Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 01:23 am BST

PDB ID	:	5HTF
Title	:	Crystal Structure of PrsA1 from Listeria monocytogenes
Authors	:	Prehna, G.; Cahoon, L.A.; Freitag, N.E.
Deposited on	:	2016-01-26
Resolution	:	2.10 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:

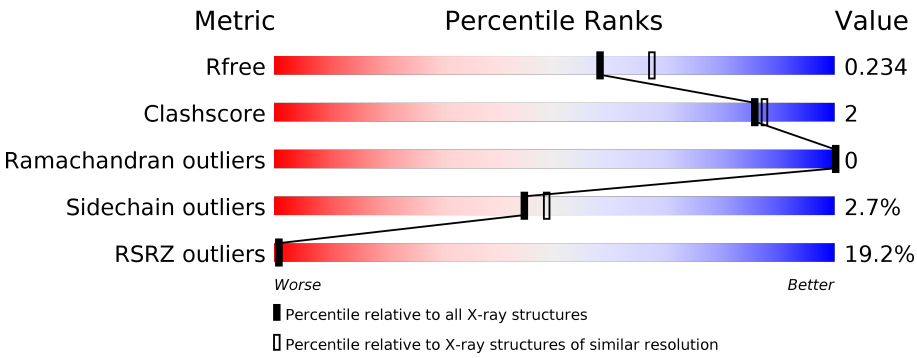
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	283	5% 89% • 7%
1	B	283	30% 82% 8% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8460 atoms, of which 4065 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.

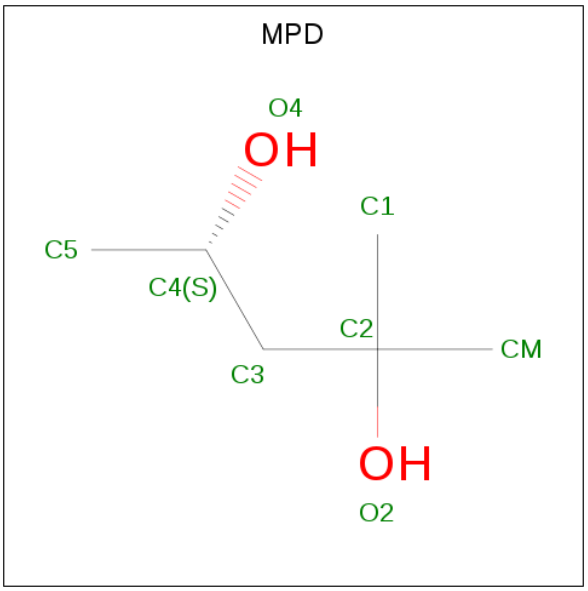
- Molecule 1 is a protein called Foldase protein PrsA 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	262	4090	1295	2030	325	435	5	0	0	0
1	B	260	4045	1280	2007	321	433	4	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP Q8Y759
A	21	ALA	-	expression tag	UNP Q8Y759
A	295	ARG	-	expression tag	UNP Q8Y759
A	296	SER	-	expression tag	UNP Q8Y759
A	297	HIS	-	expression tag	UNP Q8Y759
A	298	HIS	-	expression tag	UNP Q8Y759
A	299	HIS	-	expression tag	UNP Q8Y759
A	300	HIS	-	expression tag	UNP Q8Y759
A	301	HIS	-	expression tag	UNP Q8Y759
A	302	HIS	-	expression tag	UNP Q8Y759
B	20	MET	-	initiating methionine	UNP Q8Y759
B	21	ALA	-	expression tag	UNP Q8Y759
B	295	ARG	-	expression tag	UNP Q8Y759
B	296	SER	-	expression tag	UNP Q8Y759
B	297	HIS	-	expression tag	UNP Q8Y759
B	298	HIS	-	expression tag	UNP Q8Y759
B	299	HIS	-	expression tag	UNP Q8Y759
B	300	HIS	-	expression tag	UNP Q8Y759
B	301	HIS	-	expression tag	UNP Q8Y759
B	302	HIS	-	expression tag	UNP Q8Y759

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	22	6	14	2	0	0
			Total	C	H	O		
2	A	1	22	6	14	2	0	0

- Molecule 3 is water.

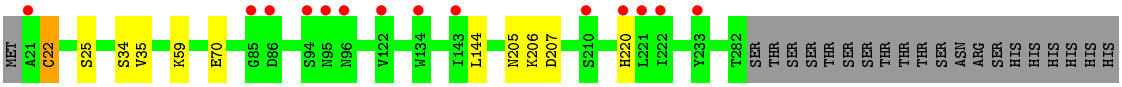
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	198	198	198	0	0
			Total	O		
3	B	83	83	83	0	0

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.

