



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 11, 2018 – 12:31 AM EST

PDB ID : 5NCD  
Title : Crystal structure of the polysaccharide deacetylase Bc1974 from *Bacillus cereus* in complex with (2S)-2-amino-5-(diaminomethylideneamino)-N-hydroxypentamide  
Authors : Giastas, P.; Andreou, A.; Eliopoulos, E.E.  
Deposited on : 2017-03-03  
Resolution : 2.45 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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
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

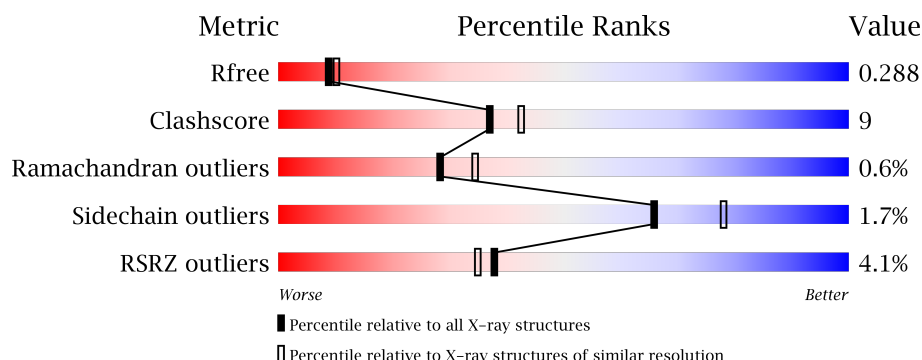
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1152 (2.46-2.42)
Clashscore	112137	1224 (2.46-2.42)
Ramachandran outliers	110173	1217 (2.46-2.42)
Sidechain outliers	110143	1217 (2.46-2.42)
RSRZ outliers	101464	1158 (2.46-2.42)

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	247	<div> <div>3%</div> <div>68%</div> <div>14%</div> <div>••</div> <div>17%</div> </div>
1	B	247	<div> <div>%</div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div>
1	C	247	<div> <div>8%</div> <div>65%</div> <div>18%</div> <div></div> <div>17%</div> </div>
1	D	247	<div> <div>2%</div> <div>67%</div> <div>16%</div> <div></div> <div>17%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CIT	B	303	-	-	-	X

## 2 Entry composition [i](#)

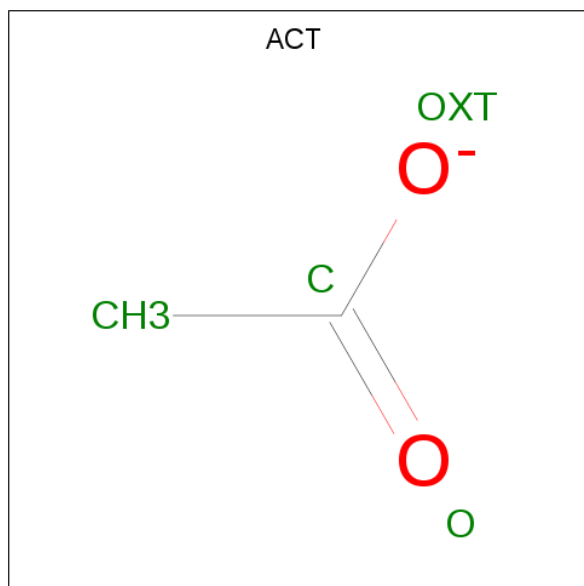
There are 6 unique types of molecules in this entry. The entry contains 6798 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptidoglycan N-acetylglucosamine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1651	1057	284	303	7			
1	B	206	Total	C	N	O	S	0	0	0
			1651	1057	284	303	7			
1	C	206	Total	C	N	O	S	0	0	0
			1645	1054	281	303	7			
1	D	206	Total	C	N	O	S	0	2	0
			1664	1066	286	305	7			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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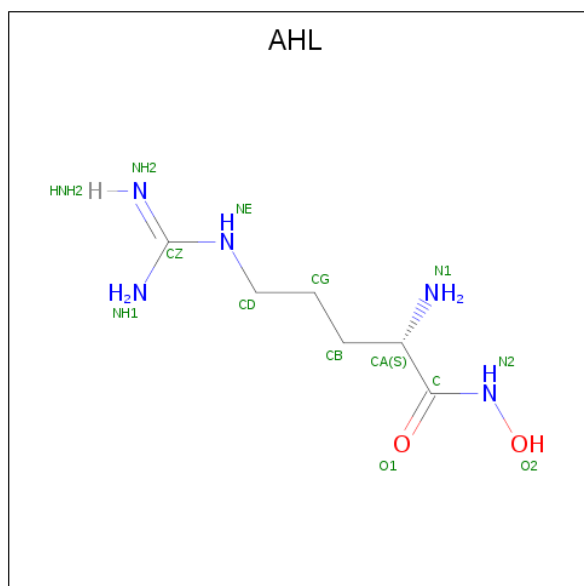
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

