Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:09 pm BST

PDB ID	:	5FQ1
Title	:	Structure of the cytoplasmic PAS domain of the Geobacillus thermodenitrificans histidine kinase CitA
Authors	:	Schomburg, B.; Giller, K.; Becker, S.
Deposited on	:	2015-12-03
Resolution	:	1.76 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 following versions of software and data (see references ①) were used in the production of this report:

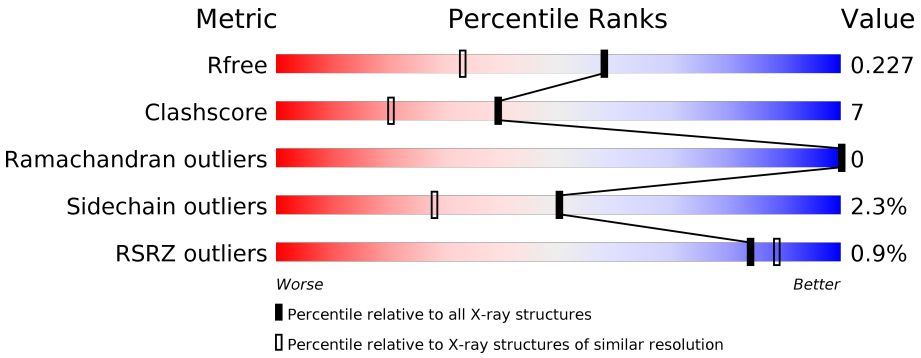
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.76 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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 <=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	112	2% 84% 14%
1	B	112	84% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	1311	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1796 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.

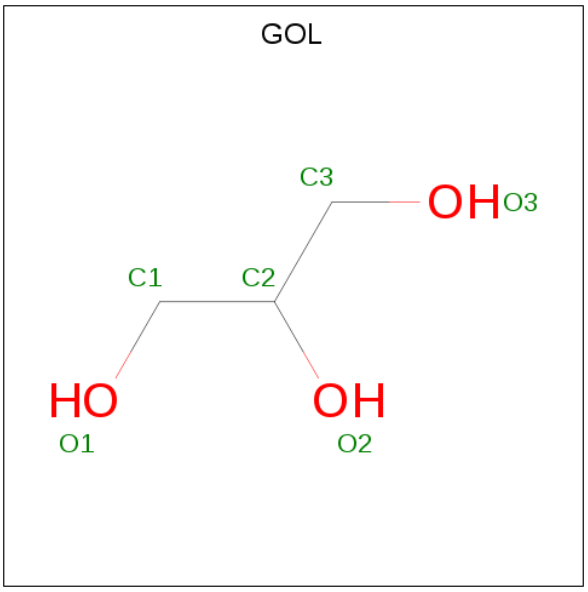
- Molecule 1 is a protein called HISTIDINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	Se	0	1	0
			848	532	150	164	2			
1	B	111	Total	C	N	O	Se	0	4	1
			858	541	148	165	4			

There are 8 discrepancies between the modelled and reference sequences:

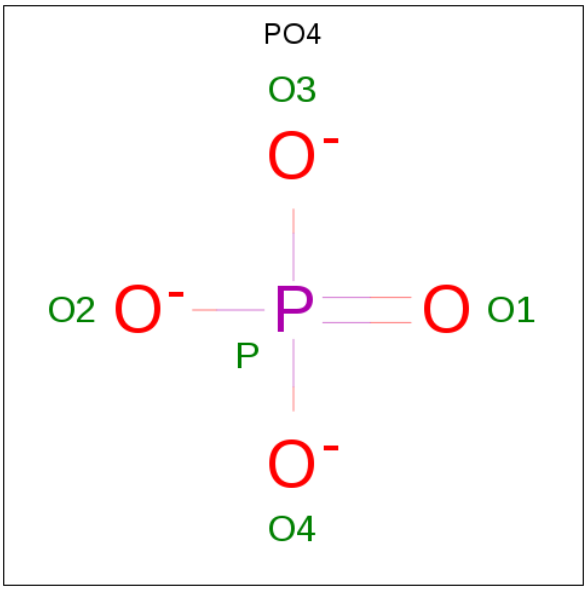
Chain	Residue	Modelled	Actual	Comment	Reference
A	198	GLY	-	expression tag	UNP A4IPE6
A	199	SER	-	expression tag	UNP A4IPE6
A	212	ALA	GLY	conflict	UNP A4IPE6
A	224	ILE	VAL	conflict	UNP A4IPE6
B	198	GLY	-	expression tag	UNP A4IPE6
B	199	SER	-	expression tag	UNP A4IPE6
B	212	ALA	GLY	conflict	UNP A4IPE6
B	224	ILE	VAL	conflict	UNP A4IPE6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	21	Total O 21 21	0	0

