



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2017 – 12:33 PM EDT

PDB ID : 1QIQ  
Title : ISOPENICILLIN N SYNTHASE FROM ASPERGILLUS NIDULANS  
(ACmC Fe COMPLEX)  
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Deposited on : 1999-06-15  
Resolution : 1.50 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

<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-20029077  
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-20029077

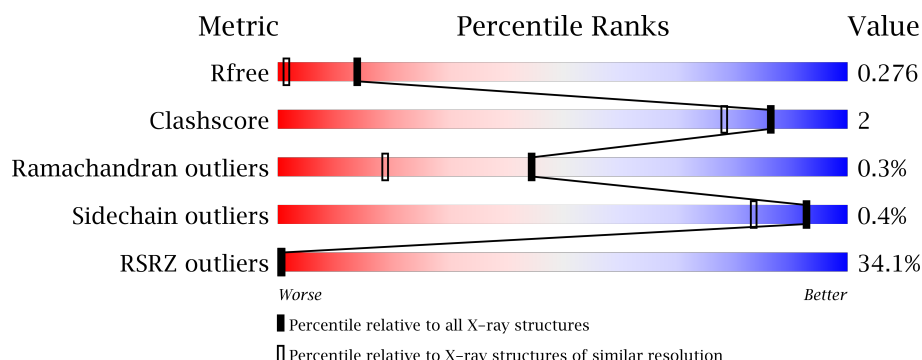
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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	331	<div> <div>34%</div> <div>92%</div> <div>7% ..</div> </div>

## 2 Entry composition [i](#)

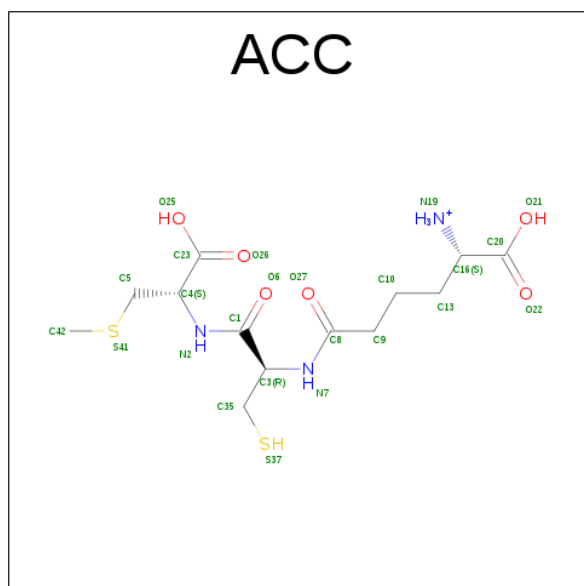
There are 5 unique types of molecules in this entry. The entry contains 3091 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ISOPENICILLIN N SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	5	0
			2651	1693	445	508	5			

- Molecule 2 is N-[N-[2-AMINO-6-OXO-HEXANOIC ACID-6-YL]CYSTEINYL]-S-METHYL CYSTEINE (three-letter code: ACC) (formula: C<sub>13</sub>H<sub>24</sub>N<sub>3</sub>O<sub>6</sub>S<sub>2</sub>).



- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

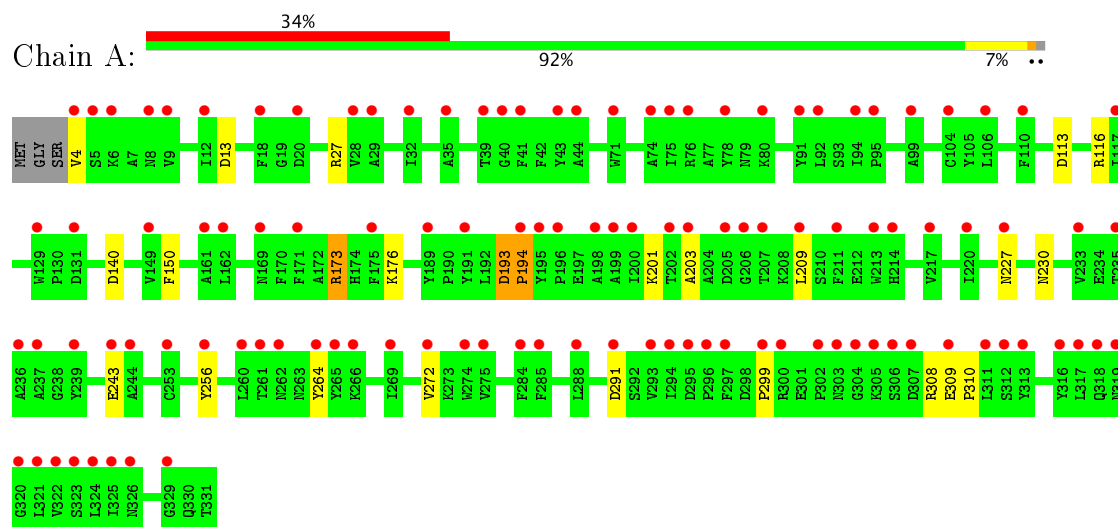
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	410	Total	O	0	0
			410	410		

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

These plots are drawn for all protein, RNA and DNA 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: ISOPENICILLIN N SYNTHASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.81Å 71.66Å 101.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.50 11.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	89.7 (25.00-1.50) 89.2 (11.99-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.173 , 0.199 0.277 , 0.276	Depositor DCC
$R_{free}$ test set	1961 reflections (4.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.0	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 72.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% 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: ACC, FE, SO4

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	0.59	0/2751	1.14	12/3744 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	CD-NE-CZ	16.22	146.30	123.60
1	A	194	PRO	N-CA-CB	8.12	113.04	103.30
1	A	27	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	A	193	ASP	CA-C-O	-7.92	103.47	120.10
1	A	194	PRO	CA-N-CD	-7.72	100.70	111.50
1	A	308	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	A	308	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	113	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	13	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	27	ARG	CD-NE-CZ	5.64	131.50	123.60
1	A	150	PHE	CB-CG-CD2	5.22	124.45	120.80
1	A	176	LYS	CA-CB-CG	5.21	124.86	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	ASP	Mainchain,Peptide

## 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	A	2651	0	2535	13	0
2	A	24	0	21	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	410	0	0	8	0
All	All	3091	0	2556	13	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 (13) 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:243[B]:GLU:CD	5:A:2317:HOH:O	2.02	0.98
1:A:291[B]:ASP:OD1	5:A:2358:HOH:O	1.82	0.97
1:A:256:TYR:HA	5:A:2332:HOH:O	1.89	0.73
1:A:243[B]:GLU:CG	5:A:2317:HOH:O	2.57	0.46
1:A:230:ASN:HD22	1:A:272:VAL:HG13	1.81	0.45
1:A:4:VAL:N	5:A:2002:HOH:O	2.50	0.44
1:A:201:LYS:HB3	5:A:2121:HOH:O	2.18	0.42
1:A:116:ARG:NH2	1:A:291[B]:ASP:OD2	2.51	0.42
1:A:309:GLU:HA	1:A:310:PRO:HD3	1.92	0.42
1:A:203:ALA:HB2	1:A:209:LEU:HD11	2.01	0.42
1:A:264:TYR:CD2	1:A:299:PRO:HG2	2.55	0.42
1:A:140:ASP:HB3	5:A:3002:HOH:O	2.20	0.42
1:A:173:ARG:NH2	5:A:2253:HOH:O	2.52	0.41

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	331/331 (100%)	319 (96%)	11 (3%)	1 (0%)	44 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	PRO

### 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	A	287/284 (101%)	286 (100%)	1 (0%)	94 86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	225	GLN
1	A	227	ASN
1	A	230	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	ACC	A	332	3	15,23,23	0.68	0	17,29,29	1.16	1 (5%)
4	SO4	A	334	-	4,4,4	0.64	0	6,6,6	0.42	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
2	ACC	A	332	3	-	0/23/31/31	0/0/0/0
4	SO4	A	334	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	332	ACC	C35-C3-N7	-3.63	106.14	111.39

