



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:00 am GMT

PDB ID : 2I6H  
Title : Structure of Protein of Unknown Function ATU0120 from *Agrobacterium tumefaciens*  
Authors : Osipiuk, J.; Xu, X.; Gu, J.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2006-08-28  
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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

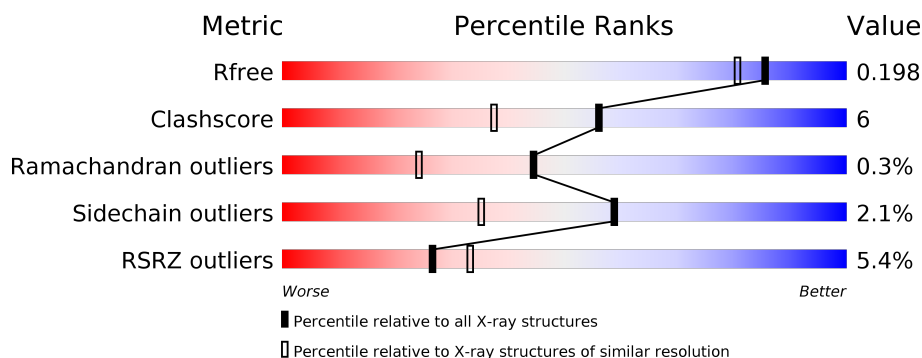
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (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. 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	207	<div> <div>3%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
1	B	207	<div> <div>6%</div> <div>73%</div> <div>11%</div> <div>15%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3673 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 Hypothetical protein Atu0120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	Se	0	14	0
			1551	981	280	285	2	3			
1	B	176	Total	C	N	O	S	Se	0	30	0
			1660	1050	296	310	2	2			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	CLONING ARTIFACT	UNP Q8UJ18
A	-20	GLY	-	CLONING ARTIFACT	UNP Q8UJ18
A	-19	SER	-	CLONING ARTIFACT	UNP Q8UJ18
A	-18	SER	-	CLONING ARTIFACT	UNP Q8UJ18
A	-17	HIS	-	EXPRESSION TAG	UNP Q8UJ18
A	-16	HIS	-	EXPRESSION TAG	UNP Q8UJ18
A	-15	HIS	-	EXPRESSION TAG	UNP Q8UJ18
A	-14	HIS	-	EXPRESSION TAG	UNP Q8UJ18
A	-13	HIS	-	EXPRESSION TAG	UNP Q8UJ18
A	-12	HIS	-	EXPRESSION TAG	UNP Q8UJ18
A	-11	SER	-	CLONING ARTIFACT	UNP Q8UJ18
A	-10	SER	-	CLONING ARTIFACT	UNP Q8UJ18
A	-9	GLY	-	CLONING ARTIFACT	UNP Q8UJ18
A	-8	ARG	-	CLONING ARTIFACT	UNP Q8UJ18
A	-7	GLU	-	CLONING ARTIFACT	UNP Q8UJ18
A	-6	ASN	-	CLONING ARTIFACT	UNP Q8UJ18
A	-5	LEU	-	CLONING ARTIFACT	UNP Q8UJ18
A	-4	TYR	-	CLONING ARTIFACT	UNP Q8UJ18
A	-3	PHE	-	CLONING ARTIFACT	UNP Q8UJ18
A	-2	GLN	-	CLONING ARTIFACT	UNP Q8UJ18
A	-1	GLY	-	CLONING ARTIFACT	UNP Q8UJ18
A	0	HIS	-	CLONING ARTIFACT	UNP Q8UJ18
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8UJ18
A	65	MSE	MET	MODIFIED RESIDUE	UNP Q8UJ18
A	82	MSE	MET	MODIFIED RESIDUE	UNP Q8UJ18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLY	-	CLONING ARTIFACT	UNP Q8UJ18
A	185	SER	-	CLONING ARTIFACT	UNP Q8UJ18
B	-21	MSE	-	CLONING ARTIFACT	UNP Q8UJ18
B	-20	GLY	-	CLONING ARTIFACT	UNP Q8UJ18
B	-19	SER	-	CLONING ARTIFACT	UNP Q8UJ18
B	-18	SER	-	CLONING ARTIFACT	UNP Q8UJ18
B	-17	HIS	-	EXPRESSION TAG	UNP Q8UJ18
B	-16	HIS	-	EXPRESSION TAG	UNP Q8UJ18
B	-15	HIS	-	EXPRESSION TAG	UNP Q8UJ18
B	-14	HIS	-	EXPRESSION TAG	UNP Q8UJ18
B	-13	HIS	-	EXPRESSION TAG	UNP Q8UJ18
B	-12	HIS	-	EXPRESSION TAG	UNP Q8UJ18
B	-11	SER	-	CLONING ARTIFACT	UNP Q8UJ18
B	-10	SER	-	CLONING ARTIFACT	UNP Q8UJ18
B	-9	GLY	-	CLONING ARTIFACT	UNP Q8UJ18
B	-8	ARG	-	CLONING ARTIFACT	UNP Q8UJ18
B	-7	GLU	-	CLONING ARTIFACT	UNP Q8UJ18
B	-6	ASN	-	CLONING ARTIFACT	UNP Q8UJ18
B	-5	LEU	-	CLONING ARTIFACT	UNP Q8UJ18
B	-4	TYR	-	CLONING ARTIFACT	UNP Q8UJ18
B	-3	PHE	-	CLONING ARTIFACT	UNP Q8UJ18
B	-2	GLN	-	CLONING ARTIFACT	UNP Q8UJ18
B	-1	GLY	-	CLONING ARTIFACT	UNP Q8UJ18
B	0	HIS	-	CLONING ARTIFACT	UNP Q8UJ18
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8UJ18
B	65	MSE	MET	MODIFIED RESIDUE	UNP Q8UJ18
B	82	MSE	MET	MODIFIED RESIDUE	UNP Q8UJ18
B	184	GLY	-	CLONING ARTIFACT	UNP Q8UJ18
B	185	SER	-	CLONING ARTIFACT	UNP Q8UJ18

