



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:27 PM UTC

PDB ID : 3S3U / pdb_00003s3u
Title : Crystal Structure of Uncleaved ThnT T282C
Authors : Schildbach, J.F.; Wright, N.T.; Buller, A.R.
Deposited on : 2011-05-18
Resolution : 1.60 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
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

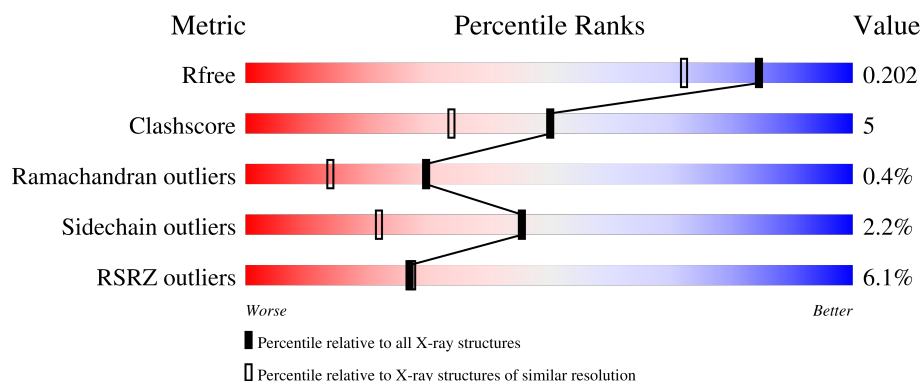
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	419	6% 78% 8% 13%
1	B	419	5% 79% 7% 14%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5923 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 cysteine transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	22	0
			2643	1640	493	508	2			
1	B	362	Total	C	N	O	S	0	12	0
			2567	1590	485	491	1			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q83XN4
A	-18	GLY	-	expression tag	UNP Q83XN4
A	-17	SER	-	expression tag	UNP Q83XN4
A	-16	SER	-	expression tag	UNP Q83XN4
A	-15	HIS	-	expression tag	UNP Q83XN4
A	-14	HIS	-	expression tag	UNP Q83XN4
A	-13	HIS	-	expression tag	UNP Q83XN4
A	-12	HIS	-	expression tag	UNP Q83XN4
A	-11	HIS	-	expression tag	UNP Q83XN4
A	-10	HIS	-	expression tag	UNP Q83XN4
A	-9	SER	-	expression tag	UNP Q83XN4
A	-8	SER	-	expression tag	UNP Q83XN4
A	-7	GLY	-	expression tag	UNP Q83XN4
A	-6	LEU	-	expression tag	UNP Q83XN4
A	-5	VAL	-	expression tag	UNP Q83XN4
A	-4	PRO	-	expression tag	UNP Q83XN4
A	-3	ARG	-	expression tag	UNP Q83XN4
A	-2	GLY	-	expression tag	UNP Q83XN4
A	-1	SER	-	expression tag	UNP Q83XN4
A	0	HIS	-	expression tag	UNP Q83XN4
A	282	CYS	THR	engineered mutation	UNP Q83XN4
B	-19	MET	-	expression tag	UNP Q83XN4
B	-18	GLY	-	expression tag	UNP Q83XN4
B	-17	SER	-	expression tag	UNP Q83XN4
B	-16	SER	-	expression tag	UNP Q83XN4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q83XN4
B	-14	HIS	-	expression tag	UNP Q83XN4
B	-13	HIS	-	expression tag	UNP Q83XN4
B	-12	HIS	-	expression tag	UNP Q83XN4
B	-11	HIS	-	expression tag	UNP Q83XN4
B	-10	HIS	-	expression tag	UNP Q83XN4
B	-9	SER	-	expression tag	UNP Q83XN4
B	-8	SER	-	expression tag	UNP Q83XN4
B	-7	GLY	-	expression tag	UNP Q83XN4
B	-6	LEU	-	expression tag	UNP Q83XN4
B	-5	VAL	-	expression tag	UNP Q83XN4
B	-4	PRO	-	expression tag	UNP Q83XN4
B	-3	ARG	-	expression tag	UNP Q83XN4
B	-2	GLY	-	expression tag	UNP Q83XN4
B	-1	SER	-	expression tag	UNP Q83XN4
B	0	HIS	-	expression tag	UNP Q83XN4
B	282	CYS	THR	engineered mutation	UNP Q83XN4

