



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:09 pm BST

PDB ID : 5NE8  
Title : Crystal structure of H307A mutant of *Thermotoga maritima* TmPEP1050 aminopeptidase  
Authors : Dutoit, R.  
Deposited on : 2017-03-10  
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

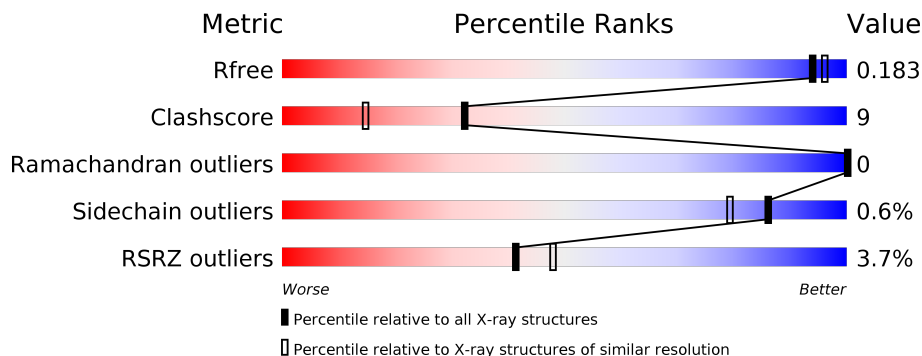
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	 3% 78% 15% • 7%
1	B	331	 4% 76% 16% • 7%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5085 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 AMINOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2381	1514	398	458	11	0	11	0
1	B	308	2369	1501	397	460	11	0	11	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	ALA	HIS	engineered mutation	UNP Q9X0E0
B	307	ALA	HIS	engineered mutation	UNP Q9X0E0

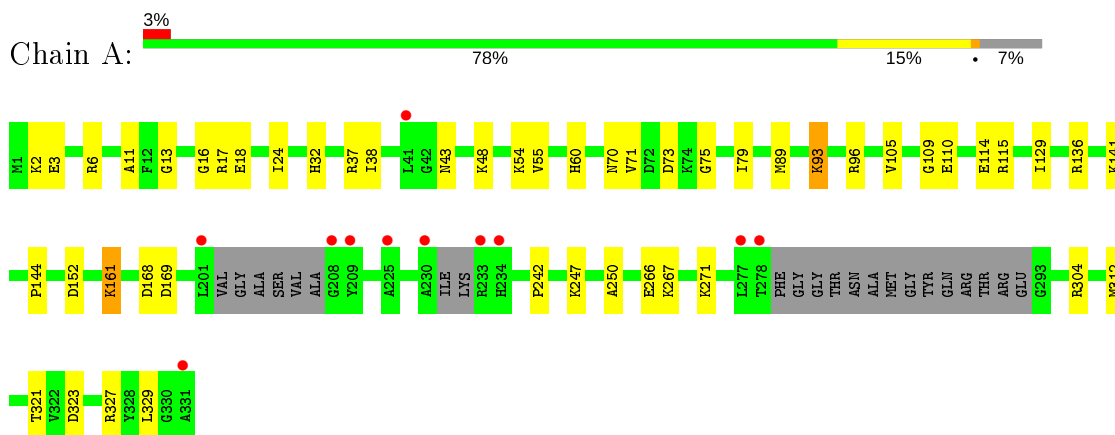
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	149	Total	O	0	0
			149	149		
2	B	186	Total	O	0	0
			186	186		