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Ca 2 2	0	0
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

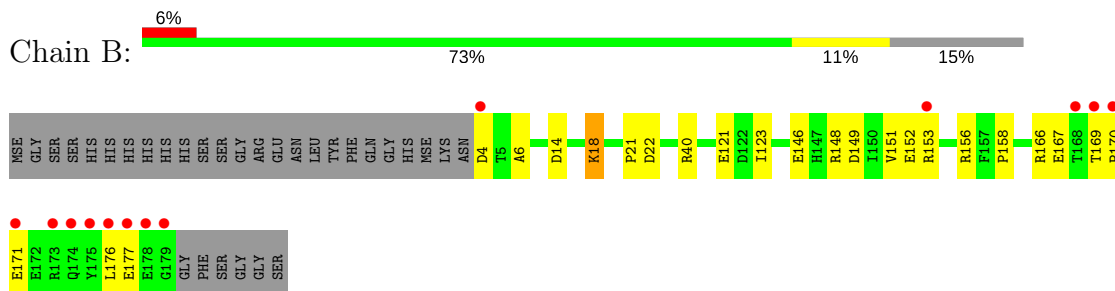
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Cl 2	0	0
3	A	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	254	Total 256	O 256	0	2
4	B	200	Total 200	O 200	0	0



- Molecule 1: Hypothetical protein Atu0120



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.49Å 101.19Å 103.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.00 – 1.75 36.90 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.00-1.75) 99.3 (36.90-1.75)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.166 , 0.199 0.165 , 0.198	Depositor DCC
$R_{free}$ test set	2138 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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](#)

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

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	0.91	3/1633 (0.2%)	0.74	0/2201
1	B	0.78	0/1736	0.71	0/2343
All	All	0.85	3/3369 (0.1%)	0.72	0/4544

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177[A]	GLU	CG-CD	7.92	1.63	1.51
1	A	177[B]	GLU	CG-CD	7.92	1.63	1.51
1	A	171	GLU	CG-CD	5.18	1.59	1.51

There are no bond angle outliers.

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	1551	0	1473	13	0
1	B	1660	0	1559	24	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	256	0	0	6	2
4	B	200	0	0	5	1
All	All	3673	0	3032	36	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 6.

