



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:47 PM UTC

PDB ID : 1JS3 / pdb_00001js3
Title : Crystal structure of dopa decarboxylase in complex with the inhibitor carbidopa
Authors : Burkhard, P.; Dominici, P.; Borri-Voltattorni, C.; Jansonius, J.N.; Malashkevich, V.N.
Deposited on : 2001-08-16
Resolution : 2.25 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

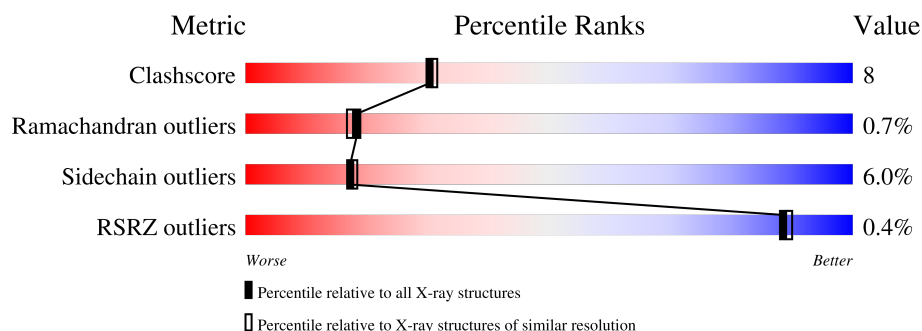
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	486	75% 19% • 5%
1	B	486	73% 20% • 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7787 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 DOPA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3625	2327	630	643	25			
1	B	464	Total	C	N	O	S	0	0	0
			3625	2327	630	643	25			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- PLP
-
- The diagram shows the chemical structure of PLP (Pyridoxal phosphate). It consists of a pyridine ring with a phosphate group attached to the 4-position and an aldehyde group attached to the 3-position. The pyridine ring is labeled with N1 (nitrogen), C2, C3, C4, C5, and C6. The phosphate group is labeled with P (phosphorus), O1P, O2P, O3P, and O4P. The aldehyde group is labeled with C4A (carbon) and O4A (oxygen). The hydroxyl group on the ring is labeled with O3 (oxygen) and C3 (carbon). The hydroxyl group on the phosphate is labeled with O3P (oxygen) and HO (hydrogen). The hydroxyl group on the aldehyde is labeled with O4A (oxygen) and C4A (carbon).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

- 142
-
- The chemical structure shows L-alanine with a 3,4-dihydroxyphenyl group. The amino group is blue, the carboxyl group is red, and the phenyl ring and its hydroxyl groups are green. Atom labels include: N (green), NH₂ (blue), NN (green), NH (blue), CB (green), CD1 (green), CE1 (green), OE1 (green), OXT (green), CA(S) (green), C (green), CG (green), CB1 (green), CD2 (green), CE2 (green), CZ (green), OH (green), O (green), and HO (red).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	10	2	4		



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			16	10	2	4		

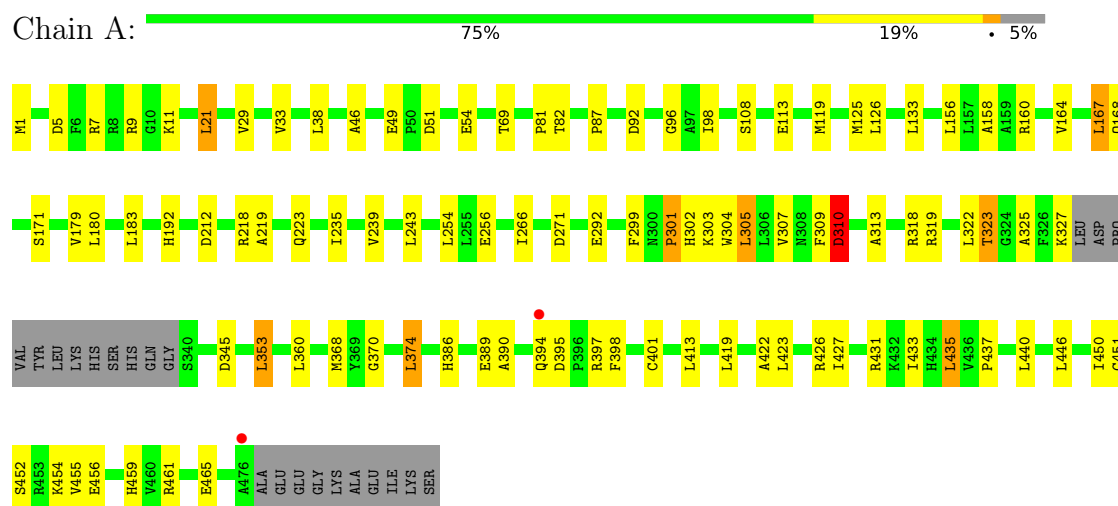
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	216	Total	O	0	0
			216	216		
5	B	239	Total	O	0	0
			239	239		

