

Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 01:08 am BST

PDB ID : 3DCI

Title: The Structure of a putative arylesterase from Agrobacterium tumefaciens str.

C58

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Deposited on : 2008-06-03

Resolution : 2.00 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

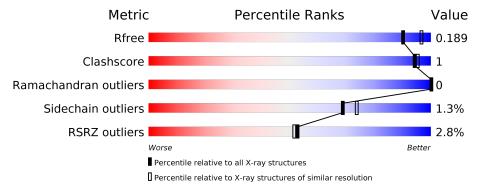
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar resolution} \\ (\#{\rm Entries, resolution range(\AA)}) \end{array}$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 >=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 <=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	232	85%	5%	10%
1	В	232	87%		10%
1	С	232	85%		10%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5138 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 Arylesterase.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace			
1	Λ	208	Total	С	N	О	S	Se	0		0
1	A	200	1548	976	281	281	4	6	0)	U
1	В	208	Total	С	N	О	S	Se	0	9	0
1	Б	200	1542	971	282	279	4	6	0		
1	C	208	Total	С	N	О	S	Se	0	0	0
1		200	1531	964	281	277	4	5	0	0	U

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	expression tag	UNP A9CF87
A	-20	GLY	-	expression tag	UNP A9CF87
A	-19	SER	-	expression tag	UNP A9CF87
A	-18	SER	-	expression tag	UNP A9CF87
A	-17	HIS	-	expression tag	UNP A9CF87
A	-16	HIS	_	expression tag	UNP A9CF87
A	-15	HIS	-	expression tag	UNP A9CF87
A	-14	HIS	-	expression tag	UNP A9CF87
A	-13	HIS	-	expression tag	UNP A9CF87
A	-12	HIS	-	expression tag	UNP A9CF87
A	-11	SER	-	expression tag	UNP A9CF87
A	-10	SER	-	expression tag	UNP A9CF87
A	-9	GLY	-	expression tag	UNP A9CF87
A	-8	ARG	-	expression tag	UNP A9CF87
A	-7	GLU	-	expression tag	UNP A9CF87
A	-6	ASN	-	expression tag	UNP A9CF87
A	-5	LEU	-	expression tag	UNP A9CF87
A	-4	TYR	-	expression tag	UNP A9CF87
A	-3	PHE	-	expression tag	UNP A9CF87
A	-2	GLN	-	expression tag	UNP A9CF87
A	-1	GLY	=	expression tag	UNP A9CF87
A	0	HIS	-	expression tag	UNP A9CF87
A	1	MSE	-	expression tag	UNP A9CF87

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Chain	Residue	Modelled Modelled	Actual	Comment	Reference
A	210	SER	_	expression tag	UNP A9CF87
В	-21	MSE	-	expression tag	UNP A9CF87
В	-20	GLY	-	expression tag	UNP A9CF87
В	-19	SER	-	expression tag	UNP A9CF87
В	-18	SER	-	expression tag	UNP A9CF87
В	-17	HIS	-	expression tag	UNP A9CF87
В	-16	HIS	-	expression tag	UNP A9CF87
В	-15	HIS	-	expression tag	UNP A9CF87
В	-14	HIS	-	expression tag	UNP A9CF87
В	-13	HIS	-	expression tag	UNP A9CF87
В	-12	HIS	-	expression tag	UNP A9CF87
В	-11	SER	-	expression tag	UNP A9CF87
В	-10	SER	_	expression tag	UNP A9CF87
В	-9	GLY	-	expression tag	UNP A9CF87
В	-8	ARG	-	expression tag	UNP A9CF87
В	-7	GLU	-	expression tag	UNP A9CF87
В	-6	ASN	-	expression tag	UNP A9CF87
В	-5	LEU	-	expression tag	UNP A9CF87
В	-4	TYR	-	expression tag	UNP A9CF87
В	-3	PHE	-	expression tag	UNP A9CF87
В	-2	GLN	_	expression tag	UNP A9CF87
В	-1	GLY	-	expression tag	UNP A9CF87
В	0	HIS	-	expression tag	UNP A9CF87
В	1	MSE	-	expression tag	UNP A9CF87
В	210	SER	-	expression tag	UNP A9CF87
С	-21	MSE	-	expression tag	UNP A9CF87
С	-20	GLY	-	expression tag	UNP A9CF87
С	-19	SER	-	expression tag	UNP A9CF87
С	-18	SER	-	expression tag	UNP A9CF87
С	-17	HIS	-	expression tag	UNP A9CF87
С	-16	HIS	-	expression tag	UNP A9CF87
С	-15	HIS	-	expression tag	UNP A9CF87
С	-14	HIS	-	expression tag	UNP A9CF87
С	-13	HIS	-	expression tag	UNP A9CF87
С	-12	HIS	_	expression tag	UNP A9CF87
С	-11	SER	-	expression tag	UNP A9CF87
С	-10	SER	-	expression tag	UNP A9CF87
С	-9	GLY	-	expression tag	UNP A9CF87
С	-8	ARG	-	expression tag	UNP A9CF87
С	-7	GLU	-	expression tag	UNP A9CF87
С	-6	ASN	-	expression tag	UNP A9CF87
С	-5	LEU	_	expression tag	UNP A9CF87

