



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:47 AM GMT

PDB ID : 3FZ8
Title : Crystal structure of glutamate decarboxylase beta from Escherichia coli: reduced Schiff base with PLP
Authors : Malashkevich, V.N.; De Biase, D.; Bossa, F.
Deposited on : 2009-01-23
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

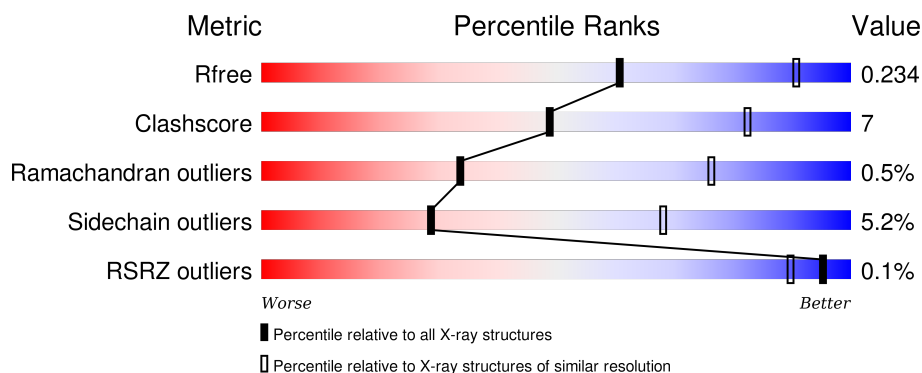
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	466	<div> <div>84%</div> <div>13% ..</div> </div>
1	B	466	<div> <div>76%</div> <div>23% ..</div> </div>
1	C	466	<div> <div>79%</div> <div>17% ..</div> </div>
1	D	466	<div> <div>77%</div> <div>19% ..</div> </div>
1	E	466	<div> <div>78%</div> <div>20% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	466	 78%18%..

2 Entry composition [i](#)

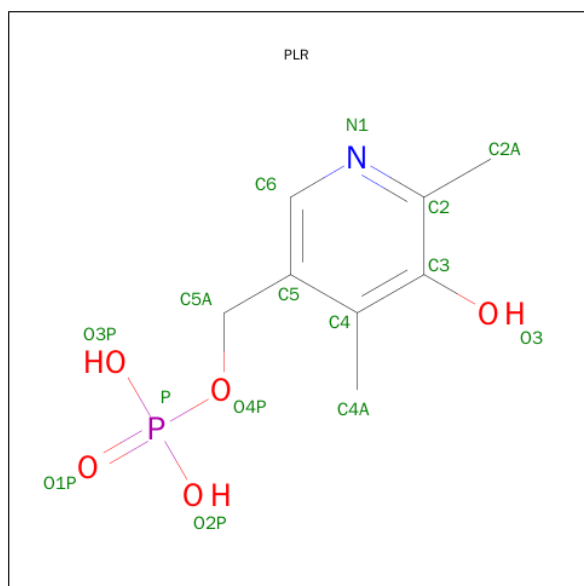
There are 3 unique types of molecules in this entry. The entry contains 21985 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate decarboxylase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	B	463	Total	C	N	O	S	0	0	0
			3681	2347	630	680	24			
1	C	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	D	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	E	464	Total	C	N	O	S	0	0	0
			3690	2353	632	681	24			
1	F	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			

- Molecule 2 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: PLR) (formula: C₈H₁₂NO₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

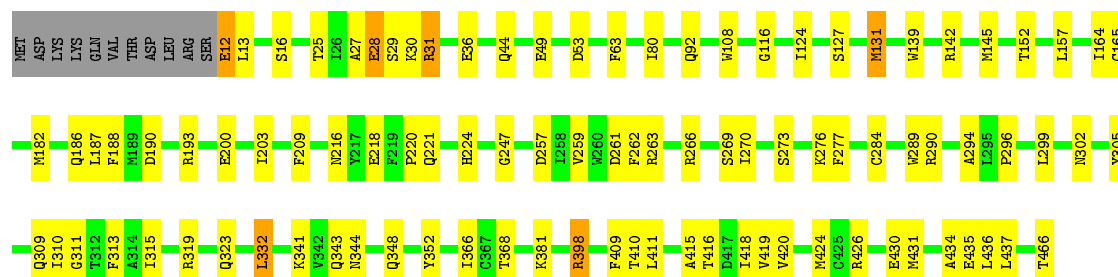
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	60	Total	O	0	0
			60	60		



