



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 03:36 AM GMT

PDB ID : 2GW1
Title : Crystal Structure of the Yeast Tom70
Authors : Wu, Y.; Sha, B.
Deposited on : 2006-05-03
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

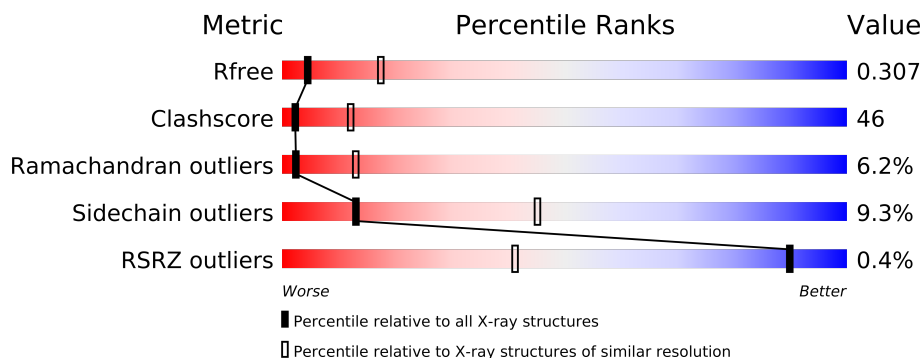
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7984 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Mitochondrial precursor proteins import receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3929	2500	642	773	14			
1	B	487	Total	C	N	O	S	0	0	0
			3929	2500	642	773	14			

- Molecule 2 is water.

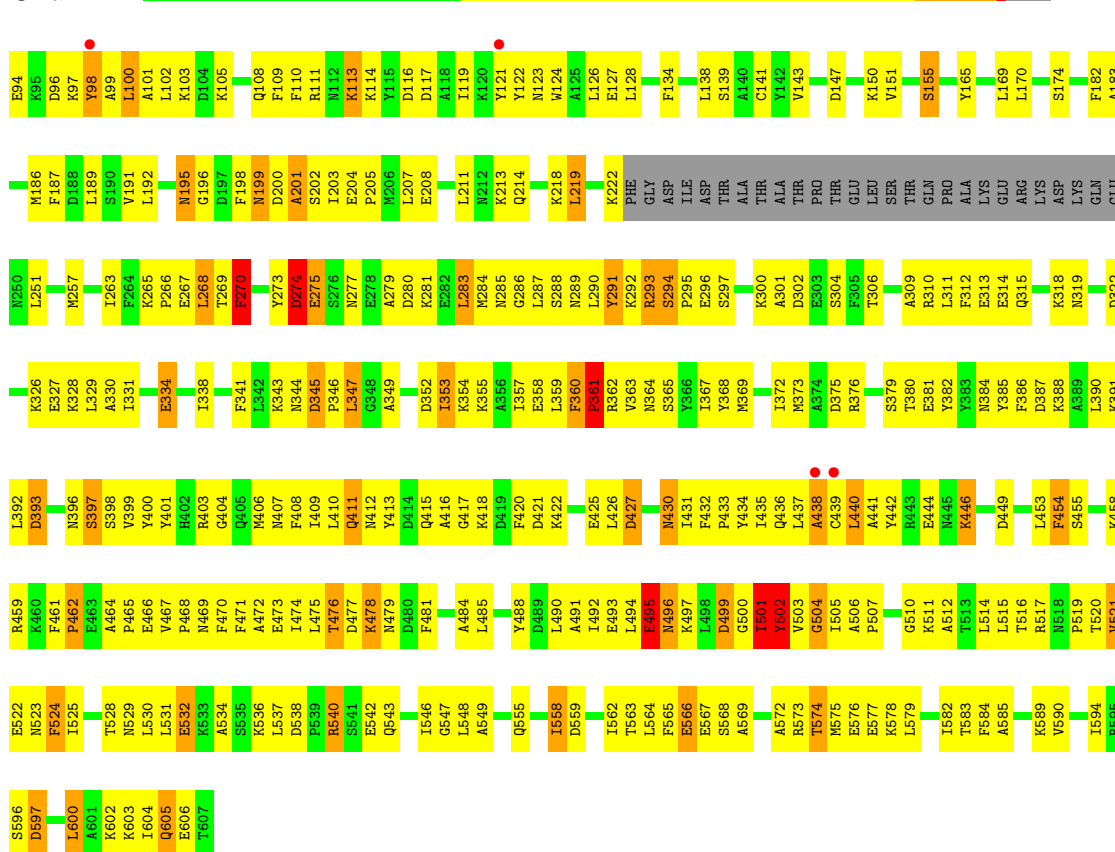
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total	O	0	0
			65	65		
2	B	61	Total	O	0	0
			61	61		

3 Residue-property plots

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.

