wwPDB X-ray Structure Validation Summary Report (i)

Oct 28, 2026 – 09:07 pm GMT

PDB ID	:	9TUP / pdb_00009tup
Title	:	Pseudomonas aeruginosa T6SS effector Tne3 in complex with its cognate immunity protein Tni3
Authors	:	Albesa-Jove, D.; Velazquez, C.; Robinson, L.A.
Deposited on	:	2026-01-08
Resolution	:	2.35 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 (1)) were used in the production of this report:

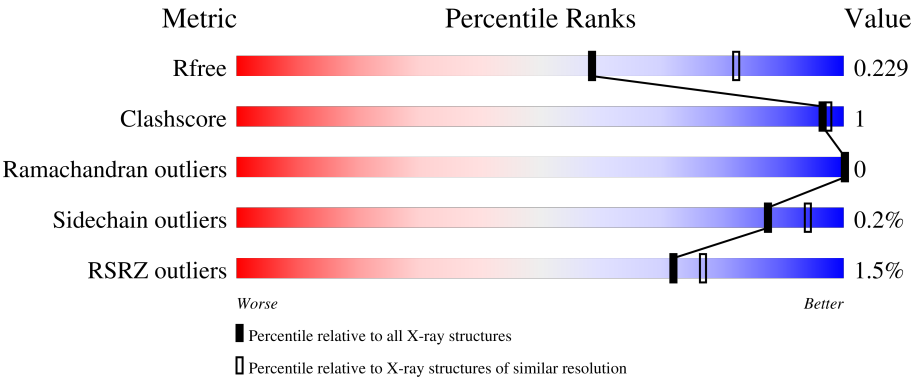
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	194	3% 85% 12%
1	C	194	% 85% 12%
2	B	177	% 95%
2	D	177	% 95%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10929 atoms, of which 5168 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 PAAR domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	170	Total	C	H	N	O	S	0	0	0
			2542	815	1252	219	251	5			
1	C	170	Total	C	H	N	O	S	0	0	0
			2539	814	1250	221	249	5			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	initiating methionine	UNP A0A6A9K0I2
A	242	GLY	-	expression tag	UNP A0A6A9K0I2
A	243	SER	-	expression tag	UNP A0A6A9K0I2
A	244	SER	-	expression tag	UNP A0A6A9K0I2
A	245	HIS	-	expression tag	UNP A0A6A9K0I2
A	246	HIS	-	expression tag	UNP A0A6A9K0I2
A	247	HIS	-	expression tag	UNP A0A6A9K0I2
A	248	HIS	-	expression tag	UNP A0A6A9K0I2
A	249	HIS	-	expression tag	UNP A0A6A9K0I2
A	250	HIS	-	expression tag	UNP A0A6A9K0I2
A	251	HIS	-	expression tag	UNP A0A6A9K0I2
A	252	HIS	-	expression tag	UNP A0A6A9K0I2
A	253	HIS	-	expression tag	UNP A0A6A9K0I2
A	254	SER	-	expression tag	UNP A0A6A9K0I2
A	255	SER	-	expression tag	UNP A0A6A9K0I2
A	256	GLY	-	expression tag	UNP A0A6A9K0I2
A	257	GLU	-	expression tag	UNP A0A6A9K0I2
A	258	ASN	-	expression tag	UNP A0A6A9K0I2
A	259	LEU	-	expression tag	UNP A0A6A9K0I2
A	260	TYR	-	expression tag	UNP A0A6A9K0I2
A	261	PHE	-	expression tag	UNP A0A6A9K0I2
A	262	GLN	-	expression tag	UNP A0A6A9K0I2
A	263	GLY	-	expression tag	UNP A0A6A9K0I2
A	264	GLY	-	expression tag	UNP A0A6A9K0I2
A	265	SER	-	expression tag	UNP A0A6A9K0I2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	241	MET	-	initiating methionine	UNP A0A6A9K0I2
C	242	GLY	-	expression tag	UNP A0A6A9K0I2
C	243	SER	-	expression tag	UNP A0A6A9K0I2
C	244	SER	-	expression tag	UNP A0A6A9K0I2
C	245	HIS	-	expression tag	UNP A0A6A9K0I2
C	246	HIS	-	expression tag	UNP A0A6A9K0I2
C	247	HIS	-	expression tag	UNP A0A6A9K0I2
C	248	HIS	-	expression tag	UNP A0A6A9K0I2
C	249	HIS	-	expression tag	UNP A0A6A9K0I2
C	250	HIS	-	expression tag	UNP A0A6A9K0I2
C	251	HIS	-	expression tag	UNP A0A6A9K0I2
C	252	HIS	-	expression tag	UNP A0A6A9K0I2
C	253	HIS	-	expression tag	UNP A0A6A9K0I2
C	254	SER	-	expression tag	UNP A0A6A9K0I2
C	255	SER	-	expression tag	UNP A0A6A9K0I2
C	256	GLY	-	expression tag	UNP A0A6A9K0I2
C	257	GLU	-	expression tag	UNP A0A6A9K0I2
C	258	ASN	-	expression tag	UNP A0A6A9K0I2
C	259	LEU	-	expression tag	UNP A0A6A9K0I2
C	260	TYR	-	expression tag	UNP A0A6A9K0I2
C	261	PHE	-	expression tag	UNP A0A6A9K0I2
C	262	GLN	-	expression tag	UNP A0A6A9K0I2
C	263	GLY	-	expression tag	UNP A0A6A9K0I2
C	264	GLY	-	expression tag	UNP A0A6A9K0I2
C	265	SER	-	expression tag	UNP A0A6A9K0I2