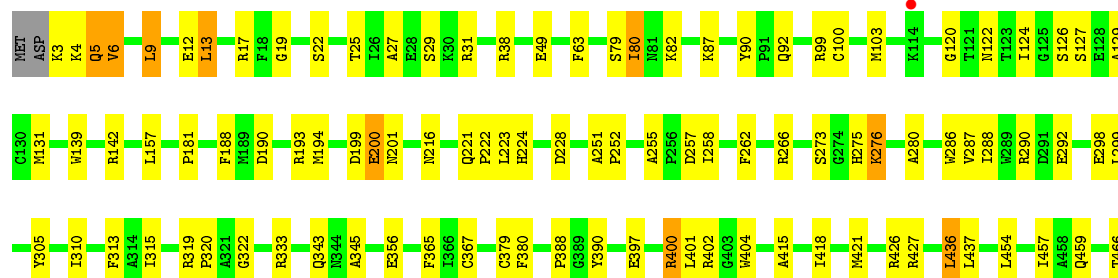
• Molecule 1: Glutamate decarboxylase beta

Chain D: 77% 19% ..



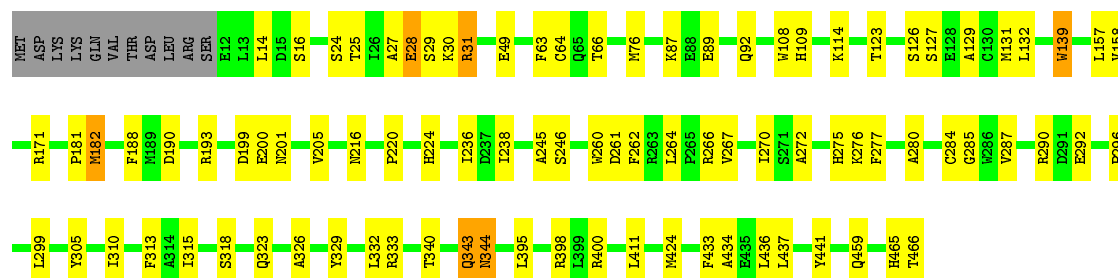
• Molecule 1: Glutamate decarboxylase beta

Chain E: 78% 20% .



• Molecule 1: Glutamate decarboxylase beta

Chain F: 78% 18% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	116.90Å 116.89Å 208.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 3.00 29.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.88-3.00) 95.4 (29.88-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.165 , 0.237 0.166 , 0.234	Depositor DCC
R_{free} test set	3072 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.6	EDS
Estimated twinning fraction	0.013 for -h,-k,l 0.041 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 60814 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21985	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PLR

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	0.61	0/3710	0.72	0/5028
1	B	0.63	0/3775	0.74	0/5115
1	C	0.64	1/3710 (0.0%)	0.76	1/5028 (0.0%)
1	D	0.62	0/3710	0.73	0/5028
1	E	0.66	2/3784 (0.1%)	0.76	2/5126 (0.0%)
1	F	0.63	0/3710	0.72	1/5028 (0.0%)
All	All	0.63	3/22399 (0.0%)	0.74	4/30353 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	276	LYS	CE-NZ	-7.00	1.31	1.49
1	E	367	CYS	CB-SG	-6.29	1.71	1.82
1	E	100	CYS	CB-SG	-5.21	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	LYS	CD-CE-NZ	8.67	131.63	111.70
1	E	157	LEU	CA-CB-CG	8.24	134.25	115.30
1	E	436	LEU	CA-CB-CG	6.66	130.62	115.30
1	F	157	LEU	CA-CB-CG	5.43	127.78	115.30

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	3616	0	3514	42	0
1	B	3681	0	3584	69	0
1	C	3616	0	3513	56	0
1	D	3616	0	3514	59	0
1	E	3690	0	3597	64	0
1	F	3616	0	3514	57	0
2	A	15	0	9	2	0
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	0	0
2	E	15	0	9	0	0
2	F	15	0	8	1	0
3	E	60	0	0	2	0
All	All	21985	0	21289	309	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 7.

The worst 5 of 309 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:D:188:PHE:HZ	1:D:216:ASN:HD22	1.02	0.99
1:E:305:TYR:HE1	1:E:310:ILE:HG13	1.35	0.90
1:F:188:PHE:HZ	1:F:216:ASN:HD22	1.20	0.86
1:E:188:PHE:HZ	1:E:216:ASN:ND2	1.74	0.85
1:E:188:PHE:HZ	1:E:216:ASN:HD22	1.20	0.85

