



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:25 PM UTC

PDB ID : 4YWH / pdb_00004ywh
Title : CRYSTAL STRUCTURE OF AN ABC TRANSPORTER SOLUTE BINDING PROTEIN (IPR025997) FROM ACTINOBACILLUS SUCCINOGENES 130Z (Asuc_0499, TARGET EFI-511068) WITH BOUND D-XYLOSE
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Deposited on : 2015-03-20
Resolution : 2.35 Å(reported)

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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)

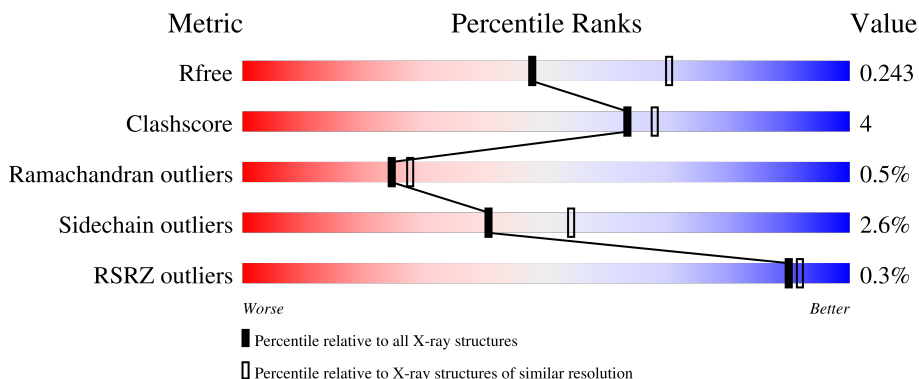
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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 $\leq 5\%$. 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	332	 82% 11% 7%
1	B	332	 84% 8% 8%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9624 atoms, of which 4752 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 ABC TRANSPORTER SOLUTE BINDING PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	310	Total	C	H	N	O	Se	0	0	0
			4752	1480	2398	401	467	6			
1	B	307	Total	C	H	N	O	Se	0	0	0
			4684	1463	2354	394	467	6			

There are 46 discrepancies between the modelled and reference sequences:

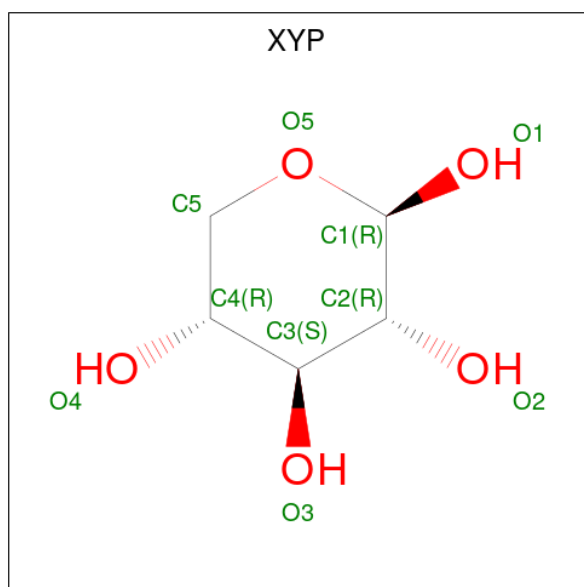
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP A6VLM7
A	2	HIS	-	expression tag	UNP A6VLM7
A	3	HIS	-	expression tag	UNP A6VLM7
A	4	HIS	-	expression tag	UNP A6VLM7
A	5	HIS	-	expression tag	UNP A6VLM7
A	6	HIS	-	expression tag	UNP A6VLM7
A	7	HIS	-	expression tag	UNP A6VLM7
A	8	SER	-	expression tag	UNP A6VLM7
A	9	SER	-	expression tag	UNP A6VLM7
A	10	GLY	-	expression tag	UNP A6VLM7
A	11	VAL	-	expression tag	UNP A6VLM7
A	12	ASP	-	expression tag	UNP A6VLM7
A	13	LEU	-	expression tag	UNP A6VLM7
A	14	GLY	-	expression tag	UNP A6VLM7
A	15	THR	-	expression tag	UNP A6VLM7
A	16	GLU	-	expression tag	UNP A6VLM7
A	17	ASN	-	expression tag	UNP A6VLM7
A	18	LEU	-	expression tag	UNP A6VLM7
A	19	TYR	-	expression tag	UNP A6VLM7
A	20	PHE	-	expression tag	UNP A6VLM7
A	21	GLN	-	expression tag	UNP A6VLM7
A	22	SER	-	expression tag	UNP A6VLM7
A	23	MSE	-	expression tag	UNP A6VLM7
B	1	MSE	-	initiating methionine	UNP A6VLM7
B	2	HIS	-	expression tag	UNP A6VLM7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	HIS	-	expression tag	UNP A6VLM7
B	4	HIS	-	expression tag	UNP A6VLM7
B	5	HIS	-	expression tag	UNP A6VLM7
B	6	HIS	-	expression tag	UNP A6VLM7
B	7	HIS	-	expression tag	UNP A6VLM7
B	8	SER	-	expression tag	UNP A6VLM7
B	9	SER	-	expression tag	UNP A6VLM7
B	10	GLY	-	expression tag	UNP A6VLM7
B	11	VAL	-	expression tag	UNP A6VLM7
B	12	ASP	-	expression tag	UNP A6VLM7
B	13	LEU	-	expression tag	UNP A6VLM7
B	14	GLY	-	expression tag	UNP A6VLM7
B	15	THR	-	expression tag	UNP A6VLM7
B	16	GLU	-	expression tag	UNP A6VLM7
B	17	ASN	-	expression tag	UNP A6VLM7
B	18	LEU	-	expression tag	UNP A6VLM7
B	19	TYR	-	expression tag	UNP A6VLM7
B	20	PHE	-	expression tag	UNP A6VLM7
B	21	GLN	-	expression tag	UNP A6VLM7
B	22	SER	-	expression tag	UNP A6VLM7
B	23	MSE	-	expression tag	UNP A6VLM7