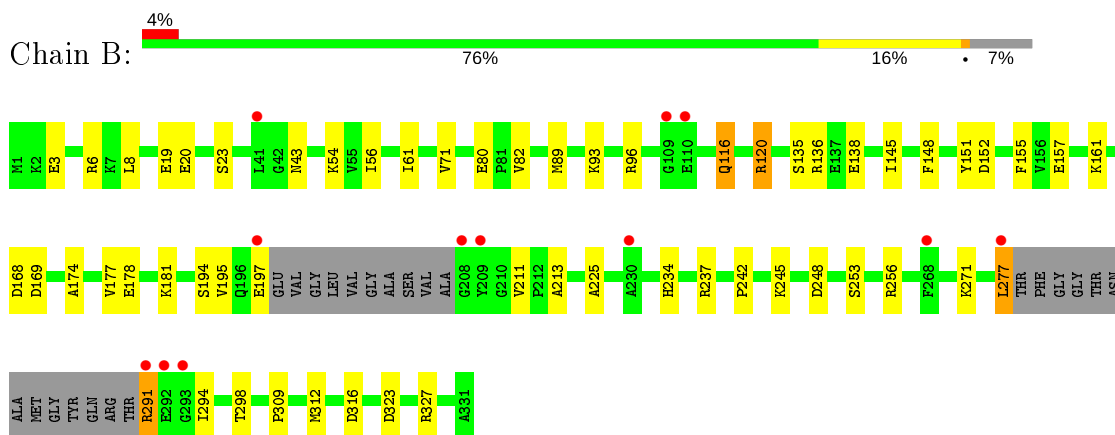
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 ( $RSRZ > 2$ ). 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: AMINOPEPTIDASE



- Molecule 1: AMINOPEPTIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.79Å 138.65Å 61.25Å 90.00° 110.51° 90.00°	Depositor
Resolution (Å)	40.11 – 1.75 40.11 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.11-1.75) 99.4 (40.11-1.75)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, $R_{free}$	0.165 , 0.185 0.169 , 0.183	Depositor DCC
$R_{free}$ test set	3355 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.367 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.400 for h,-k,-h-l	Depositor
Outliers	0 of 67094 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.54	0/2446	0.73	1/3298 (0.0%)
1	B	0.54	0/2435	0.75	2/3289 (0.1%)
All	All	0.54	0/4881	0.74	3/6587 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	B	291	ARG	CG-CD-NE	-5.48	100.30	111.80
1	A	93	LYS	CD-CE-NZ	-5.30	99.52	111.70

There are no chirality outliers.

There are no planarity outliers.

### 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	2381	0	2397	44	0
1	B	2369	0	2366	45	0
2	A	149	0	0	8	4
2	B	186	0	0	13	4
All	All	5085	0	4763	84	4

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 9.

