Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:44 PM GMT

PDB ID	:	4JDI
Title	:	Crystal structure of Serine/threonine-protein kinase PAK 4 in complex with Paktide S peptide substrate
Authors	:	Ha, B.H.; Boggon, T.J.
Deposited on	:	2013-02-25
Resolution	:	1.85 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

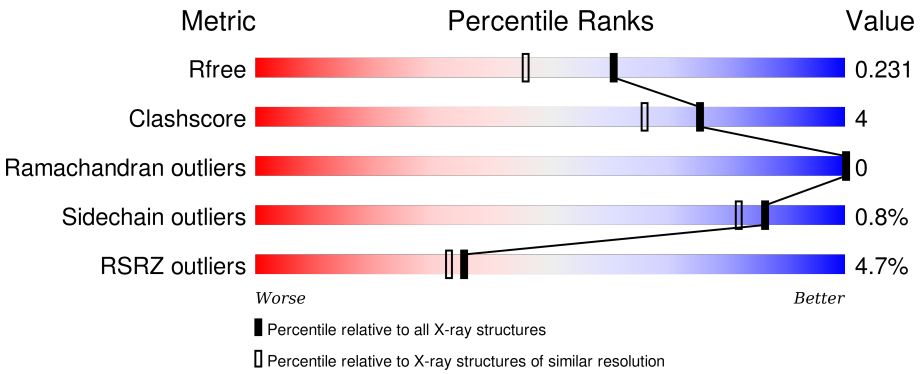
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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 <=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	346	3%, 77%, 7%, 16%
2	B	7	29%, 57%, 29%, 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2561 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 Serine/threonine-protein kinase PAK 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	290	2329	1488	408	418	1	14	0	6	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	MET	-	EXPRESSION TAG	UNP O96013
A	247	GLY	-	EXPRESSION TAG	UNP O96013
A	248	SER	-	EXPRESSION TAG	UNP O96013
A	249	SER	-	EXPRESSION TAG	UNP O96013
A	250	HIS	-	EXPRESSION TAG	UNP O96013
A	251	HIS	-	EXPRESSION TAG	UNP O96013
A	252	HIS	-	EXPRESSION TAG	UNP O96013
A	253	HIS	-	EXPRESSION TAG	UNP O96013
A	254	HIS	-	EXPRESSION TAG	UNP O96013
A	255	HIS	-	EXPRESSION TAG	UNP O96013
A	256	SER	-	EXPRESSION TAG	UNP O96013
A	257	SER	-	EXPRESSION TAG	UNP O96013
A	258	GLY	-	EXPRESSION TAG	UNP O96013
A	259	LEU	-	EXPRESSION TAG	UNP O96013
A	260	VAL	-	EXPRESSION TAG	UNP O96013
A	261	PRO	-	EXPRESSION TAG	UNP O96013
A	262	ARG	-	EXPRESSION TAG	UNP O96013
A	263	GLY	-	EXPRESSION TAG	UNP O96013
A	264	SER	-	EXPRESSION TAG	UNP O96013
A	265	HIS	-	EXPRESSION TAG	UNP O96013
A	266	MET	-	EXPRESSION TAG	UNP O96013
A	267	GLU	-	EXPRESSION TAG	UNP O96013
A	268	ASN	-	EXPRESSION TAG	UNP O96013
A	269	LEU	-	EXPRESSION TAG	UNP O96013
A	270	TYR	-	EXPRESSION TAG	UNP O96013
A	271	PHE	-	EXPRESSION TAG	UNP O96013
A	272	GLN	-	EXPRESSION TAG	UNP O96013

