



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:39 AM UTC

PDB ID : 6BGP / pdb_00006bgp
Title : Crystal Structure of Human Calpain-3 Protease Core Mutant-C129A
Authors : Ye, Q.; Campbell, R.L.; Davies, P.L.
Deposited on : 2017-10-29
Resolution : 2.75 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

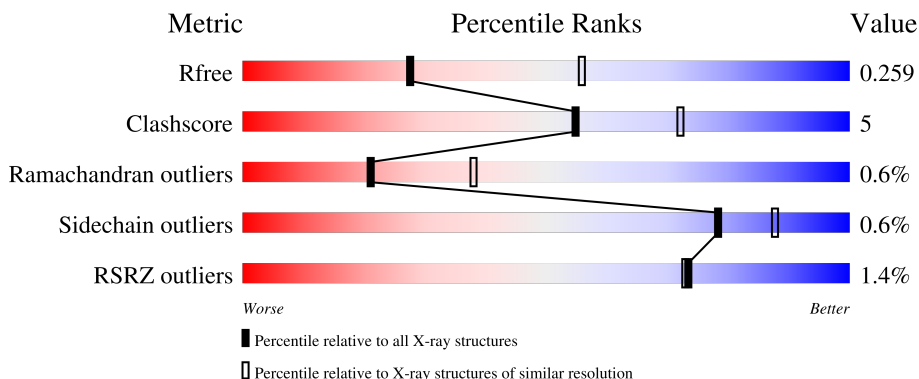
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	382	% 70% 9% 21%
1	B	382	% 73% 9% • 18%
1	C	382	% 75% 6% 18%
1	D	382	% 74% 8% • 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10316 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	303	Total	C	N	O	S	0	0	0
			2501	1610	416	461	14			
1	B	314	Total	C	N	O	S	0	0	0
			2588	1665	430	478	15			
1	C	313	Total	C	N	O	S	0	0	0
			2577	1658	430	474	15			
1	D	314	Total	C	N	O	S	0	0	0
			2588	1665	430	478	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ALA	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	ALA	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	ALA	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	ALA	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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

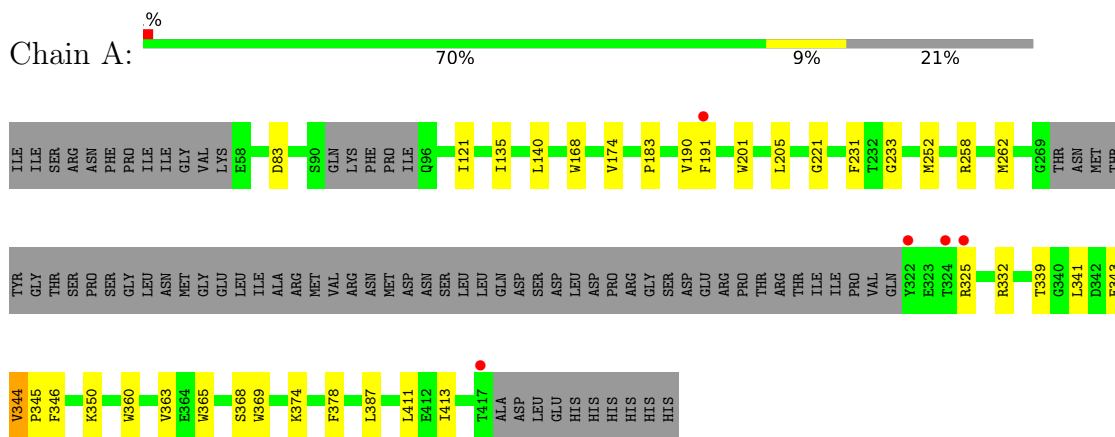
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total 14	O 14	0	0
4	B	18	Total 18	O 18	0	0
4	C	9	Total 9	O 9	0	0
4	D	9	Total 9	O 9	0	0

