



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2021 – 12:14 PM GMT

PDB ID : 7AI0  
Title : Crystal structure of human MDM2-G443T RING domain homodimer bound to UbcH5B-Ub (Crystal form 1)  
Authors : Magnussen, H.M.; Huang, D.T.  
Deposited on : 2020-09-25  
Resolution : 1.56 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

<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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

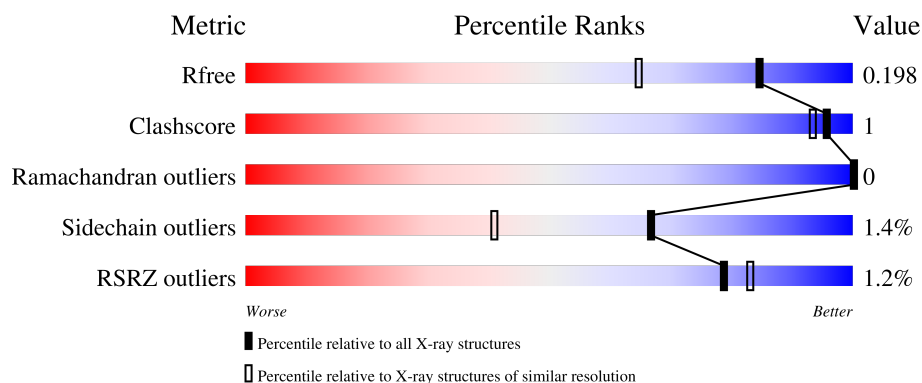
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.56 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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  $\geq 3$ , 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	AAA	75	 3% 77% 5% 17%
1	DDD	75	 3% 79% 1% 17%
2	BBB	147	 2% 97% 1% 2%
2	EEE	147	 94% 5% 1%
3	CCC	81	 93% 5% 2%

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Mol	Chain	Length	Quality of chain
3	FFF	81	 91% 5%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10086 atoms, of which 4779 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 E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	62	Total	C	H	N	O	S	30	1	0
			1019	313	529	90	78	9			
1	DDD	62	Total	C	H	N	O	S	30	1	0
			1012	311	526	89	77	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	417	GLY	-	expression tag	UNP Q00987
AAA	418	SER	-	expression tag	UNP Q00987
AAA	443	THR	GLY	engineered mutation	UNP Q00987
DDD	417	GLY	-	expression tag	UNP Q00987
DDD	418	SER	-	expression tag	UNP Q00987
DDD	443	THR	GLY	engineered mutation	UNP Q00987

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 D2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	BBB	146	Total	C	H	N	O	S	62	5	0
			2418	775	1211	212	212	8			
2	EEE	146	Total	C	H	N	O	S	64	6	0
			2446	784	1221	217	216	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	22	ARG	SER	engineered mutation	UNP P62837
BBB	85	LYS	CYS	engineered mutation	UNP P62837
EEE	22	ARG	SER	engineered mutation	UNP P62837
EEE	85	LYS	CYS	engineered mutation	UNP P62837

- Molecule 3 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	CCC	77	Total	C	H	N	O	S	31	0	0
			1214	375	619	104	115	1			
3	FFF	77	Total	C	H	N	O	S	33	2	0
			1266	389	649	108	119	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-4	GLY	-	expression tag	UNP P0CG47
CCC	-3	SER	-	expression tag	UNP P0CG47
CCC	0	SER	-	insertion	UNP P0CG47
FFF	-4	GLY	-	expression tag	UNP P0CG47
FFF	-3	SER	-	expression tag	UNP P0CG47
FFF	0	SER	-	insertion	UNP P0CG47

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	2	Total	Cl	0	0
			2	2		
4	DDD	1	Total	Cl	0	0
			1	1		
4	AAA	2	Total	Cl	0	0
			2	2		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	DDD	2	Total	Zn	0	0
			2	2		
5	AAA	2	Total	Zn	0	0
			2	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
6	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
6	EEE	1	Total	C	H	O	1	0
			10	2	6	2		
6	FFF	1	Total	C	H	O	1	0
			10	2	6	2		