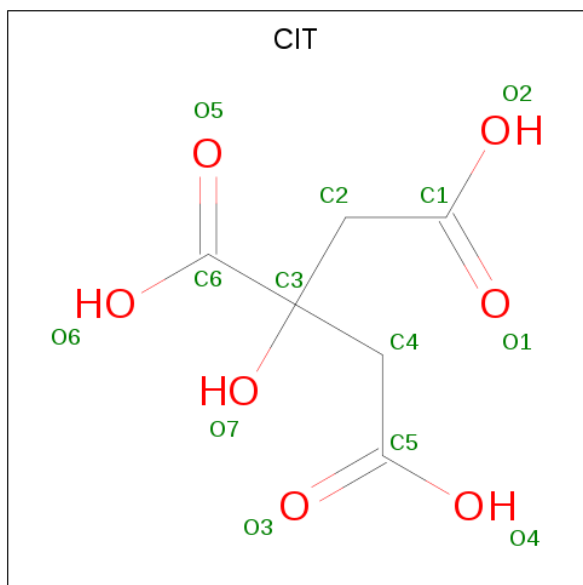
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-HYDROXY-L-ARGININAMIDE (three-letter code: AHL) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			13	6	5	2		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	B	45	Total	O	0	0
			45	45		
6	C	30	Total	O	0	0
			30	30		
6	D	31	Total	O	0	0
			31	31		



M273	YL13	PHE
	R144 R145	GLN SER
E119		ILE
	H126	THR SER
H130		PRO
		ALA
Q149		LYS
		VAL
K158		ALA
	S159	LYS
P160		GLN
		GLU
R164		ASN
	P165	VAL
P166		VAL
		GLN
S169		LEU
	M170	ALA
P171		SER
	G172	GLU
L173		GLN
		PRO
M179		LYS
	K180	VAL
V181		GLU
	V182	MET
E183		ASN
		LYS
D190		THR
		ALA
D197		PRO
		SER
Y200		ARG
	M203	PHE
D206		ASN
	L207	GLY
A208		LYS
		GLU
I212		R68
		R69
D231		Y72
	I232	K31
R233		R32
		T33
S236		N38
K245		K31
	G246	
L247		F99
	K248	F100
E249		L101
F254		D111
		L112



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.65Å 117.44Å 99.49Å 90.00° 102.92° 90.00°	Depositor
Resolution (Å)	48.48 – 2.45 48.48 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.48-2.45) 98.4 (48.48-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.226 , 0.292 0.221 , 0.288	Depositor DCC
$R_{free}$ test set	2080 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6798	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.13% 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: ZN, ACT, AHL, CIT

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	0.45	0/1696	0.62	0/2295
1	B	0.45	0/1696	0.60	1/2295 (0.0%)
1	C	0.44	0/1690	0.58	0/2288
1	D	0.43	0/1716	0.56	0/2322
All	All	0.44	0/6798	0.59	1/9200 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ASP	CB-CG-OD1	5.05	122.84	118.30

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	1651	0	1611	30	0
1	B	1651	0	1611	31	0
1	C	1645	0	1600	27	0
1	D	1664	0	1624	29	0
2	A	4	0	3	0	0
2	C	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4	0	3	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	B	13	0	14	4	0
5	B	13	0	5	2	0
6	A	39	0	0	2	0
6	B	45	0	0	6	0
6	C	30	0	0	0	0
6	D	31	0	0	2	0
All	All	6798	0	6474	117	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 9.

