Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 06:44 PM EDT

PDB ID	:	6ZDQ
Title	:	Structure of telomerase from Candida albicans in complexe with TWJ fragment of telomeric RNA
Authors	:	Zhai, L.; Rety, S.; Chen, W.F.; Auguin, D.; Xi, X.G.
Deposited on	:	2020-06-15
Resolution	:	2.98 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:

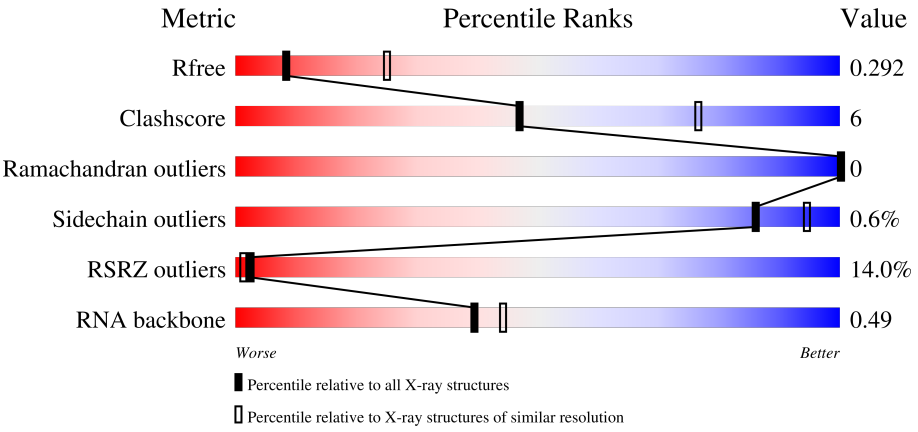
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.98 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)
RNA backbone	3102	1088 (3.26-2.70)

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 <=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	697	13% 81% 16% .
2	C	65	20% 57% 31% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6977 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	677	Total	C	N	O	S	0	0	0
			5580	3618	939	1004	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	GLU	-	expression tag	UNP A0A1D8PEA0
A	174	PHE	-	expression tag	UNP A0A1D8PEA0
A	175	HIS	-	expression tag	UNP A0A1D8PEA0
A	176	MET	-	expression tag	UNP A0A1D8PEA0
A	868	VAL	-	expression tag	UNP A0A1D8PEA0
A	869	ASP	-	expression tag	UNP A0A1D8PEA0

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	65	Total	C	N	O	P	0	0	0
			1395	623	254	453	65			

- Molecule 3 is water.

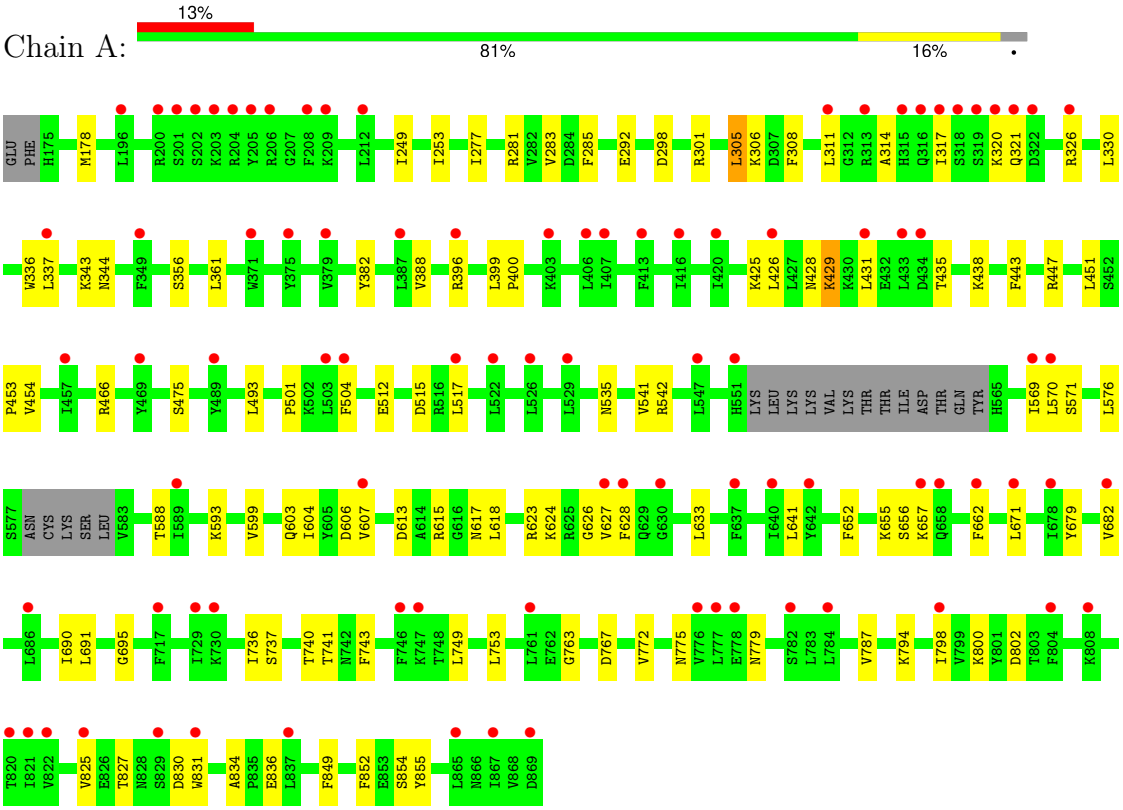
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		