3 Residue-property plots (i)

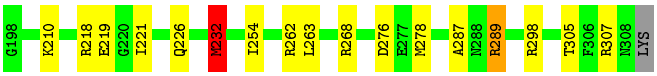
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: HISTIDINE KINASE

Chain A:

- Molecule 1: HISTIDINE KINASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	34.45Å 74.04Å 75.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.54 – 1.76 37.54 – 1.78	Depositor EDS
% Data completeness (in resolution range)	96.5 (37.54-1.76) 96.5 (37.54-1.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.185 , 0.216 0.198 , 0.227	Depositor DCC
R_{free} test set	913 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.075 for -h,l,k	Xtriage
Reported twinning fraction	0.905 for H, K, L 0.095 for -H, L, K	Depositor
Outliers	1 of 18948 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1796	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.41% 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, 0.333 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, PO4

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	0.93	0/855	1.10	3/1158 (0.3%)
1	B	0.92	0/865	1.09	9/1171 (0.8%)
All	All	0.93	0/1720	1.09	12/2329 (0.5%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	289	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	218	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	232[A]	MSE	CA-CB-CG	6.42	124.22	113.30
1	B	232[B]	MSE	CA-CB-CG	6.42	124.22	113.30
1	A	247	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	298	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	289	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	289	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	262	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	218	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	218	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	307	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	848	0	861	11	0
1	B	858	0	857	16	0
2	A	12	0	16	2	0
2	B	12	0	16	2	0
3	A	10	0	0	0	0
3	B	5	0	0	4	0
4	A	30	0	0	1	0
4	B	21	0	0	1	0
All	All	1796	0	1750	26	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 7.

All (26) 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:278[B]:MSE:HE1	3:B:1311:PO4:O4	1.48	1.11
1:B:278[B]:MSE:CE	3:B:1311:PO4:O4	2.22	0.87
1:B:276[A]:ASP:OD1	4:B:2016:HOH:O	2.06	0.72
1:B:221:ILE:HD13	1:B:305:THR:HG22	1.79	0.64
4:A:2008:HOH:O	2:B:1309:GOL:H11	1.98	0.63
1:A:213:ILE:HD11	1:B:232[A]:MSE:HE1	1.81	0.62
1:A:278:MSE:HE1	1:A:306:PHE:HE1	1.65	0.60
1:A:278:MSE:HE1	1:A:306:PHE:CE1	2.42	0.55
1:B:278[B]:MSE:SE	3:B:1311:PO4:O4	2.74	0.55
1:A:292:ILE:HD11	1:A:303[B]:VAL:CG2	2.38	0.53
1:B:219:GLU:OE2	2:B:1309:GOL:H12	2.09	0.53
1:B:278[A]:MSE:SE	1:B:289:ARG:HH21	2.43	0.52
1:B:221:ILE:CD1	1:B:305:THR:HG22	2.41	0.50
1:A:223:ALA:HB3	1:A:232:MSE:HB3	1.94	0.49
1:B:287:ALA:HA	1:B:305:THR:O	2.12	0.49
1:A:213:ILE:HD11	1:B:232[B]:MSE:HE1	1.96	0.48
1:A:278:MSE:HE2	1:A:287:ALA:HB2	1.95	0.47
2:A:1309:GOL:H11	1:B:210:LYS:NZ	2.30	0.47
1:A:244:ASP:HB3	1:A:248:ASN:HD21	1.80	0.46
1:A:292:ILE:HD11	1:A:303[B]:VAL:HG22	1.96	0.46
1:B:254[A]:ILE:CD1	1:B:263:LEU:HD12	2.46	0.45
1:B:278[A]:MSE:SE	3:B:1311:PO4:O4	2.86	0.43
1:A:220:GLY:O	1:A:305:THR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278[A]:MSE:HE3	1:B:278[A]:MSE:HB3	1.79	0.43
2:A:1309:GOL:H11	1:B:210:LYS:HZ1	1.84	0.42
1:A:223:ALA:HB2	1:A:303[B]:VAL:HG13	2.01	0.42

