



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TJW  
Title : Crystal Structure of T161D Duck Delta 2 Crystallin Mutant with bound argininosuccinate  
Authors : Sampaleanu, L.M.; Coddling, P.W.; Lobsanov, Y.D.; Tsai, M.; Smith, G.D.; Horvatin, C.; Howell, P.L.  
Deposited on : 2004-06-07  
Resolution : 2.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

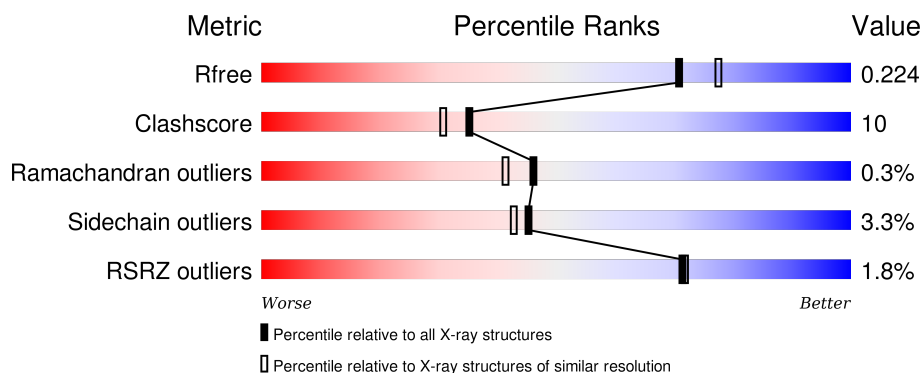
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	474	
1	B	474	
1	C	474	
1	D	474	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14819 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 Delta crystallin II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3464	2195	588	669	12			
1	B	448	Total	C	N	O	S	0	0	0
			3441	2179	581	669	12			
1	C	449	Total	C	N	O	S	0	0	0
			3456	2190	585	669	12			
1	D	449	Total	C	N	O	S	0	0	0
			3468	2194	586	676	12			

There are 28 discrepancies between the modelled and reference sequences:

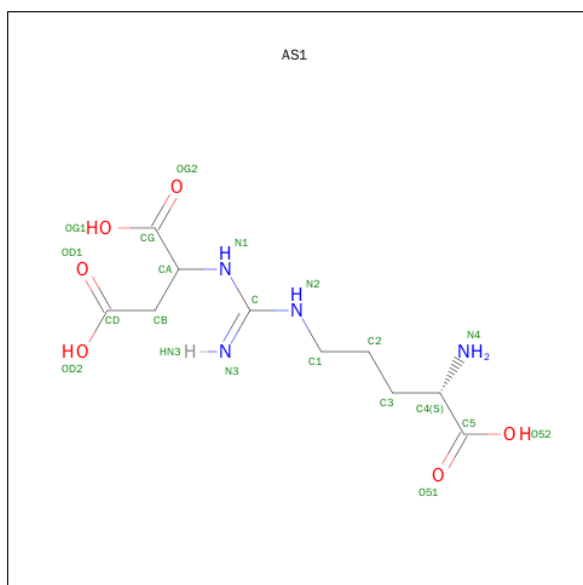
Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ASP	THR	ENGINEERED	UNP P24058
B	161	ASP	THR	ENGINEERED	UNP P24058
C	161	ASP	THR	ENGINEERED	UNP P24058
D	161	ASP	THR	ENGINEERED	UNP P24058
A	469	HIS	-	EXPRESSION TAG	UNP P24058
A	470	HIS	-	EXPRESSION TAG	UNP P24058
A	471	HIS	-	EXPRESSION TAG	UNP P24058
A	472	HIS	-	EXPRESSION TAG	UNP P24058
A	473	HIS	-	EXPRESSION TAG	UNP P24058
A	474	HIS	-	EXPRESSION TAG	UNP P24058
B	469	HIS	-	EXPRESSION TAG	UNP P24058
B	470	HIS	-	EXPRESSION TAG	UNP P24058
B	471	HIS	-	EXPRESSION TAG	UNP P24058
B	472	HIS	-	EXPRESSION TAG	UNP P24058
B	473	HIS	-	EXPRESSION TAG	UNP P24058
B	474	HIS	-	EXPRESSION TAG	UNP P24058
C	469	HIS	-	EXPRESSION TAG	UNP P24058
C	470	HIS	-	EXPRESSION TAG	UNP P24058
C	471	HIS	-	EXPRESSION TAG	UNP P24058
C	472	HIS	-	EXPRESSION TAG	UNP P24058
C	473	HIS	-	EXPRESSION TAG	UNP P24058

