



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:05 PM GMT

PDB ID : 4WSI  
Title : Crystal Structure of PALS1/Crb complex  
Authors : Wei, Z.; Li, Y.; Zhang, M.  
Deposited on : 2014-10-28  
Resolution : 2.95 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

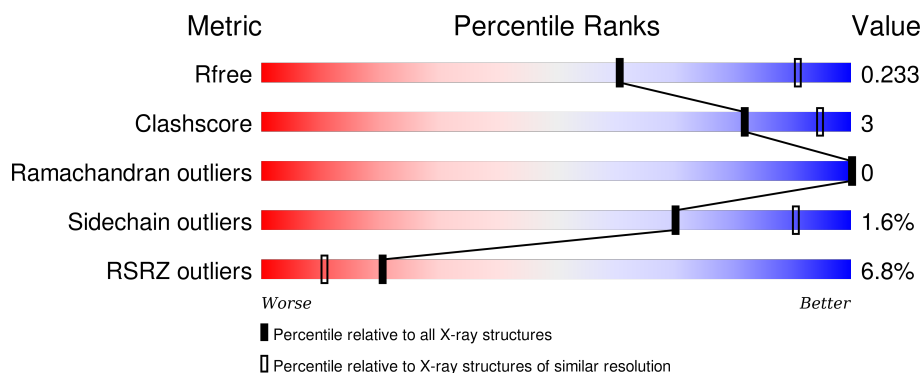
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	394	<div> <div>4%</div> <div>82% 12% 6%</div> </div>
1	B	394	<div> <div>9%</div> <div>85% 6% 9%</div> </div>
2	X	43	<div> <div>35% 7% 58%</div> </div>
2	Y	43	<div> <div>42% 58%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6042 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 MAGUK p55 subfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	1	0
			2947	1853	519	567	8			
1	B	359	Total	C	N	O	S	0	0	0
			2785	1753	484	540	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP Q8N3R9
A	233	PRO	-	expression tag	UNP Q8N3R9
A	234	GLY	-	expression tag	UNP Q8N3R9
A	235	SER	-	expression tag	UNP Q8N3R9
B	232	GLY	-	expression tag	UNP Q8N3R9
B	233	PRO	-	expression tag	UNP Q8N3R9
B	234	GLY	-	expression tag	UNP Q8N3R9
B	235	SER	-	expression tag	UNP Q8N3R9

- Molecule 2 is a protein called Protein crumbs.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	18	Total	C	N	O	S	0	0	0
			150	95	26	28	1			
2	Y	18	Total	C	N	O	S	0	0	0
			140	88	25	26	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	2104	GLY	-	expression tag	UNP P10040
X	2105	PRO	-	expression tag	UNP P10040
X	2106	GLY	-	expression tag	UNP P10040
X	2107	SER	-	expression tag	UNP P10040

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Chain	Residue	Modelled	Actual	Comment	Reference
X	2108	GLU	-	expression tag	UNP P10040
X	2109	PHE	-	expression tag	UNP P10040
Y	2104	GLY	-	expression tag	UNP P10040
Y	2105	PRO	-	expression tag	UNP P10040
Y	2106	GLY	-	expression tag	UNP P10040
Y	2107	SER	-	expression tag	UNP P10040
Y	2108	GLU	-	expression tag	UNP P10040
Y	2109	PHE	-	expression tag	UNP P10040

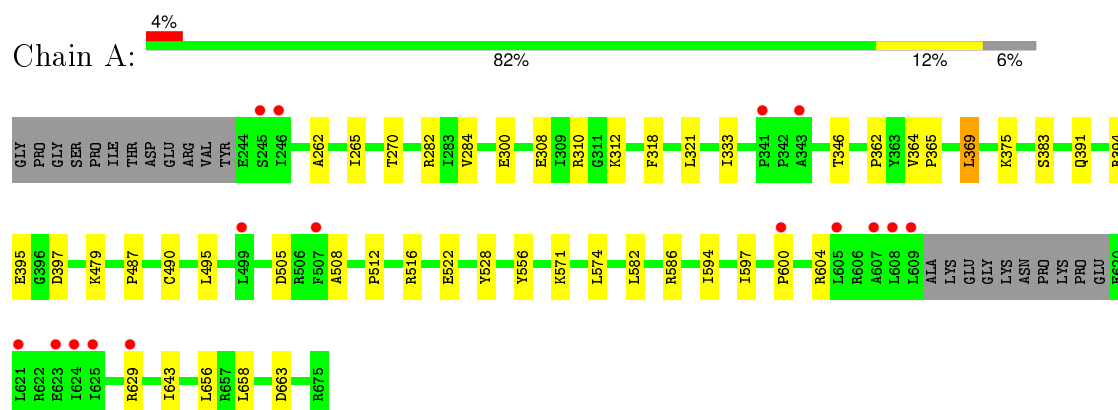
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	4	Total	O	0	0
			4	4		
3	X	1	Total	O	0	0
			1	1		

