

Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 12:28 AM EDT

PDB ID	:	6Q1H
Title	:	Structure of P. aeruginosa ATCC27853 NucC, cAAA-bound form
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Deposited on		
Resolution	:	1.45 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 (1)) were used in the production of this report:

:	FAILED
:	1.13
:	FAILED
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.35.1
	: : : :

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 1.45 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.



6Q1H

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24734 atoms, of which 11172 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1 A	240	Total	С	Η	Ν	0	\mathbf{S}	0	4	0
	A	240	3723	1209	1837	316	357	4	0		
1	В	240	Total	С	Н	Ν	0	S	0	5	0
1	D	240	3759	1218	1857	319	361	4	0		
1	С	240	Total	С	Η	Ν	0	S	0	7	0
1	U	240	3757	1220	1856	318	359	4			
1	Е	240	Total	С	Η	Ν	0	S	0	2	0
1	Ľ	240	3744	1215	1852	317	356	4	0		
1	F	240	Total	С	Η	Ν	Ο	\mathbf{S}	0	8	0
I	Ľ	240	3782	1226	1871	320	361	4		0	0
1	1 G	239	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	4	0
			3713	1206	1833	315	355	4			0

• Molecule 1 is a protein called Bacterial protein ORF C62.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	73	ASN	ASP	engineered mutation	UNP Q8GQ48
В	73	ASN	ASP	engineered mutation	UNP Q8GQ48
С	73	ASN	ASP	engineered mutation	UNP Q8GQ48
Е	73	ASN	ASP	engineered mutation	UNP Q8GQ48
F	73	ASN	ASP	engineered mutation	UNP Q8GQ48
G	73	ASN	ASP	engineered mutation	UNP Q8GQ48

• Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
0	2 D	9	Total	С	Η	Ν	0	Р	0	0	0
		ა	99	30	33	15	18	3			
0	TT	9	Total	С	Η	Ν	0	Р	0	0	0
2 П	0	99	30	33	15	18	3	0		0	

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	347	Total O 347 347	0	0
3	В	332	Total O 332 332	0	0
3	С	330	Total O 330 330	0	0
3	D	9	Total O 9 9	0	0
3	Е	356	Total O 356 356	0	0
3	F	329	Total O 329 329	0	0
3	G	348	Total O 348 348	0	0
3	Н	7	Total O 7 7	0	0

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



3 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	80.50Å 80.45 Å 262.08 Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	76.95 - 1.45	Depositor	
% Data completeness	97.4 (76.95-1.45)	Depositor	
(in resolution range)		-	
R_{merge}	0.08	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.02 (at 1.45 Å)	Xtriage	
Refinement program	PHENIX 1.15.2_3472	Depositor	
R, R_{free}	0.147 , 0.167	Depositor	
Wilson B-factor ($Å^2$)	16.8	Xtriage	
Anisotropy	0.279	Xtriage	
L-test for twinning ²	$< L > = 0.48, < L^2 > = 0.31$	Xtriage	
Estimated twinning fraction	0.015 for k,h,-l	Xtriage	
Total number of atoms	24734	wwPDB-VP	
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP	

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

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 27.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0659e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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)

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)

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.

