Full wwPDB X-ray Structure Validation Report (i)

Mar 21, 2016 – 11:21 PM EDT

PDB ID	:	5HX8
Title	:	Jak1 complex with 4-[(4-aminocyclohexyl)amino]-3-(1H-benzimidazol-2-yl)-1 H-pyridin-2-one
Authors	:	Su, H.P.
Deposited on	:	2016-01-29
Resolution	:	2.20 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:

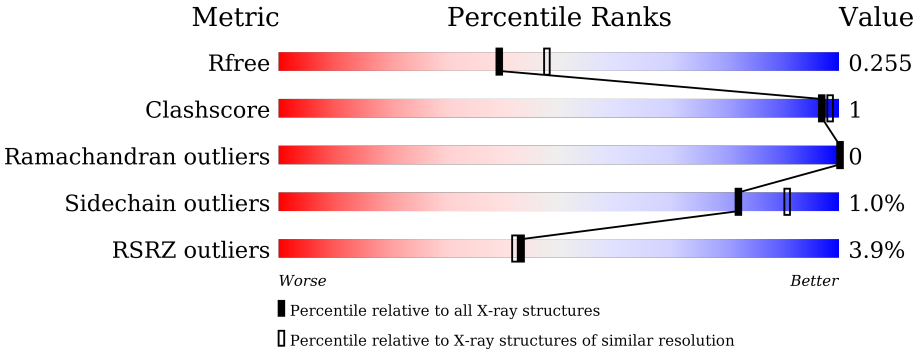
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	302	6% 94%
1	B	302	.% 87% 6% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4832 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.

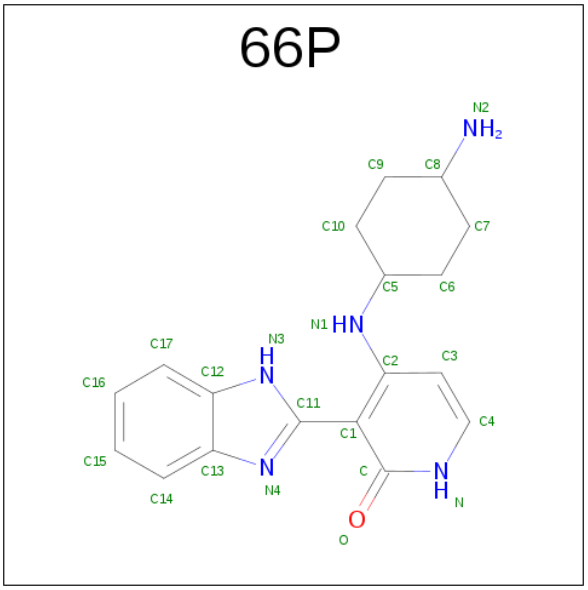
- Molecule 1 is a protein called Tyrosine-protein kinase JAK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	293	2350	1496	397	440	2	15	0	0	0
1	B	281	2287	1455	392	423	2	15	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	853	GLY	-	expression tag	UNP P23458
B	853	GLY	-	expression tag	UNP P23458

- Molecule 2 is 4-[(4-aminocyclohexyl)amino]-3-(1H-benzimidazol-2-yl)-1H-pyridin-2-one (three-letter code: 66P) (formula: $C_{18}H_{21}N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	24	18	5	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	24	18	5	1	0	0

- Molecule 3 is water.