All (84) 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:A:37[A]:ARG:NH1	2:A:401:HOH:O	2.02	0.92
1:A:96:ARG:NH1	1:A:152:ASP:OD1	2.14	0.81
1:B:197:GLU:OE1	1:B:197:GLU:N	2.15	0.79
1:B:54:LYS:NZ	2:B:407:HOH:O	2.20	0.75
1:A:115:ARG:NH1	2:A:404:HOH:O	2.17	0.74
1:B:43:ASN:OD1	1:B:195:VAL:HG22	1.87	0.74
1:B:71:VAL:O	1:B:136[A]:ARG:NH1	2.22	0.73
1:B:237:ARG:NH2	2:B:402:HOH:O	2.11	0.72
1:B:135:SER:OG	1:B:138:GLU:OE1	2.07	0.70
1:B:157:GLU:OE1	2:B:401:HOH:O	2.08	0.70
1:A:141:LYS:HA	1:B:291:ARG:NH2	2.07	0.69
1:A:96:ARG:NH2	2:A:410:HOH:O	2.29	0.66
1:B:253:SER:OG	1:B:256[B]:ARG:NH2	2.29	0.66
1:A:3[B]:GLU:OE2	1:A:6:ARG:NH1	2.29	0.65
1:B:148:PHE:O	2:B:403:HOH:O	2.14	0.64
1:A:3[B]:GLU:OE1	2:A:403:HOH:O	2.15	0.64
1:A:2:LYS:NZ	2:A:402:HOH:O	2.09	0.64
1:B:178:GLU:OE2	2:B:404:HOH:O	2.15	0.63
1:B:61:ILE:HG12	1:B:194:SER:O	1.98	0.63
1:B:20:GLU:OE2	2:B:405:HOH:O	2.17	0.58
1:B:225:ALA:HB2	1:B:234:HIS:HB2	1.85	0.57
1:A:54:LYS:HE3	1:B:145:ILE:HD13	1.86	0.57
1:A:89:MET:O	1:A:93:LYS:HG3	2.05	0.56
1:B:89:MET:O	1:B:93:LYS:HE2	2.05	0.56
1:B:177:VAL:O	1:B:181:LYS:HG3	2.06	0.56
1:A:247:LYS:HG3	1:A:250:ALA:HB2	1.87	0.55
1:A:13:GLY:HA2	1:A:17:ARG:O	2.07	0.55
1:B:6:ARG:HG3	1:B:155:PHE:HB3	1.90	0.54
1:A:144:PRO:HG3	1:B:291:ARG:HH11	1.73	0.53
1:B:3[B]:GLU:HG2	2:B:497:HOH:O	2.07	0.53
1:B:116:GLN:O	1:B:120:ARG:HG2	2.09	0.53
1:B:8:LEU:HD12	1:B:174:ALA:HB2	1.90	0.52
1:A:161:LYS:CD	1:A:161:LYS:N	2.73	0.52
1:B:248:ASP:H	1:B:277:LEU:HD21	1.75	0.52
1:B:256[B]:ARG:NE	2:B:409:HOH:O	2.32	0.51
1:B:80:GLU:OE2	2:B:406:HOH:O	2.19	0.51
1:B:225:ALA:CB	1:B:234:HIS:HB2	2.41	0.50
1:B:256[A]:ARG:HG2	2:B:409:HOH:O	2.11	0.50
1:A:242:PRO:HD2	1:A:271:LYS:O	2.12	0.50
1:B:245:LYS:HB3	1:B:298:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ALA:HB3	1:B:294:ILE:HD11	1.95	0.49
1:B:96:ARG:NH2	2:B:423:HOH:O	2.45	0.47
1:B:242:PRO:HD2	1:B:271:LYS:O	2.14	0.47
1:A:79:ILE:HG21	1:A:129:ILE:HD12	1.97	0.47
1:B:277:LEU:H	1:B:277:LEU:HD12	1.79	0.47
1:A:109:GLY:HA3	1:A:115:ARG:HG2	1.97	0.46
1:B:116:GLN:HE21	1:B:120:ARG:NH2	2.13	0.46
1:A:32:HIS:O	1:A:48:LYS:HD2	2.15	0.46
1:A:70[B]:ASN:OD1	1:A:71:VAL:N	2.47	0.45
1:A:73:ASP:HA	1:A:136[B]:ARG:HB2	1.99	0.45
1:A:323:ASP:O	1:A:327:ARG:HG2	2.17	0.45
1:B:316:ASP:N	1:B:316:ASP:OD1	2.50	0.45
1:A:11:ALA:HB2	1:A:24:ILE:HD12	1.99	0.44
1:A:267:LYS:HE3	1:A:267:LYS:HB2	1.85	0.44
1:A:60:HIS:CE1	1:A:169:ASP:HB2	2.53	0.44
1:B:19:GLU:O	1:B:23[A]:SER:OG	2.24	0.44
1:A:3[A]:GLU:OE2	1:A:6:ARG:NH1	2.51	0.44
1:A:18:GLU:N	1:A:18:GLU:OE1	2.52	0.43
1:B:234:HIS:HB3	2:B:480:HOH:O	2.17	0.43
1:A:266:GLU:OE1	2:A:405:HOH:O	2.21	0.43
1:A:73:ASP:HA	1:A:136[A]:ARG:HB2	2.01	0.43
1:A:75:GLY:O	2:A:406:HOH:O	2.21	0.43
1:A:105:VAL:HG22	1:A:129:ILE:HG12	2.01	0.43
1:B:56:ILE:HD11	1:B:211:VAL:HB	2.00	0.43
1:A:304:ARG:HB2	1:A:312:MET:HB3	2.01	0.42
1:A:55:VAL:HG11	1:A:329:LEU:HD21	2.00	0.42
1:B:168:ASP:HA	1:B:169:ASP:HA	1.80	0.42
1:A:161:LYS:HD2	1:A:161:LYS:N	2.33	0.42
1:A:3[B]:GLU:HG2	2:A:432:HOH:O	2.18	0.42
1:B:256[A]:ARG:NH1	2:B:411:HOH:O	2.33	0.42
1:B:323:ASP:O	1:B:327:ARG:HG2	2.19	0.42
1:A:168:ASP:HA	1:A:169:ASP:HA	1.82	0.42
1:A:242:PRO:HB3	1:A:321:THR:OG1	2.20	0.42
1:A:144:PRO:HG3	1:B:291:ARG:NH1	2.32	0.42
1:A:24:ILE:HD13	1:A:24:ILE:HG21	1.81	0.42
1:A:3[B]:GLU:CD	1:A:6:ARG:NH1	2.73	0.42
1:B:96:ARG:NH1	1:B:152:ASP:OD1	2.53	0.42
1:A:71:VAL:O	1:A:136[A]:ARG:NH1	2.53	0.41
1:A:16:GLY:C	1:A:17:ARG:HG2	2.41	0.41
1:A:110:GLU:H	1:A:114:GLU:CD	2.23	0.41
1:A:37[B]:ARG:NE	1:B:82:VAL:HG22	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LYS:HG2	1:B:312:MET:SD	2.61	0.40
1:A:38:ILE:HA	1:A:43:ASN:O	2.21	0.40
1:B:151:TYR:CD1	1:B:309:PRO:HG3	2.57	0.40