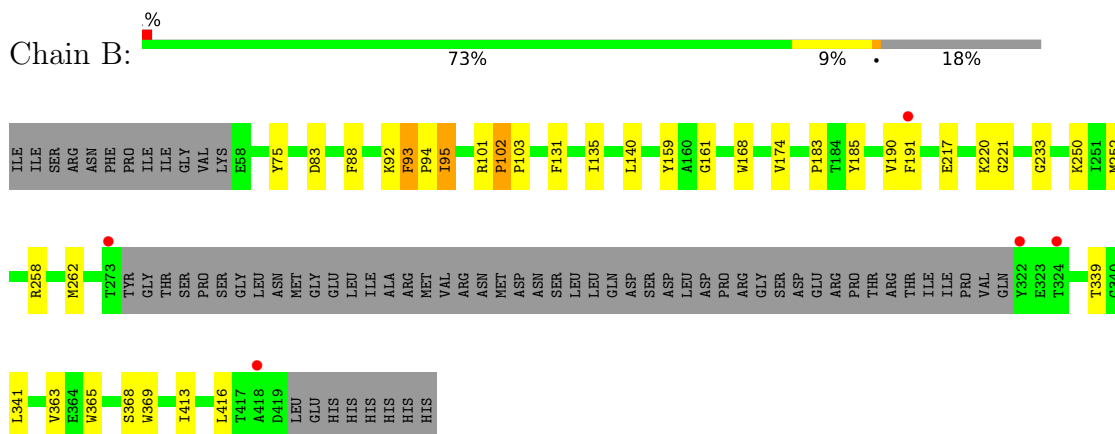
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

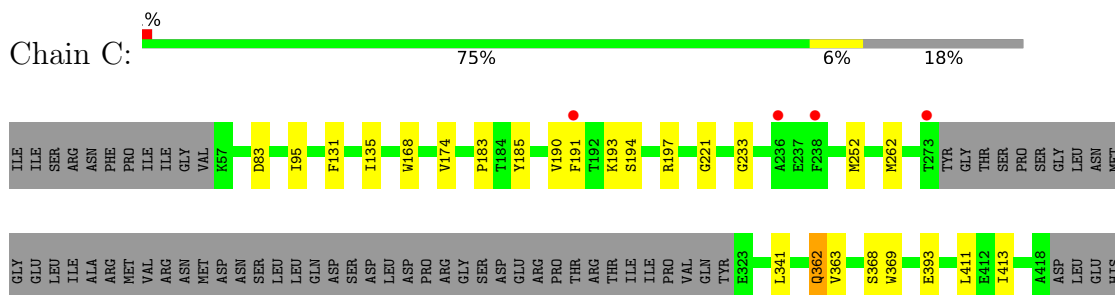
• Molecule 1: Calpain-3



• Molecule 1: Calpain-3



• Molecule 1: Calpain-3



HIS
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● Molecule 1: Calpain-3



ILE	ILE	SER	ASN	PHE	PRO	ILE	ILE	GLY	VAL	LYS	E68	D77	P78	D83	E84	T85	S90	Q91	K92	F93	P94	I95	I121	F131	I135	W168	V174	P183	V190	F191	W201	G221	G233	M252	M262	T273	TYR	GLY	THR	SER	PRO	SER
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GLY	LEU	ASN	MET	GLY	LEU	ILE	ALA	ARG	MET	VAL	ARG	ASN	MET	ASP	ASN	SER	LEU	GLN	ASP	SER	ASP	LEU	ASP	PRO	ARG	GLY	SER	ASP	GLU	ARG	PRO	THR	ARG	THR	ILE	ILE	PRO	VAL	GLN	Y322	E323	T324	R325	V331	L341	N358	V363	E364	S368	W373
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F397	W398	M399	F404	I413	D419	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.10Å 106.18Å 225.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.94 – 2.75 17.94 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (17.94-2.75) 99.5 (17.94-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.74Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.258 0.213 , 0.259	Depositor DCC
R_{free} test set	1916 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10316	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, CA

