



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:29 AM GMT

PDB ID : 2QZ6  
Title : First crystal structure of a psychrophile class C beta-lactamase  
Authors : Michaux, C.; Massant, J.; Kerff, F.; Charlier, P.; Wouters, J.  
Deposited on : 2007-08-16  
Resolution : 2.26 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  
<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

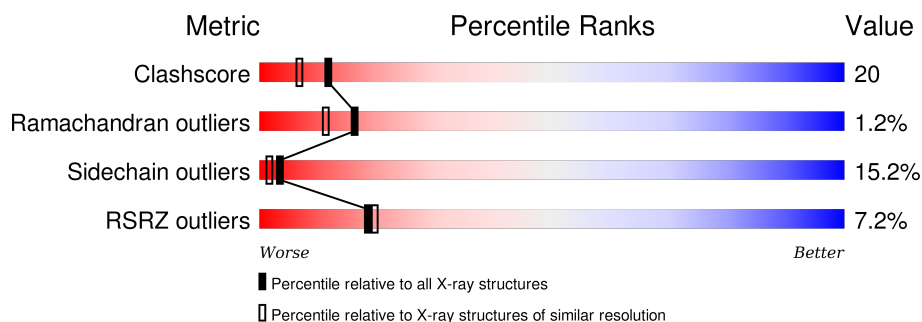
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.26 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))
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	358	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2795 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	11	0	0
			2661	1708	443	500	10			

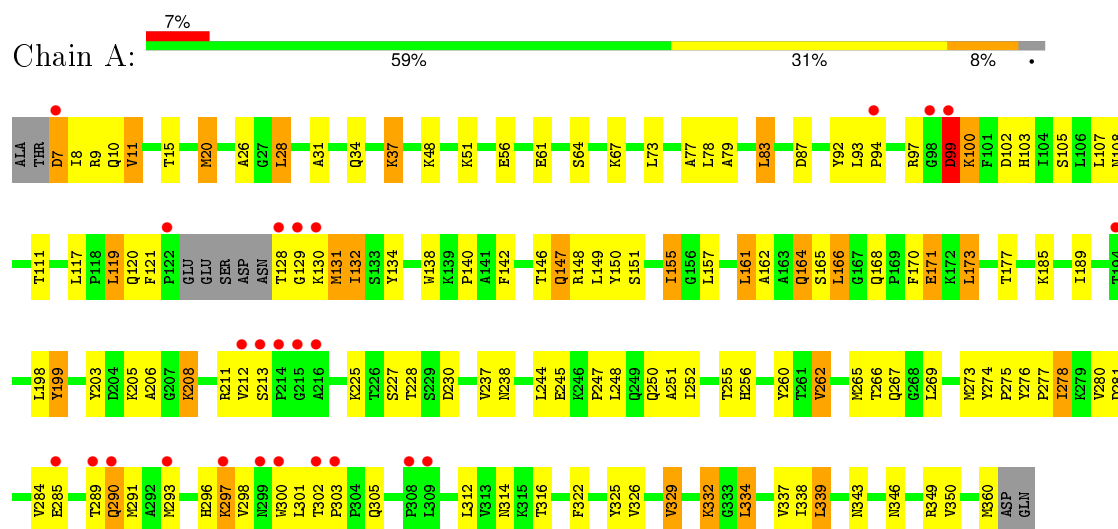
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	134	Total	O	0	0
			134	134		

### 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 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 ( $RSRZ > 2$ ). 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: Beta-lactamase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.60Å 69.70Å 53.90Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	19.12 – 2.26 19.25 – 2.26	Depositor EDS
% Data completeness (in resolution range)	95.1 (19.12-2.26) 90.1 (19.25-2.26)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.05 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.243 0.166 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	12.9	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 93.7	EDS
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 13703 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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](#)

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	0.30	0/2727	0.86	2/3711 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	TYR	CB-CG-CD2	7.46	125.48	121.00
1	A	83	LEU	CA-CB-CG	6.21	129.59	115.30

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	2661	0	2659	107	0
2	A	134	0	0	5	0
All	All	2795	0	2659	107	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 20.

