



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:14 PM UTC

PDB ID : 4THI / pdb_00004thi
Title : THIAMINASE I FROM BACILLUS THIAMINOLYTICUS WITH COVALENTLY BOUND 4-AMINO-2,5-DIMETHYLPYRIMIDINE
Authors : Campobasso, N.; Begley, T.P.; Ealick, S.E.
Deposited on : 1998-10-05
Resolution : 2.00 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)
Validation Pipeline (wwPDB-VP)	:	2.49

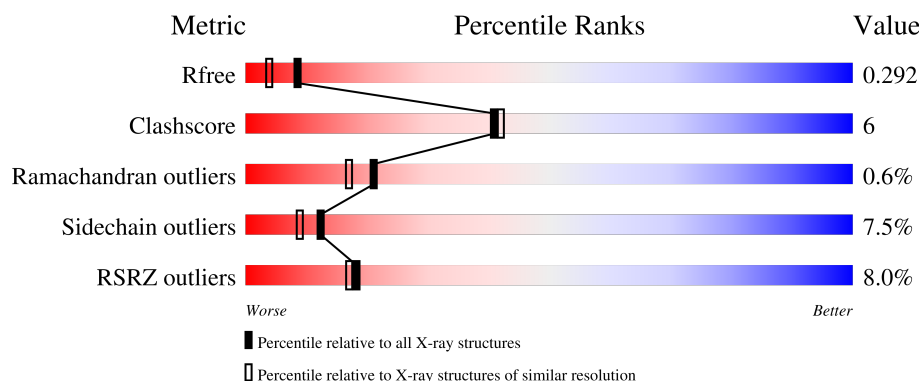
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	362	

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
2	SO4	A	372	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3000 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 PROTEIN (THIAMINASE I).

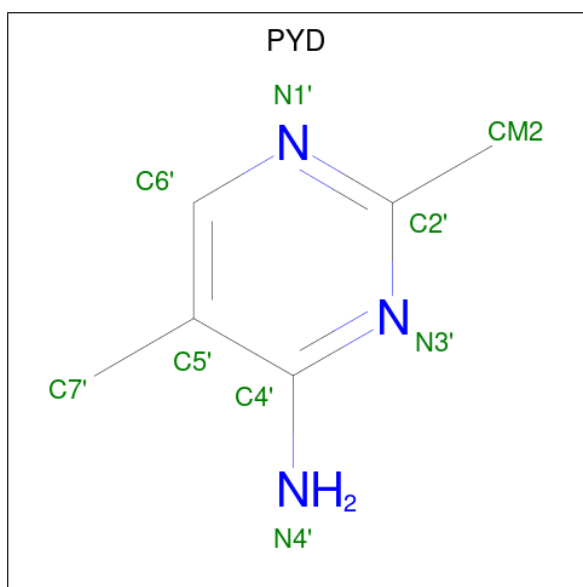
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2859	1834	472	544	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			3	2	1		

- Molecule 3 is 2,5-DIMETHYL-PYRIMIDIN-4-YLAMINE (CCD ID: PYD) (formula: C₆H₉N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	6	3		

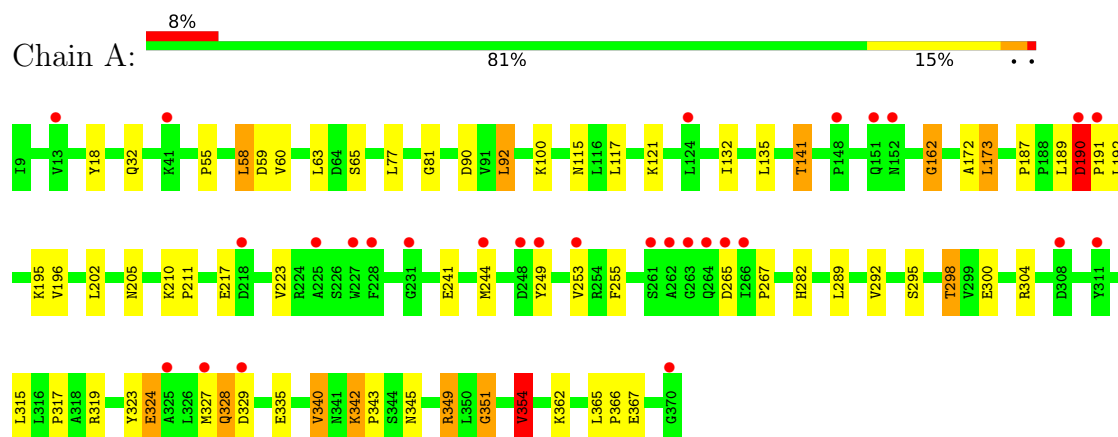
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		

