



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 3, 2018 – 10:36 AM EST

PDB ID : 6BDT  
Title : Crystal Structure of Human Calpain-3 Protease Core Mutant-C129S  
Authors : Ye, Q.; Campbell, R.L.; Davies, P.L.  
Deposited on : 2017-10-24  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	rb-20030736
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)	:	rb-20030736

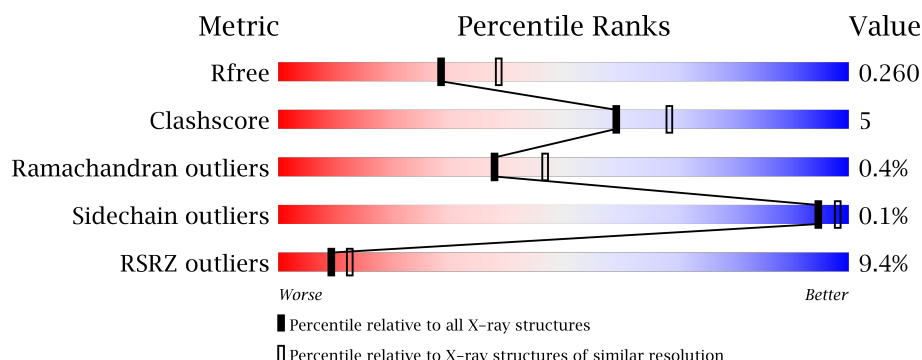
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


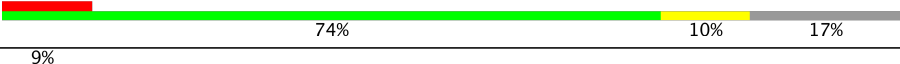

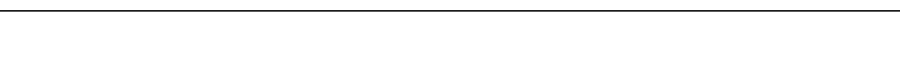
The reported resolution of this entry is 2.30 Å.

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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	382	
1	B	382	
1	C	382	
1	D	382	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10499 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 Calpain-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2530	1627	422	467	14			
1	B	318	Total	C	N	O	S	0	0	0
			2621	1686	435	485	15			
1	C	318	Total	C	N	O	S	0	0	0
			2622	1688	436	483	15			
1	D	315	Total	C	N	O	S	0	0	0
			2601	1674	431	481	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	SER	CYS	engineered mutation	UNP P20807
A	420	LEU	-	expression tag	UNP P20807
A	421	GLU	-	expression tag	UNP P20807
A	422	HIS	-	expression tag	UNP P20807
A	423	HIS	-	expression tag	UNP P20807
A	424	HIS	-	expression tag	UNP P20807
A	425	HIS	-	expression tag	UNP P20807
A	426	HIS	-	expression tag	UNP P20807
A	427	HIS	-	expression tag	UNP P20807
B	129	SER	CYS	engineered mutation	UNP P20807
B	420	LEU	-	expression tag	UNP P20807
B	421	GLU	-	expression tag	UNP P20807
B	422	HIS	-	expression tag	UNP P20807
B	423	HIS	-	expression tag	UNP P20807
B	424	HIS	-	expression tag	UNP P20807
B	425	HIS	-	expression tag	UNP P20807
B	426	HIS	-	expression tag	UNP P20807
B	427	HIS	-	expression tag	UNP P20807
C	129	SER	CYS	engineered mutation	UNP P20807
C	420	LEU	-	expression tag	UNP P20807
C	421	GLU	-	expression tag	UNP P20807

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Chain	Residue	Modelled	Actual	Comment	Reference
C	422	HIS	-	expression tag	UNP P20807
C	423	HIS	-	expression tag	UNP P20807
C	424	HIS	-	expression tag	UNP P20807
C	425	HIS	-	expression tag	UNP P20807
C	426	HIS	-	expression tag	UNP P20807
C	427	HIS	-	expression tag	UNP P20807
D	129	SER	CYS	engineered mutation	UNP P20807
D	420	LEU	-	expression tag	UNP P20807
D	421	GLU	-	expression tag	UNP P20807
D	422	HIS	-	expression tag	UNP P20807
D	423	HIS	-	expression tag	UNP P20807
D	424	HIS	-	expression tag	UNP P20807
D	425	HIS	-	expression tag	UNP P20807
D	426	HIS	-	expression tag	UNP P20807
D	427	HIS	-	expression tag	UNP P20807

- 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	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0

