



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:01 PM UTC

PDB ID : 8T3J / pdb_00008t3j
Title : Crystal structure of native exfoliative toxin C (ExhC) from *Mammaliicoccus sciuri*
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Deposited on : 2023-06-07
Resolution : 2.71 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
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

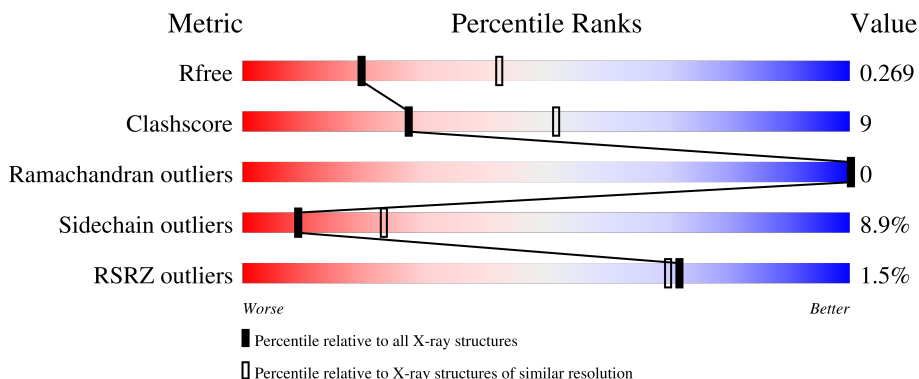
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

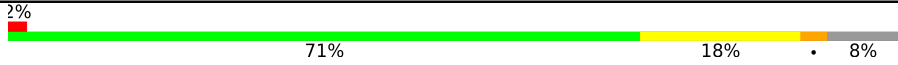
The reported resolution of this entry is 2.71 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	258	
1	B	258	
1	C	258	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10933 atoms, of which 5375 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 Exfoliative toxin C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	238	Total	C	H	N	O	S	59	0	0
			3626	1158	1794	315	358	1			
1	B	239	Total	C	H	N	O	S	59	0	0
			3644	1163	1802	317	361	1			
1	C	239	Total	C	H	N	O	S	63	0	0
			3607	1153	1779	316	358	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP F6M8N2
A	244	GLY	-	expression tag	UNP F6M8N2
A	245	GLY	-	expression tag	UNP F6M8N2
A	246	GLU	-	expression tag	UNP F6M8N2
A	247	ASN	-	expression tag	UNP F6M8N2
A	248	LEU	-	expression tag	UNP F6M8N2
A	249	TYR	-	expression tag	UNP F6M8N2
A	250	PHE	-	expression tag	UNP F6M8N2
A	251	GLN	-	expression tag	UNP F6M8N2
A	252	SER	-	expression tag	UNP F6M8N2
A	253	HIS	-	expression tag	UNP F6M8N2
A	254	HIS	-	expression tag	UNP F6M8N2
A	255	HIS	-	expression tag	UNP F6M8N2
A	256	HIS	-	expression tag	UNP F6M8N2
A	257	HIS	-	expression tag	UNP F6M8N2
A	258	HIS	-	expression tag	UNP F6M8N2
B	1	MET	-	initiating methionine	UNP F6M8N2
B	244	GLY	-	expression tag	UNP F6M8N2
B	245	GLY	-	expression tag	UNP F6M8N2
B	246	GLU	-	expression tag	UNP F6M8N2
B	247	ASN	-	expression tag	UNP F6M8N2
B	248	LEU	-	expression tag	UNP F6M8N2
B	249	TYR	-	expression tag	UNP F6M8N2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	250	PHE	-	expression tag	UNP F6M8N2
B	251	GLN	-	expression tag	UNP F6M8N2
B	252	SER	-	expression tag	UNP F6M8N2
B	253	HIS	-	expression tag	UNP F6M8N2
B	254	HIS	-	expression tag	UNP F6M8N2
B	255	HIS	-	expression tag	UNP F6M8N2
B	256	HIS	-	expression tag	UNP F6M8N2
B	257	HIS	-	expression tag	UNP F6M8N2
B	258	HIS	-	expression tag	UNP F6M8N2
C	1	MET	-	initiating methionine	UNP F6M8N2
C	244	GLY	-	expression tag	UNP F6M8N2
C	245	GLY	-	expression tag	UNP F6M8N2
C	246	GLU	-	expression tag	UNP F6M8N2
C	247	ASN	-	expression tag	UNP F6M8N2
C	248	LEU	-	expression tag	UNP F6M8N2
C	249	TYR	-	expression tag	UNP F6M8N2
C	250	PHE	-	expression tag	UNP F6M8N2
C	251	GLN	-	expression tag	UNP F6M8N2
C	252	SER	-	expression tag	UNP F6M8N2
C	253	HIS	-	expression tag	UNP F6M8N2
C	254	HIS	-	expression tag	UNP F6M8N2
C	255	HIS	-	expression tag	UNP F6M8N2
C	256	HIS	-	expression tag	UNP F6M8N2
C	257	HIS	-	expression tag	UNP F6M8N2
C	258	HIS	-	expression tag	UNP F6M8N2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	22	Total O 22 22	0	0
2	B	15	Total O 15 15	0	0
2	C	19	Total O 19 19	0	0

