



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6CXO  
Title : Complement component-9  
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Deposited on : 2018-04-03  
Resolution : 2.20 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

<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>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

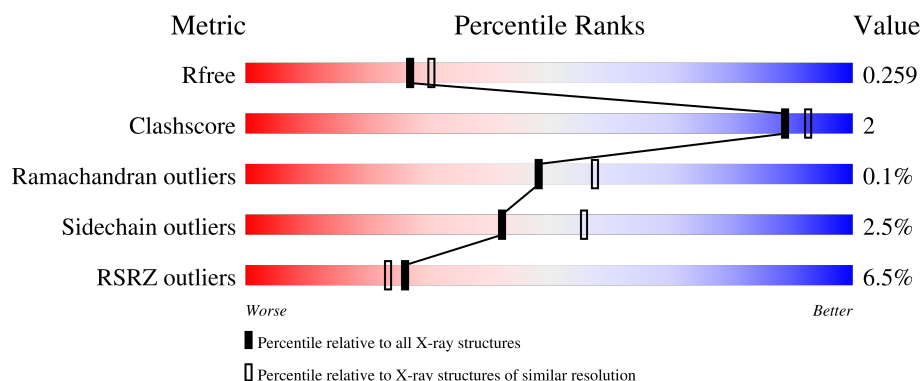
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	A	529	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>5%</div> <div>12%</div> </div> </div>
1	B	529	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7554 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 Complement component C9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3632	2280	619	703	30			
1	B	449	Total	C	N	O	S	0	0	0
			3528	2219	602	675	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ASP	-	expression tag	UNP P06683
A	28	GLU	ASN	engineered mutation	UNP P06683
A	243	ASP	ASN	engineered mutation	UNP P06683
A	397	ASP	ASN	engineered mutation	UNP P06683
B	0	ASP	-	expression tag	UNP P06683
B	28	GLU	ASN	engineered mutation	UNP P06683
B	243	ASP	ASN	engineered mutation	UNP P06683
B	397	ASP	ASN	engineered mutation	UNP P06683

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

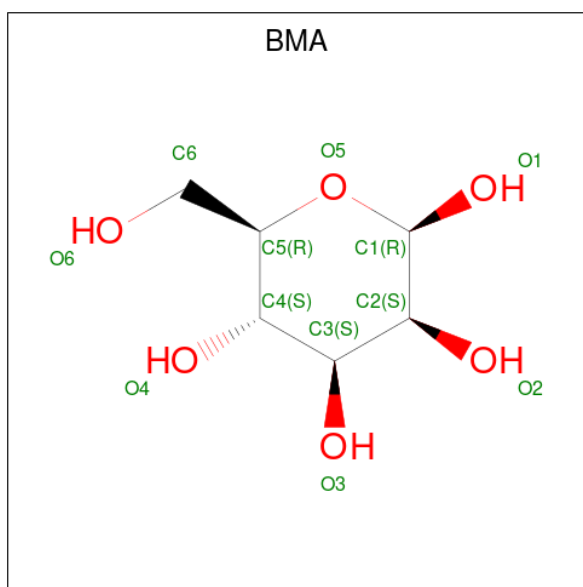


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	130	Total	O	0	0
			130	130		
7	B	205	Total	O	0	0
			205	205		



- Molecule 1: Complement component C9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.59Å 149.21Å 165.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.20 49.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.74-2.20) 98.4 (49.74-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.209 , 0.251 0.214 , 0.259	Depositor DCC
$R_{free}$ test set	3369 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.0	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, ZN, NAG, BMA, MG

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	0.49	0/3702	0.66	0/4996
1	B	0.52	0/3594	0.68	0/4839
All	All	0.51	0/7296	0.67	0/9835

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	3632	0	3416	9	0
1	B	3528	0	3362	15	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	11	0	10	0	0
7	A	130	0	0	0	0
7	B	205	0	0	0	0
All	All	7554	0	6824	25	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 2.

