WORLDWIDE wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2014 – 04:03 PM GMT

PDB ID : 3KT4

Title : Crystal structure of Tpa1 from Saccharomyces cerevisiae, a component of the messenger ribonucleoprotein complex

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Deposited on : 2009-11-24

Resolution : 2.73 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html

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1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.73 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		5.5%
RSRZ outliers		4.3%

Worse — Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
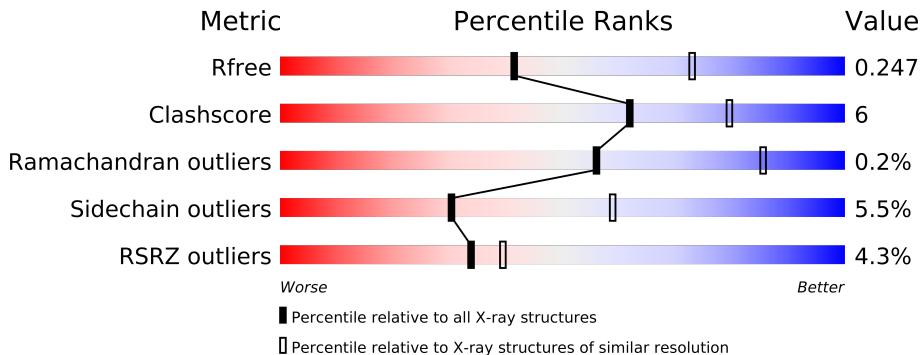
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2164 (2.78-2.70)
Clashscore	79885	2639 (2.78-2.70)
Ramachandran outliers	78287	2594 (2.78-2.70)
Sidechain outliers	78261	2595 (2.78-2.70)
RSRZ outliers	66119	2166 (2.78-2.70)

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 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	633	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4803 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 PKHD-type hydroxylase TPA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	563	Total 4603	C 2953	N 768	O 869	S 6	Se 7	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MSE	-	EXPRESSION TAG	UNP P40032
A	645	LEU	-	EXPRESSION TAG	UNP P40032
A	646	GLU	-	EXPRESSION TAG	UNP P40032
A	647	HIS	-	EXPRESSION TAG	UNP P40032
A	648	HIS	-	EXPRESSION TAG	UNP P40032
A	649	HIS	-	EXPRESSION TAG	UNP P40032
A	650	HIS	-	EXPRESSION TAG	UNP P40032
A	651	HIS	-	EXPRESSION TAG	UNP P40032
A	652	HIS	-	EXPRESSION TAG	UNP P40032

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Fe 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	199	Total 199	O 199	0	0

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: PKHD-type hydroxylase TPA1

Chain A:
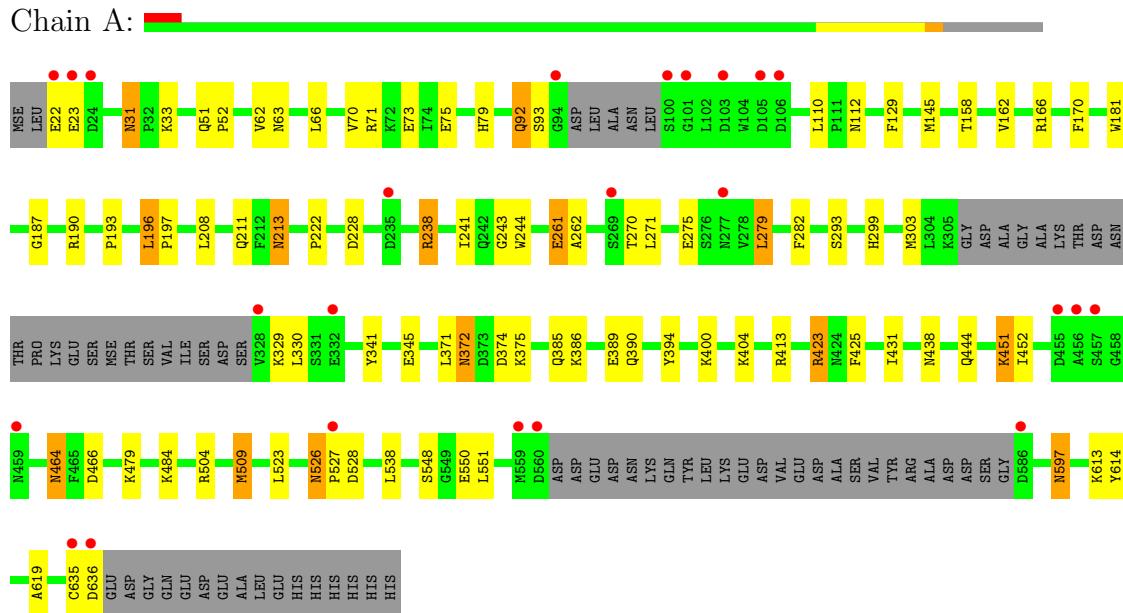
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants	136.29Å 136.29Å 83.28Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 120.00°	
Resolution (Å)	20.00 – 2.73	Depositor
	19.94 – 2.73	EDS
% Data completeness	99.8 (20.00-2.73)	Depositor
(in resolution range)	99.8 (19.94-2.73)	EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.61 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.190 , 0.247	Depositor
	0.188 , 0.247	DCC
R_{free} test set	1222 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 21.9	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 23885 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4803	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.50	0/4708	0.61	2/6349 (0.0%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	196	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	330	LEU	CA-CB-CG	5.42	127.76	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	509	MSE	Peptide