- Molecule 1: Exfoliative toxin C



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	167.09Å 167.09Å 157.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.28 – 2.71 47.28 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.28-2.71) 99.8 (47.28-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.211 , 0.270 0.212 , 0.269	Depositor DCC
R_{free} test set	1534 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10933	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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	0.64	0/1872	1.13	1/2531 (0.0%)
1	B	0.64	0/1882	1.13	1/2543 (0.0%)
1	C	0.63	0/1868	1.13	1/2527 (0.0%)
All	All	0.64	0/5622	1.13	3/7601 (0.0%)

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
1	A	0	2
1	B	0	1
1	C	0	3
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	230	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	93	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	141	LYS	CB-CA-C	5.04	117.84	109.53

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	ARG	Sidechain
1	A	48	ARG	Sidechain
1	B	90	ARG	Sidechain
1	C	112	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	C	90	ARG	Sidechain

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	1832	1794	1781	32	0
1	B	1842	1802	1789	30	0
1	C	1828	1779	1758	37	0
2	A	22	0	0	3	0
2	B	15	0	0	1	0
2	C	19	0	0	1	0
All	All	5558	5375	5328	99	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 9.

The worst 5 of 99 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:113:ASP:O	1:C:123:SER:OG	1.73	1.06
1:A:211:HIS:HE1	2:A:310:HOH:O	1.57	0.86
1:B:5:SER:N	2:B:301:HOH:O	2.18	0.76
1:C:70:ASN:HB3	1:C:72:HIS:CD2	2.32	0.65
1:C:81:PRO:O	1:C:108:ALA:HB3	1.98	0.64

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	236/258 (92%)	224 (95%)	12 (5%)	0	100	100
1	B	237/258 (92%)	226 (95%)	11 (5%)	0	100	100
1	C	237/258 (92%)	227 (96%)	10 (4%)	0	100	100
All	All	710/774 (92%)	677 (95%)	33 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	199/220 (90%)	183 (92%)	16 (8%)	11	28
1	B	200/220 (91%)	181 (90%)	19 (10%)	8	20
1	C	196/220 (89%)	178 (91%)	18 (9%)	8	22
All	All	595/660 (90%)	542 (91%)	53 (9%)	9	23

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	95	SER
1	C	15	ASN
1	C	132	GLU
1	B	113	ASP
1	B	126	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	72	HIS
1	C	211	HIS
1	C	240	GLN

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Mol	Chain	Res	Type
1	C	217	HIS
1	B	15	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	238/258 (92%)	-0.01	5 (2%) 63 61	47, 76, 125, 149	0
1	B	239/258 (92%)	0.03	2 (0%) 82 81	44, 76, 128, 148	0
1	C	239/258 (92%)	0.22	4 (1%) 69 67	44, 82, 136, 158	0
All	All	716/774 (92%)	0.08	11 (1%) 72 70	44, 78, 129, 158	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	ILE	3.8
1	A	183	PHE	3.5
1	C	183	PHE	3.1
1	C	238	LEU	3.1
1	C	242	ILE	3.1

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.