



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:26 AM UTC

PDB ID : 2Y7O / pdb_00002y7o
Title : Structure of N-terminal domain of Candida albicans als9-2 - G299W mutant
Authors : Salgado, P.S.; Burchell, L.; Cota, E.
Deposited on : 2011-01-31
Resolution : 1.75 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
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

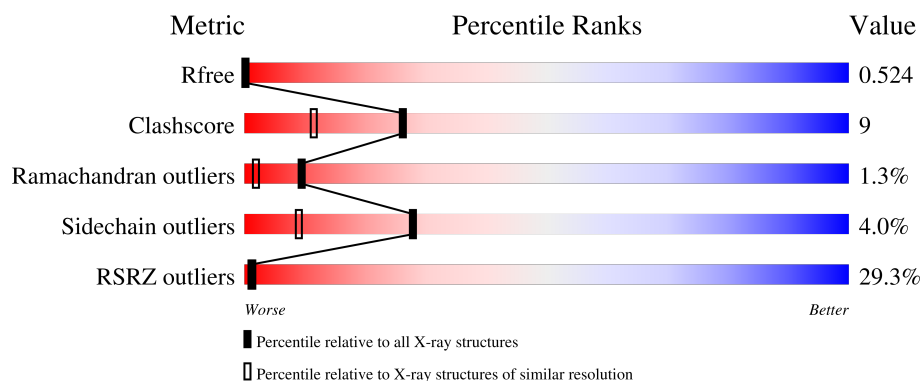
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	312	29% 87% 8% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2637 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 AGGLUTININ-LIKE ALS9 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	1	0	0
			2362	1497	365	490	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q5A8T1
A	51	THR	ASN	conflict	UNP Q5A8T1
A	212	VAL	ILE	conflict	UNP Q5A8T1
A	296	TRP	GLY	engineered mutation	UNP Q5A8T1

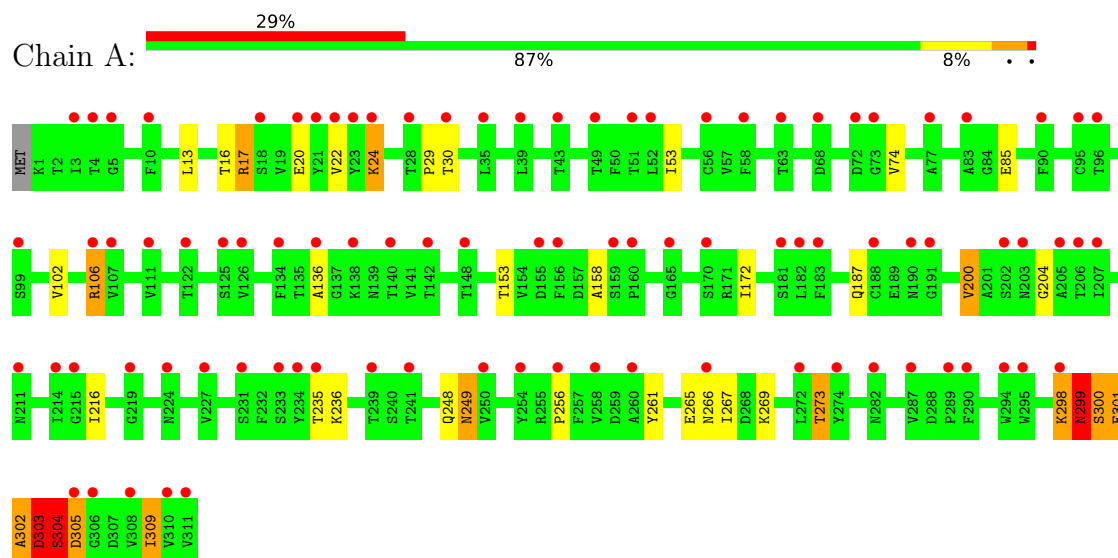
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	275	Total	O	0	0
			275	275		

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: AGGLUTININ-LIKE ALS9 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.37Å 68.31Å 89.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.51 – 1.75 36.51 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.51-1.75) 52.7 (36.51-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.39 (at 1.26Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.195 , 0.223 0.546 , 0.524	Depositor DCC
R_{free} test set	1639 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	4.4	Xtriage
Anisotropy	2.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 245.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	2637	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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	1.86	17/2420 (0.7%)	1.39	11/3314 (0.3%)

