



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 PM GMT

PDB ID : 3S3U
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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

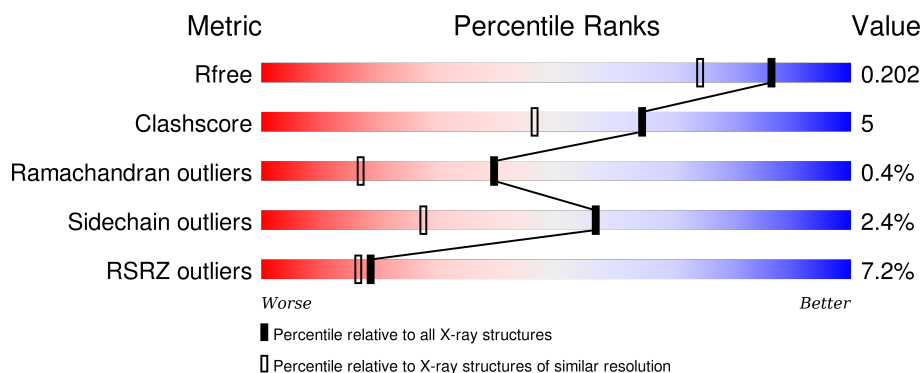
1 Overall quality at a glance

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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (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 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	419	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>13%</div> </div> </div>
1	B	419	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>14%</div> </div> </div>

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

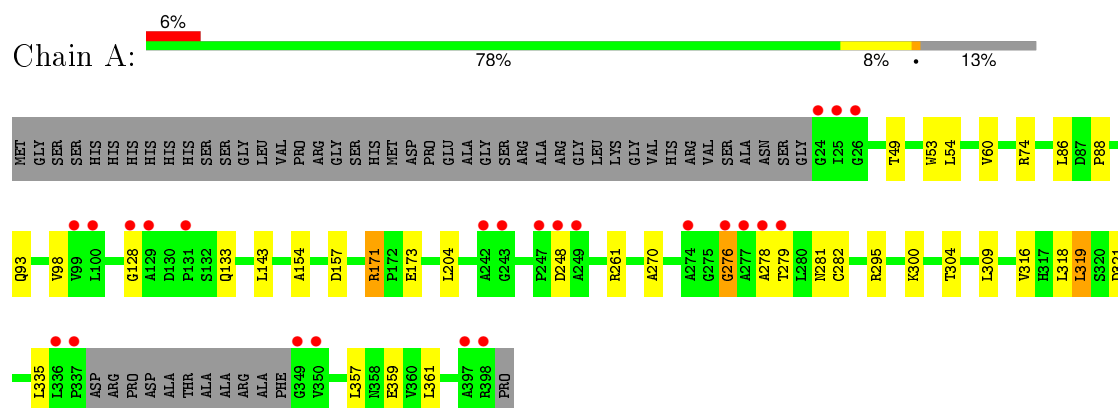
- Molecule 2 is water.

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

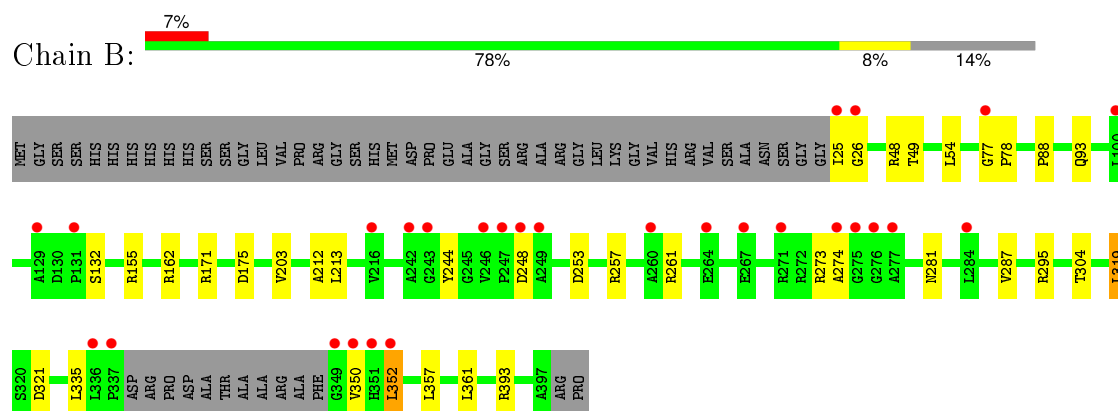
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	140.53 Å 68.65 Å 73.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.54 – 1.60 31.12 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.54-1.60) 94.4 (31.12-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.60 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.158 , 0.191 0.173 , 0.202	Depositor DCC
R_{free} test set	4524 reflections (5.32%)	DCC
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 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 89492 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.74	0/2719	0.83	5/3721 (0.1%)
1	B	0.65	0/2637	0.78	2/3607 (0.1%)
All	All	0.69	0/5356	0.80	7/7328 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74[A]	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	A	74[B]	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	B	162[A]	ARG	NE-CZ-NH1	-10.47	115.07	120.30
1	B	162[B]	ARG	NE-CZ-NH1	-10.47	115.07	120.30
1	A	74[A]	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	74[B]	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	157	ASP	CB-CG-OD1	5.91	123.61	118.30

