



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 5, 2017 – 09:18 PM EDT

PDB ID : 5TC3
Title : Structure of IMP dehydrogenase from *Ashbya gossypii* bound to ATP and GDP
Authors : Fernandez-Justel, D.; de Pereda, J.M.; Revuelta, J.L.; Buey, R.M.
Deposited on : 2016-09-14
Resolution : 2.46 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

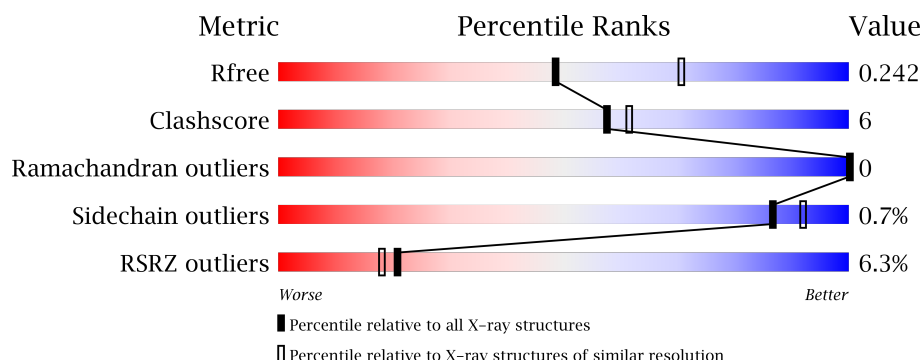
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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}	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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 $\leq 5\%$. 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	523	<div> <div>7%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
1	B	523	<div> <div>5%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14581 atoms, of which 7078 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.

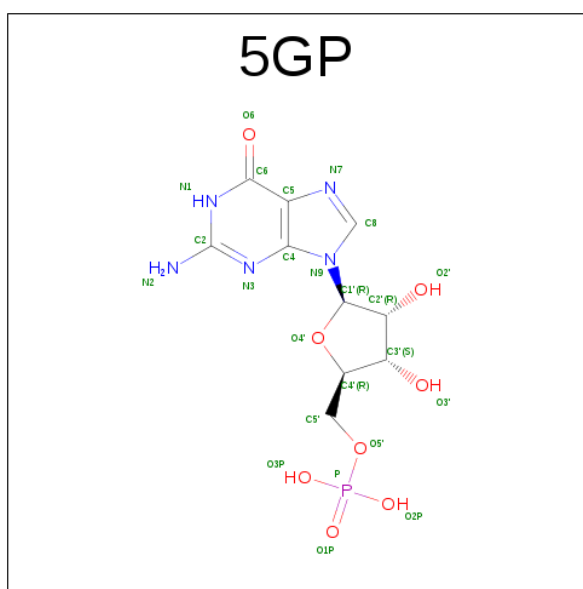
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	488	Total	C	H	N	O	S	0	0	0
			7077	2250	3491	621	693	22			
1	B	489	Total	C	H	N	O	S	0	0	0
			7054	2250	3470	616	696	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q756Z6
B	0	HIS	-	expression tag	UNP Q756Z6

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



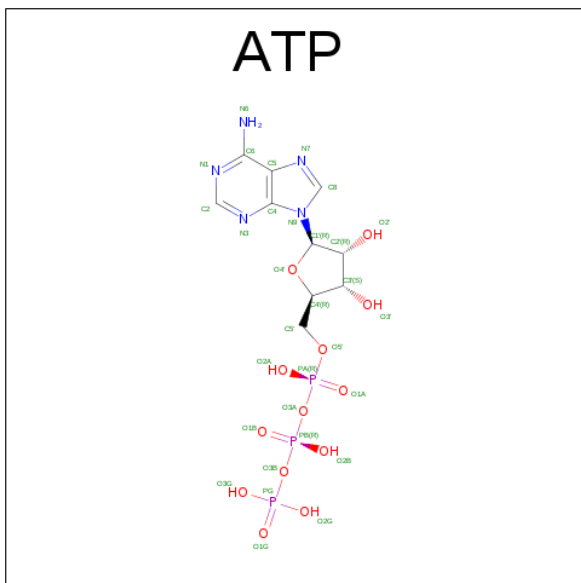
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			35	10	11	5	8	1		