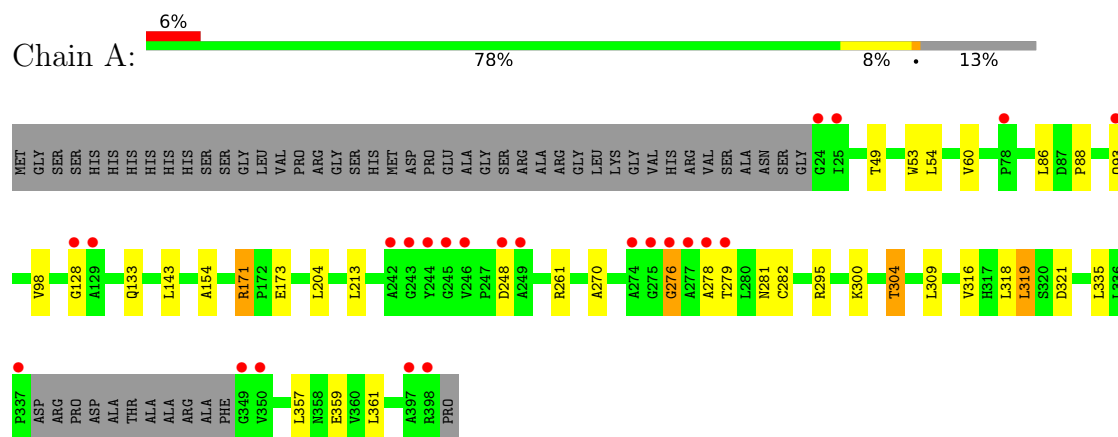
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	398	Total O 399 399	0	6
2	B	314	Total O 314 314	0	1

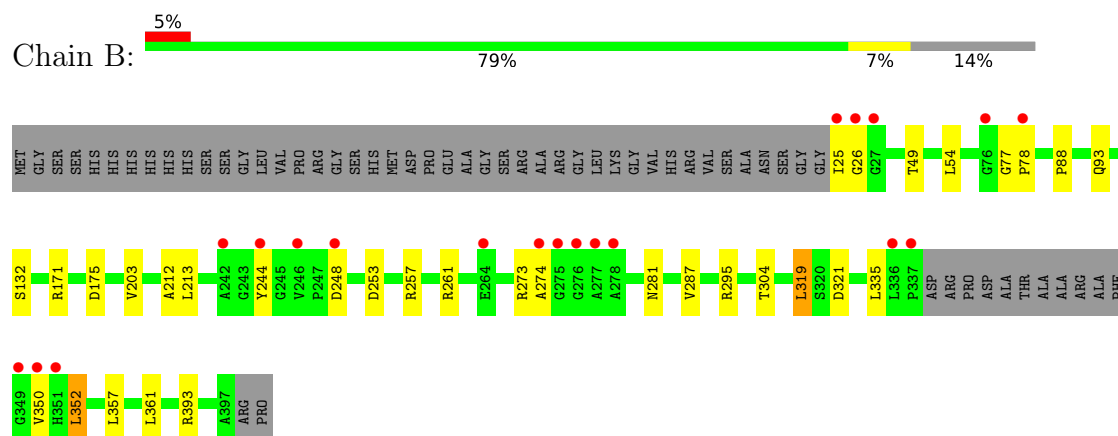
3 Residue-property plots [i](#)

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: cysteine transferase



- Molecule 1: cysteine transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.53Å 68.65Å 73.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.54 – 1.60 39.54 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.54-1.60) 94.4 (39.54-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , 0.191 0.173 , 0.202	Depositor DCC
R_{free} test set	4524 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5923	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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](#)

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	0.86	0/2719	0.92	0/3721
1	B	0.79	0/2637	0.87	0/3607
All	All	0.82	0/5356	0.89	0/7328

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	2643	0	2662	29	0
1	B	2567	0	2579	28	0
2	A	399	0	0	6	0
2	B	314	0	0	7	0
All	All	5923	0	5241	55	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 5.

