



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:05 PM UTC

PDB ID : 3G3O / pdb_00003g3o
Title : Crystal structure of the cytoplasmic tunnel domain in yeast Vtc2p
Authors : Hothorn, M.; Scheffzek, K.
Deposited on : 2009-02-02
Resolution : 2.10 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

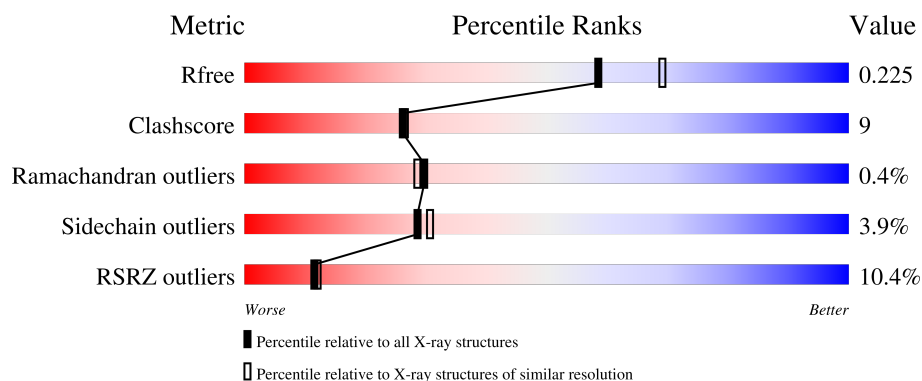
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	392	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2598 atoms, of which 34 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 Vacuolar transporter chaperone 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	H	N	O	Se	0	2	0
			2377	1519	34	399	422	3			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	MSE	-	expression tag	UNP P43585
A	163	LYS	-	expression tag	UNP P43585
A	164	HIS	-	expression tag	UNP P43585
A	165	HIS	-	expression tag	UNP P43585
A	166	HIS	-	expression tag	UNP P43585
A	167	HIS	-	expression tag	UNP P43585
A	168	HIS	-	expression tag	UNP P43585
A	169	HIS	-	expression tag	UNP P43585
A	170	PRO	-	expression tag	UNP P43585
A	171	MSE	-	expression tag	UNP P43585
A	172	SER	-	expression tag	UNP P43585
A	173	GLY	-	expression tag	UNP P43585
A	174	LEU	-	expression tag	UNP P43585
A	175	VAL	-	expression tag	UNP P43585
A	176	PRO	-	expression tag	UNP P43585
A	177	ARG	-	expression tag	UNP P43585
A	178	GLY	-	expression tag	UNP P43585
A	179	SER	-	expression tag	UNP P43585
A	180	ALA	-	expression tag	UNP P43585
A	181	MSE	-	expression tag	UNP P43585
A	182	GLY	-	expression tag	UNP P43585

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

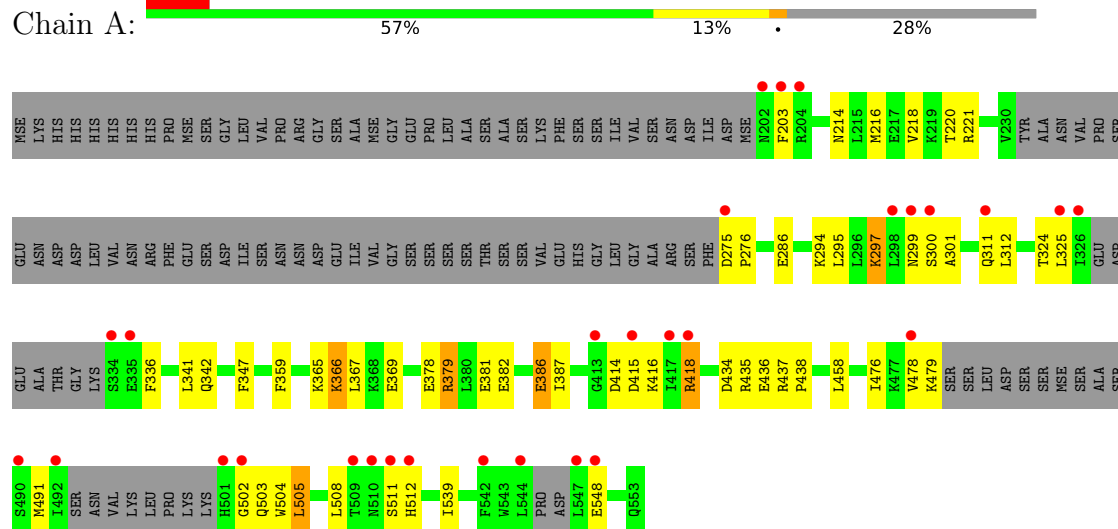


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	206	Total	O	0	0
			206	206		

- Molecule 1: Vacuolar transporter chaperone 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.20Å 74.59Å 80.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.30 – 2.10 37.30 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.30-2.10) 99.6 (37.30-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.199 , 0.236 0.192 , 0.225	Depositor DCC
R_{free} test set	1301 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2598	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.80	0/2396	0.92	2/3222 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	491	MSE	N-CA-C	5.18	117.23	108.02
1	A	504	TRP	N-CA-C	-5.08	105.93	111.82

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	2343	34	2338	44	0
2	A	15	0	0	0	0
3	A	206	0	0	8	0
All	All	2564	34	2338	44	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 9.