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.

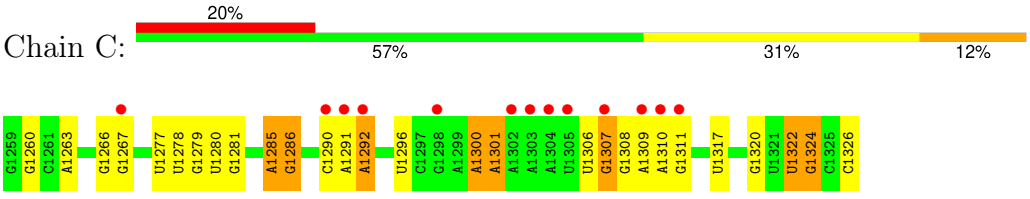
• Molecule 1: Telomerase reverse transcriptase

Chain A:



• Molecule 2: RNA

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.16Å 74.16Å 451.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.45 – 2.98 112.85 – 2.98	Depositor EDS
% Data completeness (in resolution range)	93.8 (31.45-2.98) 94.3 (112.85-2.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.238 , 0.292 0.240 , 0.292	Depositor DCC
R_{free} test set	1273 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	93.5	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 88.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6977	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.24	0/5695	0.41	0/7671
2	C	0.15	0/1562	0.69	0/2434
All	All	0.22	0/7257	0.49	0/10105

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	LYS	Peptide

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	5580	0	5719	74	0
2	C	1395	0	699	13	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6977	0	6418	83	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 6.

