Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:37 PM EDT

PDB ID	:	3WPP
Title	:	Acinetobacter sp. Tol 5 AtaA YDD-DALL3 domains in C-terminal stalk fused to GCN4 adaptors (CstalkC1iii)
Authors	:	Koiwai, K.; Hartmann, M.D.; Yoshimoto, S.; Nur 'Izzah, N.; Suzuki, A.; Linke, D.; Lupas, A.N.; Hori, K.
Deposited on	:	2014-01-15
Resolution	:	1.95 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 (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:

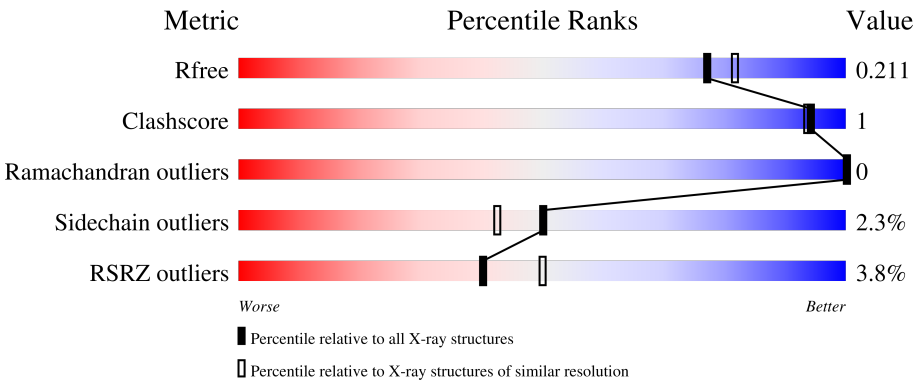
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

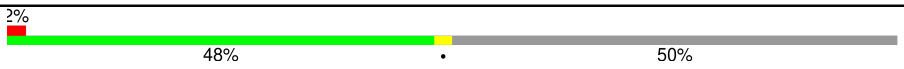
The reported resolution of this entry is 1.95 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	207	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 905 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 Trimeric autotransporter adhesin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	104	794	485	140	169	0	2	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3305	MET	-	expression tag	UNP K7ZP88
A	3306	LYS	-	expression tag	UNP K7ZP88
A	3307	GLN	-	expression tag	UNP K7ZP88
A	3308	ILE	-	expression tag	UNP K7ZP88
A	3309	GLU	-	expression tag	UNP K7ZP88
A	3310	ASP	-	expression tag	UNP K7ZP88
A	3311	LYS	-	expression tag	UNP K7ZP88
A	3312	ILE	-	expression tag	UNP K7ZP88
A	3313	GLU	-	expression tag	UNP K7ZP88
A	3314	GLU	-	expression tag	UNP K7ZP88
A	3315	ILE	-	expression tag	UNP K7ZP88
A	3316	LEU	-	expression tag	UNP K7ZP88
A	3317	SER	-	expression tag	UNP K7ZP88
A	3318	LYS	-	expression tag	UNP K7ZP88
A	3319	ILE	-	expression tag	UNP K7ZP88
A	3320	TYR	-	expression tag	UNP K7ZP88
A	3321	HIS	-	expression tag	UNP K7ZP88
A	3322	ILE	-	expression tag	UNP K7ZP88
A	3323	GLU	-	expression tag	UNP K7ZP88
A	3324	ASN	-	expression tag	UNP K7ZP88
A	3325	GLU	-	expression tag	UNP K7ZP88
A	3326	ILE	-	expression tag	UNP K7ZP88
A	3327	ALA	-	expression tag	UNP K7ZP88
A	3328	ARG	-	expression tag	UNP K7ZP88
A	3329	ILE	-	expression tag	UNP K7ZP88
A	3330	LYS	-	expression tag	UNP K7ZP88
A	3331	LYS	-	expression tag	UNP K7ZP88