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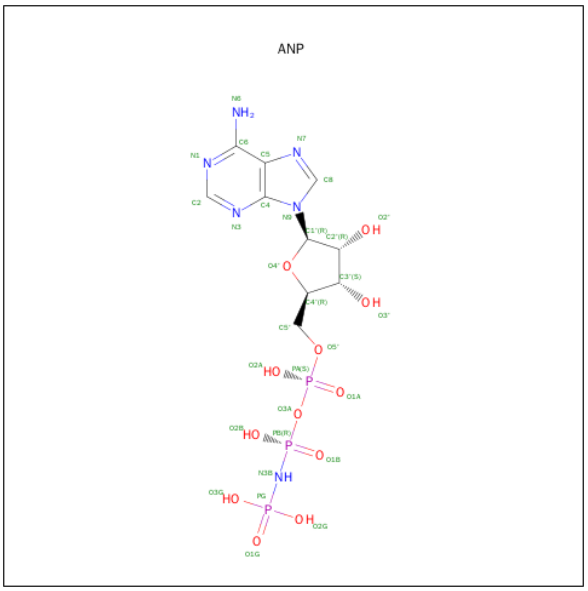
Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLY	-	EXPRESSION TAG	UNP O96013
A	274	ALA	-	EXPRESSION TAG	UNP O96013
A	275	ARG	-	EXPRESSION TAG	UNP O96013
A	276	ALA	-	EXPRESSION TAG	UNP O96013
A	277	ARG	-	EXPRESSION TAG	UNP O96013
A	278	GLN	-	EXPRESSION TAG	UNP O96013
A	279	GLU	-	EXPRESSION TAG	UNP O96013
A	280	ASN	-	EXPRESSION TAG	UNP O96013
A	281	GLY	-	EXPRESSION TAG	UNP O96013
A	282	MET	-	EXPRESSION TAG	UNP O96013
A	283	PRO	-	EXPRESSION TAG	UNP O96013
A	284	GLU	-	EXPRESSION TAG	UNP O96013
A	285	LYS	-	EXPRESSION TAG	UNP O96013

- Molecule 2 is a protein called Paktide S.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	64	38	19	7	0	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	6	9	2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

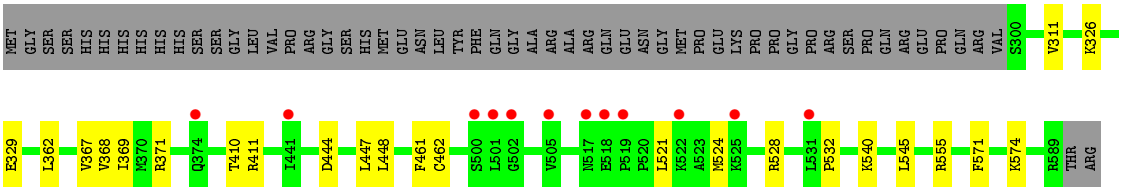
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	134	134	134	0	0
			Total	O		
5	B	5	5	5	0	0

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 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.

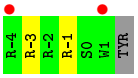
- Molecule 1: Serine/threonine-protein kinase PAK 4

Chain A:



- Molecule 2: Paktide S

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	61.91Å 61.91Å 181.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 – 1.85 29.30 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.32-1.85) 99.8 (29.30-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.233 0.192 , 0.231	Depositor DCC
R_{free} test set	1569 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 31046 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2561	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ANP, SEP

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	0.44	0/2375	0.62	0/3216
2	B	0.52	0/65	0.66	0/84
All	All	0.45	0/2440	0.62	0/3300

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	2329	0	2399	15	0
2	B	64	0	69	4	0
3	A	27	0	12	0	0
4	A	2	0	0	0	0
5	A	134	0	0	1	0
5	B	5	0	0	0	0
All	All	2561	0	2480	19	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 4.

