



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:26 AM GMT

PDB ID : 3LXP  
Title : Structural and Thermodynamic Characterization of the TYK2 and JAK3 Kinase Domains in Complex with CP-690550 and CMP-6  
Authors : Chrencik, J.E.; Benson, T.E.  
Deposited on : 2010-02-25  
Resolution : 1.65 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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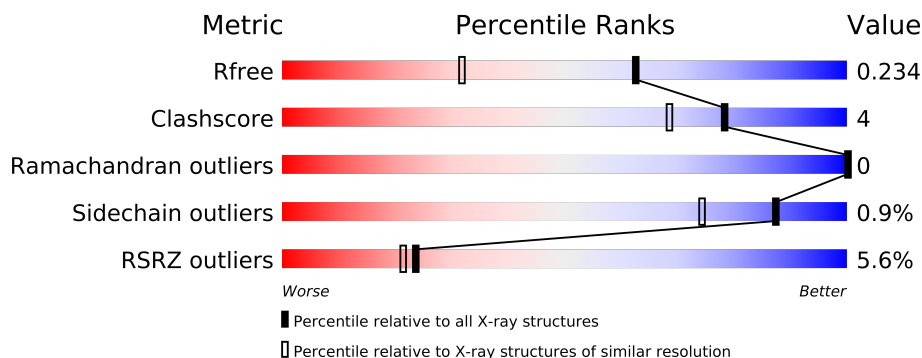
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 1.65 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))
$R_{free}$	66092	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	318	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2449 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Non-receptor tyrosine-protein kinase TYK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	286	2252	1458	372	408	1	13	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

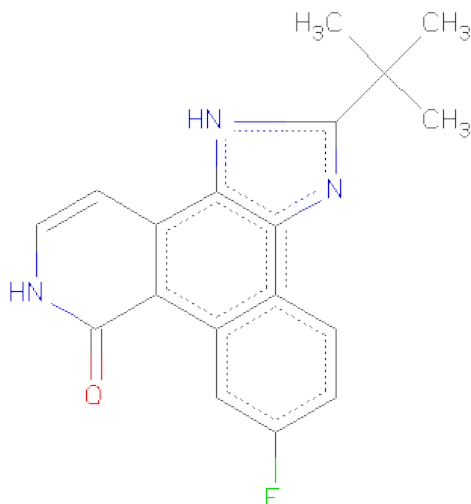
Chain	Residue	Modelled	Actual	Comment	Reference
A	865	MET	-	EXPRESSION TAG	UNP P29597
A	866	ALA	-	EXPRESSION TAG	UNP P29597
A	867	HIS	-	EXPRESSION TAG	UNP P29597
A	868	HIS	-	EXPRESSION TAG	UNP P29597
A	869	HIS	-	EXPRESSION TAG	UNP P29597
A	870	HIS	-	EXPRESSION TAG	UNP P29597
A	871	HIS	-	EXPRESSION TAG	UNP P29597
A	872	HIS	-	EXPRESSION TAG	UNP P29597
A	873	HIS	-	EXPRESSION TAG	UNP P29597
A	874	HIS	-	EXPRESSION TAG	UNP P29597
A	875	HIS	-	EXPRESSION TAG	UNP P29597
A	876	HIS	-	EXPRESSION TAG	UNP P29597
A	877	GLY	-	EXPRESSION TAG	UNP P29597
A	878	ALA	-	EXPRESSION TAG	UNP P29597
A	879	LEU	-	EXPRESSION TAG	UNP P29597
A	880	GLU	-	EXPRESSION TAG	UNP P29597
A	881	VAL	-	EXPRESSION TAG	UNP P29597
A	882	LEU	-	EXPRESSION TAG	UNP P29597
A	883	PHE	-	EXPRESSION TAG	UNP P29597
A	884	GLN	-	EXPRESSION TAG	UNP P29597
A	885	GLY	-	EXPRESSION TAG	UNP P29597
A	886	PRO	-	EXPRESSION TAG	UNP P29597
A	887	GLY	-	EXPRESSION TAG	UNP P29597
A	936	ALA	CYS	ENGINEERED	UNP P29597
A	969	ALA	GLN	ENGINEERED	UNP P29597
A	971	ALA	GLU	ENGINEERED	UNP P29597
A	972	ALA	LYS	ENGINEERED	UNP P29597

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1142	ALA	CYS	ENGINEERED	UNP P29597

- Molecule 2 is 2-TERT-BUTYL-9-FLUORO-3,6-DIHYDRO-7H-BENZ[H]-IMIDAZ[4,5-F]IS OQUINOLINE-7-ONE (three-letter code: IZA) (formula: C<sub>18</sub>H<sub>16</sub>FN<sub>3</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	23	18	1	3	1	0	0

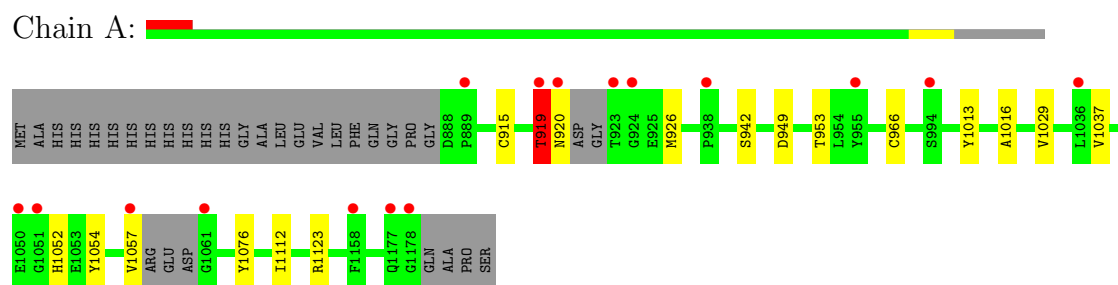
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total	O	0	0
			174	174		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Non-receptor tyrosine-protein kinase TYK2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.33Å 75.98Å 97.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.40 – 1.65 35.39 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.40-1.65) 99.7 (35.39-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.192 , 0.229 0.202 , 0.234	Depositor DCC
$R_{free}$ test set	1760 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35134 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2449	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.51	1/2295 (0.0%)	0.65	1/3113 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	966	CYS	CB-SG	-5.21	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	919	THR	CA-CB-CG2	7.55	122.97	112.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	919	THR	CB