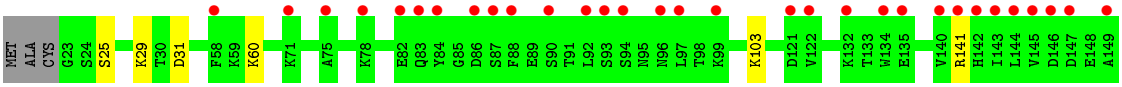
- Molecule 1: Foldase protein PrsA 1

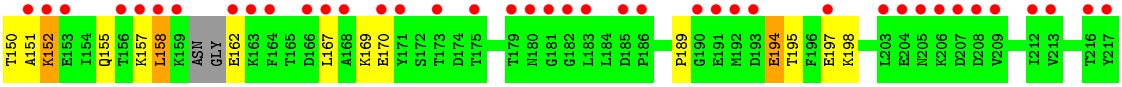
Chain A:

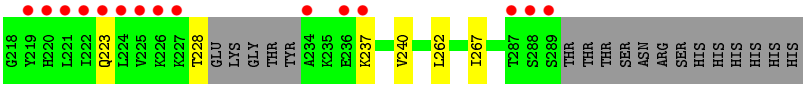


- Molecule 1: Foldase protein PrsA 1

Chain B:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.31Å 84.03Å 114.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 2.10 19.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.78-2.10) 99.7 (19.78-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.198 , 0.234 0.200 , 0.234	Depositor DCC
R_{free} test set	1864 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8460	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: MPD

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	0.25	0/2089	0.46	0/2816
1	B	0.26	0/2064	0.49	0/2781
All	All	0.26	0/4153	0.48	0/5597

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	A	2060	2030	2029	6	1
1	B	2038	2007	2003	13	1
2	A	16	28	28	1	0
3	A	198	0	0	2	0
3	B	83	0	0	2	0
All	All	4395	4065	4060	18	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 2.

All (18) 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:34:SER:O	1:B:60:LYS:NZ	2.19	0.75
1:B:151:ALA:O	1:B:155:GLN:N	2.24	0.70
1:B:29:LYS:NZ	3:B:406:HOH:O	2.34	0.57
1:A:59:LYS:NZ	3:A:504:HOH:O	2.36	0.57
1:B:158:LEU:HD23	1:B:158:LEU:H	1.73	0.54
1:A:22:CYS:SG	2:A:402:MPD:H52	2.48	0.54
1:B:141:ARG:NH1	1:B:223:GLN:OE1	2.44	0.50
1:B:237:LYS:O	1:B:240:VAL:N	2.45	0.50
1:B:262:LEU:HD11	1:B:267:ILE:HD13	1.94	0.48
1:B:152:LYS:HA	1:B:155:GLN:HB3	1.97	0.47
1:B:158:LEU:O	1:B:162:GLU:N	2.47	0.47
1:B:31:ASP:OD2	3:B:401:HOH:O	2.20	0.46
1:B:194:GLU:O	1:B:198:LYS:HG2	2.19	0.43
1:B:167:LEU:HD23	1:B:170:GLU:OE1	2.19	0.42
1:A:205:ASN:OD1	3:A:501:HOH:O	2.21	0.42
1:A:206:LYS:O	1:A:207:ASP:HB2	2.20	0.41
1:A:144:LEU:HD13	1:A:220:HIS:CE1	2.56	0.41
1:B:189:PRO:HA	1:B:197:GLU:OE2	2.21	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:70:GLU:OE2	1:B:103:LYS:NZ[4_445]	2.18	0.02

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	260/283 (92%)	256 (98%)	4 (2%)	0	100	100
1	B	254/283 (90%)	247 (97%)	7 (3%)	0	100	100
All	All	514/566 (91%)	503 (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	225/246 (92%)	222 (99%)	3 (1%)	69	75
1	B	224/246 (91%)	215 (96%)	9 (4%)	31	32
All	All	449/492 (91%)	437 (97%)	12 (3%)	44	48

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	CYS
1	A	25	SER
1	A	35	VAL
1	B	25	SER
1	B	150	THR
1	B	152	LYS
1	B	157	LYS
1	B	158	LEU
1	B	169	LYS
1	B	194	GLU
1	B	195	THR
1	B	228	THR

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)