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 [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	328/331 (99%)	1.72	112 (34%) 0 1	6, 11, 24, 30	1 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	VAL	6.1
1	A	307	ASP	4.3
1	A	296	PRO	4.3
1	A	306	SER	4.3
1	A	198	ALA	4.2
1	A	202	THR	4.1
1	A	239	TYR	4.0
1	A	325	ILE	3.9
1	A	209	LEU	3.7
1	A	264	TYR	3.7
1	A	293[A]	VAL	3.7
1	A	213	TRP	3.6
1	A	260	LEU	3.6
1	A	236	ALA	3.6
1	A	237	ALA	3.5
1	A	76	ARG	3.5
1	A	297	PHE	3.4
1	A	305	LYS	3.4
1	A	211	PHE	3.4
1	A	319	ASN	3.3
1	A	295	ASP	3.3
1	A	311	LEU	3.3
1	A	261	THR	3.2
1	A	94	ILE	3.2
1	A	117	ILE	3.2
1	A	322	VAL	3.2
1	A	110	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	274	TRP	3.1
1	A	265	TYR	3.1
1	A	220	ILE	3.0
1	A	324	LEU	3.0
1	A	207	THR	3.0
1	A	9	VAL	3.0
1	A	291[A]	ASP	3.0
1	A	169	ASN	3.0
1	A	39	THR	3.0
1	A	203	ALA	2.9
1	A	20	ASP	2.9
1	A	8	ASN	2.9
1	A	302	PRO	2.9
1	A	71	TRP	2.9
1	A	303	ASN	2.8
1	A	284	PHE	2.8
1	A	5	SER	2.8
1	A	275[A]	VAL	2.7
1	A	206	GLY	2.7
1	A	12	ILE	2.7
1	A	214	HIS	2.7
1	A	294	ILE	2.7
1	A	235	THR	2.7
1	A	6	LYS	2.7
1	A	313	TYR	2.6
1	A	316	TYR	2.6
1	A	40	GLY	2.6
1	A	243[A]	GLU	2.6
1	A	200	ILE	2.6
1	A	129	TRP	2.6
1	A	189	TYR	2.6
1	A	321	LEU	2.6
1	A	227	ASN	2.6
1	A	196	PRO	2.6
1	A	75	ILE	2.6
1	A	320	GLY	2.5
1	A	32	ILE	2.5
1	A	285	PHE	2.5
1	A	323	SER	2.5
1	A	326	ASN	2.5
1	A	80	LYS	2.5
1	A	162	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	256	TYR	2.5
1	A	205	ASP	2.4
1	A	288	LEU	2.4
1	A	28	VAL	2.4
1	A	195	TYR	2.4
1	A	299	PRO	2.4
1	A	161	ALA	2.4
1	A	253	CYS	2.4
1	A	318	GLN	2.4
1	A	269	ILE	2.4
1	A	317	LEU	2.4
1	A	312	SER	2.3
1	A	233	VAL	2.3
1	A	29	ALA	2.3
1	A	41	PHE	2.3
1	A	91	TYR	2.3
1	A	191	TYR	2.3
1	A	95	PRO	2.3
1	A	92	LEU	2.3
1	A	309	GLU	2.3
1	A	329	GLY	2.3
1	A	35	ALA	2.2
1	A	266	LYS	2.2
1	A	131	ASP	2.2
1	A	199	ALA	2.2
1	A	18	PHE	2.2
1	A	171	PHE	2.2
1	A	175	PHE	2.2
1	A	44	ALA	2.2
1	A	74	ALA	2.2
1	A	262	ASN	2.2
1	A	106	LEU	2.1
1	A	304	GLY	2.1
1	A	194	PRO	2.1
1	A	149	VAL	2.1
1	A	300	ARG	2.1
1	A	78	TYR	2.1
1	A	104	CYS	2.1
1	A	43	TYR	2.0
1	A	217	VAL	2.0
1	A	272	VAL	2.0
1	A	99	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	244	ALA	2.0

## 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(Å <sup>2</sup> )	Q<0.9
2	ACC	A	332	24/24	0.87	0.16	0.09	7,9,11,12	0
3	FE	A	333	1/1	0.86	0.14	-	8,8,8,8	0
4	SO4	A	334	5/5	0.82	0.24	-	24,24,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.