wwPDB NMR Structure Validation Summary Report

May 7, 2024 – 03:52 pm BST

PDB ID	:	2J8P
Title	:	NMR structure of C-terminal domain of human CstF-64
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Deposited on	:	2006-10-27

This is a wwPDB NMR Structure Validation Summary 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

This entry contains 30 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:530-A:572 (43)	0.87	1

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 15, 16, 17, 18, 20, 23, 27, 29, 30
2	4, 13, 22, 24, 26, 28
3	14, 19, 21, 25

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 782 atoms, of which 400 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	49	782	240	400	67	72	3	0

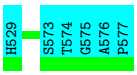
4 Residue-property plots

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: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT

Chain A:

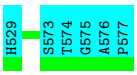


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 35 calculated structures, 30 were deposited, based on the following criterion: *STRUCTURES HAVING NO DISTANCE RESTRAINT VIOLATION LARGER THAN 0.2 A OR NO VIOLATION OF DIHEDRAL ANGLE CONSTRAINTS LARGER THAN 5 DEGREES*.

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

Software name	Classification	Version
CYANA	refinement	
ANSIG	structure solution	
TALOS	structure solution	
CYANA	structure solution	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

6.2 Too-close contacts

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

6.3 Torsion angles

6.3.1 Protein backbone

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

6.3.2 Protein sidechains

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

6.3.3 RNA

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

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

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

6.6 Ligand geometry

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

6.7 Other polymers

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