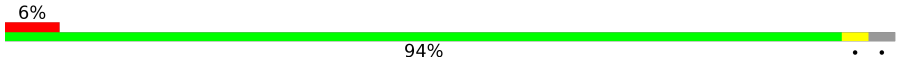
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	67	67	67	0	0
			Total	O		
3	B	80	80	80	0	0

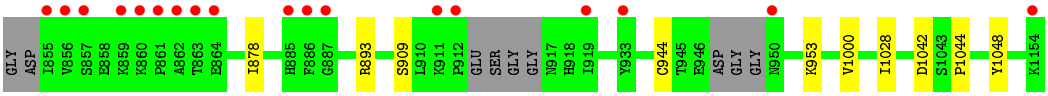
3 Residue-property plots (i)

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: Tyrosine-protein kinase JAK1

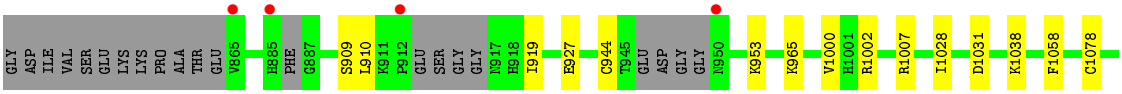
Chain A:





- Molecule 1: Tyrosine-protein kinase JAK1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.76Å 172.97Å 44.72Å 90.00° 93.60° 90.00°	Depositor
Resolution (Å)	44.63 – 2.20 43.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (44.63-2.20) 98.3 (43.22-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.20Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.197 , 0.240 0.204 , 0.255	Depositor DCC
R_{free} test set	1632 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.8	EDS
Estimated twinning fraction	0.031 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 32220 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4832	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: PTR, 66P

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	0.43	0/2364	0.64	0/3186
1	B	0.44	0/2303	0.63	0/3099
All	All	0.44	0/4667	0.64	0/6285

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	2350	0	2332	5	0
1	B	2287	0	2279	7	0
2	A	24	0	0	0	0
2	B	24	0	0	0	0
3	A	67	0	0	0	0
3	B	80	0	0	0	0
All	All	4832	0	4611	12	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 1.

All (12) 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:1000:VAL:HG13	1:A:1028:ILE:HD11	1.68	0.74
1:A:944:CYS:HB3	1:A:953:LYS:HB2	1.85	0.57
1:B:1000:VAL:HG13	1:B:1028:ILE:HD11	1.87	0.56
1:B:910:LEU:HD11	1:B:919:ILE:HA	1.88	0.55
1:B:944:CYS:HB3	1:B:953:LYS:HB2	1.93	0.51
1:A:1044:PRO:HD2	1:A:1048:TYR:CZ	2.45	0.50
1:B:965:LYS:HD2	1:B:1078:CYS:HB3	1.98	0.46
1:B:909:SER:HB3	1:B:953:LYS:HG2	1.98	0.45
1:B:1002:ARG:HA	1:B:1058:PHE:CZ	2.52	0.45
1:A:878:ILE:HD11	1:A:893:ARG:HB2	1.99	0.45
1:A:909:SER:HB3	1:A:953:LYS:HG2	2.01	0.42
1:B:1107:THR:HG23	1:B:1112:LYS:HD3	2.02	0.41

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	285/302 (94%)	277 (97%)	8 (3%)	0	100	100
1	B	272/302 (90%)	268 (98%)	4 (2%)	0	100	100
All	All	557/604 (92%)	545 (98%)	12 (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	256/267 (96%)	255 (100%)	1 (0%)	93 97
1	B	251/267 (94%)	247 (98%)	4 (2%)	70 82
All	All	507/534 (95%)	502 (99%)	5 (1%)	82 91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1042	ASP
1	B	927	GLU
1	B	1007	ARG
1	B	1031	ASP
1	B	1038	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	917	ASN
1	B	1144	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
1	PTR	A	1034	1	13,16,17	1.45	1 (7%)	19,22,24	1.21	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PTR	A	1035	1	13,16,17	1.45	2 (15%)	19,22,24	1.35	3 (15%)
1	PTR	B	1034	1	13,16,17	1.63	4 (30%)	19,22,24	1.22	2 (10%)
1	PTR	B	1035	1	13,16,17	1.42	3 (23%)	19,22,24	1.30	2 (10%)