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3332	LEU	-	expression tag	UNP K7ZP88
A	3333	ILE	-	expression tag	UNP K7ZP88
A	3475	MET	-	expression tag	UNP K7ZP88
A	3476	LYS	-	expression tag	UNP K7ZP88
A	3477	GLN	-	expression tag	UNP K7ZP88
A	3478	ILE	-	expression tag	UNP K7ZP88
A	3479	GLU	-	expression tag	UNP K7ZP88
A	3480	ASP	-	expression tag	UNP K7ZP88
A	3481	LYS	-	expression tag	UNP K7ZP88
A	3482	ILE	-	expression tag	UNP K7ZP88
A	3483	GLU	-	expression tag	UNP K7ZP88
A	3484	GLU	-	expression tag	UNP K7ZP88
A	3485	ILE	-	expression tag	UNP K7ZP88
A	3486	LEU	-	expression tag	UNP K7ZP88
A	3487	SER	-	expression tag	UNP K7ZP88
A	3488	LYS	-	expression tag	UNP K7ZP88
A	3489	ILE	-	expression tag	UNP K7ZP88
A	3490	TYR	-	expression tag	UNP K7ZP88
A	3491	HIS	-	expression tag	UNP K7ZP88
A	3492	ILE	-	expression tag	UNP K7ZP88
A	3493	GLU	-	expression tag	UNP K7ZP88
A	3494	ASN	-	expression tag	UNP K7ZP88
A	3495	GLU	-	expression tag	UNP K7ZP88
A	3496	ILE	-	expression tag	UNP K7ZP88
A	3497	ALA	-	expression tag	UNP K7ZP88
A	3498	ARG	-	expression tag	UNP K7ZP88
A	3499	ILE	-	expression tag	UNP K7ZP88
A	3500	LYS	-	expression tag	UNP K7ZP88
A	3501	LYS	-	expression tag	UNP K7ZP88
A	3502	LEU	-	expression tag	UNP K7ZP88
A	3503	ILE	-	expression tag	UNP K7ZP88
A	3504	LYS	-	expression tag	UNP K7ZP88
A	3505	LEU	-	expression tag	UNP K7ZP88
A	3506	HIS	-	expression tag	UNP K7ZP88
A	3507	HIS	-	expression tag	UNP K7ZP88
A	3508	HIS	-	expression tag	UNP K7ZP88
A	3509	HIS	-	expression tag	UNP K7ZP88
A	3510	HIS	-	expression tag	UNP K7ZP88
A	3511	HIS	-	expression tag	UNP K7ZP88

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0

- Molecule 3 is water.

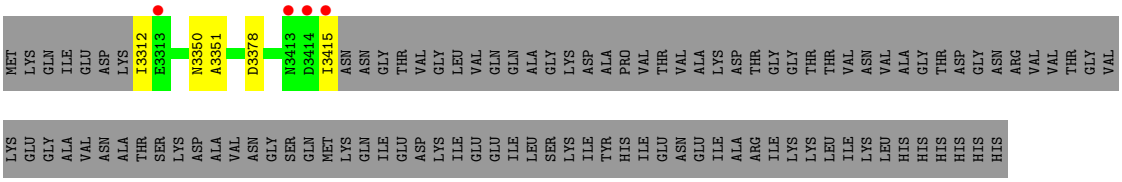
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	110	110	110	0	0

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: Trimeric autotransporter adhesin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	43.46Å 43.46Å 825.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.64 – 1.95 19.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.64-1.95) 99.8 (19.64-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.179 , 0.205 0.190 , 0.211	Depositor DCC
R_{free} test set	1160 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.968	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	905	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.57% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.59	0/804	0.70	1/1089 (0.1%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3378	ASP	CB-CG-OD1	5.57	123.31	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	794	0	790	2	0
2	A	1	0	0	0	0
3	A	110	0	0	0	0
All	All	905	0	790	2	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 (2) 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:A:3350[B]:ASN:HD22	1:A:3351:ALA:N	2.13	0.46

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	104/207 (50%)	104 (100%)	0	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	89/173 (51%)	87 (98%)	2 (2%)	52 44

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3312	ILE
1	A	3415	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3345	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	104/207 (50%)	-0.10	4 (3%) 40 50	17, 27, 77, 103	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3415	ILE	4.2
1	A	3313	GLU	3.2
1	A	3413	ASN	2.8
1	A	3414	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	A	3601	1/1	0.98	0.05	50,50,50,50	1

6.5 Other polymers (i)

There are no such residues in this entry.