



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:00 PM UTC

PDB ID : 6ZEH / pdb_00006zeh
Title : Structure of PP1-spectrin alpha II chimera [PP1(7-304) + linker (G/S)x9 + spectrin alpha II (1025-1039)] bound to Phactr1 (516-580)
Authors : Mouilleron, S.; Treisman, R.; Fedoryshchak, R.; Lee, R.; Butler, A.M.; Prechova, M.
Deposited on : 2020-06-16
Resolution : 1.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

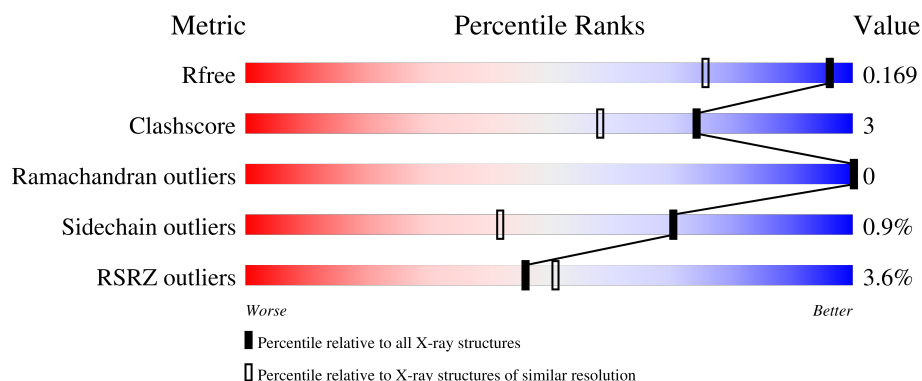
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (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 $\leq 5\%$. 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	336	3% 82% 8% 10%
1	B	336	3% 85% 7% 8%
2	C	70	4% 91% • 7%
2	D	70	4% 90% • 7%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12785 atoms, of which 6007 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 Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Spectrin alpha chain, non-erythrocytic 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	304	Total	C	H	N	O	S	0	17	0
			4928	1595	2438	418	456	21			
1	B	308	Total	C	H	N	O	S	0	11	0
			4944	1595	2454	417	456	22			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P62136
A	3	HIS	-	expression tag	UNP P62136
A	4	MET	-	expression tag	UNP P62136
A	5	GLY	-	expression tag	UNP P62136
A	6	SER	-	expression tag	UNP P62136
A	305	SER	-	linker	UNP P62136
A	306	GLY	-	linker	UNP P62136
A	307	SER	-	linker	UNP P62136
A	308	GLY	-	linker	UNP P62136
A	309	SER	-	linker	UNP P62136
A	310	GLY	-	linker	UNP P62136
A	311	SER	-	linker	UNP P62136
A	312	GLY	-	linker	UNP P62136
A	313	SER	-	linker	UNP P62136
A	314	GLY	-	linker	UNP P62136
A	315	SER	-	linker	UNP P62136
A	316	GLY	-	linker	UNP P62136
A	317	SER	-	linker	UNP P62136
A	318	GLY	-	linker	UNP P62136
A	319	SER	-	linker	UNP P62136
A	320	GLY	-	linker	UNP P62136
A	321	SER	-	linker	UNP P62136
A	322	GLY	-	linker	UNP P62136
B	2	GLY	-	expression tag	UNP P62136

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	HIS	-	expression tag	UNP P62136
B	4	MET	-	expression tag	UNP P62136
B	5	GLY	-	expression tag	UNP P62136
B	6	SER	-	expression tag	UNP P62136
B	305	SER	-	linker	UNP P62136
B	306	GLY	-	linker	UNP P62136
B	307	SER	-	linker	UNP P62136
B	308	GLY	-	linker	UNP P62136
B	309	SER	-	linker	UNP P62136
B	310	GLY	-	linker	UNP P62136
B	311	SER	-	linker	UNP P62136
B	312	GLY	-	linker	UNP P62136
B	313	SER	-	linker	UNP P62136
B	314	GLY	-	linker	UNP P62136
B	315	SER	-	linker	UNP P62136
B	316	GLY	-	linker	UNP P62136
B	317	SER	-	linker	UNP P62136
B	318	GLY	-	linker	UNP P62136
B	319	SER	-	linker	UNP P62136
B	320	GLY	-	linker	UNP P62136
B	321	SER	-	linker	UNP P62136
B	322	GLY	-	linker	UNP P62136

