



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 22, 2018 – 10:58 AM EDT

PDB ID : 6C0Y  
Title : Lysinoalanine synthase, DurN, from duramycin biosynthesis bound to duramycin  
Authors : Cogan, D.P.; Nair, S.K.  
Deposited on : 2018-01-03  
Resolution : 1.66 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

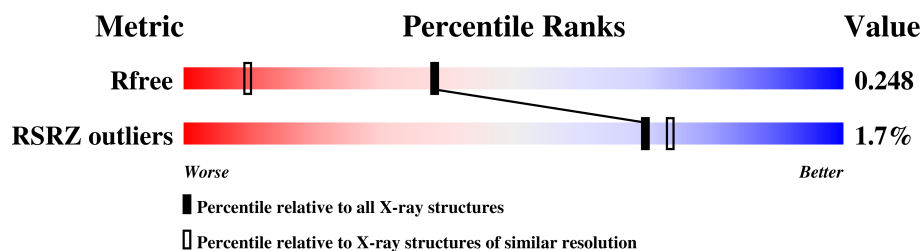
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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))
$R_{free}$	111664	1521 (1.66-1.66)
RSRZ outliers	108989	1487 (1.66-1.66)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9154 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 Lysinoalanine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	1	0
			841	534	146	158	3			
1	B	107	Total	C	N	O	S	0	2	0
			852	540	147	162	3			
1	C	108	Total	C	N	O	S	0	4	0
			880	555	156	166	3			
1	D	108	Total	C	N	O	S	0	3	0
			865	547	152	163	3			
1	E	108	Total	C	N	O	S	0	2	0
			855	540	151	161	3			
1	F	108	Total	C	N	O	S	0	2	0
			857	543	149	161	4			
1	G	108	Total	C	N	O	S	0	1	0
			851	539	147	162	3			
1	H	108	Total	C	N	O	S	0	1	0
			851	539	147	162	3			

- Molecule 2 is a protein called CYS-LYS-GLN-DAL-CYS-ALA-PHE-GLY-PRO-PHE-DBB-PHE-VAL-CYS-BH2-GLY-ASN-DBB-LYS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	19	Total	C	N	O	S	0	0	0
			140	89	23	25	3			
2	I	19	Total	C	N	O	S	0	0	0
			140	89	23	25	3			
2	J	19	Total	C	N	O	S	0	0	0
			136	86	22	25	3			
2	K	19	Total	C	N	O	S	0	0	0
			140	89	23	25	3			
2	L	18	Total	C	N	O	S	0	0	0
			130	83	21	23	3			
2	M	15	Total	C	N	O	S	0	0	0
			109	70	17	20	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	19	Total	C	N	O	S	0	0	0
			140	89	23	25	3			
2	P	19	Total	C	N	O	S	0	0	0
			136	86	22	25	3			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	K	0	0
			2	2		
3	A	2	Total	K	0	0
			2	2		
3	D	2	Total	K	0	0
			2	2		
3	C	2	Total	K	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	132	Total	O	0	0
			132	132		
4	C	166	Total	O	0	0
			166	166		
4	D	122	Total	O	0	0
			122	122		
4	E	119	Total	O	0	0
			119	119		
4	F	151	Total	O	0	0
			151	151		
4	G	148	Total	O	0	0
			148	148		
4	H	123	Total	O	0	0
			123	123		
4	O	16	Total	O	0	0
			16	16		
4	I	19	Total	O	0	0
			19	19		
4	J	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	21	Total 21	O 21	0	0
4	L	17	Total 17	O 17	0	0
4	M	9	Total 9	O 9	0	0
4	N	20	Total 20	O 20	0	0
4	P	17	Total 17	O 17	0	0

