



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:14 AM UTC

PDB ID : 9DCT / pdb\_00009dct  
Title : Structure of the TelB-associated type VII secretion system chaperone SIR\_0178  
Authors : Gkrakopoulou, P.; Kim, Y.; Whitney, J.C.  
Deposited on : 2024-08-27  
Resolution : 3.24 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](mailto: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>.

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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

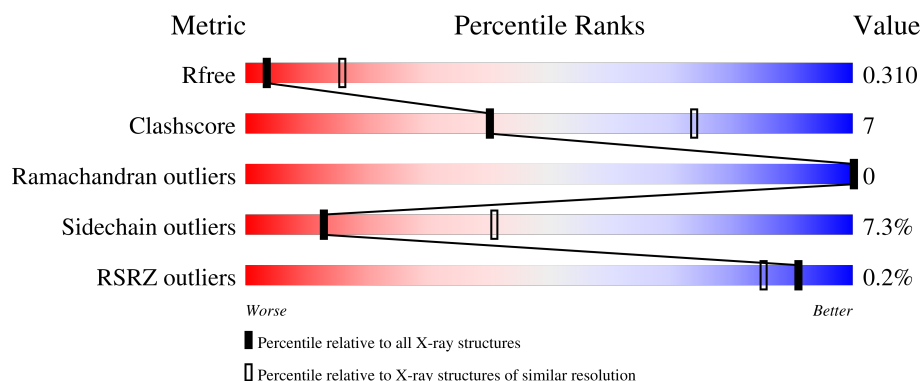
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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  $\geq 3$ , 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	251	<div> <div> <div></div> <div>69%</div> <div>20%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	251	<div> <div> <div>72%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	251	<div> <div> <div>71%</div> <div>17%</div> <div>12%</div> </div> </div>
1	D	251	<div> <div> <div>67%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7319 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 DUF4176 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1848	1210	282	350	6			
1	B	225	Total	C	N	O	S	0	0	0
			1826	1196	279	345	6			
1	C	221	Total	C	N	O	S	0	0	0
			1799	1181	274	338	6			
1	D	228	Total	C	N	O	S	0	0	0
			1845	1208	282	348	7			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP T1ZCG6
A	-12	GLY	-	expression tag	UNP T1ZCG6
A	-11	SER	-	expression tag	UNP T1ZCG6
A	-10	SER	-	expression tag	UNP T1ZCG6
A	-9	HIS	-	expression tag	UNP T1ZCG6
A	-8	HIS	-	expression tag	UNP T1ZCG6
A	-7	HIS	-	expression tag	UNP T1ZCG6
A	-6	HIS	-	expression tag	UNP T1ZCG6
A	-5	HIS	-	expression tag	UNP T1ZCG6
A	-4	HIS	-	expression tag	UNP T1ZCG6
A	-3	SER	-	expression tag	UNP T1ZCG6
A	-2	GLN	-	expression tag	UNP T1ZCG6
A	-1	ASP	-	expression tag	UNP T1ZCG6
A	0	PRO	-	expression tag	UNP T1ZCG6
B	-13	MET	-	initiating methionine	UNP T1ZCG6
B	-12	GLY	-	expression tag	UNP T1ZCG6
B	-11	SER	-	expression tag	UNP T1ZCG6
B	-10	SER	-	expression tag	UNP T1ZCG6
B	-9	HIS	-	expression tag	UNP T1ZCG6
B	-8	HIS	-	expression tag	UNP T1ZCG6
B	-7	HIS	-	expression tag	UNP T1ZCG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP T1ZCG6
B	-5	HIS	-	expression tag	UNP T1ZCG6
B	-4	HIS	-	expression tag	UNP T1ZCG6
B	-3	SER	-	expression tag	UNP T1ZCG6
B	-2	GLN	-	expression tag	UNP T1ZCG6
B	-1	ASP	-	expression tag	UNP T1ZCG6
B	0	PRO	-	expression tag	UNP T1ZCG6
C	-13	MET	-	initiating methionine	UNP T1ZCG6
C	-12	GLY	-	expression tag	UNP T1ZCG6
C	-11	SER	-	expression tag	UNP T1ZCG6
C	-10	SER	-	expression tag	UNP T1ZCG6
C	-9	HIS	-	expression tag	UNP T1ZCG6
C	-8	HIS	-	expression tag	UNP T1ZCG6
C	-7	HIS	-	expression tag	UNP T1ZCG6
C	-6	HIS	-	expression tag	UNP T1ZCG6
C	-5	HIS	-	expression tag	UNP T1ZCG6
C	-4	HIS	-	expression tag	UNP T1ZCG6
C	-3	SER	-	expression tag	UNP T1ZCG6
C	-2	GLN	-	expression tag	UNP T1ZCG6
C	-1	ASP	-	expression tag	UNP T1ZCG6
C	0	PRO	-	expression tag	UNP T1ZCG6
D	-13	MET	-	initiating methionine	UNP T1ZCG6
D	-12	GLY	-	expression tag	UNP T1ZCG6
D	-11	SER	-	expression tag	UNP T1ZCG6
D	-10	SER	-	expression tag	UNP T1ZCG6
D	-9	HIS	-	expression tag	UNP T1ZCG6
D	-8	HIS	-	expression tag	UNP T1ZCG6
D	-7	HIS	-	expression tag	UNP T1ZCG6
D	-6	HIS	-	expression tag	UNP T1ZCG6
D	-5	HIS	-	expression tag	UNP T1ZCG6
D	-4	HIS	-	expression tag	UNP T1ZCG6
D	-3	SER	-	expression tag	UNP T1ZCG6
D	-2	GLN	-	expression tag	UNP T1ZCG6
D	-1	ASP	-	expression tag	UNP T1ZCG6
D	0	PRO	-	expression tag	UNP T1ZCG6