All (107) 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:166:LEU:HD13	1:A:173:LEU:HD21	1.59	0.85
1:A:329:VAL:HG22	1:A:332:LYS:HB2	1.59	0.84
1:A:289:THR:O	1:A:293:MET:HG3	1.83	0.79
1:A:11:VAL:O	1:A:15:THR:HG23	1.85	0.77
1:A:238:ASN:HD22	1:A:256:HIS:HE1	1.29	0.77
1:A:79:ALA:HB2	1:A:250:GLN:HG2	1.74	0.69
1:A:291:MET:HA	1:A:296:HIS:HE1	1.61	0.66
1:A:326:VAL:HG22	1:A:337:VAL:HG22	1.77	0.66
1:A:157:LEU:HG	1:A:161:LEU:HD22	1.79	0.65
1:A:67:LYS:HZ3	1:A:150:TYR:HE1	1.47	0.63
1:A:67:LYS:HE2	1:A:155:ILE:HG21	1.79	0.62
1:A:245:GLU:HG3	1:A:247:PRO:HD2	1.81	0.61
1:A:281:ASP:O	1:A:285:GLU:HG3	2.00	0.61
1:A:265:MET:HG3	1:A:274:TYR:CZ	2.36	0.60
1:A:119:LEU:HD21	1:A:150:TYR:CD2	2.38	0.59
1:A:105:SER:H	1:A:108:ASN:HD22	1.49	0.59
1:A:275:PRO:O	1:A:278:ILE:HG13	2.04	0.58
1:A:37:LYS:HG3	1:A:37:LYS:O	2.03	0.57
1:A:168:GLN:HB2	1:A:173:LEU:CD1	2.34	0.57
1:A:346:ASN:HA	1:A:349:ARG:HG3	1.86	0.57
1:A:170:PHE:HD2	1:A:171:GLU:OE1	1.87	0.57
1:A:103:HIS:HB2	2:A:541:HOH:O	2.03	0.57
1:A:129:GLY:HA2	1:A:132:ILE:HB	1.87	0.57
1:A:64:SER:O	1:A:67:LYS:HG3	2.06	0.56
1:A:316:THR:HG22	1:A:325:TYR:CD1	2.41	0.56
1:A:166:LEU:CD1	1:A:173:LEU:HD21	2.35	0.55
1:A:147:GLN:HG3	1:A:297:LYS:HA	1.88	0.55
1:A:301:LEU:HD13	1:A:305:GLN:CG	2.36	0.54
1:A:26:ALA:HB2	1:A:48:LYS:HE2	1.90	0.54
1:A:73:LEU:HD11	1:A:173:LEU:HB3	1.90	0.54
1:A:168:GLN:HB2	1:A:173:LEU:HD12	1.91	0.52
1:A:20:MET:HB2	1:A:28:LEU:CD1	2.38	0.52
1:A:119:LEU:HD21	1:A:150:TYR:CE2	2.44	0.52
1:A:301:LEU:HD13	1:A:305:GLN:HG3	1.91	0.52
1:A:260:TYR:HB2	1:A:298:VAL:HG13	1.92	0.52
1:A:105:SER:H	1:A:108:ASN:ND2	2.08	0.51
1:A:131:MET:SD	1:A:132:ILE:HD13	2.50	0.51
1:A:94:PRO:HA	1:A:97:ARG:HG3	1.92	0.51
1:A:171:GLU:HG3	1:A:189:ILE:HD13	1.93	0.51
1:A:28:LEU:CD2	1:A:338:ILE:HD11	2.41	0.51
1:A:165:SER:O	1:A:165:SER:OG	2.29	0.51
1:A:117:LEU:HG	1:A:138:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:VAL:HA	2:A:597:HOH:O	2.11	0.50
1:A:298:VAL:HG12	1:A:298:VAL:O	2.13	0.49
1:A:92:TYR:HB2	1:A:161:LEU:HG	1.95	0.49
1:A:162:ALA:O	1:A:165:SER:O	2.30	0.49
1:A:290:GLN:HE21	1:A:290:GLN:N	2.11	0.48
1:A:262:VAL:HG13	1:A:298:VAL:HG22	1.95	0.48
1:A:94:PRO:O	1:A:97:ARG:HG3	2.13	0.48
1:A:93:LEU:HD12	1:A:94:PRO:HD2	1.94	0.48
1:A:171:GLU:OE1	1:A:189:ILE:HD13	2.14	0.48
1:A:289:THR:HG22	1:A:290:GLN:NE2	2.28	0.48