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	ARG	CZ-NH1	50.35	2.03	1.32
1	A	106	ARG	NE-CZ	11.54	1.45	1.33
1	A	106	ARG	CZ-NH2	10.79	1.47	1.33
1	A	304	SER	C-O	9.22	1.35	1.23
1	A	53	ILE	CA-CB	7.97	1.64	1.54
1	A	303	ASP	C-O	6.04	1.31	1.24
1	A	235	THR	N-CA	5.97	1.53	1.45
1	A	273	THR	C-O	-5.92	1.17	1.24
1	A	303	ASP	N-CA	5.65	1.53	1.46
1	A	172	ILE	CA-CB	5.60	1.60	1.54
1	A	302	ALA	C-O	5.47	1.30	1.24
1	A	74	VAL	C-O	-5.45	1.18	1.24
1	A	266	ASN	CA-C	-5.39	1.45	1.53
1	A	13	LEU	N-CA	5.34	1.53	1.46
1	A	261	TYR	N-CA	5.12	1.52	1.46
1	A	153	THR	CA-C	-5.11	1.46	1.52
1	A	187	GLN	CA-C	5.10	1.59	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	GLU	CA-C-N	-13.97	102.76	122.87
1	A	265	GLU	C-N-CA	-13.97	102.76	122.87
1	A	106	ARG	NE-CZ-NH2	-13.93	106.67	119.20
1	A	265	GLU	N-CA-C	6.56	120.50	112.23
1	A	16	THR	CA-C-N	5.90	129.14	120.82
1	A	16	THR	C-N-CA	5.90	129.14	120.82
1	A	22	VAL	N-CA-C	5.84	116.63	111.90
1	A	301	GLU	CA-C-N	-5.34	111.33	121.54
1	A	301	GLU	C-N-CA	-5.34	111.33	121.54
1	A	85	GLU	CB-CA-C	-5.13	110.64	116.54
1	A	300	SER	N-CA-C	5.11	121.68	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ARG	Sidechain

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	2362	0	2231	43	0
2	A	275	0	0	1	0
All	All	2637	0	2231	43	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 (43) 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:298:LYS:HA	1:A:299:ASN:CB	1.47	1.31
1:A:299:ASN:N	1:A:301:GLU:OE1	1.79	1.16
1:A:298:LYS:HA	1:A:299:ASN:HB2	1.18	1.14
1:A:301:GLU:O	1:A:302:ALA:HB3	1.39	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:HA	1:A:299:ASN:HB3	1.30	1.08
1:A:299:ASN:H	1:A:301:GLU:CD	1.61	1.07
1:A:298:LYS:CA	1:A:299:ASN:CB	2.38	1.02
1:A:303:ASP:CG	1:A:304:SER:H	1.66	1.01
1:A:298:LYS:NZ	1:A:300:SER:HB2	1.81	0.96
1:A:301:GLU:O	1:A:302:ALA:CB	2.12	0.93
1:A:298:LYS:CA	1:A:299:ASN:HB2	2.00	0.90
1:A:298:LYS:HG2	1:A:300:SER:N	1.87	0.90
1:A:299:ASN:O	1:A:299:ASN:ND2	2.07	0.88
1:A:298:LYS:HZ3	1:A:300:SER:HB2	1.39	0.83
1:A:298:LYS:HZ3	1:A:300:SER:CB	1.94	0.81
1:A:17:ARG:HB3	2:A:2019:HOH:O	1.80	0.80
1:A:298:LYS:HG2	1:A:300:SER:H	1.45	0.79
1:A:303:ASP:CG	1:A:304:SER:N	2.40	0.79
1:A:298:LYS:C	1:A:301:GLU:OE1	2.28	0.76
1:A:300:SER:H	1:A:301:GLU:HA	1.52	0.74
1:A:298:LYS:NZ	1:A:300:SER:CB	2.50	0.74
1:A:298:LYS:CA	1:A:299:ASN:HB3	2.14	0.71
1:A:299:ASN:HD22	1:A:299:ASN:C	1.98	0.69
1:A:299:ASN:N	1:A:301:GLU:CD	2.44	0.69
1:A:298:LYS:HD2	1:A:309:ILE:HD11	1.76	0.66
1:A:300:SER:N	1:A:301:GLU:HA	2.17	0.59
1:A:298:LYS:O	1:A:301:GLU:OE1	2.25	0.55
1:A:303:ASP:OD2	1:A:304:SER:N	2.28	0.53
1:A:204:GLY:HA3	1:A:267:ILE:HD13	1.89	0.53
1:A:200:VAL:HG13	1:A:273:THR:HB	1.91	0.52
1:A:136:ALA:HB2	1:A:158:ALA:HB2	1.96	0.48
1:A:248:GLN:O	1:A:249:ASN:O	2.32	0.47
1:A:248:GLN:O	1:A:249:ASN:C	2.57	0.45
1:A:24:LYS:HB3	1:A:24:LYS:HE3	1.85	0.44
1:A:216:ILE:HG22	1:A:256:PRO:HA	1.99	0.44
1:A:298:LYS:HZ1	1:A:303:ASP:CB	2.31	0.44
1:A:136:ALA:CB	1:A:158:ALA:HB2	2.47	0.43
1:A:298:LYS:HZ1	1:A:303:ASP:HB3	1.83	0.43
1:A:298:LYS:CG	1:A:299:ASN:HB3	2.48	0.43
1:A:267:ILE:HD12	1:A:269:LYS:O	2.19	0.43
1:A:298:LYS:HZ2	1:A:300:SER:HB2	1.74	0.42
1:A:29:PRO:HA	1:A:30:THR:HA	1.88	0.41
1:A:298:LYS:NZ	1:A:303:ASP:HB2	2.36	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	309/312 (99%)	295 (96%)	10 (3%)	4 (1%)	9 2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ASN
1	A	299	ASN
1	A	305	ASP
1	A	303	ASP

