



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Sep 16, 2019 – 12:51 PM EDT

PDB ID : 6PSY
EMDB ID: : EMD-20468
Title : Cryo-EM structure of *S. cerevisiae* Drs2p-Cdc50p in the autoinhibited apo form
Authors : Bai, L.; Li, H.
Deposited on : 2019-07-14
Resolution : 2.80 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

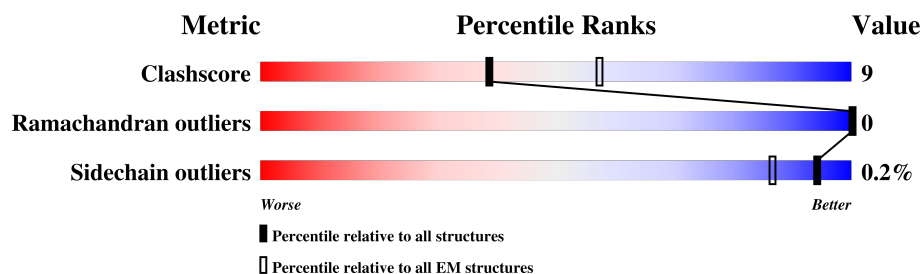
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1355	61% 19% 20%
2	E	391	70% 17% 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11540 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Probable phospholipid-transporting ATPase DRS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1090	8725	5634	1430	1623	38	0	0

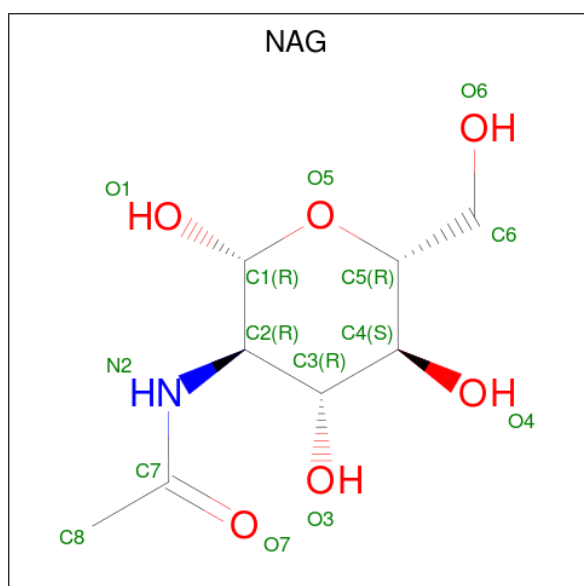
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	583	ASP	ILE	conflict	UNP P39524

- Molecule 2 is a protein called Cell division control protein 50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	339	2759	1788	457	503	11	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



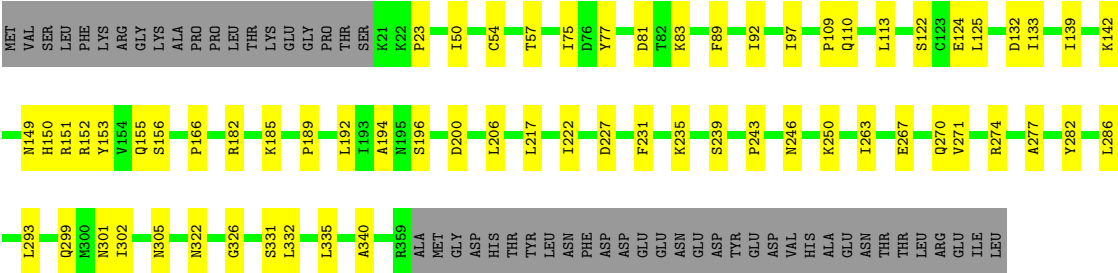
Mol	Chain	Residues	Atoms				AltConf
3	E	1	Total	C	N	O	0
			56	32	4	20	
3	E	1	Total	C	N	O	0
			56	32	4	20	
3	E	1	Total	C	N	O	0
			56	32	4	20	
3	E	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 1: Probable phospholipid-transporting ATPase DRS2



ASN
SER
ASN
ARG
PHE
SER
SER
ARG
ARG
ASP
ASP
ILE
SER
PHE
ASP
ILE

● Molecule 2: Cell division control protein 50



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	635300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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 >2	RMSZ	# Z >2
1	A	0.35	0/8912	0.62	4/12070 (0.0%)
2	E	0.36	0/2833	0.65	0/3841
All	All	0.35	0/11745	0.63	4/15911 (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
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	LEU	CA-CB-CG	7.10	131.63	115.30
1	A	629	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	363	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	746	LEU	CA-CB-CG	5.61	128.20	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	ASN	Peptide
2	E	83	LYS	Peptide

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	8725	0	8739	166	0
2	E	2759	0	2757	40	0
3	E	56	0	51	1	0
All	All	11540	0	11547	199	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.

The worst 5 of 199 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:724:ASP:O	1:A:728:LEU:HB2	1.72	0.89
1:A:914:LEU:O	1:A:918:ALA:HB3	1.73	0.86
1:A:869:THR:O	1:A:873:LEU:HB2	1.81	0.79
1:A:335:GLU:HG2	1:A:408:ARG:HE	1.52	0.74
1:A:1104:HIS:HB3	1:A:1145:ILE:HD12	1.72	0.72

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 PDB entries followed by that with respect to all EM entries.

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	1084/1355 (80%)	994 (92%)	90 (8%)	0	100	100
2	E	337/391 (86%)	309 (92%)	28 (8%)	0	100	100
All	All	1421/1746 (81%)	1303 (92%)	118 (8%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	953/1192 (80%)	951 (100%)	2 (0%)	94	98
2	E	309/355 (87%)	309 (100%)	0	100	100
All	All	1262/1547 (82%)	1260 (100%)	2 (0%)	94	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	LEU
1	A	629	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1038	GLN
1	A	1131	HIS
2	E	155	GLN
1	A	1026	GLN
2	E	246	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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
3	NAG	E	401	3,2	14,14,15	0.35	0	17,19,21	0.57	0
3	NAG	E	402	3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	E	403	2	14,14,15	0.55	0	17,19,21	0.65	1 (5%)
3	NAG	E	404	2	14,14,15	0.46	0	17,19,21	0.64	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	401	3,2	-	4/6/23/26	0/1/1/1
3	NAG	E	402	3	-	4/6/23/26	0/1/1/1
3	NAG	E	403	2	-	4/6/23/26	0/1/1/1
3	NAG	E	404	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	404	NAG	C1-O5-C5	2.25	115.26	112.20
3	E	403	NAG	C1-O5-C5	2.04	114.97	112.20

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	401	NAG	O5-C5-C6-O6
3	E	401	NAG	C4-C5-C6-O6
3	E	402	NAG	C8-C7-N2-C2
3	E	402	NAG	O7-C7-N2-C2
3	E	401	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	NAG	1	0

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.