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

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

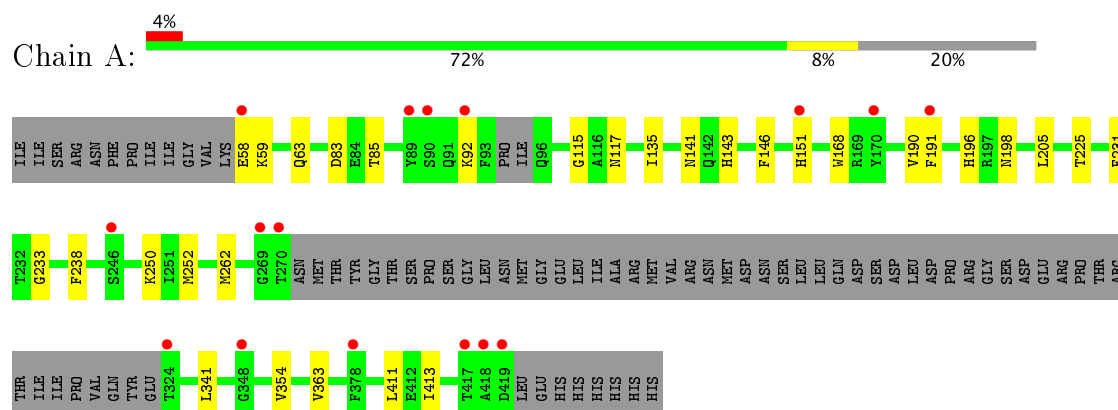
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total 39	O 39	0	0
4	B	24	Total 24	O 24	0	0
4	C	28	Total 28	O 28	0	0
4	D	22	Total 22	O 22	0	0

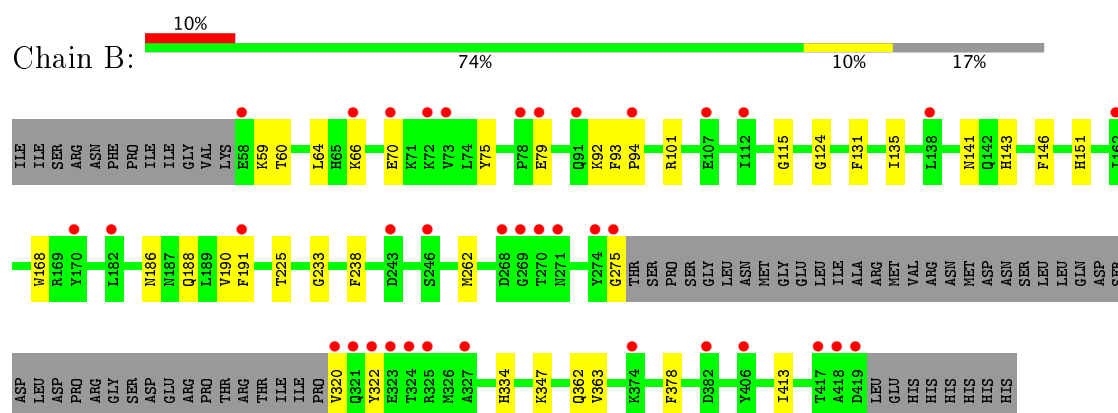
### 3 Residue-property plots

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.

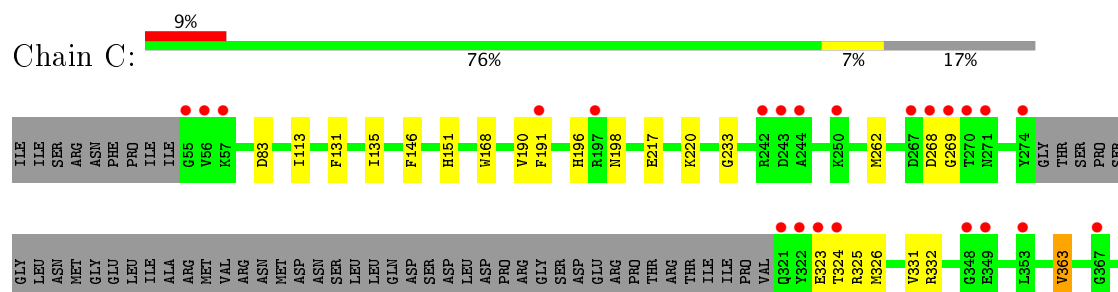
#### • Molecule 1: Calpain-3

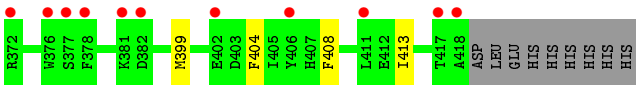


#### • Molecule 1: Calpain-3

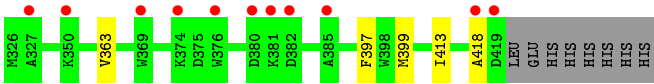
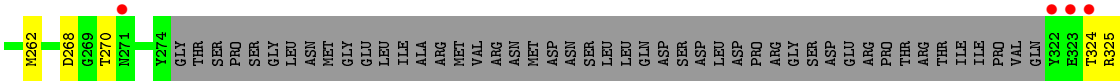
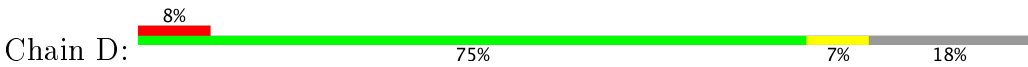


