



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:55 am BST

PDB ID : 6G7B
Title : Nt2 domain of the TssA component from the type VI secretion system of *Aeromonas hydrophila*.
Authors : Dix, S.D.; Owen, H.J.; Sun, R.; Ahmad, A.; Shastri, S.; Spiewak, H.L.; Mosby, D.J.; Harris, M.J.; Batters, S.L.; Tzokov, S.B.; Sedelnikova, S.E.; Baker, P.J.; Bullough, P.A.; Rice, D.W.; Thomas, M.S.
Deposited on : 2018-04-05
Resolution : 1.76 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

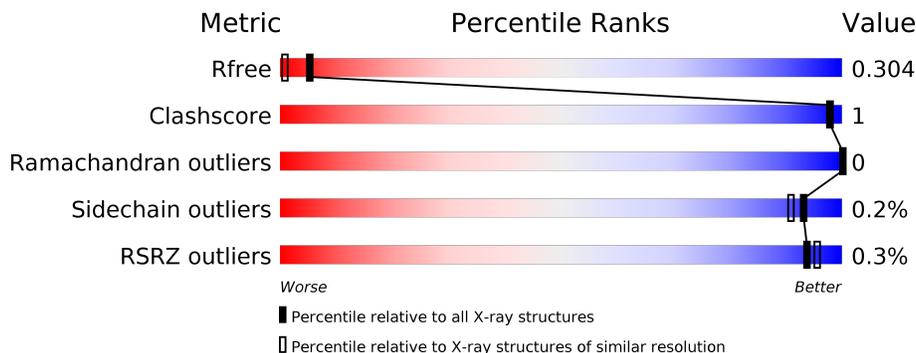
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 on 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 $\leq 5\%$. 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	382	
1	B	382	
1	C	382	
1	D	382	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4964 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 ImpA-related domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	146	1146	729	204	208	5	0	0	0
1	B	146	1146	729	204	208	5	0	0	0
1	A	146	1146	729	204	208	5	0	0	0
1	C	146	1146	729	204	208	5	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	375	LEU	-	expression tag	UNP A0KJC7
D	376	GLU	-	expression tag	UNP A0KJC7
D	377	HIS	-	expression tag	UNP A0KJC7
D	378	HIS	-	expression tag	UNP A0KJC7
D	379	HIS	-	expression tag	UNP A0KJC7
D	380	HIS	-	expression tag	UNP A0KJC7
D	381	HIS	-	expression tag	UNP A0KJC7
D	382	HIS	-	expression tag	UNP A0KJC7
B	375	LEU	-	expression tag	UNP A0KJC7
B	376	GLU	-	expression tag	UNP A0KJC7
B	377	HIS	-	expression tag	UNP A0KJC7
B	378	HIS	-	expression tag	UNP A0KJC7
B	379	HIS	-	expression tag	UNP A0KJC7
B	380	HIS	-	expression tag	UNP A0KJC7
B	381	HIS	-	expression tag	UNP A0KJC7
B	382	HIS	-	expression tag	UNP A0KJC7
A	375	LEU	-	expression tag	UNP A0KJC7
A	376	GLU	-	expression tag	UNP A0KJC7
A	377	HIS	-	expression tag	UNP A0KJC7
A	378	HIS	-	expression tag	UNP A0KJC7
A	379	HIS	-	expression tag	UNP A0KJC7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	380	HIS	-	expression tag	UNP A0KJC7
A	381	HIS	-	expression tag	UNP A0KJC7
A	382	HIS	-	expression tag	UNP A0KJC7
C	375	LEU	-	expression tag	UNP A0KJC7
C	376	GLU	-	expression tag	UNP A0KJC7
C	377	HIS	-	expression tag	UNP A0KJC7
C	378	HIS	-	expression tag	UNP A0KJC7
C	379	HIS	-	expression tag	UNP A0KJC7
C	380	HIS	-	expression tag	UNP A0KJC7
C	381	HIS	-	expression tag	UNP A0KJC7
C	382	HIS	-	expression tag	UNP A0KJC7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	88	Total O 88 88	0	0
2	B	99	Total O 99 99	0	0
2	A	105	Total O 105 105	0	0
2	C	88	Total O 88 88	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.85Å 101.32Å 78.43Å 90.00° 104.63° 90.00°	Depositor
Resolution (Å)	101.32 – 1.76 42.13 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.7 (101.32-1.76) 98.6 (42.13-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.76Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.272 , 0.306 0.268 , 0.304	Depositor DCC
R_{free} test set	2779 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtrriage
Anisotropy	0.551	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4964	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 90.36 % 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 2.3734e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

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	0.89	0/1174	0.90	4/1595 (0.3%)
1	B	0.91	0/1174	0.92	5/1595 (0.3%)
1	C	0.88	0/1174	0.95	4/1595 (0.3%)
1	D	0.88	0/1174	0.95	3/1595 (0.2%)
All	All	0.89	0/4696	0.93	16/6380 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	372	ARG	NE-CZ-NH2	9.85	125.22	120.30
1	B	372	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	C	248	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	C	311	LEU	CB-CG-CD2	-6.65	99.70	111.00
1	A	259	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	C	259	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	355	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	248	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	259	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	306	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	D	290	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	365	PHE	CB-CG-CD1	5.34	124.54	120.80
1	A	365	PHE	CB-CG-CD1	5.16	124.42	120.80
1	D	372	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	C	259	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	231	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1146	0	1132	1	0
1	B	1146	0	1132	2	0
1	C	1146	0	1132	2	0
1	D	1146	0	1132	1	0
2	A	105	0	0	0	0
2	B	99	0	0	1	0
2	C	88	0	0	0	0
2	D	88	0	0	0	0
All	All	4964	0	4528	6	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.

All (6) 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:311:LEU:HD21	1:C:320:GLY:HA3	1.79	0.64
1:B:301:GLN:NE2	2:B:401:HOH:O	2.34	0.59
1:C:301:GLN:HE21	1:C:305:GLN:HE21	1.55	0.53
1:D:297:ASN:OD1	1:D:298:ALA:N	2.46	0.47
1:B:232:ARG:O	1:B:236:GLN:HG2	2.21	0.41
1:A:348:LEU:HD12	1:A:374:LEU:HD21	2.03	0.41

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	144/382 (38%)	142 (99%)	2 (1%)	0	100	100
1	B	144/382 (38%)	142 (99%)	2 (1%)	0	100	100
1	C	144/382 (38%)	143 (99%)	1 (1%)	0	100	100
1	D	144/382 (38%)	142 (99%)	2 (1%)	0	100	100
All	All	576/1528 (38%)	569 (99%)	7 (1%)	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	115/297 (39%)	115 (100%)	0	100	100
1	B	115/297 (39%)	115 (100%)	0	100	100
1	C	115/297 (39%)	114 (99%)	1 (1%)	78	67
1	D	115/297 (39%)	115 (100%)	0	100	100
All	All	460/1188 (39%)	459 (100%)	1 (0%)	93	91

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

Mol	Chain	Res	Type
1	C	285	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	301	GLN
1	C	301	GLN
1	C	305	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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	146/382 (38%)	-0.06	0 100 100	13, 20, 38, 47	0
1	B	146/382 (38%)	-0.08	1 (0%) 87 92	13, 21, 36, 52	0
1	C	146/382 (38%)	-0.08	0 100 100	13, 21, 37, 46	0
1	D	146/382 (38%)	-0.10	1 (0%) 87 92	12, 21, 37, 54	0
All	All	584/1528 (38%)	-0.08	2 (0%) 94 95	12, 21, 37, 54	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	275	ALA	3.4
1	B	275	ALA	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.