All (55) 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:304[B]:THR:HG23	2:B:449:HOH:O	1.41	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ALA:HB3	2:A:697:HOH:O	1.52	1.06
1:B:253:ASP:HB2	1:B:257:ARG:NH2	1.79	0.95
1:B:49[B]:THR:HG21	2:B:993:HOH:O	1.67	0.95
1:A:319[B]:LEU:O	2:A:702:HOH:O	1.95	0.83
1:B:253:ASP:HB2	1:B:257:ARG:HH21	1.46	0.79
1:B:93[B]:GLN:H	1:B:93[B]:GLN:CD	1.93	0.77
1:A:49[B]:THR:HG21	2:A:691:HOH:O	1.84	0.76
1:B:25:ILE:HA	1:B:203:VAL:HG11	1.67	0.75
1:B:171:ARG:HD3	1:B:175:ASP:OD2	1.92	0.69
1:A:319[A]:LEU:HD11	1:B:357:LEU:HD23	1.75	0.69
1:B:93[B]:GLN:HG3	2:B:544:HOH:O	1.93	0.68
1:A:300:LYS:O	1:A:304[A]:THR:HG23	1.98	0.63
1:A:49[B]:THR:HG23	2:A:705:HOH:O	2.00	0.61
1:A:88:PRO:HG3	1:A:295[B]:ARG:HG2	1.83	0.60
1:B:88:PRO:HA	1:B:295[A]:ARG:CD	2.32	0.60
1:B:132:SER:HA	2:B:677:HOH:O	2.06	0.55
1:B:304[A]:THR:HG21	1:B:361:LEU:HB3	1.88	0.55
1:B:25:ILE:HA	1:B:203:VAL:CG1	2.38	0.53
1:B:88:PRO:HG3	1:B:295[A]:ARG:HG2	1.90	0.53
1:B:49[B]:THR:HG22	1:B:54:LEU:HD12	1.92	0.51
1:A:88:PRO:HA	1:A:295[B]:ARG:HD2	1.93	0.50
1:B:350:VAL:HG22	1:B:352:LEU:HD13	1.92	0.50
1:A:318[B]:LEU:O	1:A:321[B]:ASP:N	2.30	0.50
1:A:279[A]:THR:HG22	1:A:279[A]:THR:O	2.12	0.50
1:B:253:ASP:CB	1:B:257:ARG:HH21	2.22	0.49
1:B:88:PRO:HA	1:B:295[A]:ARG:HD2	1.94	0.49
1:A:60:VAL:HB	1:A:98[B]:VAL:HG22	1.95	0.49
1:A:88:PRO:HA	1:A:295[B]:ARG:CD	2.43	0.48
1:B:213:LEU:HD23	1:B:213:LEU:C	2.38	0.48
1:B:77:GLY:HA3	1:B:78:PRO:C	2.38	0.48
1:B:244:TYR:HB3	1:B:393:ARG:HD3	1.96	0.48
1:B:281:ASN:O	1:B:321[B]:ASP:HA	2.14	0.48
1:A:309:LEU:HG	1:A:316:VAL:HG11	1.98	0.46
1:B:304[B]:THR:CG2	2:B:449:HOH:O	2.24	0.46
1:A:53:TRP:CD2	1:A:154:ALA:HB1	2.51	0.45
1:A:357:LEU:HD23	1:B:319:LEU:HG	1.98	0.44
1:B:273:ARG:O	1:B:274:ALA:HB3	2.18	0.44
1:A:171:ARG:HA	1:A:171:ARG:HD2	1.64	0.44
1:A:304[A]:THR:HG21	1:A:361:LEU:HD22	2.00	0.43
1:B:257:ARG:HD2	2:B:461:HOH:O	2.19	0.43
1:A:281[A]:ASN:O	1:A:282[A]:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318[B]:LEU:O	1:A:319[B]:LEU:C	2.61	0.43
1:A:93[A]:GLN:HG3	2:A:762:HOH:O	2.19	0.42
1:A:143:LEU:HA	1:A:282[A]:CYS:HB2	2.00	0.42
1:B:212:ALA:HB2	1:B:287[B]:VAL:HG12	2.01	0.42
1:A:270:ALA:CB	1:A:276:GLY:HA2	2.49	0.42
1:A:204:LEU:HD22	1:A:359[A]:GLU:HG2	2.01	0.42
1:A:86:LEU:O	1:A:295[B]:ARG:HD3	2.20	0.41
1:A:213:LEU:C	1:A:213:LEU:HD23	2.45	0.41
1:A:128:GLY:HA3	1:A:133:GLN:OE1	2.21	0.41
1:A:49[B]:THR:HG22	1:A:54:LEU:HD12	2.02	0.41
1:A:171:ARG:HD3	2:A:546:HOH:O	2.20	0.41
1:B:49[B]:THR:HG23	2:B:739:HOH:O	2.20	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	382/419 (91%)	372 (97%)	7 (2%)	3 (1%)	16	5
1	B	370/419 (88%)	363 (98%)	6 (2%)	1 (0%)	36	20
All	All	752/838 (90%)	735 (98%)	13 (2%)	4 (0%)	30	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319[A]	LEU
1	A	319[B]	LEU
1	A	276	GLY
1	B	26	GLY

