WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary 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)

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 ⓘ

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 ⓘ

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

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 ⓘ

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.*

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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 ⓘ

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.