All (25) 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:B:200:PHE:CD2	1:B:265:PHE:HZ	2.08	0.72
1:B:276:ARG:HG2	1:B:335:GLU:HG2	1.81	0.62
1:A:176:VAL:HG23	1:A:287:ARG:HB3	1.87	0.55
1:A:502:ILE:HD11	1:A:509:CYS:HB3	1.90	0.53
4:B:603:NAG:O7	4:B:603:NAG:C1	2.57	0.51
1:B:91:ILE:HD12	1:B:95:LEU:HB2	1.92	0.51
1:A:434:ASP:HB3	1:A:437:ASP:HB2	1.93	0.50
1:B:137:GLY:HA2	1:B:324:TYR:HA	1.95	0.48
1:A:137:GLY:HA2	1:A:324:TYR:HA	1.96	0.47
1:A:140:ILE:HG22	1:A:211:PHE:HB2	1.96	0.47
1:A:140:ILE:O	1:A:209:SER:HA	2.16	0.46
1:B:130:LEU:HD12	1:B:449:PRO:HG3	1.98	0.46
1:B:101:ASN:HB2	1:B:106:TYR:CE1	2.51	0.45
1:B:502:ILE:HD11	1:B:509:CYS:HB3	1.97	0.45
1:A:125:ALA:HB1	1:A:170:ARG:HB2	1.99	0.45
1:B:200:PHE:CD2	1:B:265:PHE:CZ	2.97	0.44
1:B:19:ILE:O	1:B:53:GLY:HA3	2.18	0.43
1:A:451:LEU:HG	1:A:454:GLN:HE21	1.84	0.43
1:B:425:LYS:HA	1:B:428:ARG:HE	1.84	0.42
1:B:33:ASP:HB3	1:B:36:LEU:HB2	2.02	0.42
1:B:497:LEU:O	1:B:522:CYS:HB2	2.20	0.41
1:B:463:ILE:HD11	1:B:477:LEU:HD12	2.01	0.41
1:A:425:LYS:HG2	1:A:428:ARG:HH22	1.86	0.40
1:B:203:ILE:HD11	1:B:337:VAL:HG21	2.03	0.40
1:B:467:ILE:HG13	1:B:470:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	457/529 (86%)	444 (97%)	12 (3%)	1 (0%)	44	52
1	B	435/529 (82%)	428 (98%)	7 (2%)	0	100	100
All	All	892/1058 (84%)	872 (98%)	19 (2%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	GLU

### 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	389/469 (83%)	378 (97%)	11 (3%)	38	51
1	B	384/469 (82%)	376 (98%)	8 (2%)	48	63
All	All	773/938 (82%)	754 (98%)	19 (2%)	42	56

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PRO
1	A	94	ARG
1	A	136	TYR
1	A	249	LYS
1	A	348	LYS

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Mol	Chain	Res	Type
1	A	406	ASP
1	A	422	LEU
1	A	430	ASP
1	A	453	SER
1	A	454	GLN
1	A	520	MET
1	B	215	PHE
1	B	253	PHE
1	B	256	LYS
1	B	271	MET
1	B	364	ASP
1	B	401	ASP
1	B	406	ASP
1	B	430	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	GLN

### 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 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
4	NAG	B	603	1	14,14,15	0.43	0	17,19,21	0.29	0
6	BMA	B	605	1	11,11,12	0.53	0	15,15,17	0.61	0
6	BMA	A	605	1	11,11,12	0.43	0	15,15,17	0.39	0
4	NAG	A	603	1	14,14,15	0.37	0	17,19,21	0.29	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
4	NAG	B	603	1	-	3/6/23/26	0/1/1/1
6	BMA	B	605	1	-	1/2/19/22	1/1/1/1
6	BMA	A	605	1	-	2/2/19/22	1/1/1/1
4	NAG	A	603	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	603	NAG	C1-C2-N2-C7
4	A	603	NAG	O5-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6
4	B	603	NAG	C8-C7-N2-C2
4	B	603	NAG	O7-C7-N2-C2
6	A	605	BMA	C4-C5-C6-O6
6	A	605	BMA	O5-C5-C6-O6
6	B	605	BMA	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	605	BMA	C1-C2-C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
6	B	605	BMA	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	NAG	1	0