All (44) 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:203:PHE:CE1	1:A:479:LYS:HE3	2.12	0.85
1:A:286:GLU:HG2	3:A:65:HOH:O	1.84	0.78
1:A:203:PHE:CE2	1:A:479:LYS:HD3	2.26	0.71
1:A:203:PHE:CZ	1:A:479:LYS:HE3	2.27	0.70
1:A:325:LEU:HB2	1:A:336:PHE:CE1	2.26	0.70
1:A:216:MSE:O	1:A:220:THR:HG23	1.95	0.66
1:A:299:ASN:C	1:A:301:ALA:H	2.12	0.58
1:A:378:GLU:OE1	1:A:382:GLU:OE2	2.21	0.58
1:A:203:PHE:CZ	1:A:479:LYS:CE	2.87	0.58
1:A:203:PHE:CZ	1:A:479:LYS:HD3	2.39	0.57
1:A:203:PHE:CZ	1:A:479:LYS:CD	2.89	0.55
1:A:311:GLN:HG2	3:A:61:HOH:O	2.06	0.55
1:A:369:GLU:HG3	3:A:101:HOH:O	2.07	0.55
1:A:378:GLU:CD	1:A:382:GLU:OE2	2.52	0.52
1:A:434[B]:ASP:CG	1:A:436:GLU:O	2.52	0.52
1:A:378:GLU:OE2	1:A:382:GLU:OE2	2.28	0.50
1:A:508:LEU:O	1:A:511:SER:HB3	2.12	0.49
1:A:294:LYS:HA	1:A:301:ALA:HB1	1.94	0.49
1:A:512:HIS:CD2	1:A:512:HIS:H	2.32	0.48
1:A:295:LEU:HD23	1:A:539:ILE:HD12	1.96	0.47
1:A:214:ASN:O	1:A:218:VAL:HG23	2.15	0.46
1:A:414:ASP:OD2	1:A:416:LYS:HG3	2.16	0.46
1:A:386:GLU:HG3	1:A:387:ILE:N	2.28	0.46
1:A:379:ARG:HE	1:A:379:ARG:HA	1.81	0.45
1:A:342:GLN:HG2	3:A:571:HOH:O	2.17	0.44
1:A:414:ASP:OD2	1:A:414:ASP:C	2.60	0.44
1:A:415:ASP:O	1:A:416:LYS:C	2.62	0.43
1:A:275:ASP:N	1:A:276:PRO:HD2	2.33	0.43
1:A:502:GLY:O	1:A:505:LEU:HB2	2.18	0.43
1:A:221:ARG:NH1	3:A:30:HOH:O	2.42	0.42
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.91	0.42
1:A:299:ASN:C	1:A:301:ALA:N	2.78	0.42
1:A:312:LEU:O	3:A:579:HOH:O	2.22	0.42
1:A:347:PHE:CD2	1:A:359:PHE:HB2	2.55	0.42
1:A:434[B]:ASP:OD2	1:A:436:GLU:O	2.38	0.42
1:A:300:SER:HB3	1:A:324:THR:CG2	2.50	0.42
1:A:286:GLU:HG2	1:A:286:GLU:H	1.68	0.41
1:A:435:ARG:HG3	3:A:584:HOH:O	2.20	0.41
1:A:341:LEU:HG	1:A:387:ILE:HD12	2.03	0.41
1:A:418[A]:ARG:NH1	3:A:106:HOH:O	2.52	0.41
1:A:476:ILE:HG22	1:A:478:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ILE:HG22	1:A:478:VAL:CG2	2.51	0.41
1:A:365:LYS:HZ2	1:A:366:LYS:CE	2.33	0.40
1:A:437:ARG:N	1:A:438:PRO:CD	2.84	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	271/392 (69%)	264 (97%)	6 (2%)	1 (0%)	30 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	LYS

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	257/352 (73%)	246 (96%)	11 (4%)	26 27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	LYS
1	A	366	LYS
1	A	379	ARG
1	A	381	GLU
1	A	386	GLU
1	A	418[A]	ARG
1	A	418[B]	ARG
1	A	458	LEU
1	A	503	GLN
1	A	505	LEU
1	A	548	GLU

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

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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1000	-	4,4,4	0.37	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1001	-	4,4,4	0.54	0	6,6,6	0.78	0
2	SO4	A	1002	-	4,4,4	0.33	0	6,6,6	0.46	0

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.

No monomer is involved in short contacts.

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	278/392 (70%)	0.22	29 (10%)	11 12	15, 27, 59, 80	2 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	544	LEU	5.9
1	A	492	ILE	5.3
1	A	502	GLY	5.0
1	A	478	VAL	4.9
1	A	547	LEU	4.7
1	A	299	ASN	4.7
1	A	334	SER	4.6
1	A	490	SER	4.6
1	A	326	ILE	4.0
1	A	325	LEU	4.0
1	A	300	SER	3.6
1	A	203	PHE	3.6
1	A	510	ASN	3.6
1	A	548	GLU	3.4
1	A	511	SER	3.1
1	A	298	LEU	3.1
1	A	335	GLU	3.1
1	A	311	GLN	2.9
1	A	512	HIS	2.9
1	A	275	ASP	2.8
1	A	501	HIS	2.7
1	A	204	ARG	2.7
1	A	202	ASN	2.7
1	A	417	ILE	2.6
1	A	542	PHE	2.2
1	A	413	GLY	2.1
1	A	415	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	418[A]	ARG	2.1
1	A	509	THR	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](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1001	5/5	0.88	0.13	35,39,53,54	0
2	SO4	A	1000	5/5	0.89	0.10	52,55,59,59	0
2	SO4	A	1002	5/5	0.95	0.14	40,40,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.