

Full wwPDB X-ray Structure Validation Report (i)

Jul 4, 2023 - 01:41 am BST

PDB ID	:	80WF
Title	:	Clostridium perfringens chitinase $CP4_{3455}$ with chitosan
Authors	:	Bloch, Y.; Savvides, S.N.
Deposited on		
Resolution	:	1.30 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

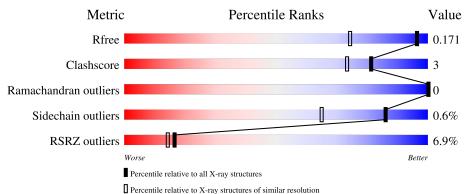
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.30 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 of 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	А	575	92%	5% •				
2	В	6	83%	17%				



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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9637 atoms, of which 4357 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.

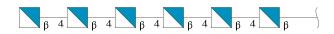
• Molecule 1 is a protein called Chitodextrinase.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace		
1	А	563	Total 8808	C 2876	Н 4287	N 738	0 887	S 20	0	11	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	44	MET	-	initiating methionine	UNP F8UNI5
А	45	GLY	-	expression tag	UNP F8UNI5
А	302	ARG	ILE	conflict	UNP F8UNI5
А	612	SER	-	expression tag	UNP F8UNI5
А	613	HIS	-	expression tag	UNP F8UNI5
А	614	HIS	-	expression tag	UNP F8UNI5
А	615	HIS	-	expression tag	UNP F8UNI5
А	616	HIS	-	expression tag	UNP F8UNI5
А	617	HIS	-	expression tag	UNP F8UNI5
А	618	HIS	-	expression tag	UNP F8UNI5

• Molecule 2 is an oligosaccharide called 2-amino-2-deoxy-beta-D-glucopyranose-(1-4)-2-amin o-2-deoxy-beta-D-glucopyranose-(1-4)-2-amino-2-deoxy-beta-D-gl



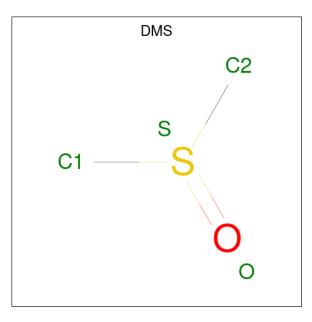
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	6	Total	C 36	Н 64	N 6	O 25	0	0	0
			101	30	04	0	$_{20}$			

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



Mol	Chain	Residues	Aton	ns	ZeroOcc	AltConf
3	А	1	Total 1	Cl 1	0	0

• Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
4	Δ	1	Total	С	Η	0	\mathbf{S}	0	0
4	A	1	10	2	6	1	1	0	U

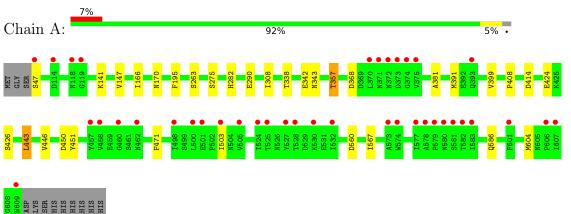
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	686	Total O 687 687	0	1



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Chitodextrinase

• Molecule 2: 2-amino-2-deoxy-beta-D-glucopyranose-(1-4)-2-amino-2-deoxy-beta-D-glucopyranos e-(1-4)-2-amino-2-deoxy-beta-D-glucopyranose-(1-4)-2-amino-2-deoxy-beta-D-glucopyranose-(1-4) -2-amino-2-deoxy-beta-D-glucopyranose-(1-4)-2-amino-2-deoxy-beta-D-glucopyranose

Chain B: 83% 17%

GCS1 GCS2 GCS3 GCS4 GCS5 GCS5 GCS6



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	50.44Å 108.50Å 111.41Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.74 - 1.30	Depositor
Resolution (A)	45.74 - 1.30	EDS
% Data completeness	$98.6\ (45.74\text{-}1.30)$	Depositor
(in resolution range)	$98.6\ (45.74\text{-}1.30)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.26 (at 1.30 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.145 , 0.170	Depositor
R, R_{free}	0.145 , 0.171	DCC
R_{free} test set	2008 reflections $(1.35%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	15.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.40 , 48.9	EDS
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9637	wwPDB-VP
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: DMS, CL, GCS

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).