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Chain	Residue	Modelled	Actual	Comment	Reference
С	-4	TYR	_	expression tag	UNP A9CF87
С	-3	PHE	-	expression tag	UNP A9CF87
С	-2	GLN	_	expression tag	UNP A9CF87
С	-1	GLY	-	expression tag	UNP A9CF87
С	0	HIS	-	expression tag	UNP A9CF87
С	1	MSE	_	expression tag	UNP A9CF87
С	210	SER	-	expression tag	UNP A9CF87

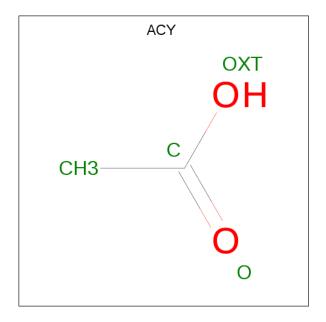
• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	8	Total Cl 8 8	0	0
3	A	8	Total Cl 8 8	0	0
3	С	6	Total Cl 6 6	0	0

• Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).





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

• Molecule 5 is water.

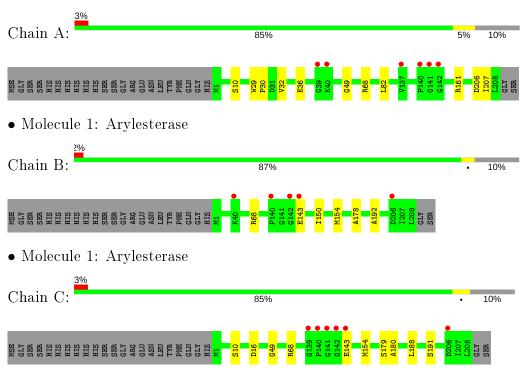
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	A	154	Total O 154 154	0	0
5	В	155	Total O 155 155	0	0
5	С	173	Total O 173 173	0	0



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: Arylesterase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	72.20Å 131.40 Å 122.33 Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.28 - 2.00	Depositor
Resolution (A)	34.28 - 2.00	EDS
% Data completeness	99.6 (34.28-2.00)	Depositor
(in resolution range)	99.6 (34.28-2.00)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.22 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
D D	0.148 , 0.184	Depositor
R, R_{free}	0.156 , 0.189	DCC
R_{free} test set	1986 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38 , 47.1	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.012 for 1/2 *h-1/2 *k,-3/2 *h-1/2 *k,-l	Xtriage
Estimated twinning fraction	0.021 for 1/2 *h + 1/2 *k, 3/2 *h - 1/2 *k, -1	Atriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5138	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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, ACY, CL

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	Boı	nd lengths	Bond angles		
MIOI	RMSZ # 2		# Z > 5	RMSZ	# Z > 5	
1	A	0.62	0/1589	0.69	0/2155	
1	В	0.71	1/1577 (0.1%)	0.73	1/2139 (0.0%)	
1	С	0.62	0/1563	0.69	1/2121 (0.0%)	
All	All	0.65	$1/4729 \ (0.0\%)$	0.71	2/6415 (0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	143	GLU	CG-CD	5.02	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	С	16	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	В	68	ARG	NE-CZ-NH1	5.27	122.94	120.30

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	1548	0	1564	6	0
1	В	1542	0	1556	2	0

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Continued	trom	mraniaone	maaa
-	110116	predidus	puyc

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	1531	0	1543	4	0
2	A	1	0	0	0	0
3	A	8	0	0	1	0
3	В	8	0	0	0	0
3	С	6	0	0	0	0
4	A	4	0	3	0	0
4	В	4	0	3	0	0
4	С	4	0	3	0	0
5	A	154	0	0	1	0
5	В	155	0	0	0	0
5	С	173	0	0	2	0
All	All	5138	0	4672	12	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 1.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	Clash overlap (Å)
1:A:161:ARG:HD2	3:A:214:CL:CL	2.42	0.56
1:C:154:MSE:HE2	5:C:443:HOH:O	2.06	0.56
1:B:150:ILE:O	1:B:154[A]:MSE:HG3	2.10	0.52
1:A:32:VAL:O	1:A:36:GLU:HG2	2.12	0.50
1:C:154:MSE:HE3	5:C:412:HOH:O	2.17	0.45
1:A:10:SER:HB3	1:A:49:GLY:HA2	2.00	0.44
1:A:82:LEU:HD13	1:A:207:ILE:HG21	2.00	0.44
1:A:161:ARG:NH2	5:A:371:HOH:O	2.47	0.43
1:B:178:ALA:HB1	1:B:192:ALA:HB1	2.02	0.41
1:C:180:ALA:HA	1:C:188:LEU:HD23	2.03	0.40
1:C:10:SER:HB3	1:C:49:GLY:HA2	2.03	0.40
1:A:29:TRP:CG	1:A:30:PRO:HD3	2.56	0.40

