



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2I1Y / pdb_00002i1y
Title : Crystal structure of the phosphatase domain of human PTP IA-2
Authors : Faber-Barata, J.; Patskovsky, Y.; Alvarado, J.; Smith, D.; Koss, J.; Wasserman, S.R.; Ozyurt, S.; Atwell, S.; Powell, A.; Kearins, M.C.; Maletic, M.; Rooney, I.; Bain, K.T.; Freeman, M.; Russell, J.C.; Thompson, D.A.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-08-15
Resolution : 2.23 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

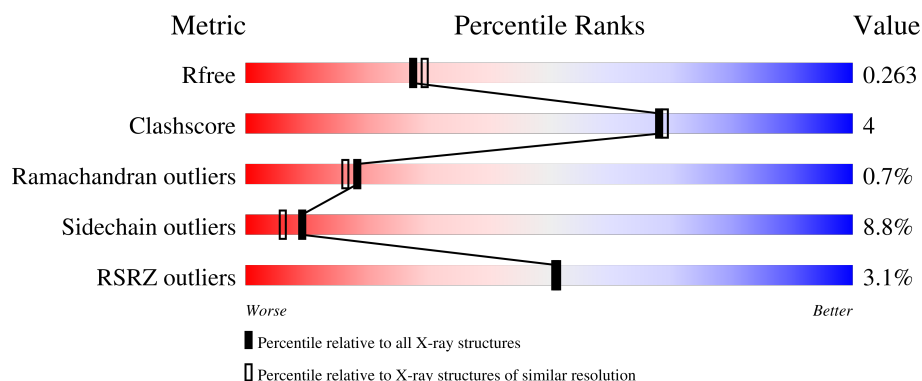
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

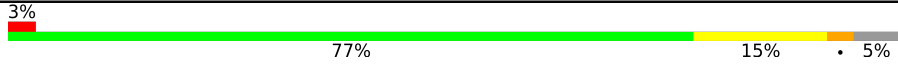
The reported resolution of this entry is 2.23 Å.

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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	301	
1	B	301	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5006 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 Receptor-type tyrosine-protein phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	6	3	0
			2325	1472	414	424	15			
1	B	290	Total	C	N	O	S	4	8	0
			2363	1498	417	430	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	679	SER	-	cloning artifact	UNP Q16849
A	680	LEU	-	cloning artifact	UNP Q16849
B	679	SER	-	cloning artifact	UNP Q16849
B	680	LEU	-	cloning artifact	UNP Q16849

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

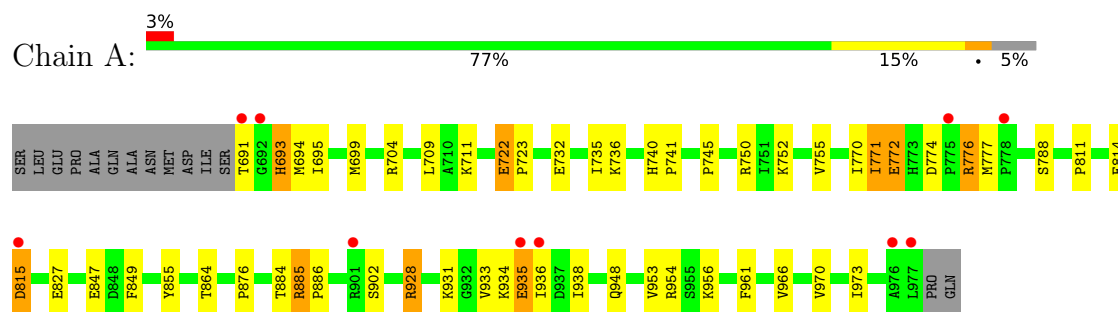
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total 157	O 157	0	0
3	B	149	Total 149	O 149	0	0

