



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 06:31 PM EDT

PDB ID : 9C9K / pdb\_00009c9k  
Title : Anti-OspA Fab 319-33  
Authors : Rudolph, M.J.; Mantis, N.  
Deposited on : 2024-06-14  
Resolution : 1.60 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

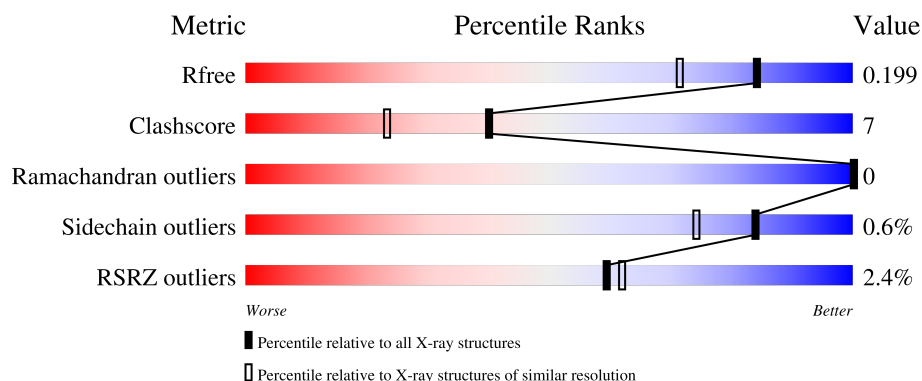
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

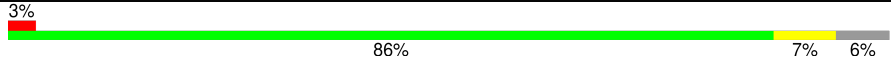
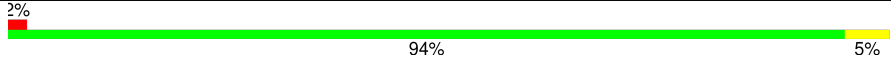
The reported resolution of this entry is 1.60 Å.

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	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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	H	223	
2	L	215	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	H	319	-	-	X	-
4	CL	H	320	-	-	X	-
4	CL	H	322	-	-	X	-
4	CL	H	324	-	-	X	-
4	CL	L	316	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6946 atoms, of which 3193 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 319-33 monoclonal Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	209	Total	C	H	N	O	S	0	7	0
			3196	1029	1582	266	309	10			

- Molecule 2 is a protein called 319-33 monoclonal Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	214	Total	C	H	N	O	S	0	8	0
			3273	1035	1611	280	340	7			

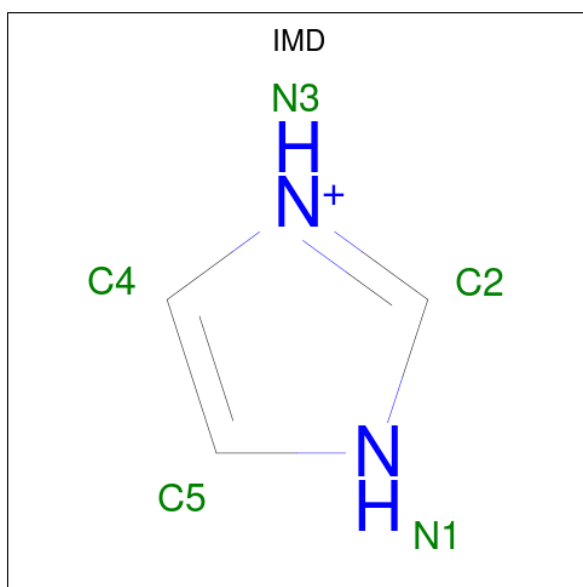
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	8	Total	Zn	0	0
			8	8		
3	L	13	Total	Zn	0	0
			13	13		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	17	Total	Cl	0	0
			17	17		
4	L	18	Total	Cl	0	0
			18	18		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	N	0	0
			5	3	2		
5	H	1	Total	C	N	0	0
			5	3	2		
5	L	1	Total	C	N	0	0
			5	3	2		
5	L	1	Total	C	N	0	0
			5	3	2		
5	L	1	Total	C	N	0	0
			5	3	2		
5	L	1	Total	C	N	0	0
			5	3	2		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			4	2	2		

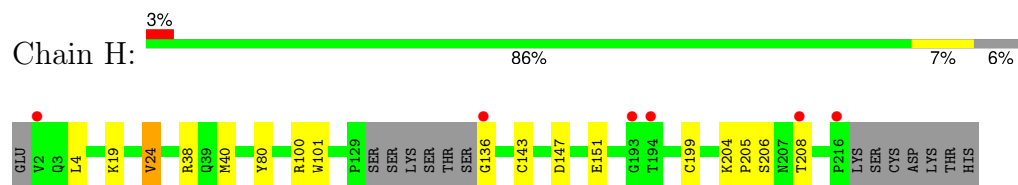
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	175	Total	O	0	0
			175	175		
7	L	207	Total	O	0	0
			207	207		

