Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 07:20 AM EDT

PDB ID	:	6UJI
Title	:	Low resolution crystal structure (5.5 A) of the anthrax toxin protective antigen heptamer prepore D425A mutant
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Deposited on	:	2019-10-03
Resolution	:	5.50 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 ⓘ 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 ⓘ) 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 5.50 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 (i)

There is only 1 type of molecule in this entry. The entry contains 53490 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 Protective antigen PA-63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3712	2316	650	740	6			
1	B	519	Total	C	N	O	S	0	0	0
			4114	2578	710	820	6			
1	C	388	Total	C	N	O	S	0	0	0
			3083	1929	539	609	6			
1	D	539	Total	C	N	O	S	0	0	0
			4265	2672	735	852	6			
1	E	516	Total	C	N	O	S	0	0	0
			4089	2564	704	815	6			
1	F	467	Total	C	N	O	S	0	0	0
			3688	2316	641	725	6			
1	G	520	Total	C	N	O	S	0	0	0
			4125	2583	710	826	6			
1	H	493	Total	C	N	O	S	0	0	0
			3894	2434	678	776	6			
1	I	529	Total	C	N	O	S	0	0	0
			4189	2622	724	837	6			
1	J	470	Total	C	N	O	S	0	0	0
			3718	2322	649	741	6			
1	K	488	Total	C	N	O	S	0	0	0
			3867	2419	673	769	6			
1	L	404	Total	C	N	O	S	0	0	0
			3189	1992	555	637	5			
1	M	473	Total	C	N	O	S	0	0	0
			3749	2345	656	742	6			
1	N	480	Total	C	N	O	S	0	0	0
			3808	2375	663	764	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	425	ALA	ASP	engineered mutation	UNP P13423

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Chain	Residue	Modelled	Actual	Comment	Reference
B	425	ALA	ASP	engineered mutation	UNP P13423
C	425	ALA	ASP	engineered mutation	UNP P13423
D	425	ALA	ASP	engineered mutation	UNP P13423
E	425	ALA	ASP	engineered mutation	UNP P13423
F	425	ALA	ASP	engineered mutation	UNP P13423
G	425	ALA	ASP	engineered mutation	UNP P13423
H	425	ALA	ASP	engineered mutation	UNP P13423
I	425	ALA	ASP	engineered mutation	UNP P13423
J	425	ALA	ASP	engineered mutation	UNP P13423
K	425	ALA	ASP	engineered mutation	UNP P13423
L	425	ALA	ASP	engineered mutation	UNP P13423
M	425	ALA	ASP	engineered mutation	UNP P13423
N	425	ALA	ASP	engineered mutation	UNP P13423

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	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	166.18Å 144.25Å 304.82Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	44.83 – 5.50	Depositor
% Data completeness (in resolution range)	99.3 (44.83-5.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 5.39Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.251 , 0.278	Depositor
Wilson B-factor (Å^2)	183.8	Xtriage
Anisotropy	0.481	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	53490	wwPDB-VP
Average B, all atoms (Å^2)	257.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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

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.