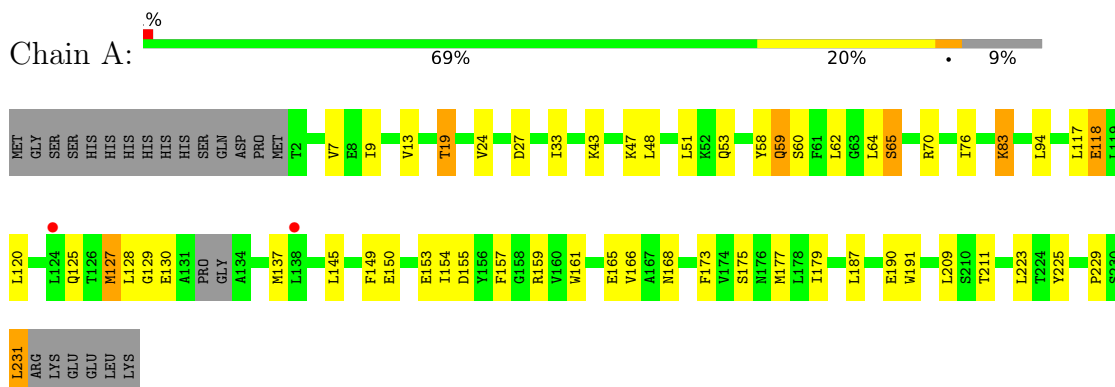
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

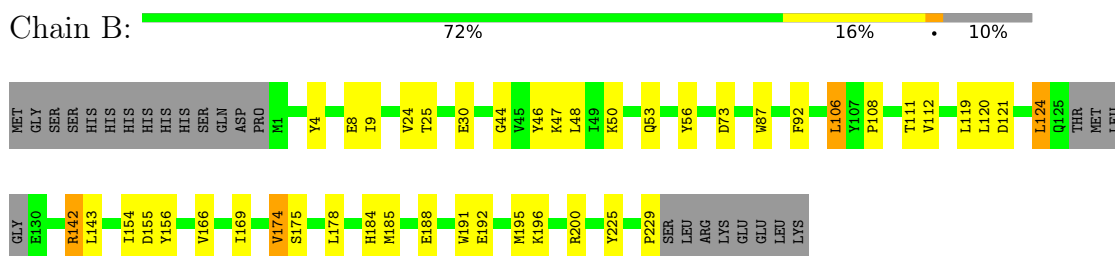
### 3 Residue-property plots [i](#)

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.