2 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	MPD	A	402	-	7,7,7	0.60	0	9,10,10	1.33	2 (22%)
2	MPD	A	401	-	7,7,7	0.32	0	9,10,10	0.43	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	MPD	A	402	-	-	2/5/5/5	-
2	MPD	A	401	-	-	2/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	402	MPD	O2-C2-C3	2.72	120.03	109.80
2	A	402	MPD	O2-C2-C1	-2.08	101.41	108.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	401	MPD	C2-C3-C4-C5
2	A	402	MPD	C2-C3-C4-C5
2	A	401	MPD	C2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	MPD	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	262/283 (92%)	0.43	14 (5%) 26 32	31, 48, 81, 124	0
1	B	260/283 (91%)	1.48	86 (33%) 0 0	34, 93, 151, 174	0
All	All	522/566 (92%)	0.95	100 (19%) 1 1	31, 56, 141, 174	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	PHE	10.0
1	B	149	ALA	7.3
1	B	236	GLU	6.6
1	B	222	ILE	6.5
1	B	143	ILE	6.4
1	B	191	GLU	6.1
1	B	217	TYR	5.8
1	B	216	THR	5.8
1	B	221	LEU	5.8
1	A	21	ALA	5.6
1	B	219	TYR	5.6
1	B	220	HIS	5.6
1	B	86	ASP	5.5
1	B	146	ASP	5.3
1	B	166	ASP	5.3
1	A	222	ILE	5.3
1	B	190	GLY	5.2
1	B	159	LYS	5.2
1	B	142	HIS	5.1
1	B	144	LEU	4.9
1	B	162	GLU	4.8
1	B	234	ALA	4.6
1	B	163	LYS	4.5
1	B	167	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	171	TYR	4.3
1	B	289	SER	4.3
1	B	156	THR	4.2
1	B	212	ILE	4.2
1	B	192	MET	4.1
1	B	83	GLN	3.8
1	B	207	ASP	3.8
1	B	88	PHE	3.7
1	B	175	THR	3.7
1	A	85	GLY	3.6
1	A	221	LEU	3.6
1	B	208	ASP	3.6
1	B	225	VAL	3.5
1	B	197	GLU	3.5
1	B	147	ASP	3.4
1	B	183	LEU	3.4
1	B	141	ARG	3.4
1	B	213	VAL	3.3
1	B	153	GLU	3.3
1	B	92	LEU	3.3
1	B	181	GLY	3.2
1	B	179	THR	3.2
1	B	97	LEU	3.1
1	B	180	ASN	3.1
1	B	93	SER	3.1
1	B	287	THR	3.1
1	A	122	VAL	3.1
1	B	182	GLY	3.0
1	B	158	LEU	3.0
1	B	94	SER	3.0
1	B	227	LYS	2.9
1	B	223	GLN	2.9
1	B	121	ASP	2.9
1	B	87	SER	2.9
1	B	145	VAL	2.9
1	B	209	VAL	2.8
1	B	82	GLU	2.7
1	B	288	SER	2.7
1	B	132	LYS	2.7
1	B	157	LYS	2.7
1	B	185	ASP	2.6
1	B	152	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	2.5
1	B	204	GLU	2.5
1	B	205	ASN	2.5
1	B	96	ASN	2.5
1	B	75	ALA	2.5
1	B	134	TRP	2.4
1	B	84	TYR	2.4
1	A	94	SER	2.4
1	B	71	LYS	2.4
1	A	96	ASN	2.3
1	B	186	PRO	2.3
1	A	210	SER	2.3
1	B	237	LYS	2.3
1	A	220	HIS	2.3
1	B	193	ASP	2.3
1	B	90	SER	2.3
1	A	86	ASP	2.3
1	A	233	TYR	2.3
1	B	168	ALA	2.2
1	A	95	ASN	2.2
1	B	226	LYS	2.2
1	A	134	TRP	2.2
1	B	135	GLU	2.2
1	B	78	LYS	2.1
1	B	170	GLU	2.1
1	B	173	THR	2.1
1	A	143	ILE	2.1
1	B	224	LEU	2.1
1	B	58	PHE	2.1
1	B	122	VAL	2.1
1	B	140	VAL	2.1
1	B	151	ALA	2.1
1	B	99	LYS	2.0
1	B	206	LYS	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 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, 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	MPD	A	401	8/8	0.74	0.33	71,101,117,121	0
2	MPD	A	402	8/8	0.93	0.32	91,126,137,137	0

6.5 Other polymers (i)

There are no such residues in this entry.