



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:50 am BST

PDB ID : 3O6W  
Title : Crystal structure of monomeric KIHxk1 in crystal form VIII (open state)  
Authors : Kuettner, E.B.; Kettner, K.; Keim, A.; Kriegel, T.M.; Strater, N.  
Deposited on : 2010-07-29  
Resolution : 1.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

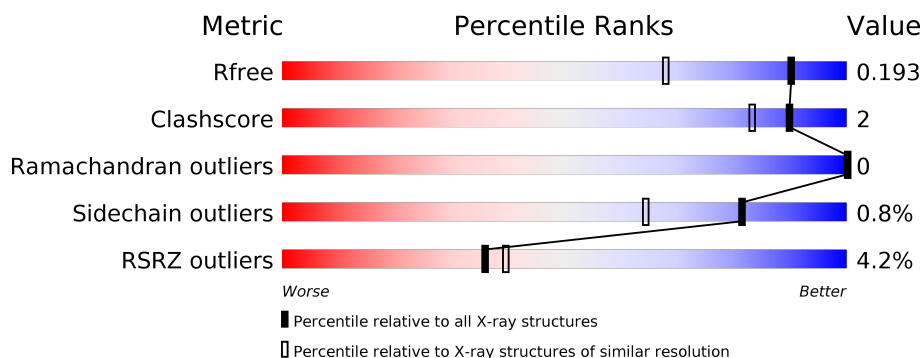
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.48 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))
$R_{free}$	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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  $\geq 3$ , 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	485	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	B	485	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8003 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 Hexokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	11	0
			3663	2325	604	719	15			
1	B	466	Total	C	N	O	S	0	16	0
			3665	2329	600	720	16			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

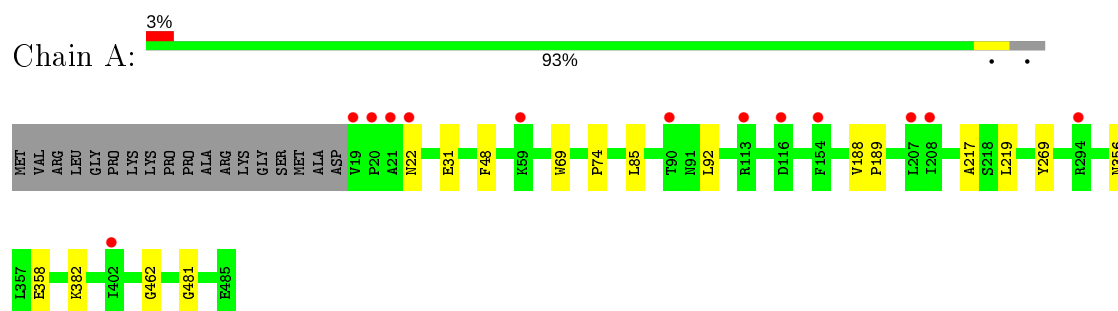
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	333	Total	O	0	0
			333	333		
4	B	297	Total	O	0	0
			297	297		

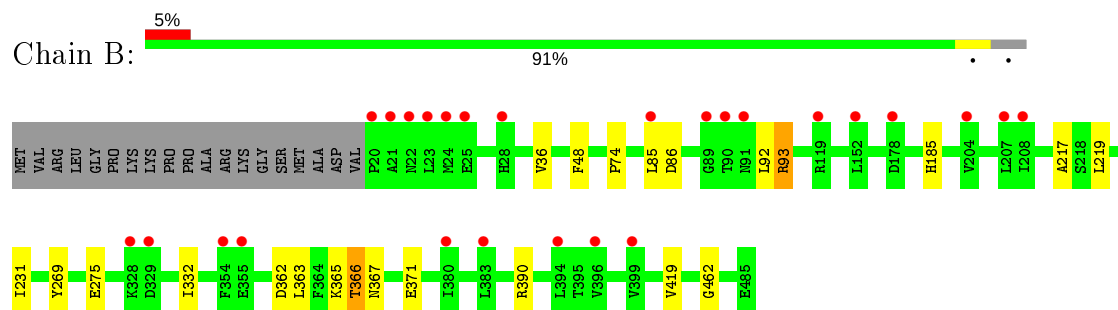
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Hexokinase



