WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 08:03 AM EDT

PDB ID	:	6UX8
Title	:	Structure of monobody 33 MLKL N-terminal domain complex
Authors	:	Birkinshaw, R.W.; Petrie, E.J.; Murphy, J.M.
Deposited on	:	2019-11-07
Resolution	:	2.50 Å(reported)

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 2.50 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 4 unique types of molecules in this entry. The entry contains 1854 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 Mixed lineage kinase domain-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1191	740	219	224	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q8NB16
A	-2	ALA	-	expression tag	UNP Q8NB16
A	-1	MET	-	expression tag	UNP Q8NB16
A	0	GLY	-	expression tag	UNP Q8NB16
A	1	SER	-	expression tag	UNP Q8NB16
A	2	GLU	-	expression tag	UNP Q8NB16
A	3	ASN	-	expression tag	UNP Q8NB16
A	4	LEU	-	expression tag	UNP Q8NB16

- Molecule 2 is a protein called Monobody.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	0	0	0
			645	416	96	133			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total 8	O 8	0	0
4	B	6	Total 6	O 6	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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.29Å 59.42Å 68.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.76 – 2.50	Depositor
% Data completeness (in resolution range)	99.5 (44.76-2.50)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.62 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.247 , 0.296	Depositor
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.691	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
Total number of atoms	1854	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.83% 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 $<|L|>$, $<L^2>$ 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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - 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.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

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.