



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:21 PM UTC

PDB ID : 6SUP / pdb_00006sup
Title : Crystal Structure of TcdB2-TccC3-Cdc42
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Deposited on : 2019-09-16
Resolution : 2.00 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
Xtrriage (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

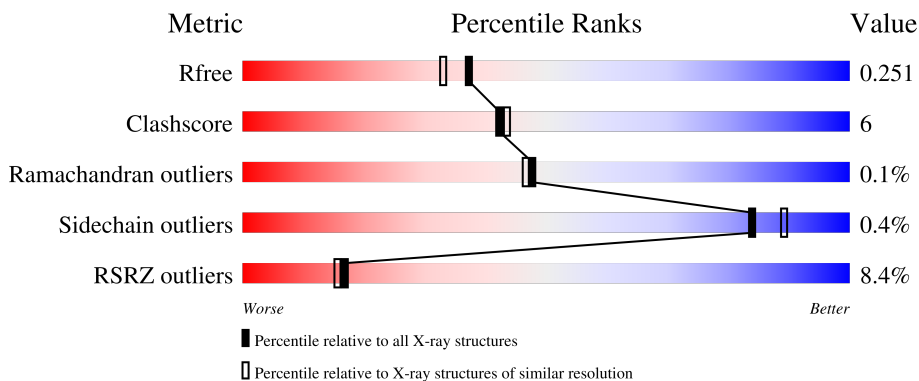
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	2128	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18283 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 TcdB2,TccC3,Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	2128	17001	10657	3017	3294	33	1	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1017	VAL	GLY	conflict	UNP Q8GF99
A	1483	ILE	-	linker	UNP Q8GF99
A	1484	ASP	-	linker	UNP Q8GF99
A	1485	PRO	-	linker	UNP Q8GF99
A	1486	LYS	-	linker	UNP Q8GF99
A	1487	LEU	-	linker	UNP Q8GF99
A	1488	TYR	-	linker	UNP Q8GF99
A	1489	GLN	-	linker	UNP Q8GF99
A	1490	LYS	-	linker	UNP Q8GF99
A	1491	THR	-	linker	UNP Q8GF99
A	1492	PRO	-	linker	UNP Q8GF99
A	1493	THR	-	linker	UNP Q8GF99
A	1494	VAL	-	linker	UNP Q8GF99
A	1495	SER	-	linker	UNP Q8GF99
A	1496	VAL	-	linker	UNP Q8GF99
A	1497	TYR	-	linker	UNP Q8GF99
A	1498	ASP	-	linker	UNP Q8GF99
A	1499	ASN	-	linker	UNP Q8GF99
A	1500	ARG	-	linker	UNP Q8GF99
A	1501	GLY	-	linker	UNP Q8GF99
A	1502	LEU	-	linker	UNP Q8GF99
A	1503	ILE	-	linker	UNP Q8GF99
A	1504	ILE	-	linker	UNP Q8GF99
A	1505	ARG	-	linker	UNP Q8GF99
A	1506	ASN	-	linker	UNP Q8GF99
A	1507	ILE	-	linker	UNP Q8GF99
A	1508	ASP	-	linker	UNP Q8GF99

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1509	PHE	-	linker	UNP Q8GF99
A	1510	HIS	-	linker	UNP Q8GF99
A	1511	ARG	-	linker	UNP Q8GF99
A	1512	THR	-	linker	UNP Q8GF99
A	1513	THR	-	linker	UNP Q8GF99

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0

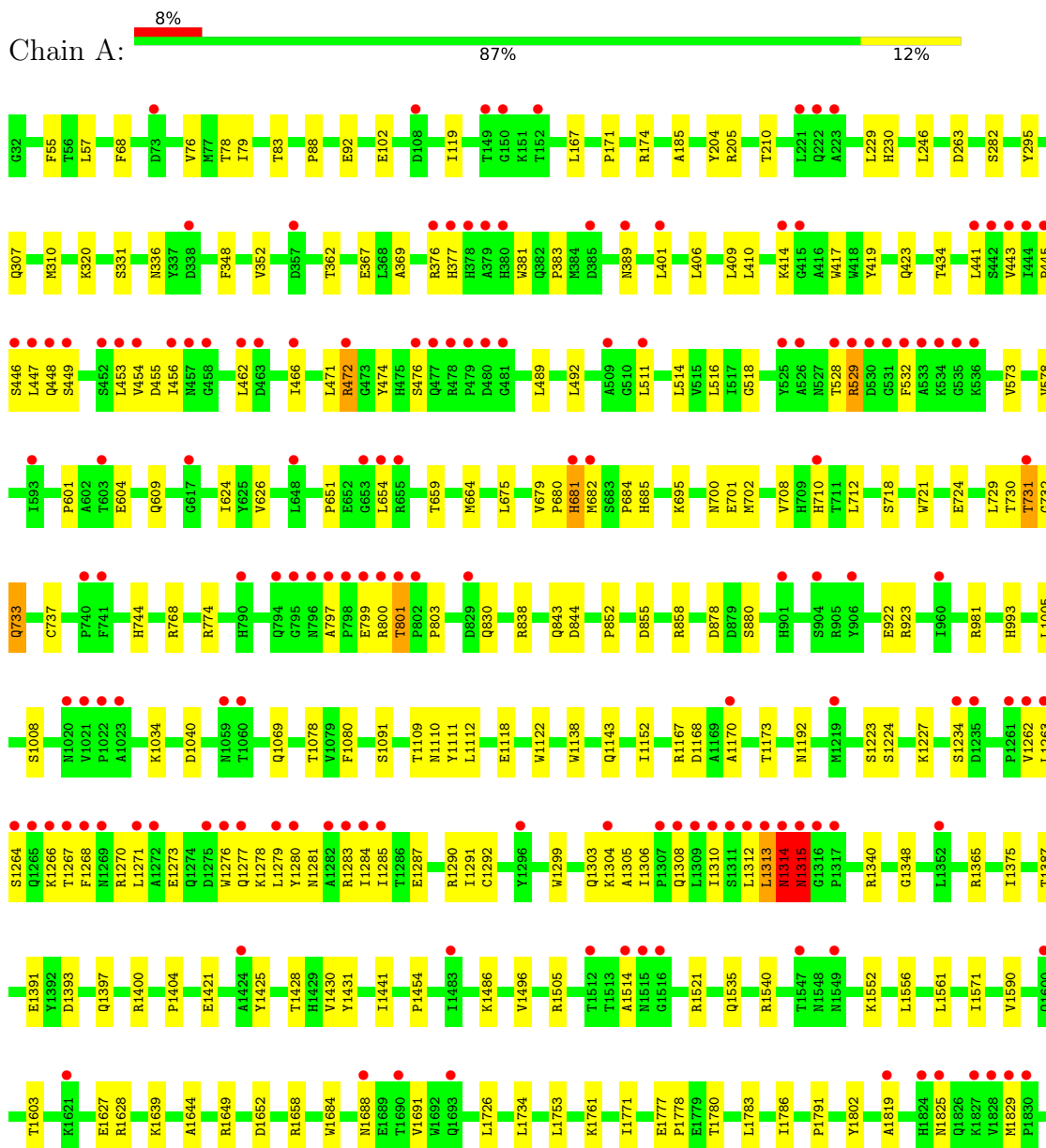
- Molecule 3 is water.