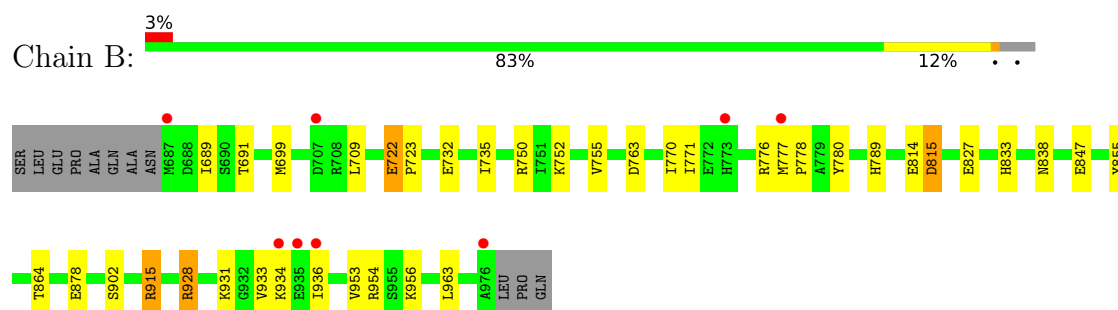
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Receptor-type tyrosine-protein phosphatase



- Molecule 1: Receptor-type tyrosine-protein phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.91Å 74.23Å 121.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 2.23 19.73 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.73-2.23) 99.3 (19.73-2.23)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.267 0.203 , 0.263	Depositor DCC
R_{free} test set	1035 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5006	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.33% 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: GOL

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	0.55	0/2388	0.87	4/3241 (0.1%)
1	B	0.55	0/2439	0.87	4/3307 (0.1%)
All	All	0.55	0/4827	0.87	8/6548 (0.1%)

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	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	938	ILE	N-CA-C	6.65	117.41	110.62
1	B	691	THR	N-CA-C	-6.38	104.42	111.82
1	B	954	ARG	N-CA-C	6.28	120.68	112.89
1	B	933	VAL	N-CA-C	-5.96	101.32	109.55
1	B	780	TYR	N-CA-C	5.77	117.95	109.24
1	A	954	ARG	N-CA-C	5.72	119.44	112.23
1	A	693	HIS	N-CA-C	-5.62	105.24	111.36
1	A	849	PHE	N-CA-C	5.40	117.47	108.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	771	ILE	Peptide

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	2325	0	2297	24	0
1	B	2363	0	2340	11	0
2	A	6	0	8	1	0
2	B	6	0	8	0	0
3	A	157	0	0	0	0
3	B	149	0	0	2	0
All	All	5006	0	4653	34	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 (34) 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:774:ASP:OD2	1:A:776:ARG:HD2	1.68	0.94
1:A:774:ASP:OD2	1:A:776:ARG:CD	2.33	0.76
1:A:691:THR:HG22	1:A:693:HIS:H	1.60	0.66
1:B:771:ILE:HG22	1:B:778:PRO:HA	1.78	0.66
1:A:691:THR:CG2	1:A:693:HIS:HB2	2.32	0.60
1:A:885:ARG:HB3	1:A:886:PRO:HD3	1.87	0.57
1:A:970:VAL:HG22	2:A:3288:GOL:H31	1.87	0.56
1:A:777:MET:HE1	1:A:931:LYS:HD3	1.88	0.54
1:A:691:THR:HG22	1:A:693:HIS:N	2.24	0.53
1:A:772:GLU:OE1	1:A:928:ARG:HD2	2.09	0.52
1:A:691:THR:HG22	1:A:693:HIS:HB2	1.92	0.50
1:A:885:ARG:CB	1:A:886:PRO:HD3	2.43	0.49
1:A:936:ILE:HG22	1:A:936:ILE:O	2.13	0.48
1:A:884:THR:HG22	1:A:961:PHE:CE1	2.48	0.48
1:B:750:ARG:HH22	1:B:763:ASP:CG	2.21	0.48
1:A:811:PRO:HG2	1:A:814:GLU:HG3	1.95	0.48
1:A:695:ILE:O	1:A:699:MET:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:TYR:OH	1:A:864:THR:HG21	2.14	0.47
1:B:789[B]:HIS:CD2	1:B:789[B]:HIS:H	2.32	0.47
1:B:814:GLU:OE2	1:B:915:ARG:NH2	2.47	0.47
1:B:699[A]:MET:HE3	1:B:963:LEU:HD12	1.97	0.47
1:A:745:PRO:HB2	1:A:750:ARG:HB3	1.97	0.46
1:A:771:ILE:HG13	1:A:948:GLN:OE1	2.17	0.45
1:B:838:ASN:HB2	1:B:855:TYR:HB3	1.99	0.45
1:B:855:TYR:OH	1:B:864:THR:HG21	2.18	0.44
1:B:928:ARG:NH2	3:B:3309:HOH:O	2.50	0.43
1:A:876:PRO:HB3	1:B:878:GLU:HG2	2.01	0.42
1:A:933:VAL:HG12	1:A:935:GLU:H	1.84	0.42
1:A:699:MET:HE1	1:A:966:VAL:HG11	2.02	0.42
1:A:740:HIS:HA	1:A:741:PRO:HD3	1.92	0.41
1:A:885:ARG:HB3	1:A:886:PRO:CD	2.50	0.41
1:B:722:GLU:HA	1:B:723:PRO:HA	1.87	0.41
1:B:833:HIS:CE1	3:B:3434:HOH:O	2.74	0.41
1:A:722:GLU:HA	1:A:723:PRO:HA	1.93	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	288/301 (96%)	277 (96%)	9 (3%)	2 (1%)	18	16
1	B	295/301 (98%)	282 (96%)	11 (4%)	2 (1%)	18	16
All	All	583/602 (97%)	559 (96%)	20 (3%)	4 (1%)	18	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	815	ASP