1:A:146:THR:O	1:A:297:LYS:HG3	2.14	0.47
1:A:255:THR:HA	1:A:269:LEU:HB2	1.96	0.47
1:A:278:ILE:HD12	1:A:278:ILE:H	1.80	0.47
1:A:173:LEU:O	1:A:177:THR:HB	2.15	0.47
1:A:291:MET:HG3	1:A:291:MET:O	2.14	0.47
1:A:251:ALA:O	1:A:255:THR:HG23	2.15	0.46
1:A:119:LEU:HA	1:A:151:SER:HA	1.97	0.46
1:A:334:LEU:HD11	1:A:360:MET:HB3	1.98	0.46
1:A:329:VAL:CG2	1:A:332:LYS:HB2	2.37	0.46
1:A:148:ARG:NH1	1:A:267:GLN:OE1	2.50	0.45
1:A:131:MET:O	1:A:134:TYR:HB3	2.16	0.45
1:A:237:VAL:HB	1:A:244:LEU:HD11	1.98	0.45
1:A:99:ASP:O	1:A:102:ASP:HB2	2.16	0.45
1:A:297:LYS:HE3	1:A:297:LYS:HB2	1.45	0.45
1:A:290:GLN:HE21	1:A:290:GLN:CA	2.30	0.45
1:A:205:LYS:HG3	1:A:206:ALA:N	2.29	0.45
1:A:164:GLN:NE2	2:A:519:HOH:O	2.50	0.45
1:A:111:THR:HB	1:A:260:TYR:CE1	2.52	0.45
1:A:100:LYS:HD2	1:A:140:PRO:HD3	1.99	0.44
1:A:314:ASN:HA	1:A:326:VAL:O	2.17	0.44
1:A:99:ASP:HB3	1:A:100:LYS:H	1.56	0.44
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.83	0.44
1:A:248:LEU:O	1:A:252:ILE:HG13	2.18	0.44
1:A:343:ASN:HB3	2:A:538:HOH:O	2.17	0.44
1:A:31:ALA:HB2	1:A:228:THR:HB	1.98	0.44
1:A:67:LYS:HD3	1:A:155:ILE:HG21	1.99	0.44
1:A:67:LYS:NZ	1:A:150:TYR:OH	2.50	0.44
1:A:28:LEU:HD22	1:A:338:ILE:HD11	1.99	0.44
1:A:73:LEU:HD21	1:A:173:LEU:CD2	2.48	0.43
1:A:99:ASP:HB3	2:A:621:HOH:O	2.18	0.43
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:NH1	1:A:211:ARG:HG3	2.34	0.43
1:A:67:LYS:CE	1:A:155:ILE:HG21	2.46	0.43
1:A:280:VAL:O	1:A:284:VAL:HG13	2.19	0.43
1:A:77:ALA:HB2	1:A:166:LEU:HD11	1.99	0.43
1:A:290:GLN:NE2	1:A:290:GLN:N	2.66	0.43
1:A:211:ARG:HH11	1:A:211:ARG:HG3	1.83	0.43
1:A:56:GLU:O	1:A:227:SER:HB2	2.19	0.42
1:A:34:GLN:HB2	1:A:360:MET:HE2	2.01	0.42
1:A:301:LEU:HD13	1:A:305:GLN:HG2	2.00	0.42
1:A:316:THR:HG22	1:A:325:TYR:HD1	1.83	0.42
1:A:61:GLU:HB2	1:A:322:PHE:CD1	2.55	0.42
1:A:339:LEU:HA	1:A:339:LEU:HD12	1.86	0.42
1:A:281:ASP:HA	1:A:284:VAL:HG22	2.03	0.41
1:A:128:THR:HG22	1:A:129:GLY:H	1.85	0.41
1:A:7:ASP:O	1:A:11:VAL:HG13	2.21	0.41
1:A:87:ASP:OD2	1:A:92:TYR:OH	2.29	0.41
1:A:48:LYS:O	1:A:51:LYS:HE3	2.21	0.41
1:A:120:GLN:HE21	1:A:121:PHE:H	1.68	0.41
1:A:301:LEU:HD22	1:A:305:GLN:HE21	1.85	0.41
1:A:120:GLN:HG3	1:A:121:PHE:N	2.36	0.41
1:A:276:TYR:CD1	1:A:277:PRO:HA	2.56	0.41
1:A:284:VAL:HG23	1:A:285:GLU:N	2.36	0.40
1:A:203:TYR:HA	1:A:208:LYS:O	2.22	0.40
1:A:8:ILE:HG23	1:A:9:ARG:N	2.35	0.40