#### • Molecule 1: Calpain-3





● Molecule 1: Calpain-3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.81Å 105.49Å 225.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.99 – 2.30 17.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (17.99-2.30) 98.4 (17.99-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.222 , 0.256 0.226 , 0.260	Depositor DCC
$R_{free}$ test set	3139 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10499	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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	0.55	0/2602	0.69	0/3518
1	B	0.60	0/2697	0.71	0/3650
1	C	0.61	0/2698	0.71	0/3650
1	D	0.59	0/2677	0.68	0/3623
All	All	0.59	0/10674	0.70	0/14441

There are no bond length outliers.

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	2530	0	2404	34	0
1	B	2621	0	2489	43	0
1	C	2622	0	2498	24	0
1	D	2601	0	2469	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	39	0	0	1	0
4	B	24	0	0	1	0
4	C	28	0	0	1	0
4	D	22	0	0	0	0
All	All	10499	0	9860	110	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 5.

The worst 5 of 110 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:146:PHE:CZ	1:B:151:HIS:HD2	1.61	1.18
1:A:58:GLU:HG2	1:A:59:LYS:H	1.20	1.05
1:A:146:PHE:CZ	1:B:151:HIS:CD2	2.50	0.99
1:B:94:PRO:HG3	1:D:94:PRO:CG	1.95	0.96
1:B:94:PRO:HG3	1:D:94:PRO:HG2	1.49	0.95

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	301/382 (79%)	293 (97%)	7 (2%)	1 (0%)	44 55
1	B	314/382 (82%)	305 (97%)	8 (2%)	1 (0%)	44 55
1	C	314/382 (82%)	307 (98%)	6 (2%)	1 (0%)	44 55
1	D	311/382 (81%)	304 (98%)	5 (2%)	2 (1%)	28 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1240/1528 (81%)	1209 (98%)	26 (2%)	5 (0%)	38	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	VAL
1	B	363	VAL
1	C	363	VAL
1	D	363	VAL
1	D	418	ALA

### 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	270/339 (80%)	269 (100%)	1 (0%)	93	97
1	B	280/339 (83%)	280 (100%)	0	100	100
1	C	280/339 (83%)	280 (100%)	0	100	100
1	D	278/339 (82%)	278 (100%)	0	100	100
All	All	1108/1356 (82%)	1107 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	198	ASN
1	B	362	GLN
1	C	198	ASN
1	B	196	HIS

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Mol	Chain	Res	Type
1	C	196	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](#)

Of 12 ligands modelled in this entry, 12 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 [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 [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	307/382 (80%)	0.31	16 (5%) 28 35	30, 52, 91, 144	0
1	B	318/382 (83%)	0.63	37 (11%) 5 8	34, 58, 101, 133	0
1	C	318/382 (83%)	0.52	34 (10%) 7 9	32, 54, 106, 130	0
1	D	315/382 (82%)	0.53	31 (9%) 8 11	30, 56, 104, 137	0
All	All	1258/1528 (82%)	0.50	118 (9%) 9 12	30, 55, 102, 144	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	ALA	8.6
1	D	418	ALA	8.4
1	B	324	THR	8.0
1	B	321	GLN	7.0
1	B	170	TYR	6.8

### 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( $\text{\AA}^2$ )	Q<0.9
2	CA	D	502	1/1	0.98	0.13	0.05	32,32,32,32	0
3	CL	C	503	1/1	0.99	0.12	-0.31	41,41,41,41	0
2	CA	C	501	1/1	0.99	0.11	-0.88	36,36,36,36	0
3	CL	B	503	1/1	0.96	0.13	-1.02	55,55,55,55	0
2	CA	D	501	1/1	0.96	0.10	-1.54	53,53,53,53	0
3	CL	D	503	1/1	0.99	0.08	-1.69	47,47,47,47	0
2	CA	B	502	1/1	0.99	0.05	-1.96	35,35,35,35	0
3	CL	A	503	1/1	0.99	0.07	-2.34	40,40,40,40	0
2	CA	A	502	1/1	0.98	0.08	-2.62	51,51,51,51	0
2	CA	C	502	1/1	0.95	0.05	-2.95	63,63,63,63	0
2	CA	B	501	1/1	0.98	0.03	-3.39	50,50,50,50	0
2	CA	A	501	1/1	0.98	0.07	-3.66	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.