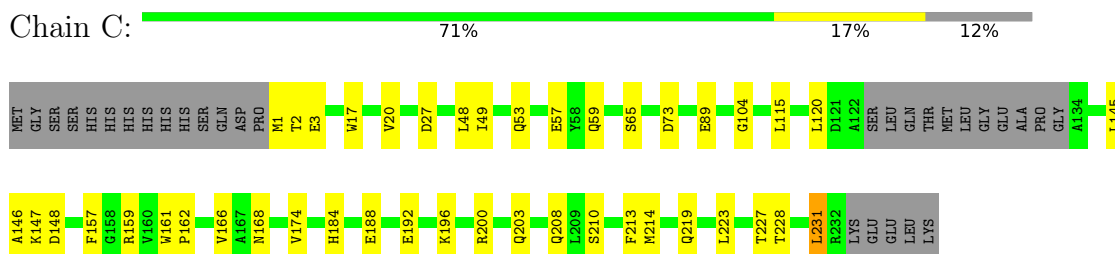
#### • Molecule 1: DUF4176 domain-containing protein



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LEU	L115	MET	GLY
ARG	D116	GLY	SER
LYS	L117	SER	SER
GLU	E118	HIS	HIS
GLU	L119	HIS	HIS
LEU	L120	HIS	HIS
LYS	L124	HIS	HIS
		HIS	HIS
		SER	
	M127	GLN	
	L128	GLN	
	G129	ASP	PRO
	GLU	ASP	PRO
	ALA	PRO	
	P132	M1	
	G133		
	A134	Y4	
	L135		
		I9	
	G140	F10	
	R141	P11	
	R142	E12	
		V13	
	L145		
	A146	W17	
	K147	P18	
	D148	T19	
	F149		
		V24	
	Y152		
		L48	
	D155	I49	
	Y156	K50	
	F157	L51	
		K52	
		Q53	
	P162		
		E57	
	V166		
		F61	
	I169		
	P170		
		L64	
	V174		
	S175		
		L67	
	L178	F68	
	I179	E69	
	K180	R70	
	L199	I76	
		L77	
	Q203	K81	
	L204		
	Q208	I86	
	L209	E89	
	A212	I99	
	S230	E114	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.81Å 69.85Å 253.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.34 – 3.24 46.34 – 3.24	Depositor EDS
% Data completeness (in resolution range)	92.0 (46.34-3.24) 92.6 (46.34-3.24)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.259 , 0.308 0.259 , 0.310	Depositor DCC
$R_{free}$ test set	941 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	123.5	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 104.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.08	0/1890	0.24	0/2566
1	B	0.08	0/1869	0.24	0/2538
1	C	0.07	0/1841	0.22	0/2499
1	D	0.08	0/1888	0.23	0/2562
All	All	0.08	0/7488	0.23	0/10165

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1848	0	1831	30	0
1	B	1826	0	1807	20	0
1	C	1799	0	1784	21	0
1	D	1845	0	1832	33	0
2	A	1	0	0	0	0
All	All	7319	0	7254	96	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 7.



The worst 5 of 96 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:B:120:LEU:HD22	1:B:178:LEU:HD21	1.79	0.63
1:C:59:GLN:HG2	1:C:65:SER:HB2	1.83	0.61
1:A:43:LYS:NZ	1:A:179:ILE:O	2.29	0.60
1:D:114:GLU:O	1:D:180:LYS:N	2.31	0.59
1:B:155:ASP:HB2	1:B:175:SER:HA	1.84	0.59

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	224/251 (89%)	210 (94%)	14 (6%)	0	100	100
1	B	221/251 (88%)	213 (96%)	8 (4%)	0	100	100
1	C	217/251 (86%)	209 (96%)	8 (4%)	0	100	100
1	D	224/251 (89%)	213 (95%)	11 (5%)	0	100	100
All	All	886/1004 (88%)	845 (95%)	41 (5%)	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	202/223 (91%)	184 (91%)	18 (9%)	9	32
1	B	199/223 (89%)	185 (93%)	14 (7%)	14	42
1	C	196/223 (88%)	186 (95%)	10 (5%)	21	52
1	D	202/223 (91%)	186 (92%)	16 (8%)	11	38
All	All	799/892 (90%)	741 (93%)	58 (7%)	13	41

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	169	ILE
1	D	147	LYS
1	C	73	ASP
1	D	142	ARG
1	D	124	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	75	GLN
1	D	53	GLN
1	D	168	ASN
1	A	184	HIS
1	A	125	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	228/251 (90%)	-0.41	2 (0%) 81 64	106, 148, 184, 197	0
1	B	225/251 (89%)	-0.43	0 100 100	94, 130, 166, 206	0
1	C	221/251 (88%)	-0.52	0 100 100	110, 140, 178, 209	0
1	D	228/251 (90%)	-0.39	0 100 100	102, 164, 207, 223	0
All	All	902/1004 (89%)	-0.44	2 (0%) 91 85	94, 145, 195, 223	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	LEU	2.2
1	A	124	LEU	2.2

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CL	A	301	1/1	0.84	0.16	138,138,138,138	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.