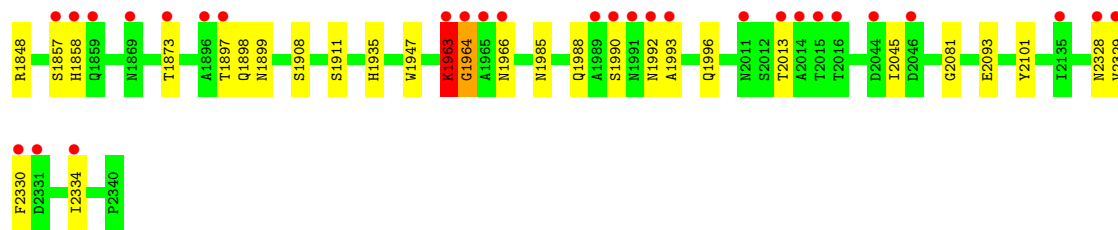
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1279	Total O 1279 1279	0	0

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: TcdB2,TccC3,Cell division control protein 42 homolog





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.35Å 156.55Å 179.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.00 48.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.17-2.00) 99.6 (48.17-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.287 , 0.320 0.214 , 0.251	Depositor DCC
R_{free} test set	9121 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtrriage
Anisotropy	0.481	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18283	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: MG

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	0.27	1/17420 (0.0%)	0.50	8/23750 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	803	PRO	C-O	-5.83	1.17	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	730	THR	CB-CA-C	-8.91	95.99	110.79
1	A	1315	ASN	N-CA-C	-7.94	103.32	113.16
1	A	681	HIS	CA-CB-CG	5.96	119.76	113.80
1	A	1964	GLY	CA-C-N	5.64	131.65	123.13
1	A	1964	GLY	C-N-CA	5.64	131.65	123.13

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	17001	0	16366	210	1
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1279	0	0	30	0
All	All	18283	0	16366	210	1

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 6.

The worst 5 of 210 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:1963:LYS:HA	1:A:1963:LYS:CE	1.91	1.01
1:A:1264:SER:OG	1:A:1315:ASN:OD1	1.78	1.00
1:A:731:THR:CG2	1:A:732:GLY:N	2.31	0.94
1:A:731:THR:HG22	1:A:732:GLY:N	1.87	0.88
1:A:731:THR:CG2	1:A:732:GLY:H	1.87	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:ASP:OD1	1:A:1825:ASN:ND2[1_655]	2.08	0.12

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	2122/2128 (100%)	2060 (97%)	59 (3%)	3 (0%)	48 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	532	PHE

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Mol	Chain	Res	Type
1	A	529	ARG
1	A	414	LYS

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	1840/1840 (100%)	1833 (100%)	7 (0%)	84 89

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1313	LEU
1	A	1314	ASN
1	A	1963	LYS
1	A	1315	ASN
1	A	733	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1781	GLN
1	A	1988	GLN
1	A	1996	GLN
1	A	1987	GLN
1	A	1314	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](#)

Of 3 ligands modelled in this entry, 3 are 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2157:LEU	C	2328:ASN	N	47.21
1	A	1471:LYS	C	1483:ILE	N	13.98

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	2128/2128 (100%)	0.43	179 (8%) 17 15	22, 36, 81, 145	1 (0%)

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	PRO	8.0
1	A	1263	LEU	7.4
1	A	1276	TRP	5.9
1	A	1829	MET	5.8
1	A	1023	ALA	5.5

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	MG	A	2401	1/1	0.95	0.09	41,41,41,41	0
2	MG	A	2403	1/1	0.95	0.06	32,32,32,32	0
2	MG	A	2402	1/1	0.98	0.06	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.