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	4603	0	4529	52	0
2	A	1	0	0	0	0
3	A	199	0	0	11	0
All	All	4803	0	4529	52	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 6.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:TRP:H	1:A:211:GLN:HE22	1.20	0.89
1:A:444:GLN:HG3	3:A:983:HOH:O	1.76	0.86
1:A:548:SER:OG	1:A:550:GLU:HG2	1.84	0.77
1:A:464:ASN:HD22	1:A:466:ASP:H	1.32	0.77
1:A:371:LEU:H	1:A:597:ASN:HD21	1.36	0.73
1:A:526:ASN:HD21	1:A:528:ASP:HB2	1.55	0.70
1:A:526:ASN:HA	3:A:972:HOH:O	1.91	0.69
1:A:526:ASN:C	1:A:526:ASN:HD22	1.95	0.69
1:A:92:GLN:HG2	3:A:936:HOH:O	1.91	0.69
1:A:423:ARG:HG2	1:A:425:PHE:CZ	2.31	0.65
1:A:62:VAL:H	1:A:213:ASN:HD21	1.43	0.65
1:A:166:ARG:HD3	1:A:244:TRP:CD1	2.32	0.64
1:A:79:HIS:HB2	3:A:932:HOH:O	1.99	0.63
1:A:145:MSE:HE3	1:A:241:ILE:HG21	1.82	0.62
1:A:413:ARG:HD3	1:A:509:MSE:HE3	1.80	0.62
1:A:394:TYR:HA	3:A:992:HOH:O	2.00	0.60
1:A:345:GLU:HB2	3:A:945:HOH:O	2.02	0.59
1:A:31:ASN:HD22	1:A:33:LYS:H	1.55	0.55
1:A:73:GLU:HB3	1:A:110:LEU:HD23	1.88	0.55
1:A:22:GLU:HA	3:A:990:HOH:O	2.08	0.52
1:A:509:MSE:SE	3:A:992:HOH:O	2.76	0.52
1:A:63:ASN:HD22	1:A:66:LEU:H	1.59	0.51
1:A:162:VAL:HG21	1:A:222:PRO:HA	1.92	0.51
1:A:464:ASN:ND2	1:A:466:ASP:H	2.06	0.50
1:A:635:CYS:O	1:A:636:ASP:HB2	2.15	0.47
1:A:190:ARG:NH1	1:A:228:ASP:OD1	2.48	0.47
1:A:451:LYS:HD3	1:A:451:LYS:HA	1.80	0.47
1:A:282:PHE:HD1	1:A:431:ILE:HG21	1.80	0.46
1:A:613:LYS:HE3	1:A:614:TYR:HB3	1.96	0.46
1:A:275:GLU:HA	1:A:279:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:293:SER:HB2	3:A:919:HOH:O	2.16	0.45
1:A:372:ASN:C	1:A:372:ASN:HD22	2.19	0.45
1:A:187:GLY:O	1:A:238:ARG:NH2	2.45	0.45
1:A:509:MSE:HE2	3:A:992:HOH:O	2.16	0.45
1:A:385:GLN:NE2	1:A:389:GLU:OE1	2.46	0.45
1:A:526:ASN:HD22	1:A:527:PRO:N	2.15	0.45
1:A:371:LEU:H	1:A:597:ASN:ND2	2.08	0.44
1:A:341:TYR:CZ	1:A:375:LYS:HE2	2.53	0.44
1:A:479:LYS:O	1:A:484:LYS:NZ	2.51	0.44
1:A:181:TRP:N	1:A:211:GLN:HE22	2.01	0.43
1:A:261:GLU:HG3	1:A:262:ALA:N	2.33	0.43
1:A:66:LEU:O	1:A:70:VAL:HG23	2.19	0.42
1:A:404:LYS:HE3	1:A:423:ARG:HB2	2.02	0.42
1:A:73:GLU:OE2	1:A:112:ASN:ND2	2.48	0.42
1:A:170:PHE:CZ	1:A:243:GLY:HA3	2.55	0.42
1:A:52:PRO:HB2	1:A:193:PRO:HA	2.02	0.42
1:A:386:LYS:HA	1:A:390:GLN:HG3	2.02	0.41
1:A:71:ARG:O	1:A:75:GLU:HG3	2.20	0.41
1:A:196:LEU:HB3	1:A:197:PRO:HD2	2.02	0.41
1:A:93:SER:HA	3:A:958:HOH:O	2.19	0.41
1:A:372:ASN:ND2	1:A:375:LYS:H	2.17	0.41
1:A:551:LEU:HD13	1:A:619:ALA:HA	2.02	0.41