There are no symmetry-related clashes.

## 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	345/358 (96%)	329 (95%)	12 (4%)	4 (1%)	16 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	A	100	LYS
1	A	166	LEU
1	A	303	PRO

### 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	282/290 (97%)	239 (85%)	43 (15%)	<b>3</b> <b>2</b>

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	GLN
1	A	11	VAL
1	A	20	MET
1	A	28	LEU
1	A	37	LYS
1	A	78	LEU
1	A	83	LEU
1	A	99	ASP
1	A	107	LEU
1	A	119	LEU
1	A	130	LYS
1	A	131	MET
1	A	132	ILE
1	A	142	PHE
1	A	147	GLN
1	A	149	LEU
1	A	155	ILE
1	A	161	LEU
1	A	164	GLN
1	A	171	GLU

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Mol	Chain	Res	Type
1	A	173	LEU
1	A	185	LYS
1	A	198	LEU
1	A	199	TYR
1	A	208	LYS
1	A	213	SER
1	A	225	LYS
1	A	230	ASP
1	A	262	VAL
1	A	266	THR
1	A	273	MET
1	A	278	ILE
1	A	290	GLN
1	A	297	LYS
1	A	300	TRP
1	A	302	THR
1	A	312	LEU
1	A	329	VAL
1	A	332	LYS
1	A	334	LEU
1	A	339	LEU
1	A	350	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	35	ASN
1	A	80	ASN
1	A	108	ASN
1	A	136	GLN
1	A	137	HIS
1	A	160	HIS
1	A	164	GLN
1	A	201	GLN
1	A	238	ASN
1	A	287	ASN
1	A	290	GLN
1	A	296	HIS
1	A	314	ASN
1	A	354	HIS

### 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 [i](#)

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	349/358 (97%)	0.17	25 (7%) 18 20	6, 17, 42, 69	4 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	THR	7.4
1	A	129	GLY	6.8
1	A	214	PRO	6.6
1	A	303	PRO	4.9
1	A	302	THR	4.8
1	A	213	SER	4.5
1	A	215	GLY	4.5
1	A	290	GLN	4.4
1	A	289	THR	4.4
1	A	7	ASP	3.7
1	A	122	PRO	3.6
1	A	309	LEU	3.5
1	A	98	GLY	3.5
1	A	299	ASN	3.5
1	A	216	ALA	3.2
1	A	308	PRO	3.2
1	A	99	ASP	2.8
1	A	130	LYS	2.6
1	A	300	TRP	2.6
1	A	194	THR	2.6
1	A	212	VAL	2.5
1	A	297	LYS	2.4
1	A	285	GLU	2.3
1	A	94	PRO	2.3
1	A	293	MET	2.3

## 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.