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Chain	Residue	Modelled	Actual	Comment	Reference
C	474	HIS	-	EXPRESSION TAG	UNP P24058
D	469	HIS	-	EXPRESSION TAG	UNP P24058
D	470	HIS	-	EXPRESSION TAG	UNP P24058
D	471	HIS	-	EXPRESSION TAG	UNP P24058
D	472	HIS	-	EXPRESSION TAG	UNP P24058
D	473	HIS	-	EXPRESSION TAG	UNP P24058
D	474	HIS	-	EXPRESSION TAG	UNP P24058

- Molecule 2 is ARGININOSUCCINATE (three-letter code: AS1) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			20	10	4	6		
2	D	1	Total	C	N	O	0	0
			20	10	4	6		
2	B	1	Total	C	N	O	0	0
			20	10	4	6		
2	A	1	Total	C	N	O	0	0
			20	10	4	6		

- Molecule 3 is water.

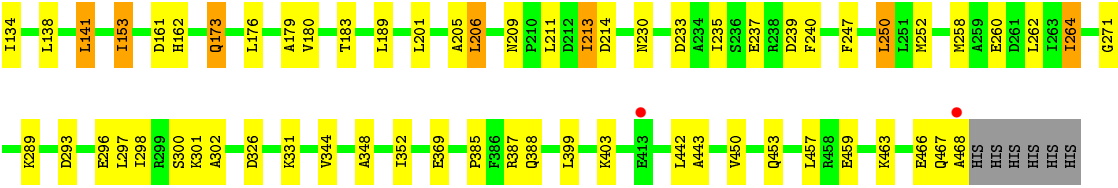
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	253	Total	O	0	0
			253	253		
3	B	196	Total	O	0	0
			196	196		

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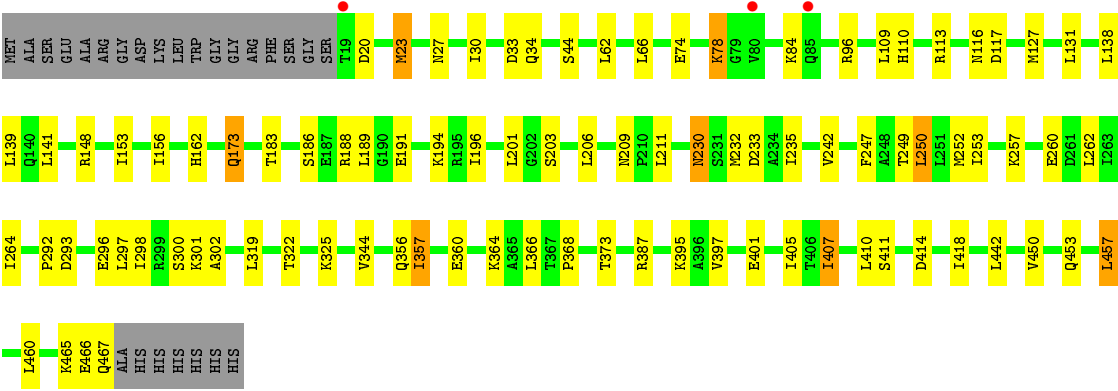
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	258	Total 258	O 258	0	0
3	D	203	Total 203	O 203	0	0





● Molecule 1: Delta crystallin II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.00 Å 98.81 Å 106.39 Å 90.00° 101.34° 90.00°	Depositor
Resolution (Å)	41.76 – 2.00 41.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.76-2.00) 99.7 (41.76-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.00 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.190 , 0.225 0.190 , 0.224	Depositor DCC
$R_{free}$ test set	12766 reflections (9.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 128294 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14819	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 3.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AS1

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	0/3509	0.62	0/4733
1	B	0.41	0/3486	0.60	0/4708
1	C	0.44	0/3501	0.62	0/4727
1	D	0.43	0/3513	0.61	0/4743
All	All	0.43	0/14009	0.61	0/18911

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	B	2	0
1	D	1	0
All	All	3	0

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	105	ILE	CB
1	B	405	ILE	CB
1	D	105	ILE	CB

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	A	3464	0	3570	64	0
1	B	3441	0	3512	76	0
1	C	3456	0	3545	72	0
1	D	3468	0	3547	75	0
2	A	20	0	14	1	0
2	B	20	0	14	0	0
2	C	20	0	14	1	0
2	D	20	0	14	1	0
3	A	253	0	0	8	0
3	B	196	0	0	5	0
3	C	258	0	0	8	0
3	D	203	0	0	5	0
All	All	14819	0	14230	276	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 10.