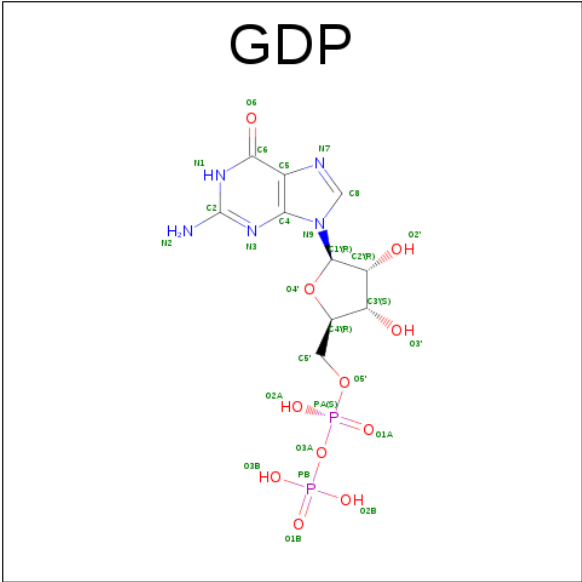
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	
			35	10	11	5	8	1	
								0	0

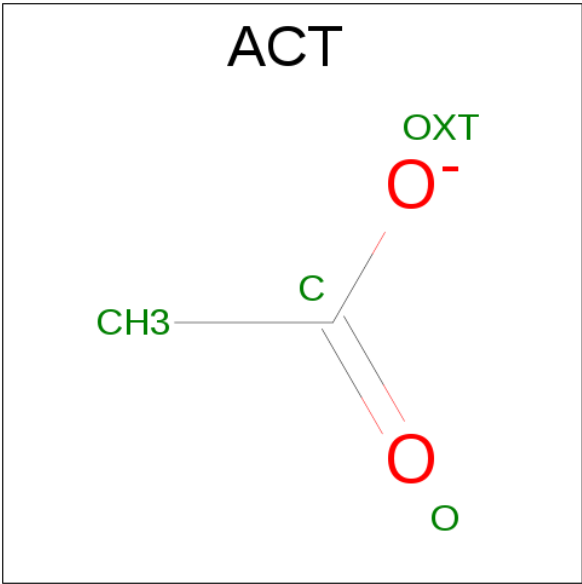
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			39	10	11	5	11	2		
4	A	1	Total	C	H	N	O	P	0	1
			80	20	24	10	22	4		
4	B	1	Total	C	H	N	O	P	0	0
			39	10	11	5	11	2		
4	B	1	Total	C	H	N	O	P	0	1
			80	20	24	10	22	4		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	23	Total	O	0	0
			23	23		

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	147.88Å 147.88Å 103.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.76 – 2.46 46.76 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.76-2.46) 99.8 (46.76-2.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.11rc1_2513: ???)	Depositor
R, R_{free}	0.216 , 0.242 0.223 , 0.242	Depositor DCC
R_{free} test set	2110 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.478 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14581	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 5GP, ATP, ACT

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	0.41	0/3633	0.54	0/4910
1	B	0.43	0/3632	0.54	0/4912
All	All	0.42	0/7265	0.54	0/9822

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

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	3586	3491	3515	39	0
1	B	3584	3470	3501	41	0
2	A	24	11	12	1	0
2	B	24	11	12	1	0
3	A	31	11	12	2	0
3	B	31	11	12	2	0
4	A	84	35	36	1	0
4	B	84	35	36	9	0
5	A	4	3	3	0	0
6	A	28	0	0	0	0
6	B	23	0	0	0	0
All	All	7503	7078	7139	81	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 6.

The worst 5 of 81 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:232:ASN:ND2	4:B:603[B]:GDP:O1B	1.56	1.39
1:B:232:ASN:HD21	4:B:603[B]:GDP:PB	1.68	1.16
1:B:232:ASN:ND2	4:B:603[B]:GDP:PB	2.31	0.97
1:B:101:CYS:O	1:B:262:ARG:NH2	1.97	0.96
1:A:500:ARG:HH21	1:A:505:GLN:HA	1.31	0.94

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	475/523 (91%)	461 (97%)	14 (3%)	0	100	100
1	B	477/523 (91%)	460 (96%)	17 (4%)	0	100	100
All	All	952/1046 (91%)	921 (97%)	31 (3%)	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	369/430 (86%)	367 (100%)	2 (0%)	91	94
1	B	368/430 (86%)	365 (99%)	3 (1%)	85	90
All	All	737/860 (86%)	732 (99%)	5 (1%)	87	92