- Molecule 2 is a protein called Chains: B,D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	174	Total	C	H	N	O	S	0	0	0
			2747	903	1342	238	261	3			
2	D	172	Total	C	H	N	O	S	0	0	0
			2706	891	1324	237	252	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	105	Total	O	0	0
			105	105		
3	D	110	Total	O	0	0
			110	110		

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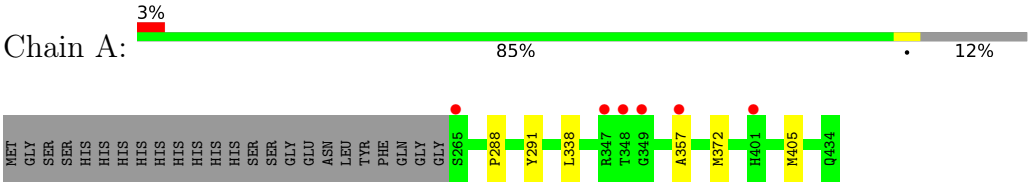
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	98	Total O 98 98	0	0

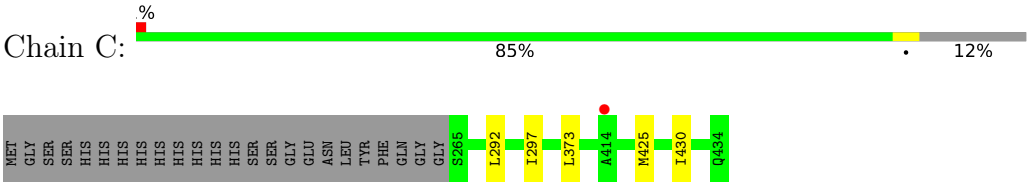
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

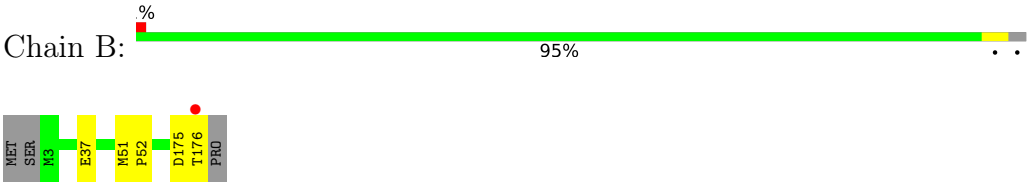
• Molecule 1: PAAR domain-containing protein



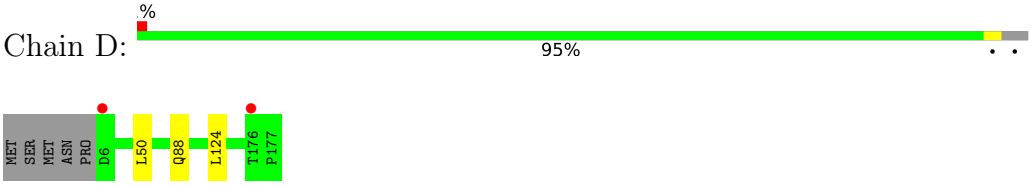
• Molecule 1: PAAR domain-containing protein



• Molecule 2: Chains: B,D



• Molecule 2: Chains: B,D



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.82Å 79.61Å 171.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.18 – 2.35 72.18 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.8 (72.18-2.35) 96.9 (72.18-2.35)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.187 , 0.229 0.188 , 0.229	Depositor DCC
R_{free} test set	1717 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10929	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.18	0/1319	0.36	0/1788
1	C	0.18	0/1318	0.36	0/1787
2	B	0.19	0/1445	0.39	0/1975
2	D	0.19	0/1422	0.40	0/1943
All	All	0.18	0/5504	0.38	0/7493

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1290	1252	1264	3	0
1	C	1289	1250	1262	3	0
2	B	1405	1342	1348	2	0
2	D	1382	1324	1330	2	0
3	A	82	0	0	0	0
3	B	105	0	0	0	0
3	C	98	0	0	0	0
3	D	110	0	0	0	0
All	All	5761	5168	5204	10	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 10 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:MET:HG3	1:C:430:ILE:HD11	1.82	0.61
1:A:357:ALA:O	1:A:405:MET:HE1	2.12	0.49
1:A:338:LEU:HD23	1:A:372:MET:HE3	1.97	0.47
2:B:175:ASP:O	2:B:176:THR:HB	2.18	0.44
1:A:288:PRO:HA	1:A:291:TYR:CE1	2.53	0.44

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	168/194 (87%)	164 (98%)	4 (2%)	0	100	100
1	C	168/194 (87%)	166 (99%)	2 (1%)	0	100	100
2	B	172/177 (97%)	170 (99%)	2 (1%)	0	100	100
2	D	170/177 (96%)	168 (99%)	2 (1%)	0	100	100
All	All	678/742 (91%)	668 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	139/162 (86%)	139 (100%)	0	100 100
1	C	138/162 (85%)	138 (100%)	0	100 100
2	B	147/152 (97%)	146 (99%)	1 (1%)	76 86
2	D	142/152 (93%)	142 (100%)	0	100 100
All	All	566/628 (90%)	565 (100%)	1 (0%)	87 94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	37	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	104	ASN
2	D	127	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	170/194 (87%)	0.06	6 (3%)	47	53	27, 39, 60, 69	0
1	C	170/194 (87%)	-0.01	1 (0%)	85	89	28, 39, 52, 60	0
2	B	174/177 (98%)	-0.30	1 (0%)	85	89	23, 32, 44, 67	0
2	D	172/177 (97%)	-0.33	2 (1%)	76	81	24, 31, 44, 69	0
All	All	686/742 (92%)	-0.14	10 (1%)	72	77	23, 35, 55, 69	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	176	THR	3.5
1	C	414	ALA	3.3
1	A	348	THR	3.2
2	D	6	ASP	2.8
1	A	347	ARG	2.6

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.