



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2018 – 02:58 PM EST

PDB ID : 4JCI  
Title : Crystal structure of csal\_2705, a putative hydroxyproline epimerase from CHROMOHALOBACTER SALEXIGENS (TARGET EFI-506486), SPACE GROUP P212121, unliganded  
Authors : Vetting, M.W.; Toro, R.; Bhosle, R.; Al Obaidi, N.F.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Stead, M.; Hillerich, B.; Love, J.; Seidel, R.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2013-02-21  
Resolution : 1.70 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
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

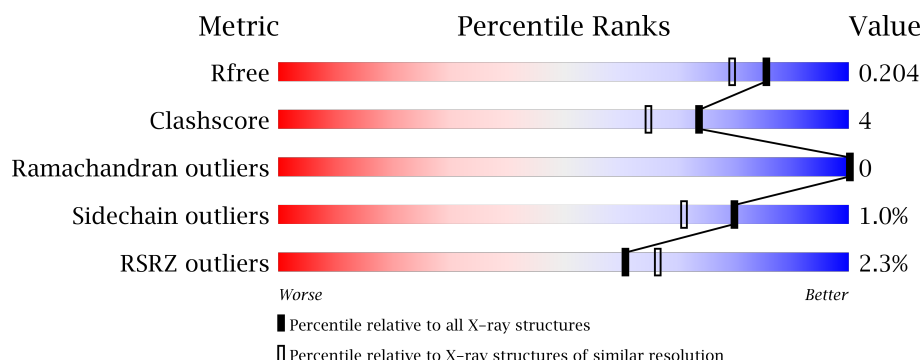
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	333	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	B	333	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9875 atoms, of which 4597 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 Proline racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	H	N	O	S	0	4	0
			4724	1500	2319	434	455	16			
1	B	308	Total	C	H	N	O	S	0	2	0
			4639	1471	2278	427	447	16			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP Q1QU06
A	-20	HIS	-	EXPRESSION TAG	UNP Q1QU06
A	-19	HIS	-	EXPRESSION TAG	UNP Q1QU06
A	-18	HIS	-	EXPRESSION TAG	UNP Q1QU06
A	-17	HIS	-	EXPRESSION TAG	UNP Q1QU06
A	-16	HIS	-	EXPRESSION TAG	UNP Q1QU06
A	-15	HIS	-	EXPRESSION TAG	UNP Q1QU06
A	-14	SER	-	EXPRESSION TAG	UNP Q1QU06
A	-13	SER	-	EXPRESSION TAG	UNP Q1QU06
A	-12	GLY	-	EXPRESSION TAG	UNP Q1QU06
A	-11	VAL	-	EXPRESSION TAG	UNP Q1QU06
A	-10	ASP	-	EXPRESSION TAG	UNP Q1QU06
A	-9	LEU	-	EXPRESSION TAG	UNP Q1QU06
A	-8	GLY	-	EXPRESSION TAG	UNP Q1QU06
A	-7	THR	-	EXPRESSION TAG	UNP Q1QU06
A	-6	GLU	-	EXPRESSION TAG	UNP Q1QU06
A	-5	ASN	-	EXPRESSION TAG	UNP Q1QU06
A	-4	LEU	-	EXPRESSION TAG	UNP Q1QU06
A	-3	TYR	-	EXPRESSION TAG	UNP Q1QU06
A	-2	PHE	-	EXPRESSION TAG	UNP Q1QU06
A	-1	GLN	-	EXPRESSION TAG	UNP Q1QU06
A	0	SER	-	EXPRESSION TAG	UNP Q1QU06
B	-21	MET	-	EXPRESSION TAG	UNP Q1QU06
B	-20	HIS	-	EXPRESSION TAG	UNP Q1QU06
B	-19	HIS	-	EXPRESSION TAG	UNP Q1QU06