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

Mol	Chain	Res	Type
1	A	280	GLN
1	A	487	ARG
1	B	232	ASN
1	B	280	GLN
1	B	487	ARG

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

Mol	Chain	Res	Type
1	B	232	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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	5GP	A	600	-	22,26,26	2.84	6 (27%)	23,40,40	1.33	3 (13%)
3	ATP	A	601	-	27,33,33	2.63	5 (18%)	25,52,52	1.75	5 (20%)
4	GDP	A	602	-	25,30,30	2.98	9 (36%)	23,47,47	1.79	5 (21%)
4	GDP	A	603[A]	-	25,30,30	3.03	9 (36%)	23,47,47	1.80	4 (17%)
4	GDP	A	603[B]	-	25,30,30	3.02	9 (36%)	23,47,47	1.83	4 (17%)
5	ACT	A	604	-	1,3,3	1.45	0	0,3,3	0.00	-
2	5GP	B	600	-	22,26,26	2.80	6 (27%)	23,40,40	1.35	3 (13%)
3	ATP	B	601	-	27,33,33	2.61	5 (18%)	25,52,52	1.65	3 (12%)
4	GDP	B	602	-	25,30,30	2.27	11 (44%)	23,47,47	2.82	7 (30%)
4	GDP	B	603[A]	-	25,30,30	3.04	10 (40%)	23,47,47	1.74	3 (13%)
4	GDP	B	603[B]	-	25,30,30	3.03	9 (36%)	23,47,47	1.71	3 (13%)

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	5GP	A	600	-	-	0/6/26/26	0/3/3/3
3	ATP	A	601	-	-	0/18/38/38	0/3/3/3
4	GDP	A	602	-	-	0/12/32/32	0/3/3/3
4	GDP	A	603[A]	-	-	0/12/32/32	0/3/3/3
4	GDP	A	603[B]	-	-	0/12/32/32	0/3/3/3
5	ACT	A	604	-	-	0/0/0/0	0/0/0/0
2	5GP	B	600	-	-	0/6/26/26	0/3/3/3
3	ATP	B	601	-	-	0/18/38/38	0/3/3/3
4	GDP	B	602	-	-	0/12/32/32	0/3/3/3
4	GDP	B	603[A]	-	-	0/12/32/32	0/3/3/3
4	GDP	B	603[B]	-	-	0/12/32/32	0/3/3/3

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	GDP	PB-O3A	-3.99	1.53	1.60
4	A	602	GDP	C2'-C1'	-3.82	1.47	1.53
4	A	603[A]	GDP	C2'-C1'	-3.78	1.47	1.53
4	A	603[B]	GDP	C2'-C1'	-3.75	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603[A]	GDP	C2'-C1'	-3.74	1.47	1.53

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603[B]	GDP	C4'-O4'-C1'	-5.74	103.66	109.77
4	A	603[A]	GDP	C4'-O4'-C1'	-5.70	103.70	109.77
4	B	603[A]	GDP	C4'-O4'-C1'	-5.57	103.84	109.77
4	B	603[B]	GDP	C4'-O4'-C1'	-5.47	103.94	109.77
4	A	602	GDP	C4'-O4'-C1'	-5.47	103.95	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	5GP	1	0
3	A	601	ATP	2	0
4	A	602	GDP	1	0
2	B	600	5GP	1	0
3	B	601	ATP	2	0
4	B	602	GDP	5	0
4	B	603[B]	GDP	4	0

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	488/523 (93%)	0.47	34 (6%)	17 15	41, 72, 111, 151	0
1	B	489/523 (93%)	0.40	28 (5%)	24 22	41, 72, 115, 149	0
All	All	977/1046 (93%)	0.43	62 (6%)	21 18	41, 72, 113, 151	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	513	LEU	7.3
1	A	513	LEU	5.4
1	A	413	THR	5.3
1	B	512	ASN	5.2
1	B	340	MET	4.9

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. 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(\AA^2)	Q<0.9
2	5GP	B	600	24/24	0.88	0.22	0.38	56,76,96,98	35
4	GDP	A	603[B]	28/28	0.82	0.20	0.19	66,71,86,87	40
4	GDP	A	603[A]	28/28	0.82	0.20	0.08	67,71,87,88	40
4	GDP	B	603[B]	28/28	0.85	0.19	-0.08	59,70,85,85	40
4	GDP	B	603[A]	28/28	0.85	0.19	-0.15	64,70,85,85	40
4	GDP	B	602	28/28	0.94	0.16	-0.18	56,64,76,77	0
3	ATP	B	601	31/31	0.94	0.16	-0.37	64,68,80,81	0
3	ATP	A	601	31/31	0.95	0.15	-0.55	67,69,83,84	0
4	GDP	A	602	28/28	0.94	0.15	-0.56	67,69,82,82	0
2	5GP	A	600	24/24	0.91	0.15	-0.68	59,85,108,110	0
5	ACT	A	604	4/4	0.95	0.09	-2.27	59,60,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.