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	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1035	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1035	1	-	0/9/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1034	PTR	CD2-CG	2.00	1.43	1.38
1	B	1035	PTR	CD1-CG	2.08	1.43	1.38
1	A	1035	PTR	CE1-CZ	2.09	1.42	1.38
1	B	1035	PTR	CE1-CZ	2.12	1.43	1.38
1	B	1034	PTR	CE2-CZ	2.23	1.43	1.38
1	B	1035	PTR	CE2-CZ	2.74	1.44	1.38
1	B	1034	PTR	CB-CA	2.86	1.59	1.53
1	A	1035	PTR	CE2-CZ	2.95	1.44	1.38
1	A	1034	PTR	CE1-CZ	2.98	1.44	1.38
1	B	1034	PTR	CE1-CZ	3.10	1.45	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1035	PTR	O-C-CA	-2.24	119.72	125.72
1	A	1035	PTR	O-C-CA	-2.20	119.83	125.72
1	A	1035	PTR	OH-CZ-CE2	2.32	126.45	119.22
1	B	1034	PTR	O2P-P-OH	2.37	113.01	105.47
1	A	1034	PTR	O2P-P-OH	2.37	113.01	105.47
1	B	1034	PTR	OH-CZ-CE1	2.57	127.22	119.22
1	B	1035	PTR	O3P-P-OH	2.58	113.70	105.47
1	A	1034	PTR	OH-CZ-CE1	2.62	127.38	119.22
1	A	1035	PTR	O2P-P-OH	2.64	113.87	105.47

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)

2 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	66P	A	1201	-	26,27,27	1.25	2 (7%)	23,38,38	1.12	2 (8%)
2	66P	B	1201	-	26,27,27	1.35	3 (11%)	23,38,38	1.15	2 (8%)

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	66P	A	1201	-	-	0/8/18/18	0/4/4/4
2	66P	B	1201	-	-	0/8/18/18	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	66P	C11-N4	-2.48	1.32	1.35
2	B	1201	66P	C11-N4	-2.42	1.32	1.35
2	B	1201	66P	C1-C2	2.25	1.46	1.41
2	A	1201	66P	C-N	4.04	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	66P	C-N	4.23	1.40	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1201	66P	C3-C4-N	-2.28	121.21	123.88
2	A	1201	66P	C3-C4-N	-2.17	121.33	123.88
2	B	1201	66P	C4-N-C	3.05	124.34	116.54
2	A	1201	66P	C4-N-C	3.10	124.49	116.54

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	291/302 (96%)	0.11	18 (6%)	24	23	31, 50, 86, 118	0
1	B	279/302 (92%)	-0.11	4 (1%)	78	77	25, 44, 71, 98	0
All	All	570/604 (94%)	0.00	22 (3%)	43	42	25, 48, 77, 118	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	855	ILE	7.2
1	A	862	ALA	5.7
1	A	860	LYS	5.2
1	B	950	ASN	4.8
1	A	911	LYS	4.0
1	A	885	HIS	3.7
1	A	887	GLY	3.6
1	A	859	LYS	3.6
1	A	1154	LYS	3.5
1	B	912	PRO	3.5
1	A	863	THR	3.4
1	B	885	HIS	3.2
1	A	861	PRO	3.2
1	A	886	PHE	3.1
1	A	864	GLU	3.0
1	B	865	VAL	3.0
1	A	912	PRO	3.0
1	A	856	VAL	2.8
1	A	857	SER	2.7
1	A	919	ILE	2.4
1	A	933	TYR	2.2
1	A	950	ASN	2.2

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	PTR	A	1034	16/17	0.84	0.15	-	62,67,74,74	0
1	PTR	B	1035	16/17	0.79	0.15	-	57,61,73,73	0
1	PTR	A	1035	16/17	0.74	0.18	-	56,64,75,75	0
1	PTR	B	1034	16/17	0.86	0.17	-	61,65,70,71	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
2	66P	A	1201	24/24	0.96	0.12	-0.30	30,33,35,37	0
2	66P	B	1201	24/24	0.96	0.10	-0.55	24,25,27,28	0

6.5 Other polymers (i)

There are no such residues in this entry.