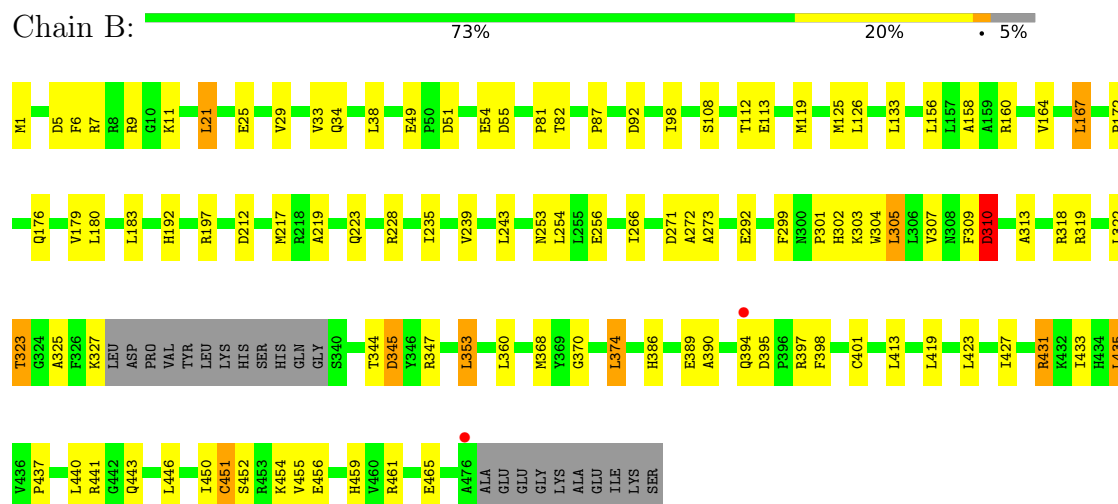
3 Residue-property plots

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: DOPA decarboxylase



• Molecule 1: DOPA decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	154.36Å 154.36Å 86.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.61 – 2.25 19.61 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.8 (19.61-2.25) 95.9 (19.61-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.26Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.144 , 0.187 0.154 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7787	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 142, PLP, SO4

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	0.55	1/3714 (0.0%)	0.99	18/5028 (0.4%)
1	B	0.55	0/3714	0.99	17/5028 (0.3%)
All	All	0.55	1/7428 (0.0%)	0.99	35/10056 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	MET	SD-CE	-5.04	1.67	1.79

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ASP	N-CA-C	-7.97	98.66	110.46
1	A	431	ARG	NE-CZ-NH2	7.78	126.20	119.20
1	A	38	LEU	N-CA-C	7.78	120.89	111.40
1	A	431	ARG	NE-CZ-NH1	-7.71	113.78	121.50
1	A	51	ASP	N-CA-C	-7.66	99.13	110.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3625	0	3606	57	0
1	B	3625	0	3606	67	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	15	0	7	2	0
3	B	15	0	7	1	0
4	A	16	0	12	1	0
4	B	16	0	12	2	0
5	A	216	0	0	3	0
5	B	239	0	0	13	0
All	All	7787	0	7250	122	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 8.