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	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
1	B	113/112 (101%)	112 (99%)	1 (1%)	0	100	100
All	All	222/224 (99%)	220 (99%)	2 (1%)	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	91/92 (99%)	90 (99%)	1 (1%)	73	60
1	B	89/92 (97%)	85 (96%)	4 (4%)	27	8
All	All	180/184 (98%)	175 (97%)	5 (3%)	50	20

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

Mol	Chain	Res	Type
1	A	240	LEU
1	B	226	GLN
1	B	232[A]	MSE
1	B	232[B]	MSE
1	B	268	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	248	ASN
1	A	271	GLN

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)

7 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	B	1310	-	5,5,5	0.29	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	B	1309	-	5,5,5	0.94	0	5,5,5	1.56	1 (20%)
3	PO4	A	1311	-	4,4,4	1.24	1 (25%)	6,6,6	1.03	0
2	GOL	A	1309	-	5,5,5	0.54	0	5,5,5	1.16	0
3	PO4	B	1311	-	4,4,4	0.84	0	6,6,6	1.71	1 (16%)
2	GOL	A	1310	-	5,5,5	0.80	0	5,5,5	1.24	1 (20%)
3	PO4	A	1312	-	4,4,4	0.64	0	6,6,6	0.69	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	B	1310	-	-	2/4/4/4	-
2	GOL	A	1310	-	-	2/4/4/4	-
2	GOL	A	1309	-	-	3/4/4/4	-
2	GOL	B	1309	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1311	PO4	P-O2	-2.16	1.48	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1311	PO4	O2-P-O1	3.36	123.19	110.89
2	A	1310	GOL	O3-C3-C2	2.31	121.27	110.20
2	B	1309	GOL	O2-C2-C1	-2.19	99.48	109.12

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1309	GOL	O1-C1-C2-C3
2	A	1310	GOL	C1-C2-C3-O3
2	A	1310	GOL	O2-C2-C3-O3
2	B	1310	GOL	O2-C2-C3-O3
2	B	1310	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	1309	GOL	O1-C1-C2-C3
2	B	1309	GOL	C1-C2-C3-O3
2	B	1309	GOL	O2-C2-C3-O3
2	A	1309	GOL	O1-C1-C2-O2
2	A	1309	GOL	C1-C2-C3-O3
2	B	1309	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1309	GOL	2	0
2	A	1309	GOL	2	0
3	B	1311	PO4	4	0

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^{th} 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	108/112 (96%)	0.11	2 (1%) 66 74	17, 28, 48, 57	0
1	B	109/112 (97%)	0.09	0 100 100	17, 28, 45, 57	0
All	All	217/224 (96%)	0.10	2 (0%) 84 89	17, 28, 46, 57	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	GLY	3.7
1	A	281	GLY	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

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. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
2	GOL	A	1309	6/6	0.77	0.18	45,47,50,54	0
2	GOL	A	1310	6/6	0.81	0.16	30,43,47,52	0
2	GOL	B	1309	6/6	0.84	0.17	26,31,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	1310	6/6	0.86	0.13	53,58,60,63	0
3	PO4	A	1312	5/5	0.88	0.23	45,47,57,59	0
3	PO4	B	1311	5/5	0.98	0.14	29,32,38,39	2
3	PO4	A	1311	5/5	0.99	0.13	27,30,34,35	0

6.5 Other polymers (i)

There are no such residues in this entry.