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### 3 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.88Å 67.42Å 69.12Å 71.51° 76.25° 72.92°	Depositor
Resolution (Å)	64.72 – 1.66 64.72 – 1.66	Depositor EDS
% Data completeness (in resolution range)	95.8 (64.72-1.66) 95.8 (64.72-1.66)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.184 , 0.242 0.198 , 0.248	Depositor DCC
$R_{free}$ test set	5255 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9861e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

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

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

31 non-standard protein/DNA/RNA residues 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	DBB	I	11	2	5,5,6	0.92	0	3,5,7	2.98	2 (66%)
2	BH2	I	15	2	5,8,9	1.40	0	4,10,12	2.22	2 (50%)
2	DBB	I	18	2	5,5,6	2.06	1 (20%)	3,5,7	4.04	3 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DAL	I	4	2	4,4,5	0.59	0	1,4,6	1.34	0
2	DBB	J	11	2	5,5,6	1.04	1 (20%)	3,5,7	2.38	1 (33%)
2	BH2	J	15	2	5,8,9	1.64	1 (20%)	4,10,12	1.75	1 (25%)
2	DBB	J	18	2	5,5,6	1.68	2 (40%)	3,5,7	3.98	2 (66%)
2	DAL	J	4	2	4,4,5	0.64	0	1,4,6	1.73	0
2	DBB	K	11	2	5,5,6	0.86	0	3,5,7	3.23	1 (33%)
2	BH2	K	15	2	5,8,9	1.97	1 (20%)	4,10,12	1.07	1 (25%)
2	DBB	K	18	2	5,5,6	1.12	0	3,5,7	0.74	0
2	DAL	K	4	2	4,4,5	0.62	0	1,4,6	0.37	0
2	DBB	L	11	2	5,5,6	0.19	0	3,5,7	1.11	0
2	BH2	L	15	2	5,8,9	1.33	0	4,10,12	2.14	2 (50%)
2	DBB	L	18	2	5,5,6	1.35	2 (40%)	3,5,7	3.23	1 (33%)
2	DAL	L	4	2	4,4,5	0.94	0	1,4,6	0.66	0
2	DBB	M	11	2	5,5,6	0.89	0	3,5,7	2.99	1 (33%)
2	BH2	M	15	2	5,8,9	1.44	1 (20%)	4,10,12	0.82	0
2	DAL	M	4	2	4,4,5	0.95	0	1,4,6	0.59	0
2	DBB	N	11	2	5,5,6	1.72	1 (20%)	3,5,7	2.71	2 (66%)
2	BH2	N	15	2	5,8,9	1.88	2 (40%)	4,10,12	0.92	0
2	DBB	N	18	2	5,5,6	6.27	1 (20%)	3,5,7	2.38	2 (66%)
2	DAL	N	4	2	4,4,5	0.59	0	1,4,6	1.02	0
2	DBB	O	11	2	5,5,6	0.32	0	3,5,7	1.68	1 (33%)
2	BH2	O	15	2	5,8,9	1.69	1 (20%)	4,10,12	1.40	1 (25%)
2	DBB	O	18	2	5,5,6	0.46	0	3,5,7	3.30	1 (33%)
2	DAL	O	4	2	4,4,5	1.20	1 (25%)	1,4,6	0.52	0
2	DBB	P	11	2	5,5,6	1.37	1 (20%)	3,5,7	0.66	0
2	BH2	P	15	2	5,8,9	1.81	2 (40%)	4,10,12	2.68	1 (25%)
2	DBB	P	18	2	5,5,6	1.66	1 (20%)	3,5,7	2.64	2 (66%)
2	DAL	P	4	2	4,4,5	0.99	0	1,4,6	0.34	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
2	DBB	I	11	2	-	0/2/4/6	0/0/0/0
2	BH2	I	15	2	-	0/4/10/12	0/0/0/0
2	DBB	I	18	2	-	0/2/4/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAL	I	4	2	-	0/0/2/4	0/0/0/0
2	DBB	J	11	2	-	0/2/4/6	0/0/0/0
2	BH2	J	15	2	-	0/4/10/12	0/0/0/0
2	DBB	J	18	2	-	0/2/4/6	0/0/0/0
2	DAL	J	4	2	-	0/0/2/4	0/0/0/0
2	DBB	K	11	2	-	0/2/4/6	0/0/0/0
2	BH2	K	15	2	-	0/4/10/12	0/0/0/0
2	DBB	K	18	2	-	0/2/4/6	0/0/0/0
2	DAL	K	4	2	-	0/0/2/4	0/0/0/0
2	DBB	L	11	2	-	0/2/4/6	0/0/0/0
2	BH2	L	15	2	-	0/4/10/12	0/0/0/0
2	DBB	L	18	2	-	0/2/4/6	0/0/0/0
2	DAL	L	4	2	-	0/0/2/4	0/0/0/0
2	DBB	M	11	2	-	0/2/4/6	0/0/0/0
2	BH2	M	15	2	-	0/4/10/12	0/0/0/0
2	DAL	M	4	2	-	0/0/2/4	0/0/0/0
2	DBB	N	11	2	-	0/2/4/6	0/0/0/0
2	BH2	N	15	2	-	0/4/10/12	0/0/0/0
2	DBB	N	18	2	-	0/2/4/6	0/0/0/0
2	DAL	N	4	2	-	0/0/2/4	0/0/0/0
2	DBB	O	11	2	-	0/2/4/6	0/0/0/0
2	BH2	O	15	2	-	0/4/10/12	0/0/0/0
2	DBB	O	18	2	-	0/2/4/6	0/0/0/0
2	DAL	O	4	2	-	0/0/2/4	0/0/0/0
2	DBB	P	11	2	-	0/2/4/6	0/0/0/0
2	BH2	P	15	2	-	0/4/10/12	0/0/0/0
2	DBB	P	18	2	-	0/2/4/6	0/0/0/0
2	DAL	P	4	2	-	0/0/2/4	0/0/0/0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	18	DBB	CA-C	-13.95	1.32	1.50
2	I	18	DBB	CA-C	-3.86	1.45	1.50
2	K	15	BH2	CA-CB	-3.74	1.47	1.54
2	N	15	BH2	CA-CB	-3.17	1.48	1.54
2	J	15	BH2	CA-CB	-3.12	1.48	1.54