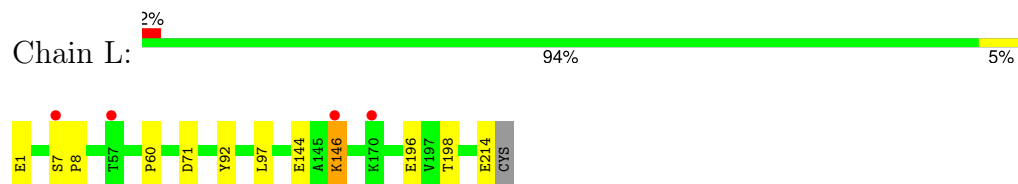
### 3 Residue-property plots [i](#)

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: 319-33 monoclonal Fab Heavy Chain



- Molecule 2: 319-33 monoclonal Fab Light Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.75Å 121.75Å 67.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 1.60 45.17 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.17-1.60) 99.8 (45.17-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.172 , 0.200 0.173 , 0.199	Depositor DCC
$R_{free}$ test set	3294 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: IMD, CL, ZN, EDO

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	H	0.37	0/1680	0.59	0/2288
2	L	0.41	0/1738	0.61	0/2358
All	All	0.39	0/3418	0.60	0/4646

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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### 5.2 Torsion angles [i](#)

#### 5.2.1 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	H	212/223 (95%)	207 (98%)	5 (2%)	0	100	100
2	L	220/215 (102%)	217 (99%)	3 (1%)	0	100	100
All	All	432/438 (99%)	424 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.2.2 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	H	184/192 (96%)	183 (100%)	1 (0%)	86	78
2	L	193/186 (104%)	192 (100%)	1 (0%)	86	78
All	All	377/378 (100%)	375 (100%)	2 (0%)	84	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	24	VAL
2	L	146	LYS

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

Mol	Chain	Res	Type
1	H	82	GLN
2	L	161	GLN

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.4 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.5 Ligand geometry

Of 64 ligands modelled in this entry, 56 are monoatomic - leaving 8 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	$\# Z  > 2$
5	IMD	H	327	3	3,5,5	0.42	0	4,5,5	0.79	0
5	IMD	L	332	3	3,5,5	0.38	0	4,5,5	0.75	0
5	IMD	L	333	3	3,5,5	0.39	0	4,5,5	0.58	0
5	IMD	L	334	3	3,5,5	0.39	0	4,5,5	0.74	0
5	IMD	L	336	3	3,5,5	0.40	0	4,5,5	0.58	0
5	IMD	H	326	3	3,5,5	0.43	0	4,5,5	0.47	0
6	EDO	L	337	-	3,3,3	0.44	0	2,2,2	0.45	0
5	IMD	L	335	3	3,5,5	0.37	0	4,5,5	0.66	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
5	IMD	H	327	3	-	-	0/1/1/1
5	IMD	L	332	3	-	-	0/1/1/1
5	IMD	L	333	3	-	-	0/1/1/1
5	IMD	L	334	3	-	-	0/1/1/1
5	IMD	L	336	3	-	-	0/1/1/1
5	IMD	H	326	3	-	-	0/1/1/1
6	EDO	L	337	-	-	1/1/1/1	-
5	IMD	L	335	3	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	337	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Other polymers [i](#)

There are no such residues in this entry.

## 5.7 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	H	209/223 (93%)	-0.04	6 (2%) 54 54	10, 33, 59, 79	4 (1%)
2	L	214/215 (99%)	-0.35	4 (1%) 66 68	8, 26, 48, 86	4 (1%)
All	All	423/438 (96%)	-0.20	10 (2%) 59 62	8, 28, 55, 86	8 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	136	GLY	3.9
1	H	193	GLY	3.6
1	H	194	THR	3.0
2	L	146	LYS	2.8
2	L	170	LYS	2.7
2	L	57	THR	2.6
1	H	216	PRO	2.6
1	H	208	THR	2.4
1	H	2	VAL	2.2
2	L	7	SER	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 oligosaccharides in this entry.