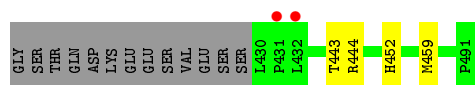
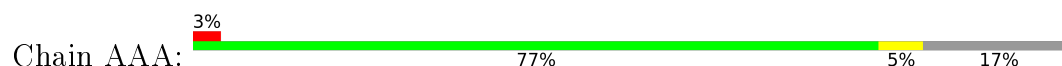
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	61	Total	O	0	0
			61	61		
7	BBB	182	Total	O	0	0
			182	182		
7	CCC	65	Total	O	0	0
			65	65		
7	DDD	51	Total	O	0	0
			51	51		
7	EEE	196	Total	O	0	0
			196	196		
7	FFF	107	Total	O	0	0
			107	107		

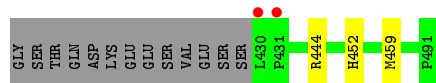
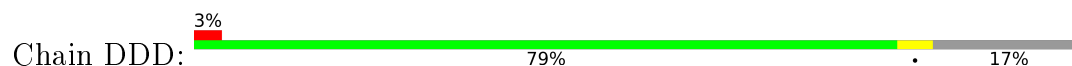
### 3 Residue-property plots [i](#)

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.

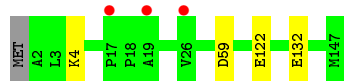
- Molecule 1: E3 ubiquitin-protein ligase Mdm2



- Molecule 1: E3 ubiquitin-protein ligase Mdm2



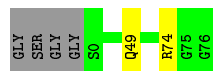
- Molecule 2: Ubiquitin-conjugating enzyme E2 D2



- Molecule 2: Ubiquitin-conjugating enzyme E2 D2



- Molecule 3: Polyubiquitin-B



- Molecule 3: Polyubiquitin-B

Chain FFF:  91% • 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.53 Å   129.53 Å   70.75 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	70.75 – 1.56 64.77 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.8 (70.75-1.56) 99.8 (64.77-1.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 1.56 Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.134 , 0.185 0.148 , 0.198	Depositor DCC
$R_{free}$ test set	4696 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, 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	AAA	0.76	0/501	0.90	1/676 (0.1%)
1	DDD	0.79	0/500	0.92	1/674 (0.1%)
2	BBB	0.85	2/1253 (0.2%)	0.95	0/1704
2	EEE	0.85	1/1269 (0.1%)	0.92	0/1726
3	CCC	0.84	0/601	0.89	0/810
3	FFF	0.89	2/626 (0.3%)	0.88	0/843
All	All	0.84	5/4750 (0.1%)	0.92	2/6433 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EEE	132	GLU	CD-OE1	7.75	1.34	1.25
2	BBB	122	GLU	CD-OE1	6.25	1.32	1.25
3	FFF	52	ASP	C-O	5.75	1.34	1.23
2	BBB	132	GLU	CD-OE1	5.56	1.31	1.25
3	FFF	64	GLU	CD-OE2	-5.10	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	444	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	DDD	444	ARG	NE-CZ-NH2	-5.31	117.65	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	AAA	490	529	520	4	0
1	DDD	486	526	518	0	0
2	BBB	1207	1211	1202	4	0
2	EEE	1225	1221	1210	4	0
3	CCC	595	619	612	1	0
3	FFF	617	649	648	1	0
4	AAA	2	0	0	0	0
4	BBB	2	0	0	0	0
4	DDD	1	0	0	0	0
5	AAA	2	0	0	0	0
5	DDD	2	0	0	0	0
6	BBB	4	6	6	0	0
6	CCC	4	6	6	0	0
6	EEE	4	6	6	0	0
6	FFF	4	6	6	0	0
7	AAA	61	0	0	0	0
7	BBB	182	0	0	0	0
7	CCC	65	0	0	1	0
7	DDD	51	0	0	0	0
7	EEE	196	0	0	0	0
7	FFF	107	0	0	1	0
All	All	5307	4779	4734	10	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 1.

