



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:48 AM EDT

PDB ID : 2B2A / pdb_00002b2a
Title : Crystal Structure of the TEN domain of the Telomerase Reverse Transcriptase
Authors : Jacobs, S.A.; Podell, E.R.; Cech, T.R.
Deposited on : 2005-09-18
Resolution : 2.22 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
Xtrriage (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

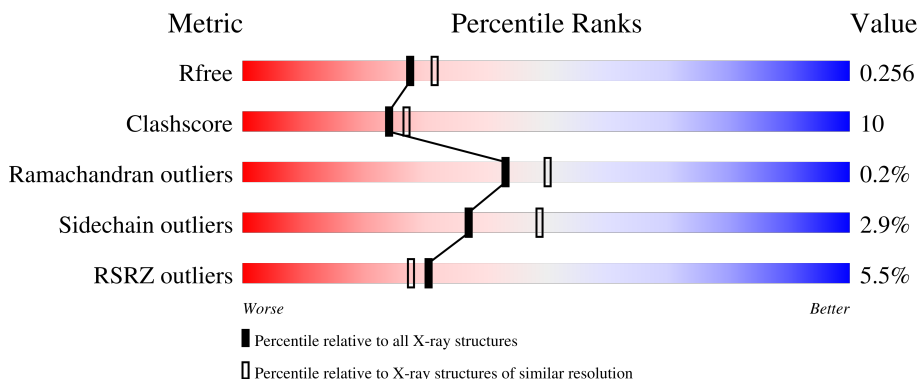
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	199	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">5% 64% 16% • 18%</p>
1	B	199	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 58%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">6% 58% 18% • 23%</p>
1	C	199	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 59% 17% • 21%</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4048 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 Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	164	1364	886	215	260	3	0	0	0
1	B	154	1281	833	200	246	2	0	0	0
1	C	157	1307	849	205	250	3	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	cloning artifact	UNP O77448
A	-6	LYS	-	cloning artifact	UNP O77448
A	-5	LYS	-	cloning artifact	UNP O77448
A	-4	HIS	-	expression tag	UNP O77448
A	-3	HIS	-	expression tag	UNP O77448
A	-2	HIS	-	expression tag	UNP O77448
A	-1	HIS	-	expression tag	UNP O77448
A	0	HIS	-	expression tag	UNP O77448
A	1	HIS	-	expression tag	UNP O77448
A	87	MET	LEU	engineered mutation	UNP O77448
B	-7	MET	-	cloning artifact	UNP O77448
B	-6	LYS	-	cloning artifact	UNP O77448
B	-5	LYS	-	cloning artifact	UNP O77448
B	-4	HIS	-	expression tag	UNP O77448
B	-3	HIS	-	expression tag	UNP O77448
B	-2	HIS	-	expression tag	UNP O77448
B	-1	HIS	-	expression tag	UNP O77448
B	0	HIS	-	expression tag	UNP O77448
B	1	HIS	-	expression tag	UNP O77448
B	87	MET	LEU	engineered mutation	UNP O77448
C	-7	MET	-	cloning artifact	UNP O77448
C	-6	LYS	-	cloning artifact	UNP O77448
C	-5	LYS	-	cloning artifact	UNP O77448

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP O77448
C	-3	HIS	-	expression tag	UNP O77448
C	-2	HIS	-	expression tag	UNP O77448
C	-1	HIS	-	expression tag	UNP O77448
C	0	HIS	-	expression tag	UNP O77448
C	1	HIS	-	expression tag	UNP O77448
C	87	MET	LEU	engineered mutation	UNP O77448

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	34	Total O 34 34	0	0
2	B	33	Total O 33 33	0	0
2	C	29	Total O 29 29	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	111.10Å 111.10Å 42.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.71 – 2.22 19.71 – 2.22	Depositor EDS
% Data completeness (in resolution range)	95.1 (19.71-2.22) 95.0 (19.71-2.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.22Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.258 0.236 , 0.256	Depositor DCC
R_{free} test set	2717 reflections (9.47%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.020 for -h,-k,l 0.028 for h,-h-k,-l 0.027 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4048	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.67% 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	0.41	0/1385	0.82	5/1867 (0.3%)
1	B	0.40	0/1299	0.82	4/1750 (0.2%)
1	C	0.38	0/1325	0.80	4/1783 (0.2%)
All	All	0.40	0/4009	0.82	13/5400 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	GLY	N-CA-C	-7.07	102.70	112.18
1	C	144	GLY	N-CA-C	-6.97	102.84	112.18
1	A	156	LEU	N-CA-C	-6.80	98.18	109.46
1	B	156	LEU	N-CA-C	-6.76	98.21	108.96
1	C	156	LEU	N-CA-C	-6.72	98.28	108.96
1	A	144	GLY	N-CA-C	-6.70	103.20	112.18
1	B	35	ASN	N-CA-C	-6.30	101.20	110.52
1	A	35	ASN	N-CA-C	-6.26	101.26	110.52
1	C	35	ASN	N-CA-C	-6.02	101.61	110.52
1	A	155	PHE	N-CA-C	5.39	118.34	109.72
1	A	45	LYS	N-CA-C	-5.37	105.47	112.23
1	B	45	LYS	N-CA-C	-5.26	105.61	112.23
1	C	45	LYS	N-CA-C	-5.03	105.89	112.23

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	1364	0	1371	26	0
1	B	1281	0	1280	34	0
1	C	1307	0	1310	30	0
2	A	34	0	0	4	0
2	B	33	0	0	6	0
2	C	29	0	0	2	0
All	All	4048	0	3961	79	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 10.