All (4) 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)
2:A:492:HOH:O	2:B:443:HOH:O[2_444]	1.86	0.34
2:A:527:HOH:O	2:B:545:HOH:O[1_556]	2.04	0.16
2:A:548:HOH:O	2:B:586:HOH:O[2_444]	2.12	0.08
2:A:445:HOH:O	2:B:580:HOH:O[1_455]	2.18	0.02

### 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	312/331 (94%)	302 (97%)	10 (3%)	0	100	100
1	B	313/331 (95%)	294 (94%)	19 (6%)	0	100	100
All	All	625/662 (94%)	596 (95%)	29 (5%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 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 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	252/272 (93%)	251 (100%)	1 (0%)	91	87
1	B	252/272 (93%)	250 (99%)	2 (1%)	81	72
All	All	504/544 (93%)	501 (99%)	3 (1%)	86	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	LYS
1	B	116	GLN
1	B	277	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	116	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](#)

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	309/331 (93%)	0.19	11 (3%) 42 49	17, 26, 47, 92	0
1	B	308/331 (93%)	0.26	12 (3%) 39 45	17, 26, 49, 80	0
All	All	617/662 (93%)	0.22	23 (3%) 41 48	17, 26, 48, 92	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	GLY	6.6
1	A	234	HIS	6.3
1	A	331	ALA	5.1
1	B	291	ARG	4.9
1	B	209	TYR	4.5
1	B	208	GLY	4.3
1	B	293	GLY	4.2
1	A	209	TYR	3.6
1	B	230	ALA	3.6
1	A	208	GLY	3.6
1	A	278	THR	3.4
1	B	277	LEU	3.3
1	B	197	GLU	3.2
1	B	292	GLU	2.8
1	A	41	LEU	2.7
1	A	277	LEU	2.7
1	A	230	ALA	2.6
1	B	41	LEU	2.5
1	B	268	PHE	2.3
1	A	201	LEU	2.1
1	A	233	ARG	2.1
1	B	110	GLU	2.0
1	A	225	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.