Mal	Chain	Bond	lengths	Bond	angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.36	0/4664	0.60	0/6347

There are no bond length outliers.

There are no bond angle outliers.

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	А	4521	4287	4261	23	1
2	В	67	64	63	2	0
3	А	1	0	0	0	0
4	А	4	6	6	1	0
5	А	687	0	0	7	0
All	All	5280	4357	4330	23	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 3.

All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:343[B]:ASN:ND2	5:A:801:HOH:O	2.11	0.80
1:A:368:ASP:OD1	2:B:6:GCS:O3	2.02	0.77
1:A:141:LYS:NZ	5:A:805:HOH:O	2.25	0.69
1:A:414:ASP:OD1	5:A:802:HOH:O	2.12	0.67
1:A:424:GLU:OE2	1:A:451:TYR:OH	2.15	0.64
1:A:368:ASP:OD2	2:B:6:GCS:N2	2.31	0.63
1:A:446:VAL:HG12	5:A:1263:HOH:O	2.00	0.62
1:A:503:ILE:HD12	1:A:604:MET:CE	2.34	0.58
1:A:408:PRO:HD3	1:A:426:SER:HB3	1.89	0.55
1:A:586:GLN:OE1	5:A:803:HOH:O	2.20	0.50
1:A:308:ILE:HG23	5:A:1157:HOH:O	2.12	0.49
1:A:503:ILE:HD12	1:A:604:MET:HE1	1.94	0.48
1:A:47:SER:N	5:A:815:HOH:O	2.48	0.47
1:A:275:SER:HB3	1:A:443:LEU:HD22	1.97	0.45
1:A:450:ASP:O	1:A:471:PHE:HA	2.17	0.44
1:A:342:GLU:O	1:A:357[A]:THR:HG23	2.17	0.43
1:A:166:ILE:C	1:A:166:ILE:HD12	2.39	0.42
1:A:141:LYS:HE3	1:A:147:VAL:O	2.19	0.42
1:A:338:THR:O	1:A:381:ALA:HA	2.21	0.41
1:A:391:MET:SD	1:A:399:VAL:CG2	3.09	0.41
1:A:282:HIS:CG	1:A:290:GLU:HB2	2.55	0.41
1:A:263[B]:SER:O	4:A:702:DMS:C1	2.69	0.41

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:170:ASN:ND2	$1:A:560:ASP:OD2[1_455]$	2.11	0.09

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		
1	А	572/575~(100%)	554 (97%)	18 (3%)	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	А	496/504~(98%)	492~(99%)	4 (1%)	81 58	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	195	PHE
1	А	357[A]	THR
1	А	357[B]	THR
1	А	443	LEU

Sometimes 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)

6 monosaccharides 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	Turne	Chain	Res	Link	Bo	Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	GCS	В	1	2	12,12,12	0.18	0	16,17,17	0.37	0	
2	GCS	В	2	2	11,11,12	0.37	0	$12,\!15,\!17$	0.68	0	
2	GCS	В	3	2	11,11,12	0.39	0	12,15,17	0.65	0	
2	GCS	В	4	2	11,11,12	0.34	0	12,15,17	0.66	0	
2	GCS	В	5	2	11,11,12	0.36	0	12,15,17	0.53	0	
2	GCS	В	6	2	11,11,12	0.28	0	$12,\!15,\!17$	0.61	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	GCS	В	1	2	-	2/2/22/22	0/1/1/1
2	GCS	В	2	2	-	0/2/19/22	0/1/1/1
2	GCS	В	3	2	-	0/2/19/22	0/1/1/1
2	GCS	В	4	2	-	0/2/19/22	0/1/1/1
2	GCS	В	5	2	-	0/2/19/22	0/1/1/1
2	GCS	В	6	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1	GCS	C4-C5-C6-O6
2	В	1	GCS	O5-C5-C6-O6

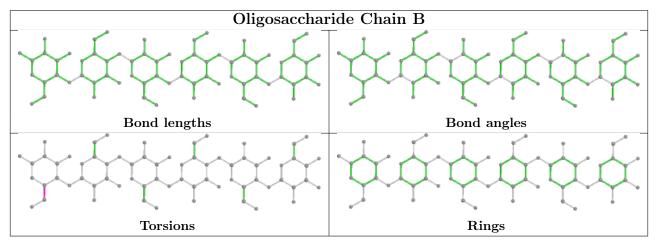
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	6	GCS	2	0



The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	Tink	Bond lengths			Bond angles		
MOI	Type	Ullalli	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	DMS	А	702	-	3,3,3	0.60	0	3,3,3	0.25	0

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.