The worst 5 of 276 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:102:ILE:HD11	1:B:106:ALA:HB2	1.42	1.00
1:A:110:HIS:HD2	1:A:113:ARG:HE	1.16	0.93
1:A:30:ILE:O	1:A:34:GLN:HG3	1.69	0.93
1:C:50:ALA:HB1	1:C:213:ILE:HD11	1.50	0.92
1:D:110:HIS:HD2	1:D:113:ARG:HE	1.17	0.92

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	447/474 (94%)	440 (98%)	6 (1%)	1 (0%)	52	48
1	B	446/474 (94%)	438 (98%)	5 (1%)	3 (1%)	26	19
1	C	447/474 (94%)	439 (98%)	7 (2%)	1 (0%)	52	48
1	D	447/474 (94%)	437 (98%)	9 (2%)	1 (0%)	52	48
All	All	1787/1896 (94%)	1754 (98%)	27 (2%)	6 (0%)	46	41

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	LEU
1	B	206	LEU
1	C	206	LEU
1	B	466	GLU
1	D	206	LEU

### 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	386/411 (94%)	374 (97%)	12 (3%)	47	46
1	B	380/411 (92%)	368 (97%)	12 (3%)	46	44
1	C	383/411 (93%)	371 (97%)	12 (3%)	47	46
1	D	386/411 (94%)	372 (96%)	14 (4%)	42	39
All	All	1535/1644 (93%)	1485 (97%)	50 (3%)	45	43

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	407	ILE
1	C	173	GLN
1	D	356	GLN

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Mol	Chain	Res	Type
1	B	465	LYS
1	C	141	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	356	GLN
1	B	464	GLN
1	D	230	ASN
1	B	388	GLN
1	A	209	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	AS1	A	1004	-	10,19,19	0.73	0	9,24,24	1.55	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AS1	B	1003	-	10,19,19	0.78	0	9,24,24	1.27	1 (11%)
2	AS1	C	1001	-	10,19,19	0.85	0	9,24,24	1.14	1 (11%)
2	AS1	D	1002	-	10,19,19	1.07	1 (10%)	9,24,24	1.10	1 (11%)

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	AS1	A	1004	-	-	0/13/23/23	0/0/0/0
2	AS1	B	1003	-	-	0/13/23/23	0/0/0/0
2	AS1	C	1001	-	-	0/13/23/23	0/0/0/0
2	AS1	D	1002	-	-	0/13/23/23	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1002	AS1	CB-CA	2.72	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1002	AS1	CA-N1-C	2.60	127.15	122.06
2	C	1001	AS1	CA-N1-C	2.92	127.78	122.06
2	B	1003	AS1	CA-N1-C	3.18	128.30	122.06
2	A	1004	AS1	CA-N1-C	4.21	130.31	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1004	AS1	1	0
2	C	1001	AS1	1	0
2	D	1002	AS1	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	449/474 (94%)	-0.15	12 (2%) 58 58	10, 19, 41, 55	0
1	B	448/474 (94%)	0.01	11 (2%) 61 61	10, 24, 40, 56	0
1	C	449/474 (94%)	-0.18	7 (1%) 74 75	10, 19, 36, 57	0
1	D	449/474 (94%)	-0.17	3 (0%) 89 89	11, 21, 37, 50	0
All	All	1795/1896 (94%)	-0.12	33 (1%) 71 72	10, 21, 39, 57	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	468	ALA	5.8
1	B	407	ILE	4.0
1	A	405	ILE	3.5
1	B	398	HIS	3.4
1	B	402	THR	3.4

### 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
2	AS1	D	1002	20/20	0.88	0.15	1.73	24,31,38,38	0
2	AS1	B	1003	20/20	0.90	0.14	1.73	15,23,35,37	0
2	AS1	C	1001	20/20	0.91	0.13	0.69	18,30,36,36	0
2	AS1	A	1004	20/20	0.94	0.10	0.16	18,24,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.