Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 11:27 pm GMT

PDB ID	:	4UOP
Title	:	Crystal structure of the lipoteichoic acid synthase LtaP from Listeria monocytogenes
Authors	:	Campeotto, I.; Freemont, P.; Grundling, A.
Deposited on	:	2014-06-06
Resolution	:	1.75 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 (i)) were used in the production of this report:

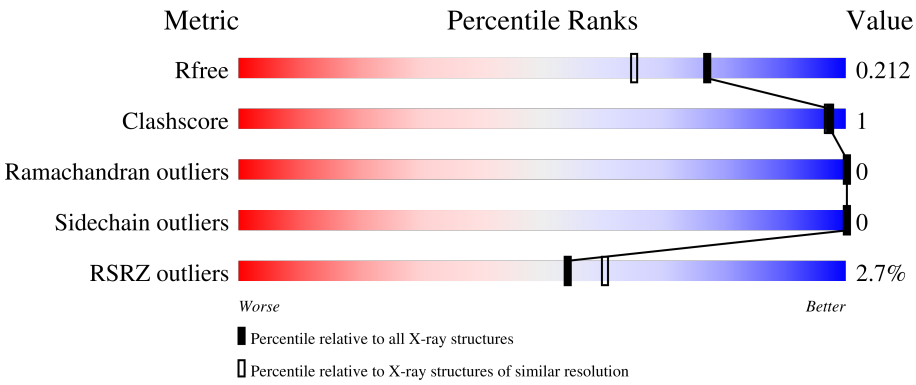
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.75 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	A	442	4% 90% • 8%
1	B	442	% 91% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7119 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 LIPOTEICHOIC ACID PRIMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	3299	2097	535	658	9	0	1	0
1	B	409	3305	2100	536	660	9	0	1	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	MET	-	expression tag	UNP Q8Y989
A	173	SER	-	expression tag	UNP Q8Y989
A	174	TYR	-	expression tag	UNP Q8Y989
A	175	TYR	-	expression tag	UNP Q8Y989
A	176	HIS	-	expression tag	UNP Q8Y989
A	177	HIS	-	expression tag	UNP Q8Y989
A	178	HIS	-	expression tag	UNP Q8Y989
A	179	HIS	-	expression tag	UNP Q8Y989
A	180	HIS	-	expression tag	UNP Q8Y989
A	181	HIS	-	expression tag	UNP Q8Y989
A	182	ASP	-	expression tag	UNP Q8Y989
A	183	TYR	-	expression tag	UNP Q8Y989
A	184	ASP	-	expression tag	UNP Q8Y989
A	185	ILE	-	expression tag	UNP Q8Y989
A	186	PRO	-	expression tag	UNP Q8Y989
A	187	THR	-	expression tag	UNP Q8Y989
A	188	THR	-	expression tag	UNP Q8Y989
A	189	GLU	-	expression tag	UNP Q8Y989
A	190	ASN	-	expression tag	UNP Q8Y989
A	191	LEU	-	expression tag	UNP Q8Y989
A	192	TYR	-	expression tag	UNP Q8Y989
A	193	PHE	-	expression tag	UNP Q8Y989
A	194	GLN	-	expression tag	UNP Q8Y989
A	195	GLY	-	expression tag	UNP Q8Y989
A	196	ALA	-	expression tag	UNP Q8Y989