The worst 5 of 10 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:AAA:443:THR:CG2	2:BBB:4:LYS:HD3	2.10	0.81
1:AAA:443:THR:HG22	2:BBB:4:LYS:HD3	1.81	0.60
1:AAA:443:THR:HG22	2:BBB:4:LYS:NZ	2.16	0.59
1:AAA:443:THR:HG23	2:BBB:4:LYS:HD3	1.93	0.48
3:FFF:49[A]:GLN:OE1	7:FFF:201:HOH:O	2.20	0.47

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	AAA	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
1	DDD	61/75 (81%)	56 (92%)	5 (8%)	0	100	100
2	BBB	149/147 (101%)	146 (98%)	3 (2%)	0	100	100
2	EEE	150/147 (102%)	148 (99%)	2 (1%)	0	100	100
3	CCC	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
3	FFF	77/81 (95%)	77 (100%)	0	0	100	100
All	All	573/606 (95%)	558 (97%)	15 (3%)	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	AAA	57/68 (84%)	55 (96%)	2 (4%)	36	9
1	DDD	57/68 (84%)	55 (96%)	2 (4%)	36	9
2	BBB	134/131 (102%)	133 (99%)	1 (1%)	84	69
2	EEE	136/131 (104%)	134 (98%)	2 (2%)	65	37
3	CCC	65/70 (93%)	64 (98%)	1 (2%)	65	37
3	FFF	70/70 (100%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	519/538 (96%)	511 (98%)	8 (2%)	67 37

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CCC	49	GLN
2	EEE	55[B]	HIS
1	DDD	459	MET
2	BBB	59	ASP
1	DDD	452	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	EEE	201	-	3,3,3	0.25	0	2,2,2	0.43	0
6	EDO	CCC	101	-	3,3,3	0.67	0	2,2,2	0.63	0
6	EDO	FFF	101	-	3,3,3	0.78	0	2,2,2	0.46	0
6	EDO	BBB	201	-	3,3,3	0.29	0	2,2,2	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	EEE	201	-	-	1/1/1/1	-
6	EDO	CCC	101	-	-	1/1/1/1	-
6	EDO	FFF	101	-	-	0/1/1/1	-
6	EDO	BBB	201	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	CCC	101	EDO	O1-C1-C2-O2
6	BBB	201	EDO	O1-C1-C2-O2
6	EEE	201	EDO	O1-C1-C2-O2

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 ⓘ

### 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	AAA	62/75 (82%)	-0.57	2 (3%) 47 55	13, 19, 38, 46	0
1	DDD	62/75 (82%)	-0.50	2 (3%) 47 55	14, 19, 32, 44	0
2	BBB	146/147 (99%)	-0.61	3 (2%) 63 69	10, 15, 34, 53	0
2	EEE	146/147 (99%)	-0.69	0 100 100	11, 15, 27, 48	0
3	CCC	77/81 (95%)	-0.34	0 100 100	13, 26, 47, 68	0
3	FFF	77/81 (95%)	-0.70	0 100 100	12, 20, 37, 44	0
All	All	570/606 (94%)	-0.59	7 (1%) 79 83	10, 18, 40, 68	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	430	LEU	4.7
1	AAA	431	PRO	3.3
2	BBB	17	PRO	3.1
2	BBB	19	ALA	3.0
2	BBB	26	VAL	2.7

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

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

### 6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	EEE	201	4/4	0.93	0.13	42,47,51,51	1
6	EDO	CCC	101	4/4	0.93	0.12	29,36,40,40	1
6	EDO	BBB	201	4/4	0.96	0.12	39,40,50,51	1
6	EDO	FFF	101	4/4	0.97	0.08	23,30,34,34	1
5	ZN	AAA	504	1/1	1.00	0.07	15,15,15,15	0
5	ZN	AAA	503	1/1	1.00	0.07	19,19,19,19	0
4	CL	BBB	202	1/1	1.00	0.09	19,19,19,19	0
5	ZN	DDD	503	1/1	1.00	0.07	14,14,14,14	0
4	CL	DDD	501	1/1	1.00	0.04	31,31,31,31	0
4	CL	BBB	203	1/1	1.00	0.05	16,16,16,16	0
4	CL	AAA	502	1/1	1.00	0.05	26,26,26,26	0
5	ZN	DDD	502	1/1	1.00	0.07	19,19,19,19	0
4	CL	AAA	501	1/1	1.00	0.04	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.