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	253/273 (93%)	247 (98%)	6 (2%)	43	19
1	B	242/273 (89%)	236 (98%)	6 (2%)	42	18
All	All	495/546 (91%)	483 (98%)	12 (2%)	45	19

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	ARG
1	A	173	GLU
1	A	248	ASP
1	A	304[A]	THR
1	A	304[B]	THR
1	A	335	LEU
1	B	248	ASP
1	B	261[A]	ARG
1	B	261[B]	ARG
1	B	319	LEU
1	B	335	LEU
1	B	352	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

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	364/419 (86%)	-0.22	24 (6%)	24 25	9, 18, 43, 62	22 (6%)
1	B	362/419 (86%)	-0.04	20 (5%)	30 31	9, 23, 51, 66	12 (3%)
All	All	726/838 (86%)	-0.13	44 (6%)	27 27	9, 20, 49, 66	34 (4%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	VAL	6.8
1	A	277	ALA	6.5
1	B	277	ALA	5.9
1	A	350	VAL	5.7
1	B	25	ILE	5.1
1	A	276	GLY	4.7
1	A	349	GLY	4.3
1	B	349	GLY	3.9
1	A	129	ALA	3.8
1	B	337	PRO	3.8
1	A	275	GLY	3.5
1	B	26	GLY	3.5
1	A	278	ALA	3.2
1	A	279[A]	THR	3.2
1	A	243	GLY	3.1
1	A	242	ALA	3.1
1	A	25	ILE	3.0
1	A	246	VAL	3.0
1	A	78	PRO	3.0
1	B	275	GLY	3.0
1	A	337	PRO	2.9
1	B	351	HIS	2.8
1	A	249	ALA	2.8
1	B	242	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	76	GLY	2.6
1	A	397	ALA	2.6
1	B	278	ALA	2.6
1	B	336	LEU	2.5
1	B	274	ALA	2.5
1	A	398	ARG	2.5
1	A	24	GLY	2.4
1	A	274	ALA	2.4
1	B	248	ASP	2.4
1	A	244	TYR	2.4
1	B	78	PRO	2.3
1	B	244	TYR	2.3
1	A	248	ASP	2.2
1	B	276	GLY	2.2
1	A	245	GLY	2.2
1	B	246	VAL	2.1
1	B	27	GLY	2.1
1	B	264	GLU	2.1
1	A	93[A]	GLN	2.0
1	A	128	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.