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: PROTEIN (THIAMINASE I)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.70Å 119.30Å 37.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.2 (30.00-2.00) 87.8 (30.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.72 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.842	Depositor
R, R_{free}	0.211 , 0.258 0.249 , 0.292	Depositor DCC
R_{free} test set	1143 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3000	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PYD

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	0.56	0/2931	1.01	19/3988 (0.5%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	MET	N-CA-C	8.01	120.73	111.11
1	A	354	VAL	CB-CA-C	-7.35	102.30	111.70
1	A	351	GLY	CA-C-N	6.23	125.92	119.56
1	A	351	GLY	C-N-CA	6.23	125.92	119.56
1	A	92	LEU	CA-C-N	6.10	125.58	119.24
1	A	92	LEU	C-N-CA	6.10	125.58	119.24
1	A	59	ASP	N-CA-C	5.85	117.46	111.14
1	A	18	TYR	N-CA-C	5.76	118.58	108.56
1	A	132	ILE	N-CA-C	5.73	118.21	111.05
1	A	162	GLY	N-CA-C	5.59	118.98	112.50
1	A	354	VAL	N-CA-C	5.51	115.97	110.23
1	A	187	PRO	N-CA-C	5.49	117.39	110.70
1	A	65	SER	N-CA-C	5.45	119.41	112.87
1	A	190	ASP	CA-C-N	-5.40	113.09	119.84
1	A	190	ASP	C-N-CA	-5.40	113.09	119.84
1	A	81	GLY	N-CA-C	-5.40	105.63	112.54
1	A	77	LEU	N-CA-C	5.33	118.69	110.42
1	A	282	HIS	CA-C-N	5.32	124.77	119.24
1	A	282	HIS	C-N-CA	5.32	124.77	119.24

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	2859	0	2811	37	0
2	A	3	0	0	0	2
3	A	9	0	8	0	0
4	A	129	0	0	4	0
All	All	3000	0	2819	37	2

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.

All (37) 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:190:ASP:HB3	1:A:191:PRO:HD3	1.56	0.84
1:A:141:THR:HB	1:A:205:ASN:HD21	1.56	0.71
1:A:328:GLN:NE2	1:A:328:GLN:H	1.88	0.70
1:A:351:GLY:O	1:A:354:VAL:HG22	1.93	0.67
1:A:141:THR:HB	1:A:205:ASN:ND2	2.09	0.66
1:A:55:PRO:HD2	1:A:58:LEU:HD12	1.79	0.64
1:A:300:GLU:O	1:A:304:ARG:HG3	1.98	0.64
1:A:328:GLN:H	1:A:328:GLN:HE21	1.46	0.63
1:A:241:GLU:HG2	1:A:315:LEU:HD23	1.80	0.62
1:A:162:GLY:HA3	1:A:362:LYS:HE2	1.83	0.61
1:A:324:GLU:HG3	4:A:471:HOH:O	1.99	0.61
1:A:317:PRO:HD2	1:A:323:TYR:CZ	2.36	0.60
1:A:241:GLU:CG	1:A:315:LEU:HD23	2.31	0.60
1:A:241:GLU:HG2	1:A:315:LEU:CD2	2.33	0.57
1:A:100:LYS:O	1:A:349:ARG:NH2	2.39	0.55
1:A:249:TYR:CE2	1:A:253:VAL:HG13	2.42	0.55
1:A:367:GLU:HG3	4:A:462:HOH:O	2.06	0.54
1:A:342:LYS:NZ	1:A:342:LYS:HB3	2.24	0.52
1:A:190:ASP:HB3	1:A:191:PRO:CD	2.32	0.52
1:A:32:GLN:HG3	1:A:298:THR:HG22	1.91	0.52
1:A:92:LEU:CD1	1:A:340:VAL:HG13	2.41	0.51
1:A:267:PRO:HB2	1:A:345:ASN:ND2	2.26	0.50
1:A:90:ASP:OD2	1:A:319:ARG:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PRO:HB2	1:A:345:ASN:HD22	1.79	0.47
1:A:295:SER:OG	1:A:298:THR:HG23	2.15	0.46
1:A:366:PRO:HD2	4:A:462:HOH:O	2.15	0.45
1:A:117:LEU:O	1:A:255:PHE:HA	2.19	0.43
1:A:342:LYS:HA	1:A:343:PRO:HD3	1.89	0.43
1:A:195:LYS:HE2	1:A:195:LYS:HB3	1.80	0.42
1:A:60:VAL:HG21	1:A:289:LEU:HD23	2.02	0.42
1:A:92:LEU:HD11	1:A:340:VAL:CG1	2.50	0.42
1:A:210:LYS:HB2	1:A:211:PRO:HD3	2.01	0.41
1:A:292:VAL:O	1:A:298:THR:HG21	2.19	0.41
1:A:172:ALA:HB3	1:A:196:VAL:HG13	2.02	0.41
1:A:292:VAL:O	1:A:298:THR:CG2	2.69	0.40
1:A:317:PRO:HD2	1:A:323:TYR:CE1	2.57	0.40
1:A:173:LEU:HD13	4:A:448:HOH:O	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:372:SO4:S	2:A:372:SO4:O3[2_555]	1.46	0.74
2:A:372:SO4:S	2:A:372:SO4:O1[2_555]	1.47	0.73