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	EXPRESSION TAG	UNP Q1QU06
B	-17	HIS	-	EXPRESSION TAG	UNP Q1QU06
B	-16	HIS	-	EXPRESSION TAG	UNP Q1QU06
B	-15	HIS	-	EXPRESSION TAG	UNP Q1QU06
B	-14	SER	-	EXPRESSION TAG	UNP Q1QU06
B	-13	SER	-	EXPRESSION TAG	UNP Q1QU06
B	-12	GLY	-	EXPRESSION TAG	UNP Q1QU06
B	-11	VAL	-	EXPRESSION TAG	UNP Q1QU06
B	-10	ASP	-	EXPRESSION TAG	UNP Q1QU06
B	-9	LEU	-	EXPRESSION TAG	UNP Q1QU06
B	-8	GLY	-	EXPRESSION TAG	UNP Q1QU06
B	-7	THR	-	EXPRESSION TAG	UNP Q1QU06
B	-6	GLU	-	EXPRESSION TAG	UNP Q1QU06
B	-5	ASN	-	EXPRESSION TAG	UNP Q1QU06
B	-4	LEU	-	EXPRESSION TAG	UNP Q1QU06
B	-3	TYR	-	EXPRESSION TAG	UNP Q1QU06
B	-2	PHE	-	EXPRESSION TAG	UNP Q1QU06
B	-1	GLN	-	EXPRESSION TAG	UNP Q1QU06
B	0	SER	-	EXPRESSION TAG	UNP Q1QU06

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

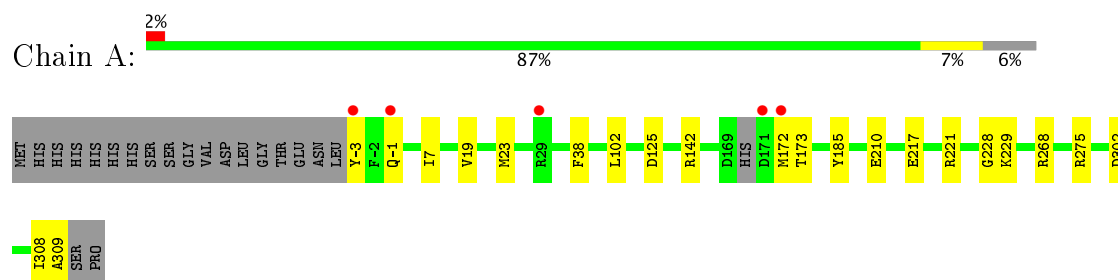
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	284	Total O 297 297	0	13
3	B	210	Total O 214 214	0	4

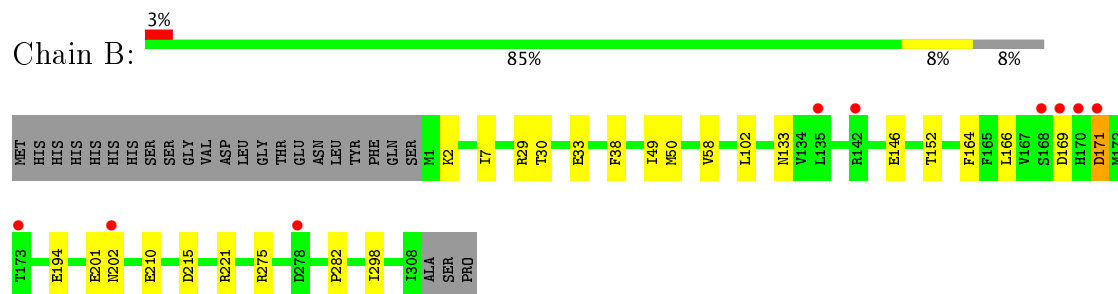
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Proline racemase



#### • Molecule 1: Proline racemase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.09 Å 54.45 Å 253.04 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.94 – 1.70 253.04 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (23.94-1.70) 96.7 (253.04-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 1.70 Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.169 , 0.205 0.169 , 0.204	Depositor DCC
$R_{free}$ test set	3629 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: NA

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	0.55	1/2475 (0.0%)	0.71	1/3358 (0.0%)
1	B	0.52	0/2422	0.67	0/3289
All	All	0.53	1/4897 (0.0%)	0.69	1/6647 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	GLU	CB-CG	-5.07	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ASP	CB-CG-OD1	5.85	123.56	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	THR	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	2405	2319	2297	15	1
1	B	2361	2278	2262	20	0
2	A	1	0	0	0	0
3	A	297	0	0	2	0
3	B	214	0	0	3	0
All	All	5278	4597	4559	35	1

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 4.