The worst 5 of 122 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:454:LYS:HE2	5:A:950:HOH:O	1.70	0.92
1:A:456:GLU:H	1:A:459:HIS:HD2	1.24	0.84
1:B:456:GLU:H	1:B:459:HIS:HD2	1.26	0.81
1:A:87:PRO:HB3	1:A:368:MET:HE3	1.66	0.77
1:B:87:PRO:HB3	1:B:368:MET:HE3	1.68	0.76

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	460/486 (95%)	445 (97%)	12 (3%)	3 (1%)	18	17
1	B	460/486 (95%)	444 (96%)	13 (3%)	3 (1%)	18	17
All	All	920/972 (95%)	889 (97%)	25 (3%)	6 (1%)	18	17

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	SER
1	A	310	ASP
1	B	108	SER
1	B	310	ASP
1	A	437	PRO

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	375/393 (95%)	353 (94%)	22 (6%)	18	18
1	B	375/393 (95%)	352 (94%)	23 (6%)	17	17
All	All	750/786 (95%)	705 (94%)	45 (6%)	17	18

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	167	LEU
1	B	323	THR
1	B	183	LEU
1	B	254	LEU
1	B	360	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	386	HIS
1	B	459	HIS
1	A	386	HIS
1	A	459	HIS
1	A	466	HIS

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 ⓘ

8 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	SO4	A	802	-	4,4,4	0.42	0	6,6,6	0.24	0
3	PLP	A	601	4	15,15,16	1.09	0	21,22,23	1.30	3 (14%)
4	142	A	701	3	14,16,16	1.21	1 (7%)	20,23,23	1.21	2 (10%)
3	PLP	B	602	4	15,15,16	1.22	1 (6%)	21,22,23	1.35	4 (19%)
2	SO4	A	803	-	4,4,4	0.39	0	6,6,6	0.13	0
4	142	B	702	3	14,16,16	1.20	1 (7%)	20,23,23	0.87	0
2	SO4	B	801	-	4,4,4	0.39	0	6,6,6	0.22	0
2	SO4	B	804	-	4,4,4	0.42	0	6,6,6	0.09	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
4	142	B	702	3	-	2/11/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	142	A	701	3	-	4/11/14/14	0/1/1/1
3	PLP	A	601	4	-	0/6/6/8	0/1/1/1
3	PLP	B	602	4	-	1/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	142	CE2-CD2	2.76	1.43	1.38
4	B	702	142	CE2-CD2	2.56	1.43	1.38
3	B	602	PLP	P-O3P	-2.02	1.47	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	142	O-C-CA	-3.61	116.30	122.78
3	A	601	PLP	C4A-C4-C5	-3.17	117.67	120.94
3	B	602	PLP	C4A-C4-C5	-3.13	117.72	120.94
3	B	602	PLP	C6-C5-C4	2.66	120.28	118.10
3	A	601	PLP	C6-C5-C4	2.50	120.15	118.10

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	142	O-C-CA-NN
4	A	701	142	O-C-CA-CB1
4	B	702	142	OXT-C-CA-CB
4	B	702	142	OXT-C-CA-CB1
3	B	602	PLP	C5A-O4P-P-O1P

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	PLP	2	0
4	A	701	142	1	0
3	B	602	PLP	1	0
4	B	702	142	2	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	464/486 (95%)	-0.69	2 (0%) 88 89	8, 20, 44, 64	0
1	B	464/486 (95%)	-0.71	2 (0%) 88 89	8, 20, 42, 65	0
All	All	928/972 (95%)	-0.70	4 (0%) 88 89	8, 20, 43, 65	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	GLN	3.1
1	A	476	ALA	2.8
1	B	394	GLN	2.4
1	B	476	ALA	2.2

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(Å ²)	Q<0.9
2	SO4	B	804	5/5	0.77	0.13	81,84,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	801	5/5	0.86	0.12	45,58,68,69	0
2	SO4	A	802	5/5	0.86	0.14	54,56,61,66	0
4	142	B	702	16/16	0.87	0.11	19,25,39,47	0
2	SO4	A	803	5/5	0.89	0.09	58,69,75,77	0
4	142	A	701	16/16	0.91	0.08	15,23,33,34	0
3	PLP	B	602	15/16	0.98	0.06	9,17,23,28	0
3	PLP	A	601	15/16	0.99	0.05	4,17,25,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.