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	453/466 (97%)	422 (93%)	27 (6%)	4 (1%)	21	64
1	B	461/466 (99%)	431 (94%)	28 (6%)	2 (0%)	39	80
1	C	453/466 (97%)	424 (94%)	27 (6%)	2 (0%)	39	80
1	D	453/466 (97%)	425 (94%)	27 (6%)	1 (0%)	52	88
1	E	462/466 (99%)	429 (93%)	28 (6%)	5 (1%)	17	58
1	F	453/466 (97%)	424 (94%)	29 (6%)	0	100	100
All	All	2735/2796 (98%)	2555 (93%)	166 (6%)	14 (0%)	34	76

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	D	28	GLU
1	A	27	ALA
1	B	186	GLN
1	C	413	GLY

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	379/390 (97%)	361 (95%)	18 (5%)	32	72
1	B	387/390 (99%)	363 (94%)	24 (6%)	23	60
1	C	379/390 (97%)	358 (94%)	21 (6%)	27	65
1	D	379/390 (97%)	359 (95%)	20 (5%)	28	67
1	E	388/390 (100%)	369 (95%)	19 (5%)	31	71
1	F	379/390 (97%)	363 (96%)	16 (4%)	36	76
All	All	2291/2340 (98%)	2173 (95%)	118 (5%)	29	68

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	309	GLN
1	D	36	GLU
1	F	246	SER
1	C	327	GLN
1	C	436	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	216	ASN
1	C	459	GLN
1	F	309	GLN
1	C	309	GLN
1	D	109	HIS

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](#)

6 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	PLR	A	500	1	15,15,15	0.91	0	21,22,22	1.43	3 (14%)
2	PLR	B	500	1	15,15,15	0.85	1 (6%)	21,22,22	1.26	3 (14%)
2	PLR	C	500	1	15,15,15	0.99	1 (6%)	21,22,22	1.38	3 (14%)
2	PLR	D	500	1	15,15,15	1.21	1 (6%)	21,22,22	1.15	2 (9%)
2	PLR	E	500	1	15,15,15	0.81	1 (6%)	21,22,22	1.33	2 (9%)
2	PLR	F	500	1	15,15,15	1.17	2 (13%)	21,22,22	1.69	5 (23%)

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	PLR	A	500	1	-	0/6/6/6	0/1/1/1
2	PLR	B	500	1	-	0/6/6/6	0/1/1/1
2	PLR	C	500	1	-	0/6/6/6	0/1/1/1
2	PLR	D	500	1	-	0/6/6/6	0/1/1/1
2	PLR	E	500	1	-	0/6/6/6	0/1/1/1
2	PLR	F	500	1	-	0/6/6/6	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	PLR	C3-C2	-3.47	1.38	1.40
2	C	500	PLR	C3-C2	-2.88	1.38	1.40
2	B	500	PLR	C3-C2	-2.55	1.39	1.40
2	F	500	PLR	C4A-C4	-2.45	1.46	1.51
2	F	500	PLR	C3-C2	-2.31	1.39	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	PLR	C4A-C4-C5	-4.35	116.35	120.88
2	E	500	PLR	O4P-P-O1P	-3.74	97.63	107.14
2	C	500	PLR	O4P-P-O1P	-3.19	99.02	107.14
2	A	500	PLR	C4A-C4-C5	-2.86	117.90	120.88
2	F	500	PLR	C2A-C2-C3	-2.71	117.77	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PLR	2	0
2	F	500	PLR	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	455/466 (97%)	-0.85	0 100 100	2, 10, 35, 53	0
1	B	463/466 (99%)	-0.84	2 (0%) 93 80	2, 9, 34, 53	0
1	C	455/466 (97%)	-0.91	0 100 100	2, 9, 34, 52	0
1	D	455/466 (97%)	-0.88	0 100 100	2, 10, 36, 52	0
1	E	464/466 (99%)	-0.90	1 (0%) 95 87	2, 8, 33, 51	0
1	F	455/466 (97%)	-0.92	0 100 100	2, 9, 34, 51	0
All	All	2747/2796 (98%)	-0.88	3 (0%) 95 90	2, 9, 35, 53	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	LYS	2.8
1	E	114	LYS	2.7
1	B	308	GLY	2.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å ²)	Q<0.9
2	PLR	D	500	15/15	0.97	0.14	0.84	3,10,14,15	0
2	PLR	E	500	15/15	0.99	0.13	-0.20	2,4,11,13	0
2	PLR	F	500	15/15	0.98	0.11	-0.27	2,5,13,14	0
2	PLR	A	500	15/15	0.99	0.13	-0.48	11,14,15,15	0
2	PLR	B	500	15/15	0.98	0.11	-0.67	3,11,13,13	0
2	PLR	C	500	15/15	0.99	0.10	-1.03	2,5,13,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.