## 6.4 Ligands

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	L	337	4/4	0.74	0.40	65,70,73,75	0
5	IMD	L	335	5/5	0.76	0.22	32,40,45,53	0
3	ZN	L	310	1/1	0.77	0.16	88,88,88,88	0
4	CL	H	319	1/1	0.78	0.19	75,75,75,75	0
3	ZN	L	309	1/1	0.82	0.14	91,91,91,91	0
4	CL	L	318	1/1	0.84	0.18	59,59,59,59	0
4	CL	L	326	1/1	0.86	0.15	57,57,57,57	0
4	CL	H	313	1/1	0.86	0.23	70,70,70,70	0
4	CL	L	324	1/1	0.86	0.19	74,74,74,74	0
4	CL	L	327	1/1	0.87	0.21	68,68,68,68	0
5	IMD	H	327	5/5	0.87	0.23	42,43,63,69	0
4	CL	H	311	1/1	0.87	0.15	53,53,53,53	0
4	CL	H	315	1/1	0.87	0.16	66,66,66,66	0
4	CL	L	317	1/1	0.88	0.11	61,61,61,61	0
4	CL	H	316	1/1	0.88	0.11	62,62,62,62	0
3	ZN	H	305	1/1	0.90	0.11	55,55,55,55	0
4	CL	H	317	1/1	0.90	0.15	46,46,46,46	0
3	ZN	H	307	1/1	0.90	0.11	62,62,62,62	0
4	CL	H	322	1/1	0.90	0.16	53,53,53,53	0
4	CL	H	324	1/1	0.90	0.23	52,52,52,52	0
4	CL	L	316	1/1	0.90	0.32	61,61,61,61	0
5	IMD	L	336	5/5	0.90	0.20	50,54,58,61	0
4	CL	H	310	1/1	0.90	0.19	51,51,51,51	0
4	CL	L	329	1/1	0.91	0.18	57,57,57,57	0
4	CL	H	321	1/1	0.92	0.16	55,55,55,55	0
3	ZN	L	313	1/1	0.94	0.09	69,69,69,69	0
4	CL	H	320	1/1	0.94	0.09	43,43,43,43	0
4	CL	H	323	1/1	0.94	0.19	45,45,45,45	0
4	CL	L	328	1/1	0.95	0.07	44,44,44,44	0
4	CL	H	309	1/1	0.95	0.10	46,46,46,46	0
4	CL	L	330	1/1	0.95	0.12	33,33,33,33	0
4	CL	H	314	1/1	0.95	0.12	57,57,57,57	0
5	IMD	L	333	5/5	0.95	0.08	22,23,24,26	0
3	ZN	L	311	1/1	0.95	0.07	36,36,36,36	1
4	CL	H	325	1/1	0.95	0.09	54,54,54,54	0
3	ZN	H	306	1/1	0.95	0.13	62,62,62,62	0
5	IMD	H	326	5/5	0.96	0.07	30,31,35,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	IMD	L	332	5/5	0.96	0.08	21,23,28,28	0
3	ZN	H	304	1/1	0.97	0.06	37,37,37,37	0
4	CL	L	322	1/1	0.97	0.09	36,36,36,36	0
5	IMD	L	334	5/5	0.97	0.08	24,25,29,34	0
4	CL	L	315	1/1	0.97	0.06	29,29,29,29	0
3	ZN	H	308	1/1	0.97	0.06	41,41,41,41	1
4	CL	H	318	1/1	0.97	0.11	45,45,45,45	0
3	ZN	L	312	1/1	0.98	0.03	27,27,27,27	1
3	ZN	L	307	1/1	0.98	0.03	31,31,31,31	1
4	CL	L	319	1/1	0.98	0.05	31,31,31,31	0
4	CL	L	320	1/1	0.98	0.05	22,22,22,22	1
3	ZN	L	308	1/1	0.98	0.12	49,49,49,49	0
3	ZN	H	301	1/1	0.98	0.05	31,31,31,31	0
4	CL	L	325	1/1	0.98	0.06	28,28,28,28	0
3	ZN	L	302	1/1	0.98	0.05	26,26,26,26	1
4	CL	H	312	1/1	0.98	0.05	29,29,29,29	0
3	ZN	L	304	1/1	0.98	0.04	33,33,33,33	1
3	ZN	L	303	1/1	0.99	0.04	25,25,25,25	1
4	CL	L	321	1/1	0.99	0.05	22,22,22,22	0
3	ZN	H	303	1/1	0.99	0.02	21,21,21,21	1
3	ZN	L	305	1/1	0.99	0.02	23,23,23,23	1
3	ZN	L	306	1/1	0.99	0.02	21,21,21,21	1
4	CL	L	314	1/1	0.99	0.04	28,28,28,28	0
3	ZN	L	301	1/1	1.00	0.04	25,25,25,25	0
4	CL	L	323	1/1	1.00	0.02	16,16,16,16	0
3	ZN	H	302	1/1	1.00	0.04	25,25,25,25	0
4	CL	L	331	1/1	1.00	0.10	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.