



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:08 am GMT

PDB ID : 5IV8
Title : The LPS Transporter LptDE from *Klebsiella pneumoniae*, core complex
Authors : Botos, I.; McCarthy, J.G.; Buchanan, S.K.
Deposited on : 2016-03-20
Resolution : 2.94 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

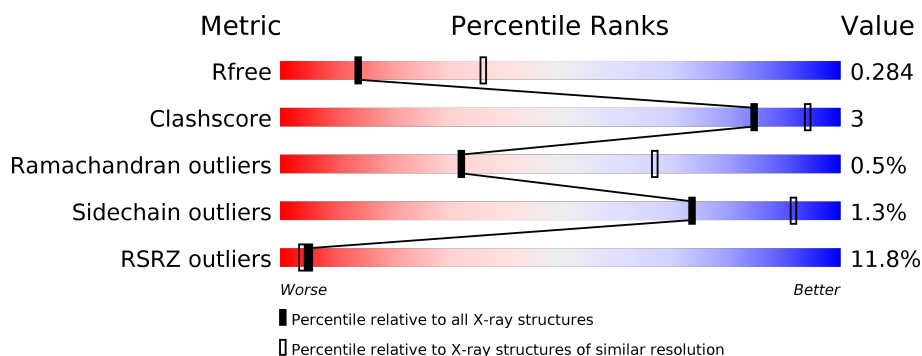
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	100719	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (2.98-2.90)

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	601	<div> <div>7%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	C	601	<div> <div>17%</div> <div>80%</div> <div>10%</div> <div>10%</div> </div>
2	B	182	<div> <div>7%</div> <div>75%</div> <div>5%</div> <div>20%</div> </div>
2	D	182	<div> <div>5%</div> <div>73%</div> <div>9%</div> <div>18%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C8E	A	801	-	-	-	X
3	C8E	A	802	-	-	-	X
3	C8E	C	801	-	-	-	X
3	C8E	C	802	-	-	-	X
3	C8E	C	803	-	-	-	X
3	C8E	C	804	-	-	-	X
3	C8E	D	201	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11347 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 LPS biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4472	2808	766	888	10			
1	C	543	Total	C	N	O	S	0	0	0
			4401	2767	749	875	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	MET	-	initiating methionine	UNP A0A0U3IWD2
A	182	SER	-	expression tag	UNP A0A0U3IWD2
A	183	ASN	-	expression tag	UNP A0A0U3IWD2
A	184	HIS	-	expression tag	UNP A0A0U3IWD2
A	185	HIS	-	expression tag	UNP A0A0U3IWD2
A	186	HIS	-	expression tag	UNP A0A0U3IWD2
A	187	HIS	-	expression tag	UNP A0A0U3IWD2
A	188	HIS	-	expression tag	UNP A0A0U3IWD2
A	189	HIS	-	expression tag	UNP A0A0U3IWD2
A	190	HIS	-	expression tag	UNP A0A0U3IWD2
A	191	HIS	-	expression tag	UNP A0A0U3IWD2
A	192	HIS	-	expression tag	UNP A0A0U3IWD2
A	193	HIS	-	expression tag	UNP A0A0U3IWD2
A	194	GLU	-	expression tag	UNP A0A0U3IWD2
A	195	ASN	-	expression tag	UNP A0A0U3IWD2
A	196	LEU	-	expression tag	UNP A0A0U3IWD2
A	197	TYR	-	expression tag	UNP A0A0U3IWD2
A	198	PHE	-	expression tag	UNP A0A0U3IWD2
A	199	GLN	-	expression tag	UNP A0A0U3IWD2
A	200	SER	-	expression tag	UNP A0A0U3IWD2
A	201	MET	-	expression tag	UNP A0A0U3IWD2
C	181	MET	-	initiating methionine	UNP A0A0U3IWD2
C	182	SER	-	expression tag	UNP A0A0U3IWD2
C	183	ASN	-	expression tag	UNP A0A0U3IWD2
C	184	HIS	-	expression tag	UNP A0A0U3IWD2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	185	HIS	-	expression tag	UNP A0A0U3IWD2
C	186	HIS	-	expression tag	UNP A0A0U3IWD2
C	187	HIS	-	expression tag	UNP A0A0U3IWD2
C	188	HIS	-	expression tag	UNP A0A0U3IWD2
C	189	HIS	-	expression tag	UNP A0A0U3IWD2
C	190	HIS	-	expression tag	UNP A0A0U3IWD2
C	191	HIS	-	expression tag	UNP A0A0U3IWD2
C	192	HIS	-	expression tag	UNP A0A0U3IWD2
C	193	HIS	-	expression tag	UNP A0A0U3IWD2
C	194	GLU	-	expression tag	UNP A0A0U3IWD2
C	195	ASN	-	expression tag	UNP A0A0U3IWD2
C	196	LEU	-	expression tag	UNP A0A0U3IWD2
C	197	TYR	-	expression tag	UNP A0A0U3IWD2
C	198	PHE	-	expression tag	UNP A0A0U3IWD2
C	199	GLN	-	expression tag	UNP A0A0U3IWD2
C	200	SER	-	expression tag	UNP A0A0U3IWD2
C	201	MET	-	expression tag	UNP A0A0U3IWD2