All (83) 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:453:PRO:HB3	1:A:541:VAL:HG11	1.61	0.83
1:A:794:LYS:HE2	1:A:798:ILE:HD13	1.72	0.71
1:A:517:LEU:HB2	1:A:626:GLY:HA3	1.77	0.66
1:A:426:LEU:HB3	1:A:431:LEU:HD11	1.80	0.63
1:A:382:TYR:OH	1:A:623:ARG:NH2	2.27	0.62
1:A:749:LEU:HB2	1:A:794:LYS:HZ3	1.65	0.61
1:A:662:PHE:HD1	1:A:671:LEU:HD12	1.66	0.60
1:A:623:ARG:NH1	1:A:626:GLY:O	2.35	0.60
1:A:517:LEU:HA	1:A:695:GLY:HA3	1.84	0.59
1:A:428:ASN:HA	1:A:429:LYS:HG2	1.84	0.57
1:A:317:ILE:HD11	1:A:326:ARG:HD2	1.86	0.56
1:A:517:LEU:HD22	1:A:641:LEU:HD23	1.87	0.56
1:A:603:GLN:HG3	1:A:633:LEU:HD12	1.87	0.56
1:A:447:ARG:HA	1:A:451:LEU:HB2	1.88	0.56
1:A:435:THR:HA	1:A:438:LYS:HG2	1.88	0.55
1:A:749:LEU:HD22	1:A:794:LYS:HD3	1.87	0.55
1:A:656:SER:N	1:A:657:LYS:HB2	2.21	0.55
1:A:852:PHE:HD2	1:A:854:SER:H	1.54	0.54
1:A:671:LEU:HD13	1:A:682:VAL:HG11	1.91	0.53
1:A:400:PRO:HB2	1:A:607:VAL:HG22	1.92	0.51
1:A:466:ARG:NH2	1:A:475:SER:O	2.43	0.51
1:A:753:LEU:HD22	1:A:787:VAL:HG23	1.93	0.51
1:A:298:ASP:HA	1:A:301:ARG:HH11	1.73	0.50
1:A:361:LEU:H	1:A:361:LEU:HD23	1.77	0.50
1:A:314:ALA:O	1:A:326:ARG:NH2	2.44	0.50
1:A:652:PHE:HA	1:A:655:LYS:HD3	1.94	0.50
1:A:396:ARG:HA	1:A:425:LYS:HG2	1.93	0.49
1:A:623:ARG:HD3	1:A:626:GLY:O	2.12	0.49
1:A:253:ILE:HD13	1:A:283:VAL:HG13	1.93	0.49
1:A:825:VAL:HG12	1:A:831:TRP:HB3	1.95	0.49
1:A:305:LEU:HD12	1:A:330:LEU:HD22	1.95	0.49
1:A:571:SER:HA	1:A:576:LEU:HB2	1.94	0.49
1:A:604:ILE:HA	1:A:627:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:GLU:OE1	1:A:836:GLU:N	2.46	0.48
1:A:320:LYS:HG2	2:C:1290:C:H4'	1.96	0.48
1:A:615:ARG:HD2	1:A:615:ARG:H	1.79	0.48
2:C:1266:G:H2'	2:C:1267:G:C8	2.49	0.48
1:A:454:VAL:HG21	1:A:599:VAL:HG11	1.96	0.47
1:A:749:LEU:HB2	1:A:794:LYS:NZ	2.27	0.47
2:C:1322:U:H2'	2:C:1324:G:C8	2.49	0.47
1:A:249:ILE:HD12	1:A:249:ILE:H	1.80	0.47
1:A:743:PHE:HB3	1:A:794:LYS:HZ2	1.80	0.47
1:A:336:TRP:HE3	1:A:337:LEU:HD12	1.79	0.47
1:A:443:PHE:CZ	1:A:447:ARG:HD2	2.50	0.47
1:A:388:VAL:HG23	1:A:624:LYS:HB2	1.97	0.46
1:A:802:ASP:OD1	2:C:1296:U:O2'	2.33	0.46
1:A:504:PHE:HB3	1:A:679:TYR:CD1	2.51	0.46
1:A:493:LEU:HD13	1:A:501:PRO:HD2	1.98	0.45
1:A:428:ASN:N	1:A:429:LYS:HA	2.32	0.45
1:A:569:ILE:HG13	1:A:570:LEU:HD12	1.98	0.45
1:A:767:ASP:N	1:A:767:ASP:OD1	2.50	0.45
1:A:399:LEU:HD22	1:A:606:ASP:HB3	1.99	0.45
1:A:512:GLU:HB3	1:A:515:ASP:HB2	1.99	0.45
2:C:1291:A:H4'	2:C:1292:A:H5'	1.98	0.45
1:A:292:GLU:HA	1:A:741:THR:HG23	1.98	0.44
1:A:736:ILE:HG22	1:A:737:SER:N	2.32	0.44
1:A:736:ILE:HG22	1:A:737:SER:H	1.82	0.44
2:C:1285:A:N6	2:C:1286:G:O6	2.51	0.44
1:A:542:ARG:HB2	1:A:588:THR:HG22	2.00	0.43
1:A:830:ASP:OD1	1:A:831:TRP:N	2.52	0.43
1:A:277:ILE:O	1:A:281:ARG:HG2	2.18	0.43
1:A:178:MET:O	1:A:344:ASN:ND2	2.52	0.43
1:A:285:PHE:HZ	1:A:343:LYS:HZ2	1.66	0.43
2:C:1263:A:H1'	2:C:1324:G:H22	1.84	0.42
1:A:623:ARG:HD2	1:A:628:PHE:CZ	2.54	0.42
1:A:849:PHE:HB3	1:A:855:TYR:HB3	2.02	0.42
2:C:1306:U:H2'	2:C:1307:G:H5"	2.01	0.42
1:A:618:LEU:HD23	1:A:618:LEU:H	1.85	0.42
1:A:306:LYS:HG2	2:C:1320:G:OP1	2.20	0.41
1:A:763:GLY:HA2	1:A:827:THR:HG21	2.01	0.41
1:A:656:SER:HA	1:A:657:LYS:C	2.41	0.41
1:A:438:LYS:HE3	1:A:438:LYS:HB2	1.93	0.41
1:A:613:ASP:OD1	1:A:617:ASN:N	2.54	0.41
2:C:1300:A:H5'	2:C:1301:A:OP2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:LYS:O	2:C:1317:U:H4'	2.21	0.41
1:A:535:ASN:HA	1:A:593:LYS:HD3	2.03	0.41
2:C:1322:U:H4'	2:C:1324:G:OP1	2.20	0.41
1:A:308:PHE:HB3	1:A:311:LEU:HG	2.03	0.41
1:A:690:ILE:HG23	1:A:691:LEU:HD12	2.03	0.41
1:A:320:LYS:HG3	1:A:321:GLN:N	2.35	0.40
2:C:1322:U:O2'	2:C:1324:G:O5'	2.37	0.40
1:A:772:VAL:HG12	1:A:775:ASN:H	1.87	0.40
1:A:831:TRP:HB2	1:A:834:ALA:HB2	2.03	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	671/697 (96%)	644 (96%)	27 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	633/653 (97%)	629 (99%)	4 (1%)	86 94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	LEU
1	A	356	SER
1	A	740	THR
1	A	779	ASN