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	18	DBB	O-C-CA	-6.02	108.43	124.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	18	DBB	O-C-CA	-5.52	109.80	124.96
2	I	18	DBB	CG-CB-CA	-5.39	100.86	113.38
2	O	18	DBB	O-C-CA	-5.30	110.40	124.96
2	K	11	DBB	O-C-CA	-5.17	110.77	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 4.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 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, 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	107/121 (88%)	-0.25	1 (0%) 84 86	15, 23, 34, 39	0
1	B	107/121 (88%)	-0.34	1 (0%) 84 86	13, 19, 28, 40	0
1	C	108/121 (89%)	-0.29	2 (1%) 66 70	12, 17, 28, 46	0
1	D	108/121 (89%)	-0.15	1 (0%) 84 86	13, 19, 32, 50	0
1	E	108/121 (89%)	-0.14	2 (1%) 66 70	13, 22, 36, 53	0
1	F	108/121 (89%)	-0.25	3 (2%) 53 53	13, 18, 32, 48	0
1	G	108/121 (89%)	-0.32	3 (2%) 53 53	11, 17, 29, 43	0
1	H	108/121 (89%)	-0.23	2 (1%) 66 70	11, 19, 36, 55	0
2	I	15/19 (78%)	0.44	1 (6%) 18 16	17, 24, 34, 42	0
2	J	15/19 (78%)	0.50	1 (6%) 18 16	14, 22, 38, 48	0
2	K	15/19 (78%)	-0.15	0 100 100	14, 20, 26, 27	0
2	L	14/19 (73%)	-0.26	0 100 100	15, 19, 22, 26	0
2	M	12/19 (63%)	0.44	0 100 100	17, 23, 35, 37	0
2	N	15/19 (78%)	-0.03	0 100 100	15, 20, 31, 34	0
2	O	15/19 (78%)	-0.29	0 100 100	12, 18, 27, 27	0
2	P	15/19 (78%)	-0.26	0 100 100	13, 20, 29, 31	0
All	All	978/1120 (87%)	-0.21	17 (1%) 70 74	11, 20, 34, 55	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	16	GLY	4.8
1	D	119	SER	4.3
2	J	19	LYS	3.7
1	F	76	GLU	3.7
1	C	63	PHE	3.6