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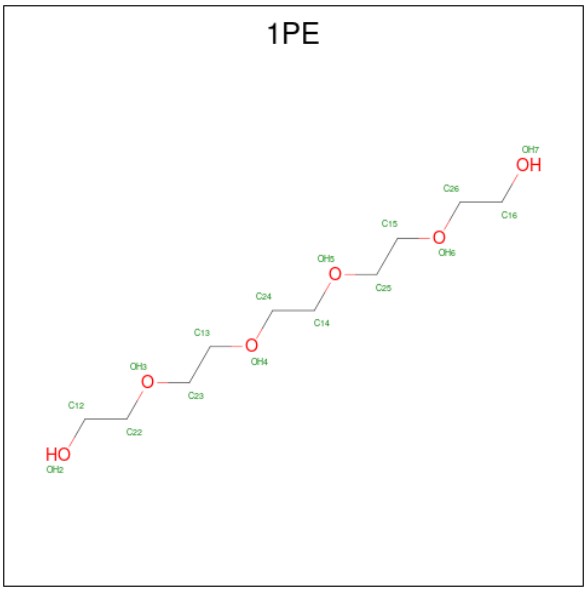
Chain	Residue	Modelled	Actual	Comment	Reference
A	197	MET	-	expression tag	UNP Q8Y989
A	198	GLY	-	expression tag	UNP Q8Y989
A	199	SER	-	expression tag	UNP Q8Y989
B	172	MET	-	expression tag	UNP Q8Y989
B	173	SER	-	expression tag	UNP Q8Y989
B	174	TYR	-	expression tag	UNP Q8Y989
B	175	TYR	-	expression tag	UNP Q8Y989
B	176	HIS	-	expression tag	UNP Q8Y989
B	177	HIS	-	expression tag	UNP Q8Y989
B	178	HIS	-	expression tag	UNP Q8Y989
B	179	HIS	-	expression tag	UNP Q8Y989
B	180	HIS	-	expression tag	UNP Q8Y989
B	181	HIS	-	expression tag	UNP Q8Y989
B	182	ASP	-	expression tag	UNP Q8Y989
B	183	TYR	-	expression tag	UNP Q8Y989
B	184	ASP	-	expression tag	UNP Q8Y989
B	185	ILE	-	expression tag	UNP Q8Y989
B	186	PRO	-	expression tag	UNP Q8Y989
B	187	THR	-	expression tag	UNP Q8Y989
B	188	THR	-	expression tag	UNP Q8Y989
B	189	GLU	-	expression tag	UNP Q8Y989
B	190	ASN	-	expression tag	UNP Q8Y989
B	191	LEU	-	expression tag	UNP Q8Y989
B	192	TYR	-	expression tag	UNP Q8Y989
B	193	PHE	-	expression tag	UNP Q8Y989
B	194	GLN	-	expression tag	UNP Q8Y989
B	195	GLY	-	expression tag	UNP Q8Y989
B	196	ALA	-	expression tag	UNP Q8Y989
B	197	MET	-	expression tag	UNP Q8Y989
B	198	GLY	-	expression tag	UNP Q8Y989
B	199	SER	-	expression tag	UNP Q8Y989

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 6 3	0	0
2	B	1	Total C O 10 6 4	0	0
2	B	1	Total C O 10 6 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	3	Total Cl 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	192	Total O 192 192	0	0

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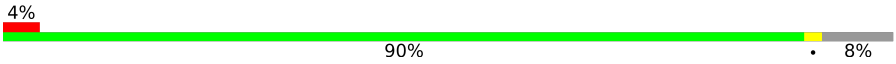
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	289	289	289	0	0

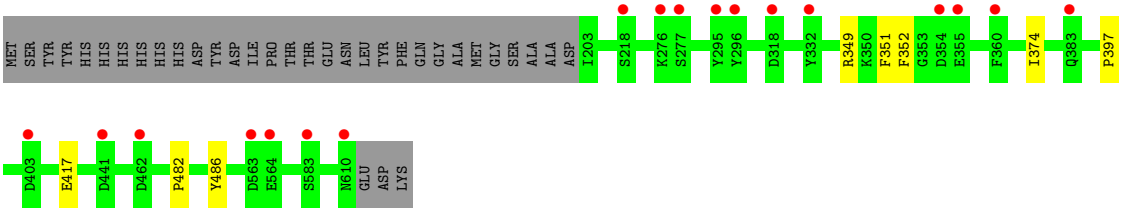
3 Residue-property plots (i)

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: LIPOTEICHOIC ACID PRIMASE

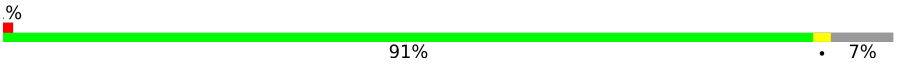
Chain A:

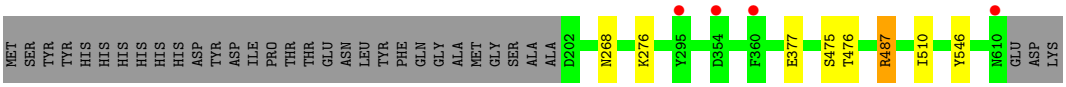




• Molecule 1: LIPOTEICHOIC ACID PRIMASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.20Å 53.70Å 85.04Å 71.63° 76.78° 65.12°	Depositor
Resolution (Å)	80.20 – 1.75 47.20 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.8 (80.20-1.75) 94.8 (47.20-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.178 , 0.207 0.187 , 0.212	Depositor DCC
R_{free} test set	3847 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7119	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