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	272/274 (99%)	261 (96%)	11 (4%)	28 9

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

Mol	Chain	Res	Type
1	A	17	ARG
1	A	20	GLU
1	A	24	LYS
1	A	102	VAL
1	A	200	VAL
1	A	236	LYS
1	A	298	LYS

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Mol	Chain	Res	Type
1	A	299	ASN
1	A	304	SER
1	A	305	ASP
1	A	309	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	A	284	ASN

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](#)

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	311/312 (99%)	1.52	91 (29%) 1 1	12, 22, 39, 63	4 (1%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	PRO	5.1
1	A	224	ASN	4.8
1	A	219	GLY	4.5
1	A	107	VAL	4.3
1	A	188	CYS	4.2
1	A	99	SER	3.9
1	A	215	GLY	3.9
1	A	295	TRP	3.9
1	A	231	SER	3.8
1	A	126	VAL	3.7
1	A	136	ALA	3.7
1	A	191	GLY	3.6
1	A	111	VAL	3.5
1	A	106	ARG	3.5
1	A	170	SER	3.5
1	A	22	VAL	3.4
1	A	56	CYS	3.4
1	A	207	ILE	3.4
1	A	287	VAL	3.4
1	A	181	SER	3.3
1	A	3	ILE	3.3
1	A	49	THR	3.3
1	A	90	PHE	3.1
1	A	310	VAL	3.1
1	A	254	TYR	3.1
1	A	39	LEU	3.1
1	A	24	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	95	CYS	3.0
1	A	234	TYR	3.0
1	A	298	LYS	3.0
1	A	241	THR	2.9
1	A	239	THR	2.8
1	A	156	PHE	2.8
1	A	272	LEU	2.7
1	A	122	THR	2.7
1	A	18	SER	2.7
1	A	10	PHE	2.7
1	A	35	LEU	2.7
1	A	306	GLY	2.7
1	A	77	ALA	2.7
1	A	73	GLY	2.6
1	A	274	TYR	2.6
1	A	182	LEU	2.6
1	A	138	LYS	2.6
1	A	58	PHE	2.6
1	A	165	GLY	2.5
1	A	202	SER	2.5
1	A	308	VAL	2.5
1	A	289	PRO	2.5
1	A	148	THR	2.5
1	A	159	SER	2.5
1	A	134	PHE	2.5
1	A	63	THR	2.5
1	A	23	TYR	2.4
1	A	206	THR	2.4
1	A	282	ASN	2.4
1	A	311	VAL	2.4
1	A	205	ALA	2.4
1	A	4	THR	2.4
1	A	28	THR	2.4
1	A	294	TRP	2.4
1	A	125	SER	2.3
1	A	155	ASP	2.3
1	A	266	ASN	2.3
1	A	203	ASN	2.3
1	A	233	SER	2.3
1	A	250	VAL	2.3
1	A	96	THR	2.3
1	A	183	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	2.2
1	A	43	THR	2.2
1	A	5	GLY	2.2
1	A	51	THR	2.2
1	A	211	ASN	2.2
1	A	227	VAL	2.2
1	A	260	ALA	2.2
1	A	142	THR	2.2
1	A	258	VAL	2.1
1	A	30	THR	2.1
1	A	68	ASP	2.1
1	A	72	ASP	2.1
1	A	21	TYR	2.1
1	A	214	ILE	2.1
1	A	83	ALA	2.1
1	A	140	THR	2.1
1	A	160	PRO	2.1
1	A	235	THR	2.1
1	A	290	PHE	2.1
1	A	20	GLU	2.0
1	A	190	ASN	2.0
1	A	305	ASP	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.