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	2643	0	2662	27	0
1	B	2567	0	2579	28	0
2	A	399	0	0	6	0
2	B	314	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5923	0	5241	53	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 (53) 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
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: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:93[B]:GLN:H	1:B:93[B]:GLN:CD	1.93	0.72
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	1:A:171:ARG:HA	1.64	0.44
1:B:213:LEU:HD23	1:B:213:LEU:C	2.38	0.43
1:A:304[A]:THR:HG21	1:A:361:LEU:HD22	2.00	0.43
1:B:77:GLY:HA3	1:B:78:PRO:C	2.38	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
1:A:143:LEU:HA	1:A:282[A]:CYS:HB2	2.00	0.42
1:A:93[A]:GLN:HG3	2:A:762:HOH:O	2.19	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: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 [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	382/419 (91%)	372 (97%)	7 (2%)	3 (1%)	24	6
1	B	370/419 (88%)	363 (98%)	6 (2%)	1 (0%)	46	23
All	All	752/838 (90%)	735 (98%)	13 (2%)	4 (0%)	39	12

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 ⓘ

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%)	249 (98%)	4 (2%)	70	47
1	B	242/273 (89%)	234 (97%)	8 (3%)	45	17
All	All	495/546 (91%)	483 (98%)	12 (2%)	57	27

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	335	LEU
1	B	48	ARG
1	B	155	ARG
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

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

5.3.3 RNA ⓘ

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](#)

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%)	0.16	24 (6%)	22 19	11, 19, 43, 62	0
1	B	362/419 (86%)	0.27	28 (7%)	16 14	14, 24, 51, 66	0
All	All	726/838 (86%)	0.22	52 (7%)	18 16	11, 21, 49, 66	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	VAL	11.5
1	B	350	VAL	11.5
1	A	277	ALA	10.0
1	B	277	ALA	8.3
1	B	25	ILE	7.9
1	B	248	ASP	6.4
1	B	276	GLY	6.0
1	A	129	ALA	5.9
1	B	274	ALA	5.0
1	A	24	GLY	5.0
1	B	337	PRO	4.8
1	A	349	GLY	4.8
1	A	337	PRO	4.7
1	B	242	ALA	4.6
1	A	278	ALA	4.0
1	A	248	ASP	3.9
1	B	275	GLY	3.9
1	B	336	LEU	3.9
1	A	249	ALA	3.8
1	B	352	LEU	3.8
1	A	25	ILE	3.8
1	A	276	GLY	3.7
1	B	129	ALA	3.7
1	A	131	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	26	GLY	3.6
1	B	249	ALA	3.5
1	B	271	ARG	3.5
1	B	247	PRO	3.4
1	A	128	GLY	3.0
1	B	131	PRO	2.8
1	A	398	ARG	2.8
1	B	243	GLY	2.8
1	B	267	GLU	2.7
1	A	274	ALA	2.7
1	B	100	LEU	2.7
1	B	349	GLY	2.7
1	A	397	ALA	2.6
1	A	336	LEU	2.6
1	B	246	VAL	2.5
1	B	351	HIS	2.5
1	A	279[A]	THR	2.5
1	B	284	LEU	2.4
1	A	26	GLY	2.4
1	A	242	ALA	2.3
1	A	247	PRO	2.3
1	A	243	GLY	2.2
1	A	99	VAL	2.2
1	B	260	ALA	2.1
1	A	100	LEU	2.1
1	B	77	GLY	2.1
1	B	264	GLU	2.1
1	B	216	VAL	2.0

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.