All (35) 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:194:GLU:OE1	3:B:502:HOH:O	1.87	0.93
1:A:142:ARG:NH2	3:A:610:HOH:O	2.02	0.93
1:B:201:GLU:O	1:B:202:ASN:OD1	1.98	0.81
1:A:19:VAL:HG11	1:A:23:MET:HG3	1.66	0.77
1:A:19:VAL:HG11	1:A:23:MET:CG	2.16	0.74
1:B:7:ILE:CD1	1:B:102:LEU:HD11	2.20	0.71
1:B:49:ILE:HG22	1:B:50:MET:CE	2.21	0.70
1:A:228:GLY:O	1:A:229:LYS:HG2	1.92	0.69
1:B:275:ARG:NH2	3:B:596:HOH:O	2.28	0.65
1:B:30:THR:HG23	1:B:33:GLU:H	1.62	0.64
1:B:146:GLU:OE2	1:B:152:THR:OG1	2.16	0.64
1:A:-3:TYR:HD2	1:A:-1:GLN:NE2	2.01	0.58
1:B:49:ILE:HG22	1:B:50:MET:HE3	1.85	0.57
1:B:49:ILE:HG22	1:B:50:MET:HE2	1.87	0.55
1:B:166:LEU:HD12	1:B:166:LEU:N	2.23	0.54
1:B:133:ASN:HB3	1:B:282:PRO:HG2	1.89	0.54
1:A:308:ILE:O	1:A:309:ALA:C	2.47	0.52
1:B:7:ILE:HD11	1:B:102:LEU:HD11	1.93	0.49
1:A:217:GLU:CB	1:A:268:ARG:HH12	2.27	0.47
1:A:19:VAL:CG1	1:A:23:MET:HG3	2.41	0.46
1:A:221:ARG:NE	3:A:697:HOH:O	2.49	0.45
1:A:-3:TYR:CD2	1:A:-1:GLN:NE2	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:CG1	1:A:23:MET:CG	2.92	0.43
1:B:58:VAL:HG22	1:B:58:VAL:O	2.17	0.43
1:B:2:LYS:HB2	1:B:298:ILE:HB	2.01	0.43
1:A:217:GLU:HB3	1:A:268:ARG:HH12	1.84	0.42
1:B:58:VAL:HG23	3:B:438:HOH:O	2.19	0.41
1:B:30:THR:CG2	1:B:33:GLU:H	2.32	0.41
1:B:171:ASP:OD2	1:B:171:ASP:N	2.54	0.41
1:B:164:PHE:CD2	1:B:210:GLU:HG3	2.56	0.41
1:A:172:MET:HG3	1:A:185:TYR:CD2	2.56	0.41
1:B:164:PHE:HD2	1:B:210:GLU:HG3	1.86	0.41
1:A:217:GLU:HB2	1:A:268:ARG:NH1	2.36	0.40
1:B:215:ASP:OD2	1:B:221:ARG:NH2	2.52	0.40
1:A:7:ILE:CD1	1:A:102:LEU:HD11	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:OD1	1:A:275[A]:ARG:HH22[3_645]	1.54	0.06

## 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	312/333 (94%)	309 (99%)	3 (1%)	0	100	100
1	B	308/333 (92%)	300 (97%)	8 (3%)	0	100	100
All	All	620/666 (93%)	609 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	251/267 (94%)	250 (100%)	1 (0%)	93	90
1	B	246/267 (92%)	242 (98%)	4 (2%)	68	53
All	All	497/534 (93%)	492 (99%)	5 (1%)	80	71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	PHE
1	B	29	ARG
1	B	38	PHE
1	B	169	ASP
1	B	171	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	312/333 (93%)	-0.12	5 (1%) 72 77	8, 18, 40, 83	0
1	B	308/333 (92%)	-0.07	9 (2%) 52 58	11, 24, 48, 76	0
All	All	620/666 (93%)	-0.09	14 (2%) 61 66	8, 21, 47, 83	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	TYR	8.5
1	A	171	ASP	5.3
1	A	-1	GLN	4.4
1	A	172	MET	4.1
1	B	278	ASP	3.8
1	B	171	ASP	3.5
1	B	168	SER	3.5
1	B	169	ASP	2.9
1	B	202	ASN	2.5
1	B	173	THR	2.4
1	B	142	ARG	2.3
1	A	29	ARG	2.1
1	B	135	LEU	2.1
1	B	170	HIS	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 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	NA	A	401	1/1	0.95	0.07	-0.73	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.