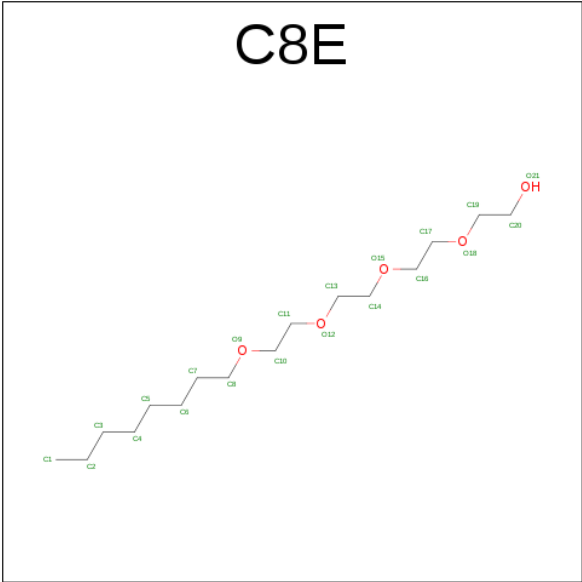
- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1140	713	201	220	6			
2	D	149	Total	C	N	O	S	0	0	0
			1164	727	205	226	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ALA	-	expression tag	UNP A0A0J4W1Y0
B	16	PRO	-	expression tag	UNP A0A0J4W1Y0
B	17	ASN	-	expression tag	UNP A0A0J4W1Y0
B	18	THR	-	expression tag	UNP A0A0J4W1Y0
B	19	SER	-	expression tag	UNP A0A0J4W1Y0
D	15	ALA	-	expression tag	UNP A0A0J4W1Y0
D	16	PRO	-	expression tag	UNP A0A0J4W1Y0
D	17	ASN	-	expression tag	UNP A0A0J4W1Y0
D	18	THR	-	expression tag	UNP A0A0J4W1Y0
D	19	SER	-	expression tag	UNP A0A0J4W1Y0

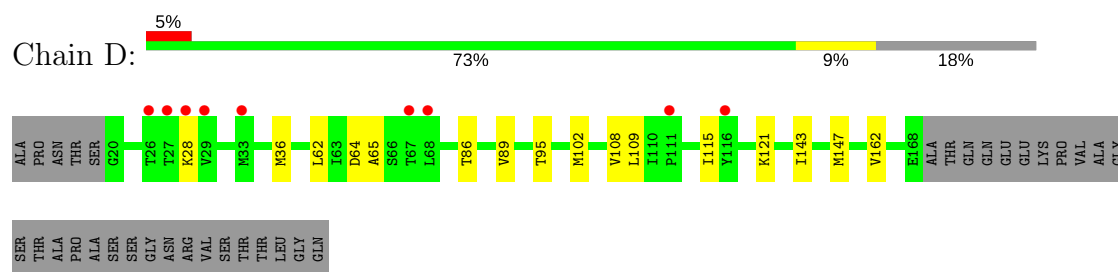
- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	D	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.02Å 173.05Å 84.76Å 90.00° 111.26° 90.00°	Depositor
Resolution (Å)	41.41 – 2.94 46.58 – 2.94	Depositor EDS
% Data completeness (in resolution range)	83.7 (41.41-2.94) 83.7 (46.58-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.235 , 0.284 0.230 , 0.284	Depositor DCC
R_{free} test set	1987 reflections (5.54%)	DCC
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11347	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: C8E

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	0.24	0/4588	0.43	0/6240
1	C	0.24	0/4517	0.45	0/6147
2	B	0.24	0/1158	0.41	0/1569
2	D	0.24	0/1183	0.41	0/1604
All	All	0.24	0/11446	0.43	0/15560