## 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	465/529 (87%)	0.58	28 (6%)	29 26	44, 70, 104, 144	0
1	B	449/529 (84%)	0.37	31 (6%)	24 22	33, 58, 96, 139	3 (0%)
All	All	914/1058 (86%)	0.48	59 (6%)	26 23	33, 65, 100, 144	3 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	ASP	9.1
1	B	205	ARG	8.7
1	B	16	PRO	5.6
1	B	116	PRO	5.0
1	A	248	PHE	4.8
1	B	184	ALA	4.4
1	A	365	LEU	4.1
1	B	433	PHE	3.9
1	A	364	ASP	3.8
1	B	389	LYS	3.7
1	A	16	PRO	3.4
1	B	204	ASN	3.3
1	A	226	GLU	3.0
1	A	471	TYR	2.9
1	A	526	GLN	2.9
1	A	207	LYS	2.8
1	B	225	PRO	2.8
1	A	200	PHE	2.8
1	B	202	ALA	2.7
1	A	433	PHE	2.7
1	B	363	MET	2.6
1	B	187	SER	2.6
1	B	215	PHE	2.6
1	B	186	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	185	ASP	2.6
1	B	197	LEU	2.6
1	B	526	GLN	2.5
1	B	394	LYS	2.5
1	B	447	ASN	2.5
1	B	121	ARG	2.5
1	B	361	PHE	2.5
1	A	395	THR	2.5
1	B	188	PHE	2.4
1	B	432	THR	2.4
1	A	225	PRO	2.3
1	A	209	SER	2.3
1	B	203	ILE	2.3
1	A	363	MET	2.3
1	A	157	GLY	2.3
1	B	516	MET	2.3
1	A	502	ILE	2.3
1	B	386	GLY	2.3
1	B	250	PHE	2.2
1	A	524	ILE	2.2
1	B	117	ARG	2.2
1	B	113	ASP	2.2
1	B	515	MET	2.2
1	A	81	ASN	2.1
1	A	515	MET	2.1
1	A	204	ASN	2.1
1	A	163	ARG	2.1
1	A	215	PHE	2.1
1	A	250	PHE	2.1
1	A	517	PHE	2.1
1	A	75	ILE	2.1
1	A	186	LYS	2.1
1	B	122	ASP	2.0
1	A	386	GLY	2.0
1	A	398	ILE	2.0

## 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 [i](#)

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
4	NAG	A	603	14/15	0.69	0.21	85,97,101,101	0
2	ZN	A	606	1/1	0.71	0.12	174,174,174,174	0
4	NAG	B	603	14/15	0.73	0.21	78,84,90,94	0
5	MG	B	604	1/1	0.79	0.38	94,94,94,94	0
5	MG	A	604	1/1	0.83	0.11	71,71,71,71	0
6	BMA	A	605	11/12	0.84	0.10	73,80,82,83	0
6	BMA	B	605	11/12	0.84	0.14	47,53,56,59	0
2	ZN	A	601	1/1	0.89	0.10	117,117,117,117	0
2	ZN	B	606	1/1	0.91	0.14	148,148,148,148	0
2	ZN	B	607	1/1	0.96	0.08	99,99,99,99	0
2	ZN	B	601	1/1	0.97	0.05	106,106,106,106	0
3	CA	A	602	1/1	0.97	0.07	65,65,65,65	0
3	CA	B	602	1/1	1.00	0.02	49,49,49,49	0

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

There are no such residues in this entry.