All (79) 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:C:168:GLN:HE22	1:C:174:LEU:H	1.29	0.80
1:A:168:GLN:HE22	1:A:174:LEU:H	1.29	0.79
1:B:177:TYR:HA	1:C:163:GLN:HG2	1.62	0.79
1:B:168:GLN:HE22	1:B:174:LEU:H	1.30	0.79
1:B:128:ARG:HB3	2:B:207:HOH:O	1.83	0.79
1:B:177:TYR:O	1:C:163:GLN:HG3	1.84	0.78
1:B:109:GLN:O	1:B:112:THR:HB	1.84	0.77
1:B:128:ARG:HG3	2:B:220:HOH:O	1.85	0.76
1:C:109:GLN:O	1:C:112:THR:HB	1.85	0.76
1:A:109:GLN:O	1:A:112:THR:HB	1.85	0.76
1:C:128:ARG:HD2	2:C:208:HOH:O	1.94	0.67
1:C:12:GLN:O	1:C:13:MET:HB2	1.95	0.64
1:B:191:ASN:O	1:C:31:LYS:HD2	1.98	0.64
1:A:51:GLU:HG2	2:A:216:HOH:O	2.00	0.60
1:B:16:ARG:HG2	1:B:164:ASN:ND2	2.16	0.60
1:A:190:ASN:HA	1:B:31:LYS:O	2.01	0.59
1:A:182:VAL:HG13	1:B:72:VAL:HG11	1.84	0.57
1:C:16:ARG:HG2	1:C:164:ASN:ND2	2.20	0.55
1:C:18:GLU:O	1:C:22:THR:HG23	2.08	0.54
1:A:18:GLU:O	1:A:22:THR:HG23	2.07	0.53
1:B:18:GLU:O	1:B:22:THR:HG23	2.09	0.53
1:A:161:VAL:HG12	1:A:162:GLU:HG3	1.90	0.53
1:C:88:THR:HG22	1:C:90:LYS:H	1.74	0.53
1:A:190:ASN:O	1:A:190:ASN:ND2	2.40	0.53
1:B:161:VAL:HG12	1:B:162:GLU:HG3	1.91	0.53
1:B:88:THR:HG22	1:B:90:LYS:H	1.75	0.52
1:C:161:VAL:HG12	1:C:162:GLU:HG3	1.92	0.52
1:B:177:TYR:O	1:C:163:GLN:CG	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ARG:HB2	1:C:19:ASP:OD2	2.10	0.51
1:A:88:THR:HG22	1:A:90:LYS:H	1.76	0.50
1:A:16:ARG:NH1	1:C:13:MET:HE3	2.29	0.48
1:B:16:ARG:HB2	1:B:19:ASP:OD2	2.14	0.48
1:A:162:GLU:HB3	1:A:163:GLN:HE21	1.77	0.48
1:B:162:GLU:HB3	1:B:163:GLN:HE21	1.78	0.48
1:A:128:ARG:HB2	1:A:131:LEU:HD12	1.96	0.48
1:A:104:GLN:O	1:A:105:ASN:HB2	2.15	0.47
1:A:16:ARG:HB2	1:A:19:ASP:OD2	2.15	0.47
1:B:45:LYS:HE2	1:B:75:TYR:O	2.16	0.46
1:C:128:ARG:HB2	1:C:131:LEU:HD12	1.97	0.46
1:B:104:GLN:O	1:B:105:ASN:HB2	2.15	0.46
1:B:190:ASN:HD21	1:C:70:ASN:HD22	1.64	0.46
1:A:133:SER:HB2	2:A:205:HOH:O	2.17	0.45
1:C:162:GLU:HB3	1:C:163:GLN:HE21	1.81	0.45
1:B:129:GLN:HB2	2:B:199:HOH:O	2.17	0.45
1:B:128:ARG:HB2	1:B:131:LEU:HD12	1.98	0.44
1:B:177:TYR:CA	1:C:163:GLN:HG2	2.41	0.44
1:C:45:LYS:HE2	1:C:75:TYR:O	2.17	0.44
1:C:87:MET:HG3	1:C:145:GLU:OE1	2.18	0.44
1:C:189:LYS:HD3	1:C:191:ASN:ND2	2.32	0.44
1:C:187:TRP:C	1:C:187:TRP:CD1	2.95	0.44
1:A:45:LYS:HE2	1:A:75:TYR:O	2.17	0.44
1:B:51:GLU:HG2	2:B:223:HOH:O	2.18	0.44
1:C:104:GLN:O	1:C:105:ASN:HB2	2.17	0.44
1:A:90:LYS:NZ	2:A:213:HOH:O	2.51	0.44
1:A:185:LYS:HB2	1:B:38:GLU:OE1	2.18	0.44
1:B:168:GLN:HE22	1:B:174:LEU:N	2.07	0.44
1:C:16:ARG:HG3	1:C:16:ARG:HH11	1.83	0.43
1:A:22:THR:HG22	1:A:25:LYS:NZ	2.34	0.43
1:C:53:ASP:OD2	1:C:54:THR:N	2.52	0.43
1:A:187:TRP:CE2	1:A:190:ASN:ND2	2.87	0.43
1:B:16:ARG:HH11	1:B:16:ARG:HG3	1.84	0.43
1:C:22:THR:HG22	1:C:25:LYS:NZ	2.33	0.43
1:B:133:SER:HB2	2:B:198:HOH:O	2.18	0.42
1:C:132:TYR:C	2:C:200:HOH:O	2.61	0.42
1:B:22:THR:HG22	1:B:25:LYS:NZ	2.34	0.42
1:A:189:LYS:O	1:A:189:LYS:HG3	2.15	0.42
1:A:107:VAL:HG21	1:A:168:GLN:HG2	2.02	0.42
1:B:98:ILE:HD13	1:B:117:PHE:HA	2.01	0.41
1:C:51:GLU:HG3	1:C:51:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:GLU:O	1:B:51:GLU:HG3	2.20	0.41
1:B:129:GLN:H	1:B:129:GLN:HG3	1.65	0.41
1:A:51:GLU:O	1:A:51:GLU:HG3	2.21	0.41
1:A:68:GLU:HG3	2:A:193:HOH:O	2.20	0.41
1:A:189:LYS:HG2	1:B:33:VAL:HG23	2.02	0.41
1:B:130:THR:HB	2:B:207:HOH:O	2.20	0.40
1:C:22:THR:HA	1:C:25:LYS:NZ	2.36	0.40
1:C:31:LYS:HE2	1:C:69:GLN:OE1	2.21	0.40
1:A:53:ASP:OD2	1:A:54:THR:N	2.54	0.40
1:B:19:ASP:O	1:B:23:VAL:HG23	2.21	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	158/199 (79%)	150 (95%)	8 (5%)	0	100	100
1	B	144/199 (72%)	140 (97%)	4 (3%)	0	100	100
1	C	147/199 (74%)	142 (97%)	4 (3%)	1 (1%)	18	18
All	All	449/597 (75%)	432 (96%)	16 (4%)	1 (0%)	43	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	13	MET