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	360/362 (99%)	351 (98%)	7 (2%)	2 (1%)	21 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ASP

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Mol	Chain	Res	Type
1	A	190	ASP

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	307/307 (100%)	284 (92%)	23 (8%)	12 9

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	63	LEU
1	A	115	ASN
1	A	121	LYS
1	A	135	LEU
1	A	141	THR
1	A	173	LEU
1	A	189	LEU
1	A	192	LEU
1	A	202	LEU
1	A	217	GLU
1	A	223	VAL
1	A	244	MET
1	A	298	THR
1	A	324	GLU
1	A	328	GLN
1	A	329	ASP
1	A	335	GLU
1	A	340	VAL
1	A	342	LYS
1	A	349	ARG
1	A	354	VAL
1	A	365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	36	GLN
1	A	115	ASN
1	A	152	ASN
1	A	205	ASN
1	A	252	GLN
1	A	320	HIS
1	A	328	GLN
1	A	345	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 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	$\# Z > 2$
3	PYD	A	371	1	9,9,9	1.66	2 (22%)	11,12,12	1.69	3 (27%)
2	SO4	A	372	-	1,2,4	2.64	1 (100%)	0,1,6	-	-

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	PYD	A	371	1	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	371	PYD	C4'-N3'	2.73	1.38	1.35
2	A	372	SO4	O1-S	2.64	1.47	1.41
3	A	371	PYD	C6'-C5'	-2.26	1.36	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	371	PYD	C5'-C6'-N1'	-3.75	121.33	125.09
3	A	371	PYD	C6'-N1'-C2'	2.55	120.26	116.07
3	A	371	PYD	CM2-C2'-N3'	2.42	120.74	117.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	372	SO4	0	2

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

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, 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	362/362 (100%)	0.74	29 (8%)	18 17	12, 20, 36, 54	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	ASP	4.3
1	A	264	GLN	3.8
1	A	191	PRO	3.6
1	A	231	GLY	3.4
1	A	263	GLY	3.3
1	A	265	ASP	3.3
1	A	262	ALA	3.2
1	A	227	TRP	2.9
1	A	308	ASP	2.9
1	A	329	ASP	2.7
1	A	253	VAL	2.6
1	A	325	ALA	2.6
1	A	249	TYR	2.6
1	A	248	ASP	2.5
1	A	41	LYS	2.4
1	A	370	GLY	2.4
1	A	151	GLN	2.4
1	A	225	ALA	2.4
1	A	266	ILE	2.3
1	A	124	LEU	2.3
1	A	148	PRO	2.1
1	A	152	ASN	2.1
1	A	13	VAL	2.1
1	A	311	TYR	2.1
1	A	218	ASP	2.1
1	A	228	PHE	2.1
1	A	244	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	261	SER	2.0
1	A	327	MET	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
3	PYD	A	371	9/9	0.88	0.10	20,20,20,20	0
2	SO4	A	372	3/5	0.97	0.08	12,12,14,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.