- Molecule 2 is beta-D-xylopyranose (CCD ID: XYP) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total	O	0	0
			85	85		
3	B	83	Total	O	0	0
			83	83		

- Molecule 1: ABC TRANSPORTER SOLUTE BINDING PROTEIN

MSE	H1S	H1S	H1S	H1S	H1S	H1S	H1S	SER	GLY	VAL	ASP	LEU	GLY	THR	ASN	LEU	Tyr	PHE	GLN	SER	
L205	N210	L230	L235	D244	Q245	A249	R253	V263	Y264	K285	P286	L293	L305	T311	D316	S317	T318	V319	I320	K321	K332
Q41	R44	K49	S72	K103	F127	E130	Y149	D158	K162	R165	M169	K170	V171	L172	Q173	P174	L175	I176	K180	I181	M201

- Molecule 1: ABC TRANSPORTER SOLUTE BINDING PROTEIN

Amino Acid	Mutations per Site (approx.)
MSE	0.95
HIS	0.75
HIS	0.75
HIS	0.75
HIS	0.75
HIS	0.75
SER	0.75
GLY	0.75
VAL	0.75
ASP	0.75
LEU	0.75
GLY	0.75
THR	0.75
ASN	0.75
LEU	0.75
Tyr	0.75
PHE	0.75
GLN	0.75
SER	0.75
MSE	0.75
LYS	0.75
D25	0.75
Q41	0.75
K42	0.75
D43	0.75
R44	0.75
D93	0.75
L110	0.75
V125	0.75
D128	0.75
K131	0.75
Y149	0.75
F150	0.75
L151	0.75
G154	0.75
R165	0.75
M169	0.75
Q173	0.75
P174	0.75
I181	0.75
D186	0.75
V192	0.75
I192	0.75
K196	0.75
A197	0.75
L198	0.75
N219	0.75
S231	0.75
Q244	0.75
D245	0.75
Y264	0.75
V310	0.75
Y331	0.75
LYS	0.75

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.80Å 37.67Å 105.34Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	24.84 – 2.35 24.84 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.2 (24.84-2.35) 94.5 (24.84-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.157 , 0.238 0.165 , 0.243	Depositor DCC
R_{free} test set	1209 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9624	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.82	1/2374 (0.0%)	0.98	1/3196 (0.0%)
1	B	0.85	0/2350	0.98	1/3169 (0.0%)
All	All	0.83	1/4724 (0.0%)	0.98	2/6365 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	ALA	CA-CB	6.80	1.64	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ASP	N-CA-C	-6.29	104.34	111.07
1	A	176	ILE	N-CA-C	-5.13	105.71	110.53

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	2354	2398	2396	24	0
1	B	2330	2354	2354	14	0
2	A	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
3	A	85	0	0	1	0
3	B	83	0	0	2	0
All	All	4872	4752	4750	38	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 4.

The worst 5 of 38 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:103:LYS:NZ	3:A:501:HOH:O	2.13	0.79
1:A:41:GLN:OE1	1:A:44:ARG:NH2	2.22	0.72
1:B:41:GLN:OE1	1:B:44:ARG:NH2	2.25	0.69
1:A:316:ASP:HA	1:A:320:ILE:CG1	2.24	0.67
1:A:245:ASP:OD1	2:A:401:XYP:O1	2.17	0.62

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	308/332 (93%)	299 (97%)	7 (2%)	2 (1%)	21	24
1	B	305/332 (92%)	295 (97%)	9 (3%)	1 (0%)	36	43
All	All	613/664 (92%)	594 (97%)	16 (3%)	3 (0%)	24	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	ASP

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Mol	Chain	Res	Type
1	A	245	ASP
1	A	266	PRO

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	254/269 (94%)	243 (96%)	11 (4%)	26	34
1	B	252/269 (94%)	250 (99%)	2 (1%)	73	84
All	All	506/538 (94%)	493 (97%)	13 (3%)	40	54

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	LEU
1	A	319	VAL
1	B	231	SER
1	A	332	LYS
1	B	181	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	61	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	XYP	B	401	-	10,10,10	1.50	2 (20%)	14,14,14	1.42	3 (21%)
2	XYP	A	401	-	10,10,10	1.46	1 (10%)	14,14,14	1.77	6 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYP	B	401	-	-	-	0/1/1/1
2	XYP	A	401	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	XYP	O5-C1	3.31	1.48	1.43
2	B	401	XYP	O5-C5	3.00	1.48	1.43
2	B	401	XYP	O5-C1	2.99	1.48	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	XYP	O5-C5-C4	-2.98	103.67	110.79
2	A	401	XYP	C5-C4-C3	2.85	113.79	109.64
2	A	401	XYP	C1-C2-C3	-2.55	105.16	110.36
2	B	401	XYP	O4-C4-C5	-2.21	104.17	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	XYP	O2-C2-C1	-2.20	104.16	109.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	XYP	2	0

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	303/332 (91%)	-0.47	1 (0%) 90 92	23, 38, 66, 99	0
1	B	301/332 (90%)	-0.53	1 (0%) 90 92	20, 36, 61, 106	0
All	All	604/664 (90%)	-0.50	2 (0%) 90 92	20, 37, 65, 106	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	ASP	2.5
1	A	311	THR	2.4

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](#)

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	XYP	A	401	10/10	0.94	0.11	17,30,41,42	0
2	XYP	B	401	10/10	0.98	0.06	20,23,27,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.