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	DBB	J	18	6/7	0.55	0.27	42,48,51,54	0
2	DBB	L	18	6/7	0.78	0.15	25,31,34,37	0
2	DBB	O	11	6/7	0.87	0.10	18,19,21,23	0
2	BH2	I	15	9/10	0.87	0.11	17,21,22,26	0
2	BH2	M	15	9/10	0.88	0.12	17,21,24,24	0
2	DBB	I	11	6/7	0.90	0.09	17,19,24,24	0
2	DBB	I	18	6/7	0.90	0.27	45,57,63,64	0
2	DBB	K	18	6/7	0.90	0.11	16,17,20,21	0
2	DBB	P	11	6/7	0.90	0.09	18,19,22,23	0
2	DBB	M	11	6/7	0.91	0.09	24,25,27,28	0
2	DBB	N	11	6/7	0.92	0.09	19,22,28,29	0
2	DBB	P	18	6/7	0.92	0.08	17,19,22,23	0
2	DAL	N	4	5/6	0.92	0.07	15,16,17,19	0
2	BH2	P	15	9/10	0.93	0.09	14,17,21,22	0
2	BH2	O	15	9/10	0.93	0.10	12,15,18,19	0
2	DBB	J	11	6/7	0.93	0.11	19,19,21,22	0
2	DAL	M	4	5/6	0.93	0.08	17,19,23,25	0
2	DAL	K	4	5/6	0.93	0.10	15,16,17,17	0
2	DBB	N	18	6/7	0.94	0.16	25,29,32,37	0
2	DBB	O	18	6/7	0.94	0.10	20,22,23,23	0
2	DAL	L	4	5/6	0.94	0.07	14,15,15,16	0
2	BH2	J	15	9/10	0.95	0.08	14,17,19,23	0
2	DBB	K	11	6/7	0.95	0.08	17,17,19,20	0
2	DAL	I	4	5/6	0.95	0.06	16,17,19,21	0
2	DAL	P	4	5/6	0.95	0.07	15,15,17,17	0
2	BH2	L	15	9/10	0.95	0.07	15,16,20,23	0
2	BH2	K	15	9/10	0.96	0.06	13,16,18,21	0
2	BH2	N	15	9/10	0.96	0.07	15,16,18,18	0
2	DBB	L	11	6/7	0.96	0.06	16,18,19,19	0
2	DAL	J	4	5/6	0.97	0.07	14,17,18,21	0
2	DAL	O	4	5/6	0.98	0.05	13,13,14,14	0

## 5.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.4 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, 95<sup>th</sup> 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
3	K	A	201	1/1	0.98	0.09	18,18,18,18	0
3	K	B	202	1/1	0.98	0.07	15,15,15,15	0
3	K	D	201	1/1	0.99	0.08	17,17,17,17	0
3	K	C	201	1/1	1.00	0.05	12,12,12,12	0
3	K	A	202	1/1	1.00	0.08	15,15,15,15	0
3	K	B	201	1/1	1.00	0.07	15,15,15,15	0
3	K	C	202	1/1	1.00	0.07	14,14,14,14	0
3	K	D	202	1/1	1.00	0.07	14,14,14,14	0

## 5.5 Other polymers [i](#)

There are no such residues in this entry.