- Molecule 1: Hexokinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.54Å 93.59Å 114.29Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	29.12 – 1.48 27.23 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.12-1.48) 99.7 (27.23-1.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.167 , 0.184 0.179 , 0.193	Depositor DCC
$R_{free}$ test set	1723 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8003	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<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.

## 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: GOL, 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	0.60	0/3795	0.71	0/5137
1	B	0.56	0/3820	0.67	1/5170 (0.0%)
All	All	0.58	0/7615	0.69	1/10307 (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	B	93	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	3663	0	3634	12	0
1	B	3665	0	3637	15	0
2	A	12	0	16	0	0
2	B	18	0	24	2	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	333	0	0	0	0
4	B	297	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8003	0	7311	27	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 2.

All (27) 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:85:LEU:HD11	1:B:92[B]:LEU:HD21	1.43	1.00
1:B:185:HIS:HD2	2:B:488:GOL:H31	1.43	0.84
1:A:85:LEU:HD11	1:A:92:LEU:HD11	1.68	0.75
1:B:85:LEU:HD11	1:B:92[B]:LEU:CD2	2.18	0.72
1:B:185:HIS:CD2	2:B:488:GOL:H31	2.25	0.72
1:A:356[B]:ASN:ND2	1:A:358:GLU:HG3	2.07	0.68
1:B:363:LEU:HD12	1:B:367:ASN:HD22	1.62	0.64
1:B:362:ASP:O	1:B:366:THR:HG23	1.97	0.63
1:A:356[B]:ASN:ND2	1:A:358:GLU:CG	2.66	0.59
1:B:275:GLU:CG	4:B:632:HOH:O	2.52	0.57
1:B:365:LYS:HE2	1:B:371:GLU:HG2	1.89	0.55
1:B:275:GLU:HG2	4:B:632:HOH:O	2.10	0.51
1:B:363:LEU:HD12	1:B:367:ASN:ND2	2.27	0.49
1:B:86:ASP:HB3	1:B:93:ARG:HB3	1.96	0.48
1:A:31:GLU:OE2	1:A:382:LYS:HE2	2.15	0.47
1:A:217:ALA:HB2	1:A:462:GLY:HA2	1.97	0.46
1:B:231:ILE:HG22	1:B:419:VAL:HB	1.98	0.45
1:B:74:PRO:HD2	1:B:219:LEU:HD23	1.97	0.45
1:A:85:LEU:HD11	1:A:92:LEU:CD1	2.45	0.43
1:B:217:ALA:HB2	1:B:462:GLY:HA2	2.01	0.42
1:A:69:TRP:CE3	1:A:481:GLY:HA2	2.55	0.42
1:A:217:ALA:HB2	1:A:462:GLY:CA	2.50	0.41
1:A:22:ASN:ND2	1:A:22:ASN:H	2.19	0.41
1:A:74:PRO:HD2	1:A:219:LEU:HD23	2.03	0.41
1:A:356[B]:ASN:HD22	1:A:358:GLU:CG	2.34	0.40
1:B:36[A]:VAL:CG2	1:B:390:ARG:HG3	2.51	0.40
1:A:188:VAL:HB	1:A:189:PRO:HD3	2.03	0.40

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	476/485 (98%)	464 (98%)	12 (2%)	0	100	100
1	B	480/485 (99%)	468 (98%)	12 (2%)	0	100	100
All	All	956/970 (99%)	932 (98%)	24 (2%)	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	409/412 (99%)	407 (100%)	2 (0%)	88	77
1	B	413/412 (100%)	409 (99%)	4 (1%)	76	54
All	All	822/824 (100%)	816 (99%)	6 (1%)	81	68

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	269	TYR
1	B	48	PHE
1	B	269	TYR
1	B	332	ILE
1	B	366	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	62	ASN
1	A	110	ASN
1	A	439	ASN
1	B	185	HIS
1	B	367	ASN
1	B	439	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 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	$\# Z  > 2$
2	GOL	B	487	-	5,5,5	0.43	0	5,5,5	0.84	0
3	PO4	B	490	-	4,4,4	0.92	0	6,6,6	0.43	0
2	GOL	B	488	-	5,5,5	0.33	0	5,5,5	0.39	0
3	PO4	B	489	-	4,4,4	0.93	0	6,6,6	1.41	1 (16%)
3	PO4	A	488	-	4,4,4	1.01	0	6,6,6	1.36	0
2	GOL	B	486	-	5,5,5	0.33	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	487	-	5,5,5	0.33	0	5,5,5	0.53	0
2	GOL	A	486	-	5,5,5	0.38	0	5,5,5	0.47	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	GOL	A	487	-	-	2/4/4/4	-
2	GOL	B	487	-	-	0/4/4/4	-
2	GOL	A	486	-	-	0/4/4/4	-
2	GOL	B	488	-	-	2/4/4/4	-
2	GOL	B	486	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	489	PO4	O3-P-O2	2.65	116.48	107.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	488	GOL	C1-C2-C3-O3
2	B	488	GOL	O2-C2-C3-O3
2	A	487	GOL	C1-C2-C3-O3
2	A	487	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	488	GOL	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	467/485 (96%)	0.13	13 (2%) 53 57	12, 20, 37, 52	0
1	B	466/485 (96%)	0.25	26 (5%) 24 26	13, 22, 48, 77	0
All	All	933/970 (96%)	0.19	39 (4%) 36 39	12, 21, 43, 77	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	VAL	7.3
1	B	22	ASN	6.8
1	B	21	ALA	6.5
1	A	22	ASN	6.1
1	B	354	PHE	5.9
1	A	21	ALA	5.5
1	B	20	PRO	3.9
1	A	113	ARG	3.3
1	B	28	HIS	3.2
1	B	329	ASP	3.1
1	A	20	PRO	2.9
1	A	116	ASP	2.7
1	A	90	THR	2.7
1	B	89	GLY	2.6
1	A	402	ILE	2.5
1	B	23	LEU	2.5
1	A	208	ILE	2.4
1	B	119	ARG	2.4
1	B	396	VAL	2.4
1	B	328	LYS	2.3
1	B	208	ILE	2.3
1	B	383	LEU	2.3
1	B	24[A]	MET	2.3
1	B	91	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	90	THR	2.2
1	B	25	GLU	2.2
1	A	207	LEU	2.2
1	B	152	LEU	2.2
1	B	394	LEU	2.2
1	B	355	GLU	2.2
1	B	207	LEU	2.1
1	B	380	ILE	2.1
1	A	294	ARG	2.1
1	B	85	LEU	2.1
1	B	204	VAL	2.0
1	B	399	VAL	2.0
1	A	59	LYS	2.0
1	B	178	ASP	2.0
1	A	154	PHE	2.0

## 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. 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	GOL	B	488	6/6	0.71	0.21	37,51,53,53	0
2	GOL	A	487	6/6	0.90	0.10	31,32,38,44	0
2	GOL	B	487	6/6	0.91	0.09	25,28,43,43	0
3	PO4	B	490	5/5	0.94	0.14	20,28,29,30	5
2	GOL	A	486	6/6	0.94	0.12	20,22,26,29	0
3	PO4	A	488	5/5	0.95	0.08	19,25,32,32	5
2	GOL	B	486	6/6	0.95	0.10	22,23,30,33	0
3	PO4	B	489	5/5	0.95	0.12	22,24,36,39	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.