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: CL, 1PE, MG

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	0.39	0/3384	0.58	0/4586
1	B	0.44	0/3390	0.61	2/4594 (0.0%)
All	All	0.42	0/6774	0.60	2/9180 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	487	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	B	487	ARG	NE-CZ-NH1	8.42	124.51	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	3299	0	3139	5	0
1	B	3305	0	3144	7	0
2	A	9	0	10	0	0
2	B	20	0	26	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	192	0	0	0	0
5	B	289	0	0	1	0
All	All	7119	0	6319	10	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 (10) 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:349:ARG:O	1:A:352:PHE:O	2.10	0.69
1:A:417:GLU:OE2	1:B:276:LYS:HE2	2.06	0.56
1:B:475:SER:OG	2:B:1615:1PE:H231	2.09	0.53
1:B:268:ASN:N	4:B:1613:CL:CL	2.71	0.49
1:B:476:THR:OG1	1:B:487:ARG:NH2	2.46	0.48
1:A:397:PRO:HB3	1:B:546:TYR:CE2	2.50	0.46
1:A:482:PRO:HB2	1:A:486:TYR:CE1	2.53	0.44
1:B:377:GLU:HG2	5:B:2159:HOH:O	2.18	0.44
1:B:510:ILE:HD11	4:B:1612:CL:CL	2.57	0.42
1:A:351:PHE:CZ	1:A:374:ILE:HD11	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 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	407/442 (92%)	395 (97%)	12 (3%)	0	100	100
1	B	408/442 (92%)	397 (97%)	11 (3%)	0	100	100
All	All	815/884 (92%)	792 (97%)	23 (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	A	367/395 (93%)	367 (100%)	0	100	100
1	B	368/395 (93%)	368 (100%)	0	100	100
All	All	735/790 (93%)	735 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	561	GLN
1	B	561	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 5 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	1PE	B	1614	-	9,9,15	0.42	0	8,8,14	0.63	0
2	1PE	A	1611	-	8,8,15	0.61	0	7,7,14	0.26	0
2	1PE	B	1615	-	9,9,15	0.64	0	8,8,14	0.54	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	1PE	B	1614	-	-	0/7/7/13	-
2	1PE	A	1611	-	-	1/6/6/13	-
2	1PE	B	1615	-	-	5/7/7/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1615	1PE	OH4-C13-C23-OH3
2	B	1615	1PE	OH2-C12-C22-OH3
2	B	1615	1PE	OH5-C14-C24-OH4
2	A	1611	1PE	C12-C22-OH3-C23
2	B	1615	1PE	C13-C23-OH3-C22
2	B	1615	1PE	C23-C13-OH4-C24

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1615	1PE	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, 95th 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^2)	Q<0.9
1	A	408/442 (92%)	0.16	18 (4%)	34	40	19, 33, 52, 73	0
1	B	409/442 (92%)	-0.07	4 (0%)	82	87	15, 25, 40, 62	0
All	All	817/884 (92%)	0.04	22 (2%)	54	60	15, 28, 50, 73	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	TYR	5.2
1	B	360	PHE	4.4
1	A	296	TYR	4.3
1	A	318	ASP	4.1
1	A	360	PHE	3.9
1	B	610	ASN	3.8
1	A	295	TYR	3.7
1	A	277	SER	3.5
1	A	610	ASN	3.4
1	A	564	GLU	3.3
1	A	354	ASP	3.2
1	A	403	ASP	2.7
1	A	276	LYS	2.6
1	A	563	ASP	2.6
1	A	355	GLU	2.5
1	A	218	SER	2.5
1	A	332	TYR	2.4
1	A	583	SER	2.3
1	A	462	ASP	2.2
1	A	441	ASP	2.1
1	B	354	ASP	2.1
1	A	383	GLN	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 monosaccharides 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, 95th 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
2	1PE	B	1615	10/16	0.85	0.19	50,60,60,61	0
2	1PE	A	1611	9/16	0.89	0.11	42,44,46,47	0
2	1PE	B	1614	10/16	0.93	0.13	30,35,41,43	0
4	CL	B	1611	1/1	0.98	0.07	43,43,43,43	0
4	CL	B	1612	1/1	0.98	0.17	45,45,45,45	0
4	CL	B	1613	1/1	0.98	0.18	44,44,44,44	0
3	MG	A	1612	1/1	0.99	0.08	22,22,22,22	0
3	MG	B	1616	1/1	1.00	0.18	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.