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	4472	0	4149	21	0
1	C	4401	0	4074	27	0
2	B	1140	0	1147	5	0
2	D	1164	0	1175	8	0
3	A	63	0	102	2	0
3	C	84	0	136	1	0
3	D	21	0	34	0	0
4	A	2	0	0	0	0
All	All	11347	0	10817	60	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 60 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:C:642:ARG:HE	1:C:646:ARG:HD3	1.52	0.74
1:C:646:ARG:HA	1:C:685:SER:O	1.91	0.70
1:C:251:ALA:HB3	1:C:254:PHE:HB2	1.78	0.64
1:A:774:ILE:HG13	1:A:775:LEU:HD12	1.82	0.62
2:D:109:LEU:HG	2:D:115:ILE:HG22	1.83	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	548/601 (91%)	510 (93%)	35 (6%)	3 (0%)	32	67
1	C	539/601 (90%)	497 (92%)	38 (7%)	4 (1%)	25	59
2	B	142/182 (78%)	139 (98%)	3 (2%)	0	100	100
2	D	147/182 (81%)	141 (96%)	6 (4%)	0	100	100
All	All	1376/1566 (88%)	1287 (94%)	82 (6%)	7 (0%)	32	67

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	666	SER
1	A	365	GLN
1	C	629	ASP
1	C	365	GLN
1	C	239	GLY

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	480/526 (91%)	474 (99%)	6 (1%)	73	91
1	C	473/526 (90%)	464 (98%)	9 (2%)	62	86
2	B	127/156 (81%)	127 (100%)	0	100	100
2	D	131/156 (84%)	130 (99%)	1 (1%)	85	95
All	All	1211/1364 (89%)	1195 (99%)	16 (1%)	73	91

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	394	ASP
1	C	421	ASN
1	C	677	ILE
1	C	290	TYR
1	C	692	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	91	GLN

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

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	$\# Z > 2$
3	C8E	A	801	-	20,20,20	0.39	0	19,19,19	0.33	0
3	C8E	A	802	-	20,20,20	0.38	0	19,19,19	0.40	0
3	C8E	A	803	-	20,20,20	0.38	0	19,19,19	0.37	0
3	C8E	C	801	-	20,20,20	0.38	0	19,19,19	0.35	0
3	C8E	C	802	-	20,20,20	0.38	0	19,19,19	0.40	0
3	C8E	C	803	-	20,20,20	0.37	0	19,19,19	0.40	0
3	C8E	C	804	-	20,20,20	0.38	0	19,19,19	0.38	0
3	C8E	D	201	-	20,20,20	0.39	0	19,19,19	0.35	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
3	C8E	A	801	-	-	0/18/18/18	0/0/0/0
3	C8E	A	802	-	-	0/18/18/18	0/0/0/0
3	C8E	A	803	-	-	0/18/18/18	0/0/0/0
3	C8E	C	801	-	-	0/18/18/18	0/0/0/0
3	C8E	C	802	-	-	0/18/18/18	0/0/0/0
3	C8E	C	803	-	-	0/18/18/18	0/0/0/0
3	C8E	C	804	-	-	0/18/18/18	0/0/0/0
3	C8E	D	201	-	-	0/18/18/18	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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
3	A	801	C8E	2	0
3	C	801	C8E	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	552/601 (91%)	0.43	41 (7%) 15 12	14, 62, 120, 154	0
1	C	543/601 (90%)	0.85	101 (18%) 1 1	21, 72, 157, 211	0
2	B	146/182 (80%)	0.54	13 (8%) 10 8	21, 63, 126, 164	0
2	D	149/182 (81%)	0.41	9 (6%) 23 19	29, 62, 134, 180	0
All	All	1390/1566 (88%)	0.60	164 (11%) 5 4	14, 65, 144, 211	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	753	ILE	8.0
1	C	688	ILE	7.3
1	C	723	ILE	6.4
1	C	301	HIS	6.2
1	A	722	ALA	6.1

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(\AA^2)	Q<0.9
3	C8E	D	201	21/21	0.88	0.38	9.46	19,62,96,105	0
3	C8E	C	803	21/21	0.86	0.31	5.67	42,80,130,132	0
3	C8E	C	804	21/21	0.92	0.34	5.25	28,45,61,65	0
3	C8E	A	802	21/21	0.89	0.39	4.31	22,53,94,110	0
3	C8E	A	801	21/21	0.88	0.30	3.41	31,69,97,99	0
3	C8E	C	802	21/21	0.92	0.26	3.12	22,48,72,79	0
3	C8E	C	801	21/21	0.93	0.27	2.30	16,46,75,84	0
3	C8E	A	803	21/21	0.76	0.29	1.82	32,74,93,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.