wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 03:17 pm GMT

PDB ID	:	6SUP
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 (i) 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 (i)) were used in the production of this report:

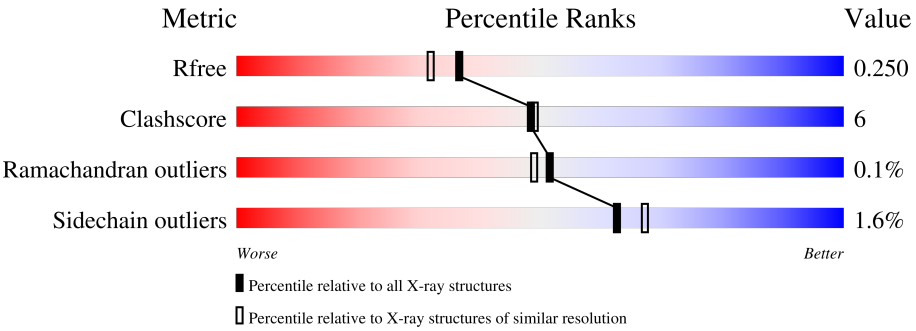
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	2128	87% 13%

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
1	A	2128	Total	C	N	O	S	1	0	0
			17001	10657	3017	3294	33			

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

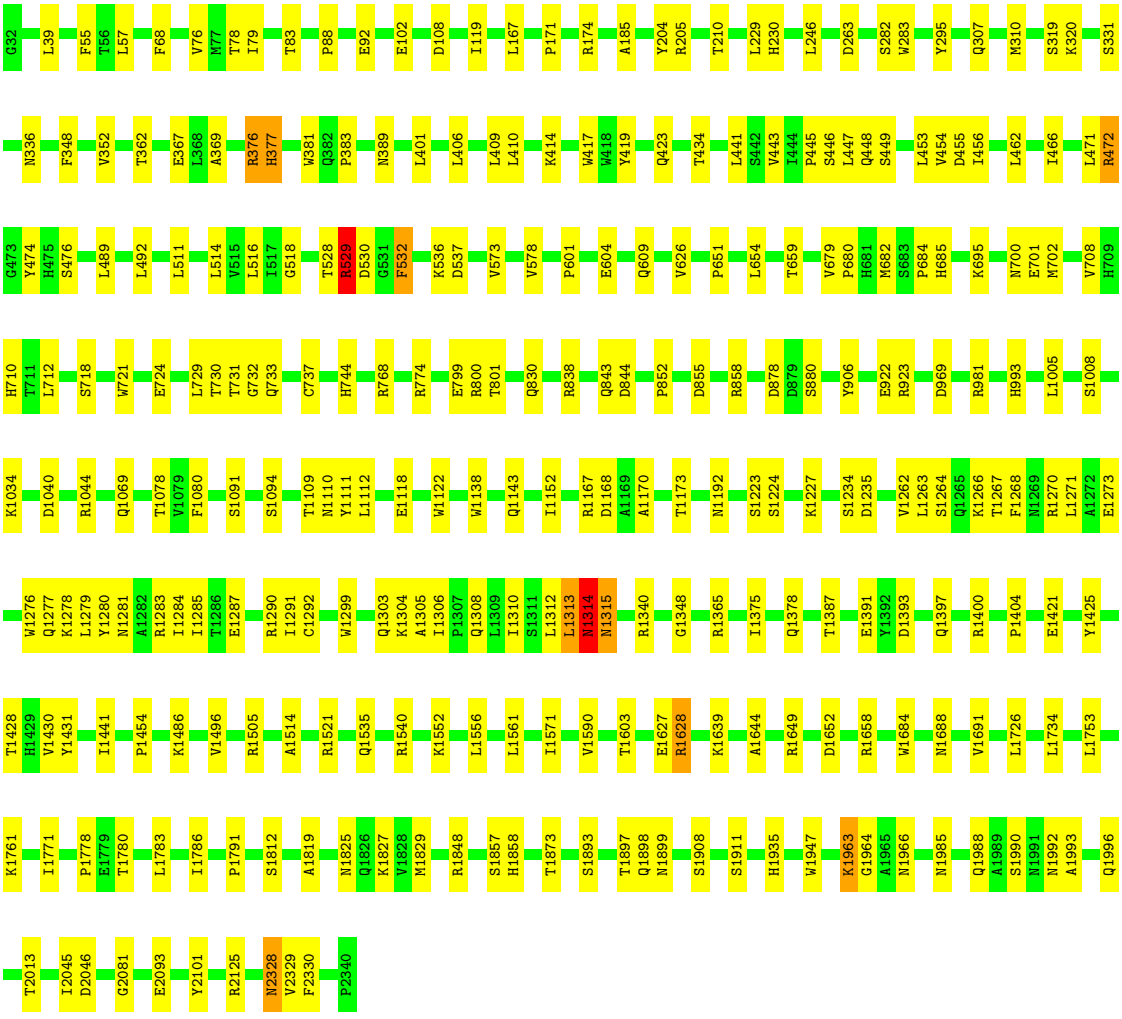
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1279	Total	O	0	0
			1279	1279		

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. 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. 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

Chain A:



4 Data and refinement statistics (i)

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 48.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.17-2.00) 99.6 (48.34-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.287 , 0.320 0.212 , 0.250	Depositor DCC
R_{free} test set	9121 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18283	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 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.33	0/17420	0.55	2/23750 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	730	THR	CB-CA-C	-5.78	95.99	111.60
1	A	1314	ASN	CB-CA-C	5.11	120.61	110.40

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	17001	0	16366	201	1
2	A	3	0	0	0	0
3	A	1279	0	0	29	0
All	All	18283	0	16366	201	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 201 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%)	51 49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	532	PHE
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%)	1811 (98%)	29 (2%)	62 67

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1044	ARG
1	A	2125	ARG
1	A	1313	LEU
1	A	1893	SER
1	A	1235	ASP

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	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 monosaccharides 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.