- Molecule 2 is a protein called Phosphatase and actin regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	65	Total	C	H	N	O	S	0	4	0
			1146	359	576	106	104	1			
2	D	65	Total	C	H	N	O	S	0	2	0
			1093	345	539	106	102	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	511	GLY	-	expression tag	UNP Q4VY12
C	512	PRO	-	expression tag	UNP Q4VY12
C	513	LEU	-	expression tag	UNP Q4VY12
C	514	GLY	-	expression tag	UNP Q4VY12
C	515	SER	-	expression tag	UNP Q4VY12
D	511	GLY	-	expression tag	UNP Q4VY12
D	512	PRO	-	expression tag	UNP Q4VY12
D	513	LEU	-	expression tag	UNP Q4VY12

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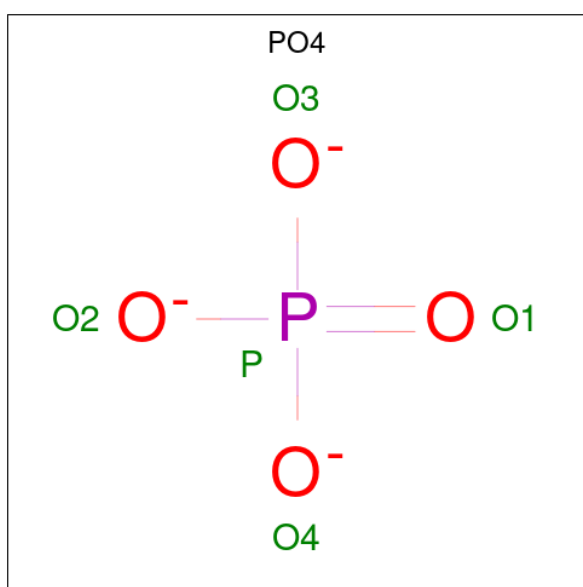
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Chain	Residue	Modelled	Actual	Comment	Reference
D	514	GLY	-	expression tag	UNP Q4VY12
D	515	SER	-	expression tag	UNP Q4VY12

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

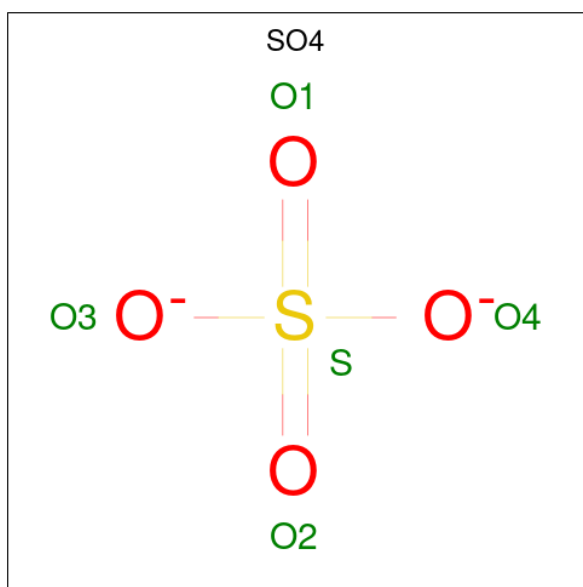
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

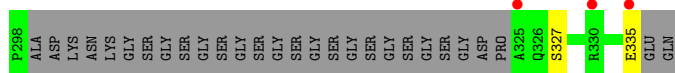


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	256	Total	O	0	0
			256	256		
6	C	85	Total	O	0	0
			85	85		
6	B	246	Total	O	0	0
			246	246		
6	D	68	Total	O	0	0
			68	68		

- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Spectrin alpha chain, non-erythrocytic 1



SER
GLY
SER
GLY
SER
GLY
SER
GLY
SER
GLY
SER
GLY
SER
GLY
SER
GLY
SER
GLY
ASP
PRO
ALA
Q326
S327
E331
E335
E336
Q337

GLY
PRO
LEU
GLY
SER
R516
K517
I518
L519
I520
K540
P580

GLY
PRO
LEU
GLY
SER
R516
R521
F522
S523
Q532
D533
R576
P580

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.50Å 122.39Å 69.34Å 90.00° 92.18° 90.00°	Depositor
Resolution (Å)	69.29 – 1.30 69.29 – 1.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (69.29-1.30) 99.4 (69.29-1.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.18_3845, PHENIX 1.18_3845	Depositor
R, R_{free}	0.137 , 0.169 0.137 , 0.169	Depositor DCC
R_{free} test set	9653 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	1.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12785	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: MN, SO4, PO4

