



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:17 PM UTC

PDB ID : 6ZD1 / pdb_00006zd1
Title : Structure of apo telomerase from Candida Tropicalis
Authors : Zhai, L.; Rety, S.; Chen, W.F.; Auguin, D.; Xi, X.G.
Deposited on : 2020-06-13
Resolution : 2.47 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

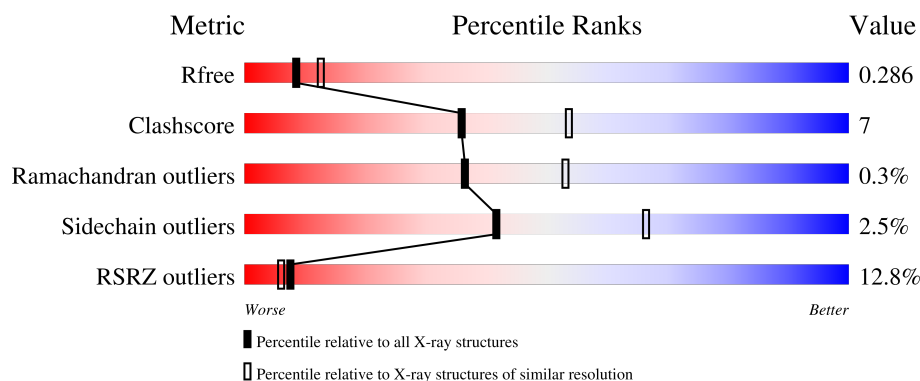
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	705	11% 76% 14% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5305 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
1	A	645	Total	C	N	O	S	Se	0	0	0
			5291	3410	893	967	10	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	880	VAL	-	expression tag	UNP C5MCQ7
A	881	ASP	-	expression tag	UNP C5MCQ7

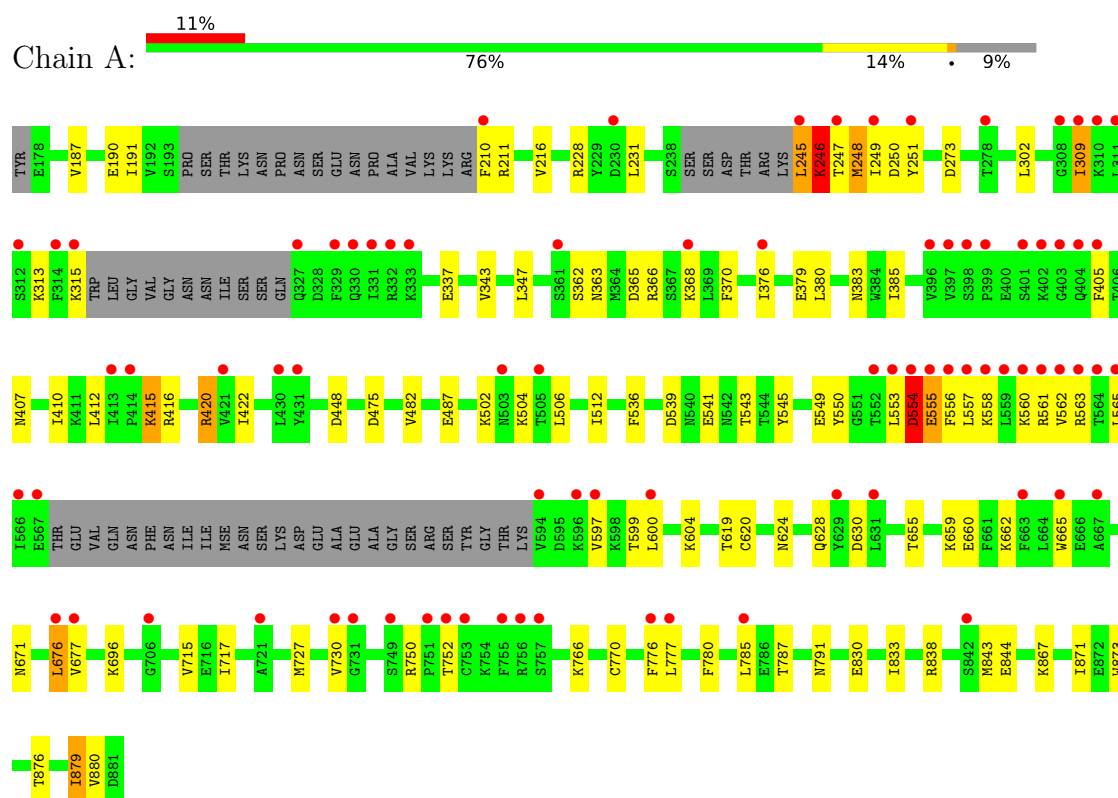
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		