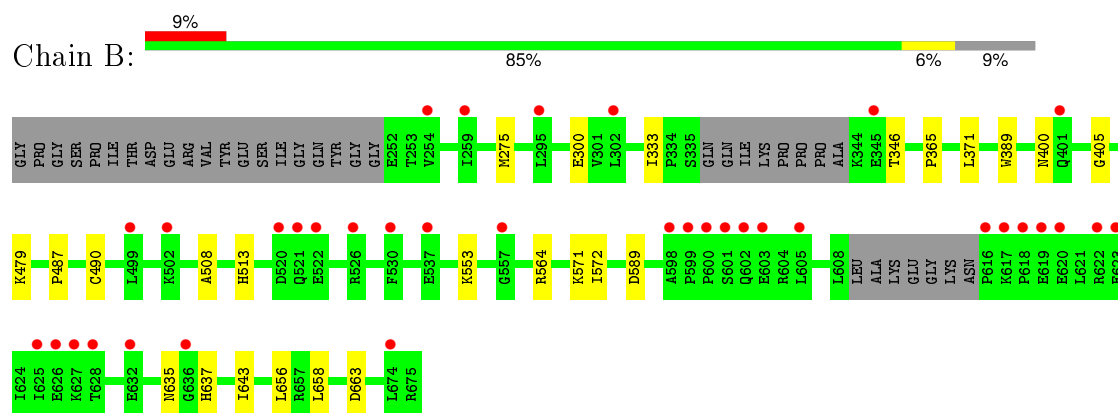
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

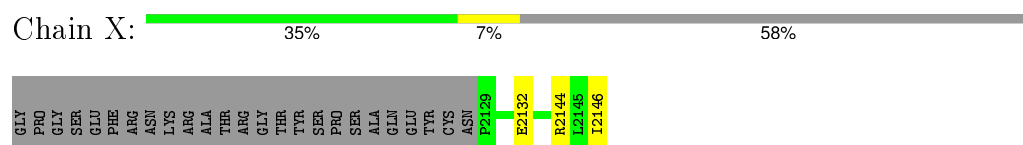
- Molecule 1: MAGUK p55 subfamily member 5



- Molecule 1: MAGUK p55 subfamily member 5



- Molecule 2: Protein crumbs



- Molecule 2: Protein crumbs



GLY	PRO	GLY	SER	GLU	PHE	ARG	ASN	LYS	ARG	ALA	THR	ARG	GLY	THR	TYR	SER	PRO	SER	ALA	GLN	GLU	TYR	CYS	ASN	P2129	12146
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.93Å 111.93Å 223.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.52 – 2.95 49.91 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.52-2.95) 94.2 (49.91-2.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.11 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.207 , 0.235 0.204 , 0.233	Depositor DCC
$R_{free}$ test set	1448 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.7	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 30435 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.23	0/3005	0.42	0/4071
1	B	0.22	0/2839	0.40	0/3853
2	X	0.22	0/153	0.41	0/205
2	Y	0.21	0/143	0.41	0/193
All	All	0.22	0/6140	0.41	0/8322

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	2947	0	2875	26	0
1	B	2785	0	2671	12	0
2	X	150	0	157	4	0
2	Y	140	0	135	0	0
3	A	15	0	0	1	0
3	B	4	0	0	0	0
3	X	1	0	0	1	0
All	All	6042	0	5838	38	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 3.