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	0.48	0/2599	0.67	1/3512 (0.0%)
1	B	0.51	0/2588	0.70	0/3494
2	C	0.37	0/593	0.55	0/796
2	D	0.39	0/577	0.55	0/775
All	All	0.47	0/6357	0.66	1/8577 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	HIS	CA-CB-CG	5.20	119.00	113.80

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	2490	2438	2390	20	0
1	B	2490	2454	2422	17	0
2	C	570	576	576	1	0
2	D	554	539	529	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	B	5	0	0	1	0
6	A	256	0	0	5	0
6	B	246	0	0	5	0
6	C	85	0	0	0	0
6	D	68	0	0	0	0
All	All	6778	6007	5917	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.

The worst 5 of 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:B:75[B]:LEU:HD21	6:B:627:HOH:O	1.87	0.74
1:B:195:VAL:HG21	6:B:745:HOH:O	1.98	0.64
1:A:127[B]:CYS:SG	1:A:195:VAL:HG21	2.38	0.63
1:B:101[B]:LEU:CD1	1:B:143:ARG:HG3	2.31	0.61
1:B:101[B]:LEU:HD12	1:B:143:ARG:HG3	1.82	0.60

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	317/336 (94%)	306 (96%)	11 (4%)	0	100	100
1	B	315/336 (94%)	304 (96%)	11 (4%)	0	100	100
2	C	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
2	D	65/70 (93%)	64 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	764/812 (94%)	740 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	272/287 (95%)	270 (99%)	2 (1%)	76	50
1	B	276/287 (96%)	273 (99%)	3 (1%)	65	33
2	C	62/61 (102%)	62 (100%)	0	100	100
2	D	58/61 (95%)	57 (98%)	1 (2%)	53	17
All	All	668/696 (96%)	662 (99%)	6 (1%)	70	42

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	246	ARG
1	B	335	GLU
2	D	521	ARG
1	A	335	GLU
1	A	246	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	117	ASN
1	A	237	HIS
1	A	262	GLN
1	B	117	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 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	$\# Z > 2$
5	SO4	B	504	-	4,4,4	0.41	0	6,6,6	0.45	0
4	PO4	B	503	3	4,4,4	0.85	0	6,6,6	1.66	2 (33%)
4	PO4	A	503	3	4,4,4	1.31	1 (25%)	6,6,6	1.05	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	PO4	P-O3	-2.20	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	PO4	O3-P-O1	-2.78	101.11	110.95
4	B	503	PO4	O4-P-O3	2.57	115.90	107.91

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
5	B	504	SO4	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	304/336 (90%)	-0.18	10 (3%)	49	55	6, 16, 32, 46	10 (3%)
1	B	308/336 (91%)	-0.16	11 (3%)	46	51	7, 16, 32, 49	8 (2%)
2	C	65/70 (92%)	0.04	3 (4%)	37	43	10, 20, 34, 43	4 (6%)
2	D	65/70 (92%)	0.23	3 (4%)	37	43	10, 24, 36, 41	1 (1%)
All	All	742/812 (91%)	-0.12	27 (3%)	46	51	6, 17, 33, 49	23 (3%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	GLY	6.1
1	A	325	ALA	5.0
1	A	7	LEU	4.1
1	A	6	SER	3.5
1	B	3	HIS	3.5

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	SO4	B	504	5/5	0.96	0.14	13,27,30,31	0
4	PO4	A	503	5/5	0.99	0.04	9,10,11,12	0
3	MN	B	501	1/1	1.00	0.01	9,9,9,9	0
3	MN	B	502	1/1	1.00	0.01	10,10,10,10	0
3	MN	A	501	1/1	1.00	0.02	8,8,8,8	0
4	PO4	B	503	5/5	1.00	0.02	10,10,11,11	0
3	MN	A	502	1/1	1.00	0.01	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.