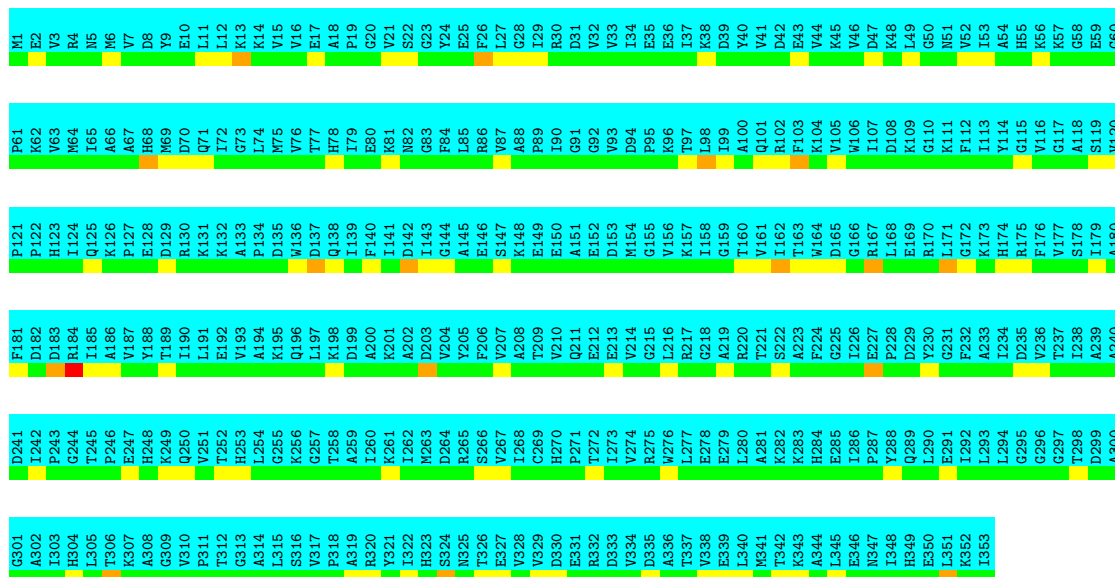
Chain I:



- Molecule 1: Tetrahedral aminopeptidase

Chain J:

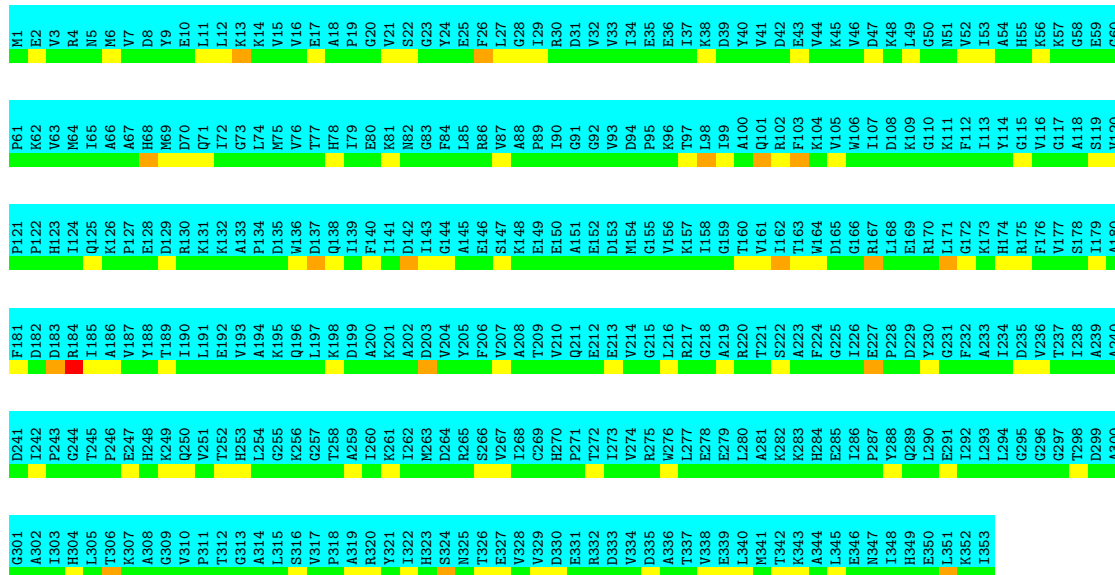
100%



- Molecule 1: Tetrahedral aminopeptidase

Chain K:

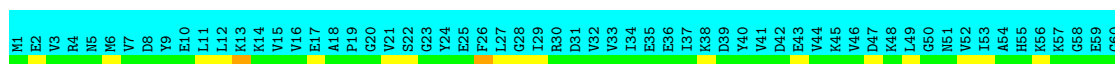
100%



- Molecule 1: Tetrahedral aminopeptidase

Chain L:

100%



P61	P121	F181	D241	G301
K62	P122	D182	I242	A302
M63	H123	D183	P243	I303
M64	I124	R184	G244	H304
I65	K125	I185	T245	L305
A66	K126	A186	P246	T306
A67	P127	V187	E247	K307
H68	E128	Y188	H248	A308
M69	D129	T189	K249	G309
D70	R130	I190	Q250	V310
Q71	K131	L191	V251	P311
I72	K132	E192	T252	T312
G73	A133	V193	H253	G313
L74	P134	A194	L254	A314
M75	D135	K195	G255	L315
W76	W136	Q196	K256	S316
T77	D137	L197	G257	V317
H78	Q138	K198	T258	P318
I79	I139	D199	A259	A319
F80	F140	A200	I260	R320
K81	I141	K201	K261	Y321
N82	D142	A202	I262	I322
G83	I143	D203	M263	H323
F84	G144	V204	D264	S324
L85	A145	V205	R265	N325
R86	E146	F206	S266	T326
H87	S147	V207	T267	E327
A88	K148	A208	I268	V328
P89	E149	T209	C269	V329
I90	E150	V210	H270	D330
G91	A151	Q211	P271	E331
E92	E152	E212	T272	R332
N93	D153	E213	I273	D333
D94	M154	V214	V274	V334
P95	G155	G215	R275	D335
K96	V156	L216	W276	A336
T97	K157	R217	L277	T337
L98	I158	G218	E278	V338
I99	G159	A219	E279	F339
A100	T160	R220	L280	L340
Q101	V161	T221	A281	K341
R102	I162	S222	K282	T342
F103	T163	A223	H283	K343
K104	W164	F224	H284	A344
V105	D165	G225	E285	L345
W106	G166	I226	I286	E346
I107	R167	E227	P287	N347
D108	L168	P228	Y288	I348
K109	E169	D229	Q289	H349
G110	R170	Y230	L290	E350
K111	L171	G231	E291	L351
F112	G172	F232	I292	K352
I113	K173	A233	L293	I353
Y114	H174	I234	L294	
G115	R175	D235	G295	
V116	F176	V236	G296	
G117	V177	T237	G297	
A118	S178	I238	T298	
S119	I179	A239	D299	
V120	A180	A240	A300	

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%)

The following table shows the completeness of the chemical shift assignments for the full 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	¹ H	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%)

7.1.4 Statistically unusual chemical shifts [i](#)

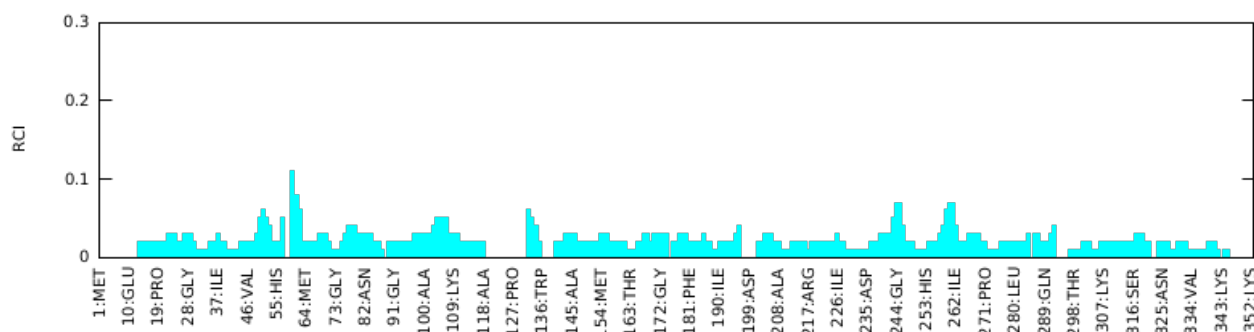
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

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

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

7.2.2 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 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	241	0.06 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	282	0.16 ± 0.17	None needed (< 0.5 ppm)
^{15}N	289	1.24 ± 0.40	Should be applied

7.2.3 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%)
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%)

The following table shows the completeness of the chemical shift assignments for the full 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	¹ H	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:

