wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 07:43 PM EDT

PDB ID	:	6O3X
Title	:	Crystal structure of yeast Nrd1 CID in complex with Sen1 NIM2
Authors	:	Zhang, Y.; Tong, L.
Deposited on	:	2019-02-27
Resolution	:	1.99 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.

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)	:	2.35.1

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 1.99 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 (i)

There are 4 unique types of molecules in this entry. The entry contains 3823 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 Protein NRD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	148	1167	733	203	226	5	0	0	0
1	B	138	1098	697	188	208	5	0	0	0
1	C	146	1152	724	199	224	5	0	0	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP P53617
A	-14	GLY	-	expression tag	UNP P53617
A	-13	SER	-	expression tag	UNP P53617
A	-12	SER	-	expression tag	UNP P53617
A	-11	HIS	-	expression tag	UNP P53617
A	-10	HIS	-	expression tag	UNP P53617
A	-9	HIS	-	expression tag	UNP P53617
A	-8	HIS	-	expression tag	UNP P53617
A	-7	HIS	-	expression tag	UNP P53617
A	-6	HIS	-	expression tag	UNP P53617
A	-5	SER	-	expression tag	UNP P53617
A	-4	SER	-	expression tag	UNP P53617
A	-3	GLY	-	expression tag	UNP P53617
A	-2	LEU	-	expression tag	UNP P53617
A	-1	VAL	-	expression tag	UNP P53617
A	0	PRO	-	expression tag	UNP P53617
A	1	ARG	-	expression tag	UNP P53617
A	2	GLY	-	expression tag	UNP P53617
A	3	SER	-	expression tag	UNP P53617
A	4	HIS	-	expression tag	UNP P53617
A	5	MET	-	expression tag	UNP P53617
B	-15	MET	-	initiating methionine	UNP P53617
B	-14	GLY	-	expression tag	UNP P53617

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	SER	-	expression tag	UNP P53617
B	-12	SER	-	expression tag	UNP P53617
B	-11	HIS	-	expression tag	UNP P53617
B	-10	HIS	-	expression tag	UNP P53617
B	-9	HIS	-	expression tag	UNP P53617
B	-8	HIS	-	expression tag	UNP P53617
B	-7	HIS	-	expression tag	UNP P53617
B	-6	HIS	-	expression tag	UNP P53617
B	-5	SER	-	expression tag	UNP P53617
B	-4	SER	-	expression tag	UNP P53617
B	-3	GLY	-	expression tag	UNP P53617
B	-2	LEU	-	expression tag	UNP P53617
B	-1	VAL	-	expression tag	UNP P53617
B	0	PRO	-	expression tag	UNP P53617
B	1	ARG	-	expression tag	UNP P53617
B	2	GLY	-	expression tag	UNP P53617
B	3	SER	-	expression tag	UNP P53617
B	4	HIS	-	expression tag	UNP P53617
B	5	MET	-	expression tag	UNP P53617
C	-15	MET	-	initiating methionine	UNP P53617
C	-14	GLY	-	expression tag	UNP P53617
C	-13	SER	-	expression tag	UNP P53617
C	-12	SER	-	expression tag	UNP P53617
C	-11	HIS	-	expression tag	UNP P53617
C	-10	HIS	-	expression tag	UNP P53617
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C	-5	SER	-	expression tag	UNP P53617
C	-4	SER	-	expression tag	UNP P53617
C	-3	GLY	-	expression tag	UNP P53617
C	-2	LEU	-	expression tag	UNP P53617
C	-1	VAL	-	expression tag	UNP P53617
C	0	PRO	-	expression tag	UNP P53617
C	1	ARG	-	expression tag	UNP P53617
C	2	GLY	-	expression tag	UNP P53617
C	3	SER	-	expression tag	UNP P53617
C	4	HIS	-	expression tag	UNP P53617
C	5	MET	-	expression tag	UNP P53617

- Molecule 2 is a protein called Helicase SEN1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	6	48	29	6	13	0	0	0
2	E	6	48	29	6	13	0	0	0
2	F	6	48	29	6	13	0	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	125	125	125	0	0
4	B	51	51	51	0	0
4	C	72	72	72	0	0
4	D	7	7	7	0	0
4	E	2	2	2	0	0
4	F	3	3	3	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	98.69Å 102.40Å 115.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 1.99	Depositor
% Data completeness (in resolution range)	98.1 (49.34-1.99)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.226	Depositor
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.574	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.075 for -k,-h,-l	Xtriage
Total number of atoms	3823	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.97% 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.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore 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 monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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 (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)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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