

Full wwPDB NMR Structure Validation Report (i)

May 7, 2024 – 03:58 pm BST

PDB ID : 2CKC

Title : Solution structures of the BRK domains of the human Chromo Helicase Do-

main 7 and 8, reveals structural similarity with GYF domain suggesting a role

in protein interaction

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Folkers, G.E.

Deposited on : 2006-04-14

This is a Full wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

MolProbity : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

wwPDB-RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

wwPDB-ShiftChecker : v1.2

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.



2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues				
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model	
1	A:2565-A:2604 (40)	0.38	13	

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 6 clusters. No single-model clusters were found.

Cluster number	Models	
1	1, 4, 8, 9, 12, 13, 14, 18, 21, 23	
2	2, 6, 15, 17, 19	
3	3, 7, 16, 24	
4	11, 22	
5	10, 25	
6	5, 20	



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 961 atoms, of which 479 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7.

Mol	Chain	Residues	Atoms			Trace			
1	Λ	60	Total	С	Н	N	О	S	0
	60	961	309	479	78	94	1	U	

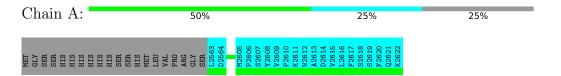


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7

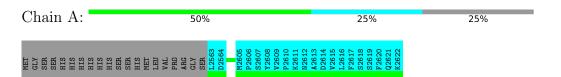


4.2 Scores per residue for each member of the ensemble

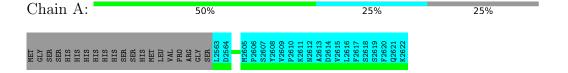
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

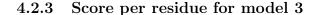
• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



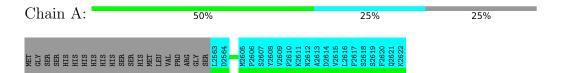
4.2.2 Score per residue for model 2





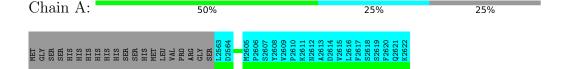


• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



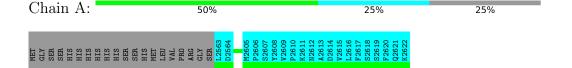
4.2.4 Score per residue for model 4

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



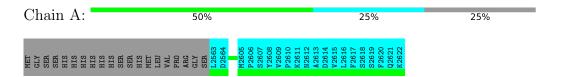
4.2.5 Score per residue for model 5

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7

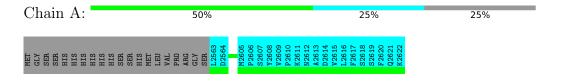


4.2.6 Score per residue for model 6

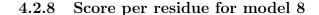
• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



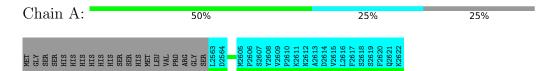
4.2.7 Score per residue for model 7





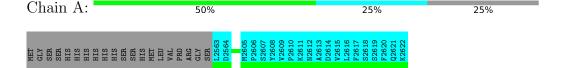






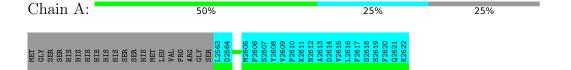
4.2.9 Score per residue for model 9

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



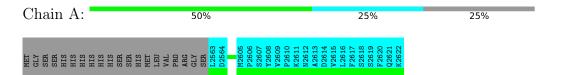
4.2.10 Score per residue for model 10

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7

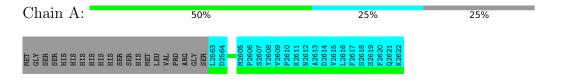


4.2.11 Score per residue for model 11

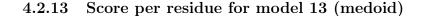
• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



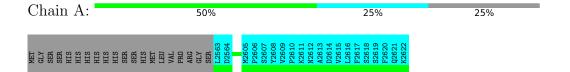
4.2.12 Score per residue for model 12





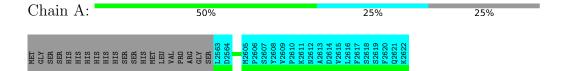


• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



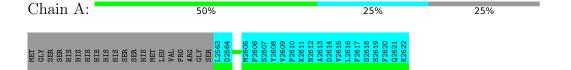
4.2.14 Score per residue for model 14

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



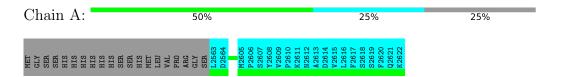
4.2.15 Score per residue for model 15

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



4.2.16 Score per residue for model 16

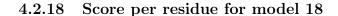
• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



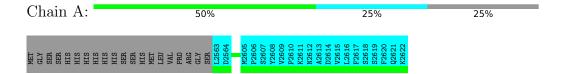
4.2.17 Score per residue for model 17





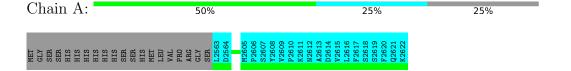


• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



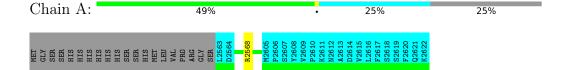
4.2.19 Score per residue for model 19

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



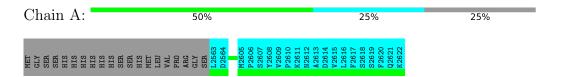
4.2.20 Score per residue for model 20

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7

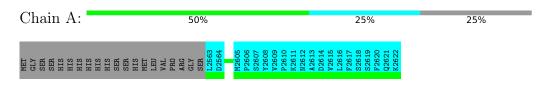


4.2.21 Score per residue for model 21

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



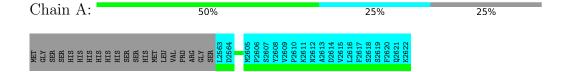
4.2.22 Score per residue for model 22





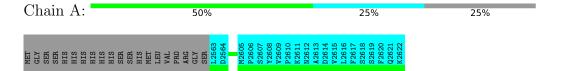
4.2.23 Score per residue for model 23

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



4.2.24 Score per residue for model 24

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7



4.2.25 Score per residue for model 25

• Molecule 1: CHROMODOMAIN-HELICASE-DNA-BINDING PROTEIN 7

Chain A: 50% 25% 25% 25% 25% 25%



Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: CANDID IN CYANA.

Of the 50 calculated structures, 25 were deposited, based on the following criterion: LEAST RESTRAINT VIOLATION.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	
Sparky	structure solution	

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts (i)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA (i)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates (i)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry (i)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers (i)

MolProbity failed to run properly - this section will have to be empty.



6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