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: Telomerase reverse transcriptase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	65.80Å 65.80Å 387.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.78 – 2.47 43.78 – 2.47	Depositor EDS
% Data completeness (in resolution range)	85.1 (43.78-2.47) 85.4 (43.78-2.47)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.246 , 0.284 0.250 , 0.286	Depositor DCC
R_{free} test set	1417 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5305	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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	0.22	0/5370	0.44	6/7196 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	246	LYS	N-CA-C	7.23	124.63	113.28
1	A	245	LEU	CA-C-N	6.01	137.08	126.45
1	A	245	LEU	C-N-CA	6.01	137.08	126.45
1	A	561	ARG	CA-C-N	5.35	131.60	121.97
1	A	561	ARG	C-N-CA	5.35	131.60	121.97
1	A	248	MSE	N-CA-C	5.23	117.72	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	LYS	Peptide

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	5291	0	5436	78	0
2	A	14	0	0	0	0
All	All	5305	0	5436	78	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 (78) 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:676:LEU:HD23	1:A:730:VAL:HG21	1.32	1.08
1:A:415:LYS:HG3	1:A:420:ARG:HG3	1.59	0.84
1:A:366:ARG:HD3	1:A:776:PHE:CZ	2.15	0.80
1:A:248:MSE:HE1	1:A:380:LEU:HD22	1.66	0.78
1:A:245:LEU:C	1:A:246:LYS:HG3	2.12	0.75
1:A:363:ASN:H	1:A:366:ARG:HE	1.35	0.74
1:A:624:ASN:HD22	1:A:628:GLN:HB2	1.51	0.73
1:A:717:ILE:HG12	1:A:727:MSE:HE3	1.73	0.69
1:A:420:ARG:HE	1:A:422:ILE:HD11	1.59	0.67
1:A:676:LEU:HD23	1:A:730:VAL:CG2	2.18	0.67
1:A:415:LYS:HG3	1:A:420:ARG:CG	2.26	0.65
1:A:228:ARG:HD2	1:A:231:LEU:HD23	1.77	0.64
1:A:302:LEU:HD13	1:A:337:GLU:HB3	1.79	0.64
1:A:245:LEU:O	1:A:246:LYS:HG3	1.99	0.62
1:A:482:VAL:HG13	1:A:487:GLU:HB3	1.82	0.62
1:A:365:ASP:OD2	1:A:368:LYS:NZ	2.31	0.62
1:A:873:TRP:O	1:A:876:THR:HG22	2.01	0.61
1:A:363:ASN:N	1:A:366:ARG:HE	2.00	0.60
1:A:777:LEU:HD22	1:A:791:ASN:ND2	2.17	0.59
1:A:379:GLU:OE1	1:A:383:ASN:ND2	2.33	0.58
1:A:553:LEU:HD22	1:A:838:ARG:HA	1.85	0.58
1:A:553:LEU:HA	1:A:843:MSE:HE2	1.84	0.58
1:A:624:ASN:ND2	1:A:628:GLN:HB2	2.20	0.56
1:A:766:LYS:NZ	1:A:770:CYS:SG	2.68	0.56
1:A:556:PHE:O	1:A:560:LYS:N	2.38	0.55
1:A:362:SER:OG	1:A:415:LYS:HG2	2.07	0.55
1:A:565:LEU:HD12	1:A:830:GLU:HA	1.88	0.55