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2252	0	2155	15	0
2	A	23	0	16	1	0
3	A	174	0	0	1	1
All	All	2449	0	2171	16	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (16) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:919:THR:HG23	1:A:920:ASN:C	1.60	1.21
1:A:919:THR:CG2	1:A:920:ASN:HA	2.12	0.80
1:A:919:THR:HG23	1:A:920:ASN:CA	2.14	0.78
1:A:919:THR:HG22	1:A:920:ASN:HA	1.66	0.76
1:A:919:THR:CG2	1:A:920:ASN:CA	2.66	0.73
1:A:919:THR:CG2	1:A:920:ASN:C	2.51	0.71
1:A:1052:HIS:ND1	1:A:1054:PTR:O1P	2.24	0.70
1:A:915:CYS:HA	1:A:926:MET:HE2	1.80	0.63
2:A:1183:IZA:O0	2:A:1183:IZA:H7	2.03	0.57
1:A:949:ASP:O	1:A:953:THR:HG23	2.14	0.48
1:A:919:THR:HB	3:A:73:HOH:O	2.12	0.47
1:A:1029:VAL:HG13	1:A:1037:VAL:HG13	2.00	0.44
1:A:1112:ILE:HG23	1:A:1123:ARG:HD2	1.99	0.43
1:A:1057:VAL:HG12	1:A:1076:TYR:C	2.39	0.43
1:A:1013:TYR:O	1:A:1016:ALA:HB3	2.21	0.41
1:A:915:CYS:SG	1:A:926:MET:CE	3.09	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:245:HOH:O	3:A:328:HOH:O[3_544]	2.14	0.06



## 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	279/318 (88%)	273 (98%)	6 (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	226/270 (84%)	224 (99%)	2 (1%)	87	74

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	919	THR
1	A	942	SER

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

Mol	Chain	Res	Type
1	A	1116	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	PTR	A	1054	1	16,16,17	4.25	2 (12%)	20,22,24	0.90	1 (5%)

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
1	PTR	A	1054	1	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1054	PTR	O-C	15.00	1.21	1.11
1	A	1054	PTR	OH-CZ	-6.61	1.23	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1054	PTR	P-OH-CZ	2.31	130.06	123.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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	IZA	A	1183	-	26,26,26	1.75	6 (23%)	38,41,41	2.64	16 (42%)

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	IZA	A	1183	-	-	0/3/6/6	0/0/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1183	IZA	C14-C2	-4.79	1.48	1.51
2	A	1183	IZA	C3-C0	-2.83	1.39	1.45
2	A	1183	IZA	C2-N0	2.61	1.38	1.33
2	A	1183	IZA	C9-C10	-2.40	1.38	1.41
2	A	1183	IZA	C11-C10	2.37	1.48	1.39
2	A	1183	IZA	C1-C0	-2.01	1.38	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1183	IZA	C3-C0-C1	-6.50	117.91	121.86
2	A	1183	IZA	C14-C2-N1	6.08	127.51	123.14
2	A	1183	IZA	C17-C14-C2	-5.62	104.29	109.39
2	A	1183	IZA	C9-C1-C0	5.30	122.86	119.94
2	A	1183	IZA	C16-C14-C2	4.30	113.30	109.39
2	A	1183	IZA	C4-C3-C0	-4.14	117.35	122.84
2	A	1183	IZA	C15-C14-C2	3.79	112.83	109.39
2	A	1183	IZA	C6-C7-C8	3.72	121.42	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1183	IZA	C5-C6-C7	-2.97	120.61	123.73
2	A	1183	IZA	C13-C9-C1	-2.74	119.19	123.78
2	A	1183	IZA	C4-C3-C8	2.46	121.89	118.62
2	A	1183	IZA	C2-N1-C0	2.30	105.82	103.33
2	A	1183	IZA	C13-C9-C10	2.13	122.45	117.91
2	A	1183	IZA	C8-C10-C9	2.13	120.46	118.14
2	A	1183	IZA	C3-C0-N1	2.12	131.74	127.63
2	A	1183	IZA	C7-C8-C3	-2.09	116.69	118.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	286/318 (89%)	0.19	16 (5%) 24 21	10, 19, 31, 40	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1178	GLY	7.7
1	A	1057	VAL	4.5
1	A	923	THR	4.4
1	A	919	THR	4.4
1	A	1177	GLN	3.8
1	A	924	GLY	3.1
1	A	994	SER	3.0
1	A	920	ASN	2.8
1	A	938	PRO	2.8
1	A	1158	PHE	2.5
1	A	1061	GLY	2.4
1	A	1036	LEU	2.3
1	A	955	TYR	2.2
1	A	1050	GLU	2.1
1	A	889	PRO	2.0
1	A	1051	GLY	2.0

### 6.2 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. 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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PTR	A	1054	16/17	0.14	0.58	23,29,43,44	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IZA	A	1183	23/23	0.09	0.03	14,15,17,18	0

### 6.5 Other polymers

There are no such residues in this entry.