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	0.63	0/2573	0.81	3/3480 (0.1%)
1	B	0.66	0/2663	0.83	4/3604 (0.1%)
1	C	0.58	0/2651	0.81	2/3586 (0.1%)
1	D	0.80	0/2663	0.87	4/3604 (0.1%)
All	All	0.67	0/10550	0.83	13/14274 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	363	VAL	N-CA-CB	-8.37	102.51	111.46
1	A	344	VAL	CA-C-N	-7.71	110.20	119.84
1	A	344	VAL	C-N-CA	-7.71	110.20	119.84
1	B	93	PHE	CA-C-N	6.54	126.67	119.87
1	B	93	PHE	C-N-CA	6.54	126.67	119.87

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	2501	0	2373	35	0
1	B	2588	0	2460	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2577	0	2460	16	0
1	D	2588	0	2460	19	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
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	0	1	0
4	B	18	0	0	1	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
All	All	10316	0	9753	96	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 96 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:325:ARG:HD2	1:A:332:ARG:H	1.18	1.05
1:D:83:ASP:OD1	1:D:85:THR:HG22	1.69	0.92
1:B:102:PRO:HB2	1:B:103:PRO:HD3	1.57	0.85
1:B:365:TRP:HZ3	1:B:368:SER:O	1.62	0.83
1:A:365:TRP:HZ3	1:A:368:SER:O	1.63	0.81

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	297/382 (78%)	287 (97%)	8 (3%)	2 (1%)	18	34
1	B	310/382 (81%)	299 (96%)	9 (3%)	2 (1%)	21	38
1	C	309/382 (81%)	300 (97%)	8 (3%)	1 (0%)	36	56
1	D	310/382 (81%)	300 (97%)	8 (3%)	2 (1%)	21	38
All	All	1226/1528 (80%)	1186 (97%)	33 (3%)	7 (1%)	21	38

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	GLY
1	B	221	GLY
1	C	221	GLY
1	A	363	VAL
1	D	363	VAL

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	266/338 (79%)	263 (99%)	3 (1%)	65	79
1	B	276/338 (82%)	274 (99%)	2 (1%)	76	86
1	C	275/338 (81%)	274 (100%)	1 (0%)	84	91
1	D	276/338 (82%)	275 (100%)	1 (0%)	84	91
All	All	1093/1352 (81%)	1086 (99%)	7 (1%)	78	88

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	95	ILE
1	B	174	VAL
1	D	174	VAL
1	C	174	VAL
1	A	374	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	158	ASN
1	C	389	HIS
1	C	186	ASN
1	C	158	ASN
1	C	271	ASN

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 oligosaccharides 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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	303/382 (79%)	-0.23	5 (1%) 69 67	35, 59, 96, 144	0
1	B	314/382 (82%)	-0.09	5 (1%) 70 69	37, 62, 107, 150	0
1	C	313/382 (81%)	-0.11	4 (1%) 75 75	37, 65, 114, 142	0
1	D	314/382 (82%)	-0.04	3 (0%) 79 79	33, 65, 122, 149	0
All	All	1244/1528 (81%)	-0.12	17 (1%) 73 73	33, 62, 111, 150	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	238	PHE	3.2
1	B	322	TYR	2.9
1	B	273	THR	2.8
1	A	325	ARG	2.8
1	D	273	THR	2.6

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	C	503	1/1	0.96	0.05	46,46,46,46	0
3	CL	A	503	1/1	0.97	0.05	47,47,47,47	0
3	CL	B	503	1/1	0.97	0.04	58,58,58,58	0
2	CA	D	502	1/1	0.97	0.05	54,54,54,54	0
2	CA	B	502	1/1	0.98	0.02	57,57,57,57	0
2	CA	C	501	1/1	0.98	0.05	41,41,41,41	0
2	CA	A	501	1/1	0.98	0.03	41,41,41,41	0
3	CL	D	503	1/1	0.98	0.03	52,52,52,52	0
2	CA	B	501	1/1	0.99	0.02	41,41,41,41	0
2	CA	C	502	1/1	0.99	0.03	72,72,72,72	0
2	CA	D	501	1/1	0.99	0.04	37,37,37,37	0
2	CA	A	502	1/1	0.99	0.02	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.