All (38) 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:318:PHE:HB2	2:X:2144:ARG:HG2	1.74	0.69
1:A:586:ARG:NH1	3:A:714:HOH:O	2.36	0.59
1:B:479:LYS:NZ	1:B:663:ASP:OD1	2.32	0.57
1:B:371:LEU:HB2	1:B:405:GLY:HA3	1.88	0.56
1:A:508:ALA:HB2	1:A:571:LYS:HE3	1.87	0.55
1:A:479:LYS:NZ	1:A:663:ASP:OD1	2.40	0.52
1:A:321:LEU:HD22	2:X:2146:ILE:HB	1.91	0.51
1:B:508:ALA:HB2	1:B:571:LYS:HD3	1.92	0.51
1:A:505:ASP:N	1:A:505:ASP:OD1	2.35	0.49
2:X:2144:ARG:NH1	3:X:2201:HOH:O	2.47	0.48
1:B:643:ILE:HD11	1:B:658:LEU:HD12	1.96	0.47
1:A:582:LEU:HD22	1:A:594:ILE:HD13	1.97	0.46
1:A:516:ARG:NH2	1:A:522:GLU:OE1	2.49	0.46
1:B:487:PRO:HB2	1:B:490:CYS:SG	2.57	0.45
1:A:362:PRO:HG3	1:A:629:ARG:HG2	1.99	0.45
1:B:564:ARG:NH2	1:B:589:ASP:OD1	2.47	0.44
1:A:284:VAL:HG21	1:A:369:LEU:HD21	1.99	0.44
1:B:365:PRO:HD3	1:B:389:TRP:CE2	2.53	0.44
1:A:556:TYR:CZ	2:X:2132:GLU:HG2	2.53	0.44
1:A:512:PRO:HG2	1:A:528:TYR:CD1	2.54	0.43
1:A:375:LYS:NZ	1:B:635:ASN:HB3	2.33	0.43
1:A:383:SER:HB3	1:A:391:GLN:HB2	2.01	0.43
1:B:300:GLU:HB3	1:B:333:ILE:HB	2.00	0.43
1:A:364:VAL:HA	1:A:365:PRO:HD3	1.79	0.42
1:A:643:ILE:HD11	1:A:658:LEU:HD12	2.01	0.42
1:A:394:ARG:O	1:A:397:ASP:HB2	2.19	0.42
1:B:275:MET:HG3	1:B:553:LYS:HE3	2.01	0.42
1:A:487:PRO:HB2	1:A:490:CYS:SG	2.59	0.42
1:A:516:ARG:HD3	1:A:556:TYR:OH	2.20	0.41
1:A:600:PRO:HB2	1:A:604:ARG:HB3	2.02	0.41
1:A:300:GLU:HB3	1:A:333:ILE:HB	2.01	0.41
1:A:512:PRO:HG2	1:A:528:TYR:CE1	2.56	0.41
1:B:479:LYS:HB3	1:B:572:ILE:HG12	2.03	0.41
1:B:400:ASN:OD1	1:B:400:ASN:N	2.53	0.41
1:A:270:THR:OG1	1:A:282:ARG:HB3	2.21	0.41
1:A:308:GLU:O	1:A:312:LYS:HE2	2.21	0.41
1:A:495:LEU:HD12	1:A:597:ILE:HD13	2.03	0.41
1:A:262:ALA:HB3	1:A:265:ILE:HB	2.02	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	369/394 (94%)	354 (96%)	15 (4%)	0	100	100
1	B	353/394 (90%)	339 (96%)	14 (4%)	0	100	100
2	X	16/43 (37%)	16 (100%)	0	0	100	100
2	Y	16/43 (37%)	16 (100%)	0	0	100	100
All	All	754/874 (86%)	725 (96%)	29 (4%)	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	317/346 (92%)	311 (98%)	6 (2%)	65	89
1	B	295/346 (85%)	291 (99%)	4 (1%)	74	92
2	X	18/38 (47%)	18 (100%)	0	100	100
2	Y	15/38 (40%)	15 (100%)	0	100	100
All	All	645/768 (84%)	635 (98%)	10 (2%)	70	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	ARG
1	A	346	THR

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Mol	Chain	Res	Type
1	A	369	LEU
1	A	395	GLU
1	A	574	LEU
1	A	656	LEU
1	B	346	THR
1	B	513	HIS
1	B	637	HIS
1	B	656	LEU

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](#)

There are no ligands in this entry.

### 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

### 6.1 Protein, DNA and RNA chains

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	372/394 (94%)	0.41	16 (4%) 39 23	44, 70, 153, 175	0
1	B	359/394 (91%)	0.55	36 (10%) 9 5	54, 93, 173, 200	0
2	X	18/43 (41%)	0.25	0 100 100	60, 72, 89, 111	0
2	Y	18/43 (41%)	-0.01	0 100 100	71, 126, 153, 157	0
All	All	767/874 (87%)	0.46	52 (6%) 20 11	44, 81, 160, 200	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	PRO	5.9
1	A	609	LEU	5.5
1	A	608	LEU	5.3
1	B	521	GLN	5.0
1	B	598	ALA	4.6
1	B	520	ASP	4.6
1	B	616	PRO	4.6
1	B	601	SER	4.5
1	A	624	ILE	4.3
1	B	599	PRO	4.3
1	B	605	LEU	3.9
1	A	245	SER	3.9
1	A	625	ILE	3.8
1	A	623	GLU	3.7
1	B	618	PRO	3.5
1	A	600	PRO	3.4
1	B	499	LEU	3.3
1	B	617	LYS	2.9
1	B	401	GLN	2.9
1	B	623	GLU	2.7
1	B	522	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	619	GLU	2.7
1	A	605	LEU	2.7
1	A	629	ARG	2.6
1	B	259	ILE	2.5
1	A	343	ALA	2.5
1	B	345	GLU	2.5
1	B	628	THR	2.5
1	A	507	PHE	2.4
1	A	621	LEU	2.3
1	B	627	LYS	2.3
1	B	254	VAL	2.3
1	A	607	ALA	2.3
1	B	620	GLU	2.3
1	B	625	ILE	2.3
1	B	636	GLY	2.3
1	B	626	GLU	2.2
1	A	499	LEU	2.2
1	B	502	LYS	2.2
1	A	246	ILE	2.2
1	A	341	PRO	2.2
1	B	295	LEU	2.2
1	B	526	ARG	2.2
1	B	530	PHE	2.1
1	B	537	GLU	2.1
1	B	674	LEU	2.1
1	B	622	ARG	2.1
1	B	302	LEU	2.1
1	B	602	GLN	2.0
1	B	557	GLY	2.0
1	B	603	GLU	2.0
1	B	632	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.