All (19) 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:A:311[A]:VAL:HG12	1:A:367:VAL:HG11	1.63	0.81
1:A:369:ILE:HG13	1:A:462:CYS:SG	2.38	0.64
1:A:411:ARG:HH22	1:A:540:LYS:NZ	1.97	0.63
1:A:528:ARG:O	1:A:555:ARG:NH2	2.31	0.60
2:B:-3:ARG:HH11	2:B:-1:ARG:HD2	1.68	0.58
1:A:411:ARG:HH22	1:A:540:LYS:HZ3	1.52	0.57
1:A:368:VAL:HA	1:A:371:ARG:HG2	1.90	0.54
2:B:-3:ARG:HG3	2:B:-1:ARG:H	1.75	0.52
1:A:411:ARG:NH2	1:A:540:LYS:NZ	2.58	0.52
1:A:326:LYS:CE	1:A:329:GLU:HG3	2.43	0.48
1:A:521:LEU:HA	1:A:524:MET:HE2	1.97	0.46
2:B:-3:ARG:NH1	2:B:-1:ARG:HD2	2.31	0.45
1:A:574:LYS:NZ	5:A:1180:HOH:O	2.44	0.44
1:A:362[A]:LEU:HD23	1:A:461:PHE:CD1	2.52	0.44
2:B:-1:ARG:NE	2:B:-1:ARG:HA	2.32	0.43
1:A:447:LEU:C	1:A:448[B]:LEU:HD12	2.39	0.43
1:A:545[A]:LEU:HD13	1:A:571:PHE:CZ	2.54	0.42
1:A:532:PRO:HG3	1:A:555:ARG:HG3	2.03	0.41
1:A:521:LEU:H	1:A:521:LEU:HD22	1.86	0.40

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	292/346 (84%)	286 (98%)	6 (2%)	0	100	100
2	B	4/7 (57%)	4 (100%)	0	0	100	100
All	All	296/353 (84%)	290 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	258/300 (86%)	256 (99%)	2 (1%)	86 82
2	B	6/7 (86%)	6 (100%)	0	100 100
All	All	264/307 (86%)	262 (99%)	2 (1%)	86 82

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

Mol	Chain	Res	Type
1	A	410	THR
1	A	444	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	SEP	A	474	1	8,9,10	0.60	0	8,12,14	1.37	1 (12%)

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	SEP	A	474	1	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	474	SEP	O3P-P-O1P	2.24	117.79	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	ANP	A	1000	4	22,29,33	1.47	5 (22%)	24,45,52	1.99	3 (12%)

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	ANP	A	1000	4	-	0/9/32/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	ANP	C2-N3	2.03	1.35	1.32
3	A	1000	ANP	PB-O3A	2.16	1.61	1.59
3	A	1000	ANP	O4'-C1'	2.52	1.44	1.41
3	A	1000	ANP	C5-C4	3.21	1.47	1.40
3	A	1000	ANP	PB-O1B	3.63	1.50	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1000	ANP	N3-C2-N1	-7.09	123.47	128.89
3	A	1000	ANP	C2'-C1'-N9	-4.13	107.99	114.29
3	A	1000	ANP	C4-C5-N7	-2.21	107.45	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	289/346 (83%)	0.19	12 (4%)	40	37	22, 34, 52, 58	0
2	B	6/7 (85%)	1.51	2 (33%)	0	0	35, 49, 52, 57	0
All	All	295/353 (83%)	0.21	14 (4%)	35	33	22, 34, 52, 58	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	-4	ARG	4.3
1	A	441	ILE	3.7
1	A	519	PRO	3.7
2	B	1	TRP	3.3
1	A	501	LEU	3.2
1	A	525	LYS	3.1
1	A	531	LEU	2.9
1	A	517	ASN	2.6
1	A	518	GLU	2.6
1	A	522	LYS	2.6
1	A	500	SER	2.6
1	A	505	VAL	2.3
1	A	374	GLN	2.1
1	A	502	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SEP	A	474	10/11	0.99	0.07	-	29,31,32,33	0

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
4	MG	A	1001	1/1	0.93	0.20	1.00	40,40,40,40	0
3	ANP	A	1000	27/31	0.96	0.08	-0.91	26,30,33,36	8
4	MG	A	1002	1/1	0.97	0.04	-2.94	28,28,28,28	1

6.5 Other polymers (i)

There are no such residues in this entry.