



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4AKX / pdb_00004akx
Title : Structure of the heterodimeric complex ExoU-SpcU from the type III secretion system (T3SS) of *Pseudomonas aeruginosa*
Authors : Gendrin, C.; Contreras-Martel, C.; Bouillot, S.; Elsen, S.; Lemaire, D.; Skoufias, D.A.; Huber, P.; Attree, I.; Dessen, A.
Deposited on : 2012-02-29
Resolution : 2.94 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

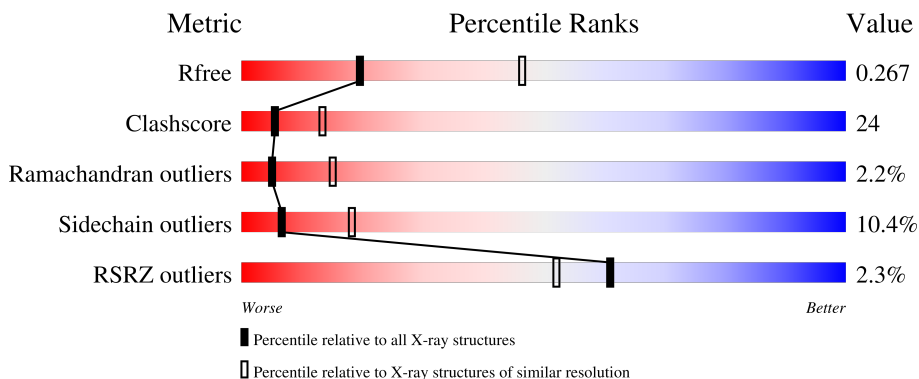
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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 $\leq 5\%$. 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	127	2% 47% 43% 5%
2	B	660	2% 48% 30% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5059 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 SPCU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	Se	0	1	0
			943	602	165	173	3			

- Molecule 2 is a protein called EXOU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	534	Total	C	N	O	Se	0	1	0
			4078	2531	738	796	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	GLY	-	expression tag	UNP Q02IF1
B	29	SER	-	expression tag	UNP Q02IF1

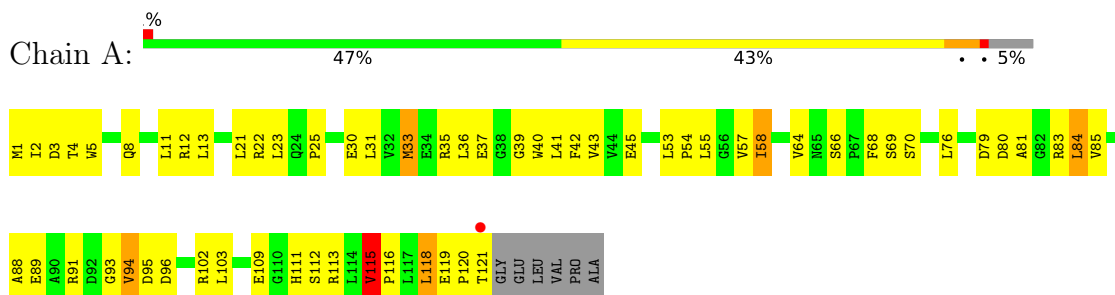
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	29	Total	O	0	0
			29	29		

3 Residue-property plots

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: SPCU



• Molecule 2: EXOU



F615	P616	S617	L618	Y619	R620	Q623	P624	D625	S626	L631	R632	E636	R639	T642	S643	P644	L651	I654	Y658	S659	A660	R661	GLY	PHE	LEU	ARG	PHE	GLY	LYS	PRO	LEU	SER	S672	T673	E676	M677	A678	K679	E685	PHE	THR
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.89Å 52.80Å 121.81Å 90.00° 127.18° 90.00°	Depositor
Resolution (Å)	97.05 – 2.94 97.05 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.7 (97.05-2.94) 98.7 (97.05-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.208 , 0.264 0.207 , 0.267	Depositor DCC
R_{free} test set	840 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5059	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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.

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	0.94	0/962	0.96	3/1312 (0.2%)
2	B	0.88	2/4119 (0.0%)	0.95	5/5545 (0.1%)
All	All	0.89	2/5081 (0.0%)	0.95	8/6857 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	327	SER	CB-OG	9.71	1.61	1.42
2	B	377	GLU	C-O	7.17	1.37	1.23

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	654	ILE	N-CA-C	6.87	117.02	110.42
2	B	575	GLN	N-CA-C	-5.29	105.59	111.36
2	B	106	SER	N-CA-C	5.24	117.03	108.55
1	A	58	ILE	CB-CA-C	-5.21	105.21	112.04
1	A	115	VAL	CA-C-N	-5.15	114.44	119.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	319	PHE	Peptide

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	943	0	961	58	0
2	B	4078	0	4115	187	0
3	A	9	0	0	2	0
3	B	29	0	0	3	0
All	All	5059	0	5076	239	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 24.

The worst 5 of 239 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:1[A]:MSE:SE	1:A:1[A]:MSE:CE	2.14	1.45
1:A:21:LEU:HB2	1:A:33:MSE:HE3	1.21	1.20
1:A:119:GLU:HB3	1:A:120:PRO:HD3	1.35	1.08
2:B:221:GLU:HB3	2:B:222:PRO:HD2	1.35	1.06
2:B:453:HIS:CE1	2:B:457:ARG:HH11	1.73	1.05

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	119/127 (94%)	108 (91%)	9 (8%)	2 (2%)	7	20
2	B	519/660 (79%)	468 (90%)	39 (8%)	12 (2%)	5	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	638/787 (81%)	576 (90%)	48 (8%)	14 (2%)	5	15

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
2	B	319	PHE
2	B	153	SER
2	B	324	GLN
2	B	412	LEU

5.3.2 Protein sidechains ⓘ

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	102/103 (99%)	94 (92%)	8 (8%)	11	28
2	B	440/517 (85%)	392 (89%)	48 (11%)	6	17
All	All	542/620 (87%)	486 (90%)	56 (10%)	7	18

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	279	ILE
2	B	677	MSE
2	B	423	VAL
2	B	672	SER
2	B	631	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	567	HIS
2	B	623	GLN
2	B	598	GLN

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Mol	Chain	Res	Type
2	B	411	GLN
2	B	566	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 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 [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	119/127 (93%)	-0.35	1 (0%) 82 77	50, 76, 130, 190	0
2	B	521/660 (78%)	-0.08	14 (2%) 56 47	33, 98, 175, 206	1 (0%)
All	All	640/787 (81%)	-0.13	15 (2%) 61 52	33, 94, 174, 206	1 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	347	VAL	3.3
2	B	322	VAL	2.9
2	B	658	TYR	2.7
2	B	294	PRO	2.6
2	B	202	ILE	2.6

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 oligosaccharides 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.