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	154/189 (82%)	148 (96%)	6 (4%)	28	37
1	B	144/189 (76%)	141 (98%)	3 (2%)	47	61
1	C	147/189 (78%)	143 (97%)	4 (3%)	39	52
All	All	445/567 (78%)	432 (97%)	13 (3%)	37	49

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	69	GLN
1	A	112	THR
1	A	163	GLN
1	A	189	LYS
1	A	190	ASN
1	B	69	GLN
1	B	112	THR
1	B	163	GLN
1	C	48	GLN
1	C	69	GLN
1	C	112	THR
1	C	163	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	74	ASN
1	A	77	GLN
1	A	91	GLN
1	A	163	GLN
1	A	168	GLN
1	A	190	ASN
1	B	48	GLN
1	B	74	ASN
1	B	77	GLN
1	B	91	GLN
1	B	163	GLN

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Mol	Chain	Res	Type
1	B	168	GLN
1	B	190	ASN
1	C	12	GLN
1	C	48	GLN
1	C	74	ASN
1	C	77	GLN
1	C	91	GLN
1	C	163	GLN
1	C	168	GLN
1	C	191	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](#)

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	164/199 (82%)	0.37	10 (6%) 27 24	18, 35, 55, 70	0
1	B	154/199 (77%)	0.43	12 (7%) 19 16	19, 36, 56, 71	0
1	C	157/199 (78%)	0.39	4 (2%) 58 56	22, 37, 59, 69	0
All	All	475/597 (79%)	0.40	26 (5%) 30 28	18, 36, 57, 71	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	GLN	3.9
1	A	13	MET	3.8
1	B	121	TYR	3.8
1	C	121	TYR	3.4
1	A	121	TYR	3.3
1	B	163	GLN	3.2
1	A	77	GLN	3.0
1	A	128	ARG	2.8
1	A	190	ASN	2.7
1	B	77	GLN	2.7
1	B	53	ASP	2.7
1	B	175	ASN	2.7
1	C	163	GLN	2.5
1	B	120	GLU	2.5
1	B	87	MET	2.5
1	C	77	GLN	2.5
1	A	164	ASN	2.3
1	A	162	GLU	2.3
1	B	164	ASN	2.2
1	A	53	ASP	2.1
1	A	90	LYS	2.1
1	B	101	GLY	2.1
1	B	112	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	120	GLU	2.1
1	B	128	ARG	2.1
1	B	48	GLN	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.