1 monomer is involved in 1 short contact:

	Mol	Chain	Res	Type	Clashes	Symm-Clashes
ſ	4	А	702	DMS	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^{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>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	563/575~(97%)	0.02	39 (6%) 16 14	11, 19, 42, 68	0

All (39) RSRZ outliers are listed below:

Mol			Type	RSRZ	
1	А	370	LEU	7.1	
1	А	574	TRP	6.1	
1	А	583	ILE	5.5	
1	А	371	ASN	5.0	
1	А	373	ASP	4.9	
1	А	527	TYR	4.9	
1	А	532	ILE	4.8	
1	А	372	ASN	4.4	
1	А	581	SER	4.3	
1	А	114	ASP	4.2	
1	А	580	ASN	4.1	
1	А	457	TYR	4.0	
1	А	582	THR	3.9	
1	А	609	ASN	3.9	
1	А	577	ILE	3.8	
1	А	573	ALA	3.7	
1	А	374	GLY	3.6	
1	А	47	SER	3.6	
1	А	118	ASN	3.6	
1	А	607	ILE	3.6	
1	А	505	VAL	3.5	
1	А	460	GLY	3.4	
1	А	525	THR	3.0	
1	А	462	ASN	3.0	
1	А	498	ILE	3.0	
1	А	503	ILE	3.0	
1	A	501	GLU	2.7	

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Mol	Chain	Res Type		RSRZ	
1	А	458	VAL	2.7	
1	А	578	ALA	2.6	
1	А	524	ILE	2.5	
1	А	579	PRO	2.5	
1	А	393	GLN	2.4	
1	А	119	GLY	2.3	
1	А	375	VAL	2.3	
1	А	601	PHE	2.2	
1	А	500	LEU	2.2	
1	А	606	PRO	2.2	
1	А	528	THR	2.1	
1	А	530	LYS	2.0	

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6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

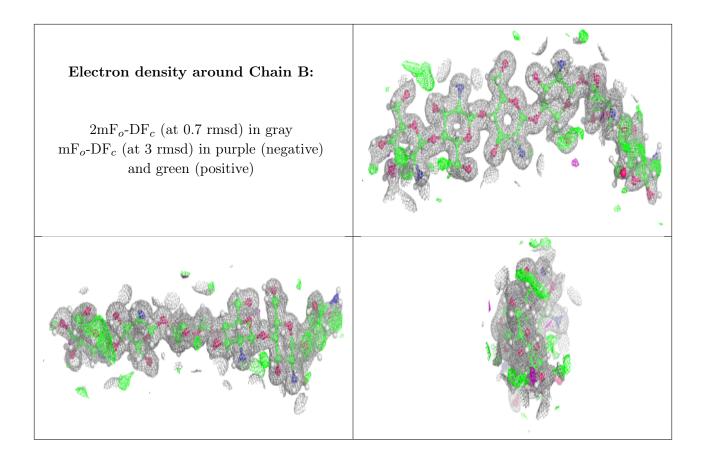
6.3 Carbohydrates (i)

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	GCS	В	1	12/12	0.56	0.20	$28,\!30,\!36,\!36$	24
2	GCS	В	6	11/12	0.79	0.17	$30,\!41,\!49,\!52$	0
2	GCS	В	2	11/12	0.94	0.08	20,25,31,38	0
2	GCS	В	5	11/12	0.95	0.06	16,21,33,34	0
2	GCS	В	3	11/12	0.97	0.06	17,19,23,23	0
2	GCS	В	4	11/12	0.98	0.04	15,19,23,24	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





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	$B-factors(Å^2)$	Q < 0.9
4	DMS	А	702	4/4	0.97	0.09	$23,\!28,\!32,\!32$	0
3	CL	А	701	1/1	1.00	0.03	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.