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Mol	Chain	Res	Type
1	A	953	VAL
1	B	815	ASP
1	B	953	VAL

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	252/261 (97%)	228 (90%)	24 (10%)	8	5
1	B	258/261 (99%)	238 (92%)	20 (8%)	11	8
All	All	510/522 (98%)	466 (91%)	44 (9%)	9	6

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	694	MET
1	A	704	ARG
1	A	709	LEU
1	A	711	LYS
1	A	722	GLU
1	A	732	GLU
1	A	735	ILE
1	A	736	LYS
1	A	752	LYS
1	A	755	VAL
1	A	770	ILE
1	A	772	GLU
1	A	776	ARG
1	A	788	SER
1	A	815	ASP
1	A	827	GLU
1	A	847	GLU
1	A	885	ARG
1	A	902	SER
1	A	928	ARG

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Mol	Chain	Res	Type
1	A	934	LYS
1	A	935	GLU
1	A	956	LYS
1	A	973	ILE
1	B	689	ILE
1	B	709	LEU
1	B	722	GLU
1	B	732	GLU
1	B	735	ILE
1	B	752	LYS
1	B	755	VAL
1	B	770	ILE
1	B	776	ARG
1	B	777	MET
1	B	815	ASP
1	B	827	GLU
1	B	847	GLU
1	B	902	SER
1	B	915	ARG
1	B	928	ARG
1	B	931	LYS
1	B	934	LYS
1	B	936	ILE
1	B	956	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	730	GLN
1	A	944	HIS
1	B	833	HIS
1	B	860	GLN

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 [i](#)

There are no oligosaccharides 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	GOL	A	3288	-	5,5,5	0.37	0	5,5,5	0.18	0
2	GOL	B	3287	-	5,5,5	0.40	0	5,5,5	0.26	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	3288	-	-	0/4/4/4	-
2	GOL	B	3287	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3287	GOL	O1-C1-C2-O2
2	B	3287	GOL	O1-C1-C2-C3
2	B	3287	GOL	C1-C2-C3-O3
2	B	3287	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3288	GOL	1	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	287/301 (95%)	-0.16	10 (3%)	47 46	8, 26, 57, 92	6 (2%)
1	B	290/301 (96%)	-0.15	8 (2%)	55 55	3, 26, 59, 83	10 (3%)
All	All	577/602 (95%)	-0.16	18 (3%)	51 51	3, 26, 59, 92	16 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	934	LYS	3.0
1	B	976	ALA	2.6
1	A	976	ALA	2.6
1	A	901	ARG	2.6
1	A	936	ILE	2.6
1	B	777	MET	2.5
1	B	936	ILE	2.5
1	B	773	HIS	2.5
1	A	778	PRO	2.4
1	B	935	GLU	2.4
1	A	815	ASP	2.3
1	B	687	MET	2.3
1	A	692	GLY	2.3
1	A	691	THR	2.2
1	B	707[A]	ASP	2.2
1	A	977	LEU	2.1
1	A	775	PRO	2.1
1	A	935	GLU	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	3287	6/6	0.85	0.12	38,50,55,59	0
2	GOL	A	3288	6/6	0.86	0.13	39,62,66,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.