Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 08:53 am GMT

PDB ID	:	2WQ3
Title	:	GCN4 leucine zipper mutant with three IxxNTxx motifs coordinating chloride and nitrate
Authors	:	Hartmann, M.D.; Hernandez Alvarez, B.; Lupas, A.N.
Deposited on	:	2009-08-12
Resolution	:	1.22 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 (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
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.22 Å.

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

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α, β, γ	56.67Å 56.67Å 56.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.14 – 1.22	Depositor
% Data completeness (in resolution range)	99.4 (23.14-1.22)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.22Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.141 , 0.200	Depositor
Wilson B-factor (Å^2)	11.9	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.056 for -l,-k,-h	Xtriage
Total number of atoms	345	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality (i)

3.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

3.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

3.3 Torsion angles (i)

3.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

3.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

3.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

There are no non-standard protein/DNA/RNA residues in this entry.

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

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.

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data (i)

4.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

4.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

4.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

4.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.