The worst 5 of 117 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:128:MET:SD	6:B:408:HOH:O	2.14	1.05
1:C:117:ASN:HD22	1:C:156:ILE:HB	1.32	0.91
1:A:69:LYS:HB2	1:A:252:TYR:HA	1.66	0.76
1:B:228:LEU:HD21	4:B:301:AHN:N1	2.02	0.74
1:C:88:ASN:OD1	1:C:115:ARG:NH2	2.20	0.74

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	204/247 (83%)	193 (95%)	9 (4%)	2 (1%)	18 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	204/247 (83%)	194 (95%)	10 (5%)	0	100	100
1	C	204/247 (83%)	193 (95%)	8 (4%)	3 (2%)	12	11
1	D	206/247 (83%)	194 (94%)	12 (6%)	0	100	100
All	All	818/988 (83%)	774 (95%)	39 (5%)	5 (1%)	28	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	127	SER
1	C	190	ASP
1	C	241	PRO
1	C	204	PRO

### 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	173/208 (83%)	167 (96%)	6 (4%)	41	56
1	B	173/208 (83%)	170 (98%)	3 (2%)	66	78
1	C	172/208 (83%)	170 (99%)	2 (1%)	75	85
1	D	175/208 (84%)	174 (99%)	1 (1%)	89	93
All	All	693/832 (83%)	681 (98%)	12 (2%)	66	78

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	GLU
1	B	189	TRP
1	C	189	TRP
1	A	245	LYS
1	B	266	ASN

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

Mol	Chain	Res	Type
1	B	266	ASN
1	C	117	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
2	ACT	A	301	3	1,3,3	2.21	1 (100%)	0,3,3	0.00	-
4	AHL	B	301	3	12,12,12	0.97	2 (16%)	10,14,14	0.64	0
5	CIT	B	303	-	3,12,12	1.25	0	3,17,17	2.23	2 (66%)
2	ACT	C	301	3	1,3,3	1.73	0	0,3,3	0.00	-
2	ACT	D	301	3	1,3,3	2.26	1 (100%)	0,3,3	0.00	-

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
2	ACT	A	301	3	-	0/0/0/0	0/0/0/0
4	AHL	B	301	3	-	0/13/13/13	0/0/0/0
5	CIT	B	303	-	-	0/6/16/16	0/0/0/0
2	ACT	C	301	3	-	0/0/0/0	0/0/0/0
2	ACT	D	301	3	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	AHL	CZ-NH1	-2.01	1.26	1.34
2	A	301	ACT	CH3-C	2.21	1.51	1.48
2	D	301	ACT	CH3-C	2.26	1.51	1.48
4	B	301	AHL	CZ-NH2	2.50	1.42	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	303	CIT	C3-C4-C5	-3.04	110.20	114.95
5	B	303	CIT	C3-C2-C1	2.30	118.54	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	AHL	4	0
5	B	303	CIT	2	0
2	C	301	ACT	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 [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	206/247 (83%)	0.60	8 (3%) 40 36	37, 58, 93, 140	0
1	B	206/247 (83%)	0.48	3 (1%) 74 72	34, 55, 74, 112	0
1	C	206/247 (83%)	0.75	19 (9%) 10 8	39, 60, 96, 113	0
1	D	206/247 (83%)	0.55	4 (1%) 67 64	32, 54, 72, 104	0
All	All	824/988 (83%)	0.59	34 (4%) 38 35	32, 57, 92, 140	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ARG	4.2
1	C	204	PRO	3.5
1	C	245	LYS	3.4
1	A	197	ASP	3.2
1	C	252	TYR	3.1

### 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 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
5	CIT	B	303	13/13	0.78	0.28	3.12	74,85,93,96	0
3	ZN	C	302	1/1	0.95	0.24	1.82	79,79,79,79	0
2	ACT	D	301	4/4	0.83	0.21	1.68	52,54,60,63	0
4	AHL	B	301	13/13	0.90	0.23	1.12	53,65,80,82	0
3	ZN	B	302	1/1	0.98	0.23	1.06	79,79,79,79	0
2	ACT	A	301	4/4	0.89	0.20	0.41	50,56,63,65	0
3	ZN	D	302	1/1	0.98	0.17	-0.19	76,76,76,76	0
2	ACT	C	301	4/4	0.90	0.17	-0.73	44,55,59,60	0
3	ZN	A	302	1/1	0.94	0.12	-2.50	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.