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	555/633 (88%)	536 (97%)	18 (3%)	1 (0%)	56	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLU

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	513/564 (91%)	485 (94%)	28 (6%)	30	59

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	51	GLN
1	A	92	GLN
1	A	129	PHE
1	A	158	THR
1	A	208	LEU
1	A	213	ASN
1	A	238	ARG
1	A	261	GLU
1	A	270	THR
1	A	271	LEU
1	A	279	LEU
1	A	299	HIS
1	A	303	MSE
1	A	329	LYS
1	A	372	ASN
1	A	374	ASP
1	A	400	LYS
1	A	423	ARG
1	A	438	ASN
1	A	451	LYS
1	A	452	ILE
1	A	464	ASN
1	A	504	ARG
1	A	523	LEU
1	A	526	ASN
1	A	538	LEU
1	A	597	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	40	GLN
1	A	51	GLN
1	A	54	ASN
1	A	63	ASN
1	A	211	GLN
1	A	213	ASN
1	A	249	GLN
1	A	295	HIS
1	A	299	HIS
1	A	372	ASN
1	A	390	GLN
1	A	438	ASN
1	A	464	ASN
1	A	499	GLN
1	A	526	ASN
1	A	597	ASN

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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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	563/633 (88%)	-0.05	24 (4%)	34	39	21, 34, 60, 76	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	VAL	6.9
1	A	94	GLY	4.9
1	A	23	GLU	4.6
1	A	636	ASP	4.1
1	A	100	SER	3.9
1	A	586	ASP	3.7
1	A	459	ASN	3.7
1	A	22	GLU	3.6
1	A	455	ASP	3.6
1	A	101	GLY	3.4
1	A	277	ASN	3.0
1	A	635	CYS	3.0
1	A	456	ALA	2.8
1	A	457	SER	2.8
1	A	24	ASP	2.7
1	A	105	ASP	2.6
1	A	527	PRO	2.6
1	A	560	ASP	2.5
1	A	332	GLU	2.5
1	A	269	SER	2.3
1	A	103	ASP	2.3
1	A	106	ASP	2.3
1	A	235	ASP	2.2
1	A	559	MSE	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE	A	701	1/1	0.07	-5.55	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.