



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 05:04 AM EDT

PDB ID : 6UUJ
Title : Structure of PE5-PPE4-EspG3 complex from the type VII (ESX-3) secretion system, space group P212121
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Deposited on : 2019-10-30
Resolution : 3.00 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 ⓘ 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**
Xtrriage (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 3.00 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 28770 atoms, of which 14231 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 PE family immunomodulator PE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	A	73	966	301	483	85	97	0	0	0
1	D	71	944	294	472	83	95	0	0	0
1	G	74	982	306	492	86	98	0	0	0
1	J	71	944	294	472	83	95	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP L7N695
A	4	ALA	-	expression tag	UNP L7N695
A	5	MET	-	expression tag	UNP L7N695
D	3	GLY	-	expression tag	UNP L7N695
D	4	ALA	-	expression tag	UNP L7N695
D	5	MET	-	expression tag	UNP L7N695
G	3	GLY	-	expression tag	UNP L7N695
G	4	ALA	-	expression tag	UNP L7N695
G	5	MET	-	expression tag	UNP L7N695
J	3	GLY	-	expression tag	UNP L7N695
J	4	ALA	-	expression tag	UNP L7N695
J	5	MET	-	expression tag	UNP L7N695

- Molecule 2 is a protein called PPE family protein PPE4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	164	2309	757	1134	194	220	4	0	0	0
2	E	163	2299	754	1129	193	219	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	H	162	Total	C	H	N	O	S	0	0	0
			2288	751	1124	192	217	4			
2	K	163	Total	C	H	N	O	S	0	0	0
			2298	754	1129	193	218	4			

- Molecule 3 is a protein called ESX-3 secretion-associated protein EspG3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	C	259	Total	C	H	N	O	S	0	0	0
			3934	1264	1949	340	375	6			
3	F	259	Total	C	H	N	O	S	0	0	0
			3934	1264	1949	340	375	6			
3	I	259	Total	C	H	N	O	S	0	0	0
			3934	1264	1949	340	375	6			
3	L	259	Total	C	H	N	O	S	0	0	0
			3934	1264	1949	340	375	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	MET	-	initiating methionine	UNP B2HNX0
C	4	ALA	-	expression tag	UNP B2HNX0
F	3	MET	-	initiating methionine	UNP B2HNX0
F	4	ALA	-	expression tag	UNP B2HNX0
I	3	MET	-	initiating methionine	UNP B2HNX0
I	4	ALA	-	expression tag	UNP B2HNX0
L	3	MET	-	initiating methionine	UNP B2HNX0
L	4	ALA	-	expression tag	UNP B2HNX0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		
4	I	1	Total	O	0	0
			1	1		
4	J	1	Total	O	0	0
			1	1		

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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.27Å 158.63Å 209.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.52 – 3.00	Depositor
% Data completeness (in resolution range)	98.8 (39.52-3.00)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.266 , 0.301	Depositor
Wilson B-factor (Å ²)	85.8	Xtrriage
Anisotropy	0.604	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	28770	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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

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.