1:A:539:ASP:OD2	1:A:545:TYR:OH	2.23	0.54
1:A:776:PHE:CE1	1:A:777:LEU:HG	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:GLU:HA	1:A:604:LYS:HD3	1.90	0.53
1:A:247:THR:OG1	1:A:250:ASP:OD2	2.27	0.52
1:A:624:ASN:ND2	1:A:630:ASP:OD2	2.43	0.52
1:A:539:ASP:O	1:A:543:THR:OG1	2.28	0.51
1:A:750:ARG:HG2	1:A:752:THR:H	1.75	0.51
1:A:363:ASN:H	1:A:366:ARG:NE	2.05	0.50
1:A:660:GLU:HB3	1:A:696:LYS:CE	2.41	0.50
1:A:624:ASN:ND2	1:A:628:GLN:OE1	2.45	0.50
1:A:549:GLU:HB2	1:A:600:LEU:HG	1.94	0.50
1:A:313:LYS:H	1:A:315:LYS:NZ	2.10	0.49
1:A:867:LYS:HB2	1:A:871:ILE:HD13	1.95	0.49
1:A:273:ASP:HB2	1:A:315:LYS:HE3	1.95	0.49
1:A:662:LYS:HA	1:A:665:TRP:CZ3	2.49	0.48
1:A:562:VAL:HG22	1:A:563:ARG:H	1.78	0.48
1:A:553:LEU:HG	1:A:557:LEU:HD21	1.96	0.48
1:A:554:ASP:HA	1:A:557:LEU:CD1	2.43	0.48
1:A:407:ASN:ND2	1:A:619:THR:OG1	2.47	0.47
1:A:504:LYS:HD3	1:A:504:LYS:HA	1.74	0.46
1:A:363:ASN:O	1:A:366:ARG:NE	2.49	0.46
1:A:655:THR:HG22	1:A:659:LYS:HE2	1.98	0.45
1:A:660:GLU:HB3	1:A:696:LYS:HZ1	1.81	0.45
1:A:368:LYS:HB3	1:A:370:PHE:CZ	2.51	0.45
1:A:309:ILE:H	1:A:309:ILE:HG12	1.64	0.45
1:A:660:GLU:HB3	1:A:696:LYS:NZ	2.32	0.45
1:A:343:VAL:O	1:A:347:LEU:HB2	2.18	0.44
1:A:777:LEU:HD23	1:A:777:LEU:HA	1.79	0.44
1:A:780:PHE:CZ	1:A:785:LEU:HG	2.52	0.44
1:A:554:ASP:HA	1:A:557:LEU:HG	2.00	0.44
1:A:210:PHE:HB3	1:A:211:ARG:H	1.62	0.44
1:A:216:VAL:HG21	1:A:315:LYS:HA	2.00	0.43
1:A:776:PHE:CD1	1:A:777:LEU:HG	2.52	0.43
1:A:597:VAL:HG12	1:A:599:THR:HG23	2.00	0.43
1:A:245:LEU:HA	1:A:251:TYR:OH	2.20	0.42
1:A:502:LYS:HE2	1:A:502:LYS:HB2	1.81	0.42
1:A:554:ASP:N	1:A:554:ASP:OD1	2.51	0.42
1:A:787:THR:O	1:A:791:ASN:ND2	2.52	0.42
1:A:554:ASP:HB3	1:A:558:LYS:HD2	2.02	0.42
1:A:405:PHE:HZ	1:A:448:ASP:HB3	1.85	0.42
1:A:187:VAL:O	1:A:191:ILE:HG13	2.20	0.42
1:A:550:TYR:CE2	1:A:844:GLU:HG3	2.55	0.42
1:A:506:LEU:HD12	1:A:506:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PHE:HB3	1:A:604:LYS:HE3	2.01	0.41
1:A:553:LEU:C	1:A:555:GLU:H	2.27	0.41
1:A:385:ILE:HG13	1:A:412:LEU:HD11	2.01	0.41
1:A:565:LEU:HD11	1:A:833:ILE:HG13	2.03	0.41
1:A:715:VAL:HG12	1:A:727:MSE:HE2	2.03	0.41
1:A:410:ILE:HD11	1:A:620:CYS:SG	2.61	0.41
1:A:376:ILE:HD12	1:A:376:ILE:HA	1.94	0.40
1:A:879:ILE:H	1:A:879:ILE:HG13	1.55	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	635/705 (90%)	617 (97%)	16 (2%)	2 (0%)	36 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	VAL
1	A	554	ASP