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 r	number	of	residues	for	which	the	backbone	conformation	was
analysed, and the total numb	er of	residues								

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentil	es
1	A	$209/232 \; (90\%)$	203 (97%)	6 (3%)	0	100 100	0
1	В	$208/232 \; (90\%)$	202 (97%)	6 (3%)	0	100 100	0
1	С	$206/232 \ (89\%)$	197 (96%)	9 (4%)	0	100 100	0
All	All	623/696 (90%)	602 (97%)	21 (3%)	0	100 100	0

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	Percer	$_{ m tiles}$
1	A	157/168 (94%)	155 (99%)	2 (1%)	69	74
1	В	156/168 (93%)	156 (100%)	0	100	100
1	С	154/168 (92%)	150 (97%)	4 (3%)	46	48
All	All	467/504 (93%)	461 (99%)	6 (1%)	69	74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	206	ASP
1	С	68	ARG
1	С	143	GLU
1	С	179	SER
1	С	191	SER

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 26 ligands modelled in this entry, 23 are monoatomic - leaving 3 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		В	ond len	$\overline{ ext{gths}}$	Е	ond ang	gles
WIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACY	С	217	-	1,3,3	2.50	1 (100%)	0,3,3	0.00	1
4	ACY	В	219	-	1,3,3	2.34	1 (100%)	0,3,3	0.00	-
4	ACY	A	220	-	1,3,3	2.71	1 (100%)	0,3,3	0.00	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
4	A	220	ACY	СН3-С	2.71	1.52	1.48
4	С	217	ACY	СН3-С	2.50	1.51	1.48
4	В	219	ACY	СН3-С	2.34	1.51	1.48

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 (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^{th} 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>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	$203/232 \ (87\%)$	0.06	6 (2%) 50 49	23, 28, 36, 39	0
1	В	203/232 (87%)	-0.26	5 (2%) 57 56	22, 26, 35, 41	0
1	С	203/232 (87%)	-0.07	6 (2%) 50 49	21, 26, 34, 45	0
All	All	609/696 (87%)	-0.09	17 (2%) 53 51	21, 27, 36, 45	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	140	PRO	7.5
1	A	140	PRO	6.4
1	С	142	GLY	3.7
1	С	141	GLY	3.6
1	С	139	GLY	3.6
1	С	206	ASP	3.3
1	A	141	GLY	3.2
1	A	40	LYS	3.2
1	В	143	GLU	3.1
1	В	142	GLY	3.0
1	В	40	LYS	2.9
1	В	140	PRO	2.9
1	A	142	GLY	2.8
1	С	143	GLU	2.4
1	A	39	GLY	2.4
1	В	206	ASP	2.2
1	A	137	VAL	2.2

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. The B-factors column lists the minimum, median, 95^{th} 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	${f B-factors}({f \AA}^2)$	Q < 0.9
3	CL	A	214	1/1	0.84	0.36	79,79,79,79	0
3	CL	A	216	1/1	0.85	0.13	48,48,48,48	0
3	CL	A	218	1/1	0.87	0.12	45,45,45,45	0
3	CL	В	218	1/1	0.88	0.12	60,60,60,60	0
3	CL	A	212	1/1	0.94	0.09	36,36,36,36	0
4	ACY	В	219	4/4	0.95	0.15	25,28,29,30	0
3	CL	В	214	1/1	0.95	0.08	43,43,43,43	0
4	ACY	С	217	4/4	0.96	0.15	23,27,28,28	0
3	CL	В	211	1/1	0.96	0.18	41,41,41,41	0
4	ACY	A	220	4/4	0.96	0.15	29,31,32,33	0
3	CL	В	212	1/1	0.97	0.29	49,49,49,49	0
3	CL	С	213	1/1	0.97	0.11	36,36,36,36	0
3	CL	A	217	1/1	0.97	0.13	46,46,46,46	0
3	CL	С	216	1/1	0.98	0.19	31,31,31,31	0
3	CL	A	213	1/1	0.98	0.10	33,33,33,33	0
3	CL	С	212	1/1	0.98	0.17	32,32,32,32	0
3	CL	A	211	1/1	0.98	0.05	29,29,29,29	0
3	CL	В	217	1/1	0.98	0.11	36,36,36,36	0
3	CL	С	211	1/1	0.99	0.08	27,27,27,27	0
3	CL	С	214	1/1	0.99	0.16	32,32,32,32	1
3	CL	В	213	1/1	0.99	0.14	30,30,30,30	0
3	CL	В	216	1/1	0.99	0.08	28,28,28,28	0
3	CL	С	215	1/1	0.99	0.11	30,30,30,30	0
2	ZN	A	219	1/1	0.99	0.08	32,32,32,32	0
3	CL	A	215	1/1	0.99	0.09	30,30,30,30	0
3	CL	В	215	1/1	0.99	0.14	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.

