W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 05:03 AM EDT

PDB ID	:	6MI3
Title	:	Structure of NEMO(51-112) with N- and C-terminal coiled-coil adaptors.
Authors	:	Pellegrini, M.; Barczewski, A.H.; Mierke, D.F.; Ragusa, M.J.
Deposited on	:	2018-09-19
Resolution	:	1.78 Å(reported)

This is a wwPDB X-ray 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/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.

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 1.78 Å.

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

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2227 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 NF-kB ESSENTIAL MODULATOR,NF-kappa-B essential modulator,NF-kB ESSENTIAL MODULATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total 1011	C 630	N 185	O 194	S 2	0	0	0
1	B	124	Total 1033	C 643	N 192	O 196	S 2	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ALA	GLU	engineered mutation	UNP Q9Y6K9
A	57	ALA	GLU	engineered mutation	UNP Q9Y6K9
A	76	ALA	CYS	engineered mutation	UNP Q9Y6K9
A	95	SER	CYS	engineered mutation	UNP Q9Y6K9
B	56	ALA	GLU	engineered mutation	UNP Q9Y6K9
B	57	ALA	GLU	engineered mutation	UNP Q9Y6K9
B	76	ALA	CYS	engineered mutation	UNP Q9Y6K9
B	95	SER	CYS	engineered mutation	UNP Q9Y6K9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	112	Total 112	O 112	0	0
2	B	71	Total 71	O 71	0	0

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

3   Data and refinement statistics   ⓘ

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.48Å 33.62Å 76.87Å 90.00° 115.04° 90.00°	Depositor
Resolution (Å)	37.75 – 1.78	Depositor
% Data completeness (in resolution range)	67.6 (37.75-1.78)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 1.78Å)	Xtriage
Refinement program	PHENIX dev_2849	Depositor
R, R_{free}	0.243 , 0.266	Depositor
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.038	Xtriage
L-test for twinning[2]	$< \lvert L \rvert > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Total number of atoms	2227	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

4.2 Too-close contacts ⓘ

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

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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

4.3.2 Protein sidechains ⓘ

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

4.3.3 RNA ⓘ

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

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

There are no ligands in this entry.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

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

5.4 Ligands ⓘ

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

5.5 Other polymers ⓘ

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