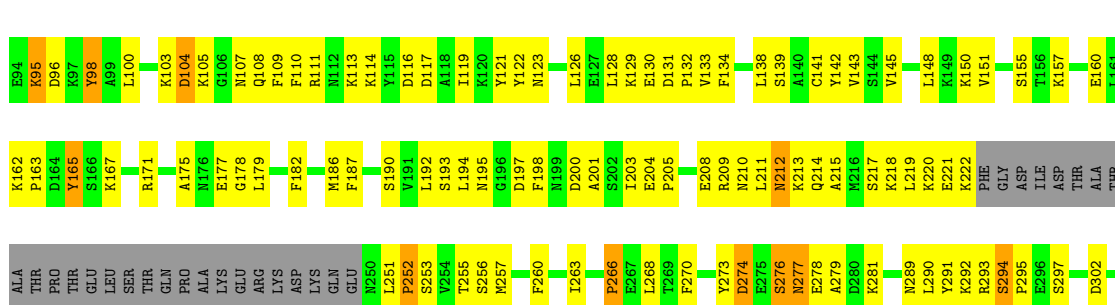
- Molecule 1: Mitochondrial precursor proteins import receptor

Chain A:



- Molecule 1: Mitochondrial precursor proteins import receptor

Chain B:



E577	K511	K446	Y382	L311
K578	L514	F447	Y383	L316
L579	L515	D448	N384	
Q580	T516	D449	Y385	
	R517	C450	F386	D322
A585	N518		D387	E323
E586	P519	L453		K324
A587	T520	F454	L390	
	V521		K391	E327
V590	E522	K458	L392	K328
Q591	N523		D393	L329
	P524	F461	S394	A330
T594	I525	P462	Y395	T331
R595	I526	E463	N396	S332
S596	A527	A464		L333
D597	T528	P465	V399	E334
P598	N529	E466	Y400	H335
V599	L530	V467	Y401	T336
L600	L531	P468	H402	C337
A601	E532	N469	K403	T338
	E533	F470	Q404	F339
	A534		Q405	K340
	K535	E473	M406	F341
	S536	I474	N407	L342
	K537	L475	F408	K343
	L537	T476	I409	N344
	D538	D477	L410	D345
	P539	K478	Q411	P346
	R540	N479	N412	L347
	S541	D480	Y413	G348
		F481	Y414	
		D482	D414	A349
	K545	K483		
	I546	A484	G417	D352
	L548	L485	K418	T353
	A549	K486	D419	K354
	Q550	Q487	F420	K355
	M551	Y488	D421	A356
	K552	D489	K422	T357
	L553	L490	A423	
	Q554	A491	K424	F360
	E556	I492	E425	P361
	D557	E493	L426	R362
	L558	L494	D427	V363
	D559	E495		N364
	E560	N496	M430	
		K497	I431	T367
		L498	F432	Y368
	T563	D499	P433	K369
	L564	G500	Y434	A370
	P565	I501	I435	L371
	E566	Y502	Q436	I372
	E567	V503	L437	K373
	S568	Q504	A374	A374
		I505	C439	D375
		A506	L440	R376
	L571	A507	A441	N377
	A572	P507	Y442	B378
		L508	R443	S379
	M575	V509	E444	T380
	E576		N445	E381

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.88Å 168.60Å 82.99Å 90.00° 102.59° 90.00°	Depositor
Resolution (Å)	46.17 – 3.00 46.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.17-3.00) 94.8 (46.17-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.316 0.254 , 0.307	Depositor DCC
R_{free} test set	1128 reflections (4.83%)	DCC
Wilson B-factor (Å ²)	83.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 25246 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7984	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.29	0/3999	0.53	1/5379 (0.0%)
1	B	0.29	0/3999	0.51	0/5379
All	All	0.29	0/7998	0.52	1/10758 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	GLU	N-CA-C	-5.31	96.66	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3929	0	3885	383	0
1	B	3929	0	3885	357	0
2	A	65	0	0	22	0
2	B	61	0	0	25	0
All	All	7984	0	7770	726	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 46.

The worst 5 of 726 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:439:CYS:SG	1:B:442:TYR:HB2	2.02	0.99
1:A:478:LYS:HE3	1:A:478:LYS:HA	1.45	0.98
1:B:148:LEU:HB3	1:B:179:LEU:HD11	1.46	0.96
1:B:255:THR:HG22	2:B:660:HOH:O	1.66	0.93
1:B:344:ASN:O	1:B:345:ASP:HB3	1.66	0.93

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	483/514 (94%)	377 (78%)	81 (17%)	25 (5%)	3	18
1	B	483/514 (94%)	385 (80%)	63 (13%)	35 (7%)	2	8
All	All	966/1028 (94%)	762 (79%)	144 (15%)	60 (6%)	2	13

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	201	ALA
1	A	274	ASP
1	A	361	PRO
1	A	397	SER

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	425/448 (95%)	380 (89%)	45 (11%)	10	36
1	B	425/448 (95%)	391 (92%)	34 (8%)	17	53
All	All	850/896 (95%)	771 (91%)	79 (9%)	13	45

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	536	LYS
1	A	605	GLN
1	B	538	ASP
1	A	540	ARG
1	A	566	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	605	GLN
1	B	212	ASN
1	B	555	GLN
1	B	123	ASN
1	B	214	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	487/514 (94%)	-0.08	4 (0%) 83 26	40, 76, 125, 154	0
1	B	487/514 (94%)	-0.13	0 100 100	36, 74, 123, 162	0
All	All	974/1028 (94%)	-0.11	4 (0%) 90 41	36, 75, 125, 162	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TYR	2.9
1	A	439	CYS	2.5
1	A	121	TYR	2.3
1	A	438	ALA	2.1

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 ⓘ

There are no such residues in this entry.