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	64/65 (98%)	18 (28%)	1 (1%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	1260	G
2	C	1277	U
2	C	1278	U
2	C	1279	G
2	C	1280	U
2	C	1281	G
2	C	1285	A
2	C	1286	G
2	C	1292	A
2	C	1300	A
2	C	1301	A
2	C	1307	G
2	C	1308	G
2	C	1309	A
2	C	1310	A
2	C	1311	G
2	C	1324	G
2	C	1326	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	1322	U

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 monosaccharides 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, 95^{th} 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	677/697 (97%)	0.85	91 (13%)	3 1	79, 119, 168, 211	0
2	C	65/65 (100%)	1.10	13 (20%)	1 0	102, 144, 215, 259	0
All	All	742/762 (97%)	0.87	104 (14%)	2 1	79, 121, 175, 259	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	SER	6.1
1	A	203	LYS	5.8
1	A	317	ILE	5.2
2	C	1307	G	5.0
1	A	318	SER	4.8
1	A	313	ARG	4.6
1	A	551	HIS	4.6
1	A	426	LEU	4.3
2	C	1311	G	4.3
1	A	570	LEU	4.2
1	A	547	LEU	4.1
1	A	396	ARG	4.0
2	C	1303	A	4.0
1	A	831	TRP	4.0
1	A	628	PHE	3.7
2	C	1302	A	3.6
1	A	627	VAL	3.6
1	A	517	LEU	3.6
1	A	200	ARG	3.5
1	A	206	ARG	3.5
1	A	319	SER	3.3
1	A	202	SER	3.2
1	A	433	LEU	3.2
1	A	503	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	379	VAL	3.2
1	A	522	LEU	3.1
1	A	403	LYS	3.1
1	A	678	ILE	3.1
1	A	825	VAL	3.1
1	A	642	TYR	3.1
1	A	322	ASP	3.0
1	A	607	VAL	3.0
1	A	406	LEU	2.9
1	A	682	VAL	2.9
2	C	1304	A	2.9
1	A	431	LEU	2.9
1	A	686	LEU	2.8
1	A	717	PHE	2.8
1	A	413	PHE	2.8
1	A	375	TYR	2.8
2	C	1309	A	2.8
1	A	777	LEU	2.8
1	A	420	ILE	2.8
1	A	387	LEU	2.7
1	A	746	PHE	2.7
1	A	808	LYS	2.7
2	C	1310	A	2.7
1	A	489	TYR	2.7
1	A	867	ILE	2.7
1	A	349	PHE	2.7
1	A	529	LEU	2.6
1	A	730	LYS	2.6
1	A	657	LYS	2.6
1	A	416	ILE	2.6
1	A	457	ILE	2.6
1	A	320	LYS	2.5
1	A	820	THR	2.5
1	A	630	GLY	2.5
1	A	821	ILE	2.5
1	A	569	ILE	2.5
1	A	469	TYR	2.4
1	A	526	LEU	2.4
2	C	1298	G	2.4
1	A	315	HIS	2.4
1	A	205	TYR	2.4
1	A	337	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	316	GLN	2.4
1	A	869	ASP	2.4
1	A	829	SER	2.3
1	A	209	LYS	2.3
2	C	1305	U	2.3
1	A	204	ARG	2.3
1	A	778	GLU	2.3
2	C	1292	A	2.3
1	A	662	PHE	2.3
1	A	837	LEU	2.3
1	A	326	ARG	2.2
1	A	761	LEU	2.2
2	C	1291	A	2.2
1	A	729	ILE	2.2
1	A	212	LEU	2.2
1	A	658	GLN	2.2
1	A	311	LEU	2.2
2	C	1290	C	2.2
1	A	784	LEU	2.1
1	A	589	ILE	2.1
1	A	798	ILE	2.1
2	C	1267	G	2.1
1	A	822	VAL	2.1
1	A	747	LYS	2.1
1	A	804	PHE	2.1
1	A	371	TRP	2.1
1	A	208	PHE	2.1
1	A	407	ILE	2.1
1	A	640	ILE	2.1
1	A	504	PHE	2.1
1	A	671	LEU	2.1
1	A	865	LEU	2.0
1	A	434	ASP	2.0
1	A	782	SER	2.0
1	A	776	VAL	2.0
1	A	321	GLN	2.0
1	A	637	PHE	2.0
1	A	196	LEU	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 monosaccharides 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.