wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	3LMF
Title	:	Crystal Structure of Nmul_A1745 protein from Nitrosospira multiformis, Northeast Structural Genomics Consortium Target NmR72
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Deposited on	:	2010-01-29
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

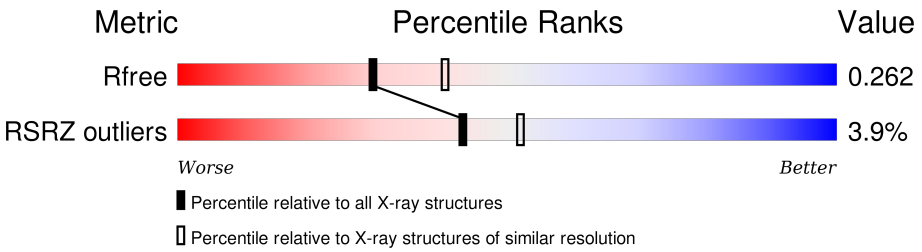
MolProbity	:	FAILED
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk26765
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 854 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	109	822	489	152	158	16	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	LEU	-	EXPRESSION TAG	UNP Q2Y879
A	115	GLU	-	EXPRESSION TAG	UNP Q2Y879
A	116	HIS	-	EXPRESSION TAG	UNP Q2Y879
A	117	HIS	-	EXPRESSION TAG	UNP Q2Y879
A	118	HIS	-	EXPRESSION TAG	UNP Q2Y879
A	119	HIS	-	EXPRESSION TAG	UNP Q2Y879
A	120	HIS	-	EXPRESSION TAG	UNP Q2Y879
A	121	HIS	-	EXPRESSION TAG	UNP Q2Y879

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	32	32	32	0	0

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3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	94.42Å 94.42Å 72.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 2.30 47.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.2 (19.80-2.30) 95.4 (47.21-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	9.71 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2 &XtalView	Depositor
R, R_{free}	0.209 , 0.247 0.226 , 0.262	Depositor DCC
R_{free} test set	436 reflections (5.48%)	DCC
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 15711 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	854	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

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

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

4.5 Carbohydrates (i)

There are no carbohydrates in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

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 (i)

5.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	102/121 (84%)	0.09	4 (3%) 43 52	16, 29, 52, 77	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	GLN	3.2
1	A	7	THR	3.0
1	A	92	ASP	2.1
1	A	90	GLN	2.1

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

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

5.3 Carbohydrates (i)

There are no carbohydrates in this entry.

5.4 Ligands (i)

There are no ligands in this entry.

5.5 Other polymers (i)

There are no such residues in this entry.