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	599/640 (94%)	584 (98%)	15 (2%)	42 66

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	GLU
1	A	246	LYS
1	A	249	ILE
1	A	309	ILE
1	A	415	LYS
1	A	416	ARG
1	A	420	ARG
1	A	475	ASP
1	A	512	ILE
1	A	554	ASP
1	A	555	GLU
1	A	671	ASN
1	A	676	LEU
1	A	879	ILE
1	A	880	VAL

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	428	GLN
1	A	546	HIS
1	A	624	ASN
1	A	628	GLN
1	A	711	HIS
1	A	764	ASN
1	A	767	GLN
1	A	791	ASN
1	A	826	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	634/705 (89%)	0.82	81 (12%) 7 6	48, 79, 117, 144	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	PHE	5.2
1	A	564	THR	5.0
1	A	210	PHE	4.2
1	A	597	VAL	4.2
1	A	309	ILE	4.1
1	A	594	VAL	4.1
1	A	631	LEU	4.1
1	A	557	LEU	3.9
1	A	777	LEU	3.9
1	A	676	LEU	3.8
1	A	554	ASP	3.8
1	A	565	LEU	3.7
1	A	245	LEU	3.7
1	A	562	VAL	3.6
1	A	314	PHE	3.5
1	A	329	PHE	3.5
1	A	567	GLU	3.4
1	A	753	CYS	3.4
1	A	721	ALA	3.4
1	A	553	LEU	3.3
1	A	755	PHE	3.2
1	A	757	SER	3.1
1	A	559	LEU	3.1
1	A	401	SER	3.1
1	A	315	LYS	3.0
1	A	667	ALA	3.0
1	A	399	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	421	VAL	2.8
1	A	677	VAL	2.8
1	A	310	LYS	2.8
1	A	842	SER	2.7
1	A	330	GLN	2.7
1	A	414	PRO	2.6
1	A	751	PRO	2.6
1	A	596	LYS	2.6
1	A	331	ILE	2.6
1	A	333	LYS	2.6
1	A	566	ILE	2.5
1	A	397	VAL	2.5
1	A	561	ARG	2.5
1	A	249	ILE	2.5
1	A	247	THR	2.5
1	A	505	THR	2.5
1	A	558	LYS	2.4
1	A	311	LEU	2.4
1	A	600	LEU	2.4
1	A	251	TYR	2.4
1	A	629	TYR	2.4
1	A	332	ARG	2.4
1	A	404	GLN	2.4
1	A	756	ARG	2.4
1	A	503	ASN	2.4
1	A	403	GLY	2.3
1	A	731	GLY	2.3
1	A	776	PHE	2.3
1	A	555	GLU	2.3
1	A	665	TRP	2.3
1	A	563	ARG	2.3
1	A	405	PHE	2.2
1	A	749	SER	2.2
1	A	560	LYS	2.2
1	A	376	ILE	2.2
1	A	398	SER	2.2
1	A	402	LYS	2.2
1	A	730	VAL	2.1
1	A	278	THR	2.1
1	A	706	GLY	2.1
1	A	785	LEU	2.1
1	A	663	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLN	2.1
1	A	430	LEU	2.1
1	A	368	LYS	2.1
1	A	396	VAL	2.1
1	A	552	THR	2.1
1	A	413	ILE	2.1
1	A	431	TYR	2.1
1	A	308	GLY	2.1
1	A	752	THR	2.0
1	A	230	ASP	2.0
1	A	312	SER	2.0
1	A	361	SER	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.