All (36) 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[B]:ASP:OD2	4:A:660:HOH:O	1.77	1.03
1:B:22:ASP:HB2	4:B:706:HOH:O	1.61	0.99
1:A:90[A]:ARG:HD3	1:A:120:ALA:HB2	1.46	0.94
1:B:156[B]:ARG:O	1:B:158:PRO:HD3	1.75	0.86
1:B:123:ILE:HD11	1:B:152[A]:GLU:HG2	1.59	0.83
1:B:167[A]:GLU:O	4:B:660:HOH:O	2.05	0.73
1:B:14:ASP:O	1:B:18:LYS:HD3	1.90	0.72
1:A:43:HIS:HD2	1:A:67:LEU:O	1.75	0.70
1:A:98[A]:ARG:HG3	4:A:602:HOH:O	1.92	0.69
1:B:4:ASP:HA	4:B:705:HOH:O	1.94	0.67
1:B:149:ASP:O	1:B:153[B]:ARG:HG3	1.98	0.63
1:A:22:ASP:OD1	4:A:721:HOH:O	2.16	0.60
1:A:134[B]:GLN:HB2	1:A:135:PRO:HD3	1.89	0.55
1:B:121:GLU:OE2	1:B:156[A]:ARG:HB2	2.07	0.53
1:B:171[B]:GLU:HB2	4:B:676:HOH:O	2.08	0.52
1:B:123:ILE:CD1	1:B:152[A]:GLU:HG2	2.36	0.51
1:B:153[B]:ARG:NH1	1:B:153[B]:ARG:HG2	2.26	0.50
1:B:158:PRO:HB2	1:B:176[A]:LEU:HD21	1.92	0.50
1:A:98[B]:ARG:CZ	4:A:620:HOH:O	2.60	0.49
1:B:148:ARG:O	1:B:152[A]:GLU:HG3	2.13	0.49
1:B:169[B]:THR:HB	1:B:170[B]:PRO:HD2	1.94	0.49
1:A:90[A]:ARG:HD3	1:A:120:ALA:CB	2.31	0.48
1:B:156[B]:ARG:NH2	1:B:167[B]:GLU:O	2.44	0.47
1:A:1:MSE:HA	4:A:641:HOH:O	2.15	0.47
1:A:130:CYS:O	1:A:134[B]:GLN:HG2	2.14	0.47
1:B:121:GLU:CD	1:B:156[A]:ARG:HB2	2.37	0.45
1:B:151[B]:VAL:O	1:B:152[B]:GLU:C	2.56	0.44
1:B:156[A]:ARG:NH1	1:B:166:ARG:HD2	2.33	0.43
1:B:149:ASP:O	1:B:153[B]:ARG:CG	2.65	0.43
1:B:153[A]:ARG:HD2	4:B:621:HOH:O	2.19	0.43
1:B:153[B]:ARG:HH11	1:B:153[B]:ARG:CG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD23	1:B:21:PRO:HG2	2.02	0.42
1:B:4:ASP:OD2	1:B:6:ALA:HB3	2.19	0.42
1:B:158:PRO:HD2	3:B:506:CL:CL	2.58	0.41
1:A:98[B]:ARG:NH2	4:A:620:HOH:O	2.53	0.41
1:A:43:HIS:CD2	1:A:67:LEU:O	2.65	0.40

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)
4:A:595:HOH:O	4:A:660:HOH:O[1_655]	1.65	0.55
4:A:691:HOH:O	4:B:686:HOH:O[3_645]	1.93	0.27

## 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	191/207 (92%)	190 (100%)	1 (0%)	0	100	100
1	B	203/207 (98%)	199 (98%)	2 (1%)	2 (1%)	18	4
All	All	394/414 (95%)	389 (99%)	3 (1%)	2 (0%)	44	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	177[A]	GLU
1	B	177[B]	GLU

### 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	159/163 (98%)	156 (98%)	3 (2%)	62	41
1	B	170/163 (104%)	166 (98%)	4 (2%)	54	30
All	All	329/326 (101%)	322 (98%)	7 (2%)	59	35

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	PHE
1	A	40	ARG
1	A	174	GLN
1	B	18	LYS
1	B	40	ARG
1	B	146[A]	GLU
1	B	146[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	B	134	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

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 [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	176/207 (85%)	-0.38	6 (3%)	46	52	9, 13, 30, 38	0
1	B	174/207 (84%)	-0.01	13 (7%)	15	20	9, 14, 24, 38	1 (0%)
All	All	350/414 (84%)	-0.20	19 (5%)	26	33	9, 13, 29, 38	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179[A]	GLY	8.1
1	A	177[A]	GLU	4.9
1	B	170[A]	PRO	4.6
1	B	178[A]	GLU	4.4
1	B	176[A]	LEU	3.8
1	B	174[A]	GLN	3.8
1	A	178	GLU	3.7
1	B	175[A]	TYR	3.6
1	A	174	GLN	3.5
1	A	170	PRO	3.4
1	B	177[A]	GLU	3.2
1	B	4	ASP	3.1
1	B	153[A]	ARG	3.0
1	B	168[A]	THR	2.7
1	B	173[A]	ARG	2.4
1	B	169[A]	THR	2.4
1	A	173	ARG	2.2
1	B	171[A]	GLU	2.2
1	A	26[A]	ASP	2.1

### 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](#)

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
3	CL	A	505	1/1	0.99	0.09	-0.81	23,23,23,23	0
3	CL	B	506	1/1	0.99	0.10	-1.27	29,29,29,29	0
2	CA	B	502	1/1	0.99	0.04	-2.45	14,14,14,14	1
2	CA	A	501	1/1	1.00	0.02	-8.08	15,15,15,15	0
2	CA	B	503	1/1	0.99	0.04	-	19,19,19,19	1
3	CL	B	504	1/1	0.99	0.06	-	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.