



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 09:50 pm GMT

PDB ID : 5W2L  
Title : Structure of a central domain of human Ctc1  
Authors : Rice, C.; Skordalakes, E.  
Deposited on : 2017-06-06  
Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

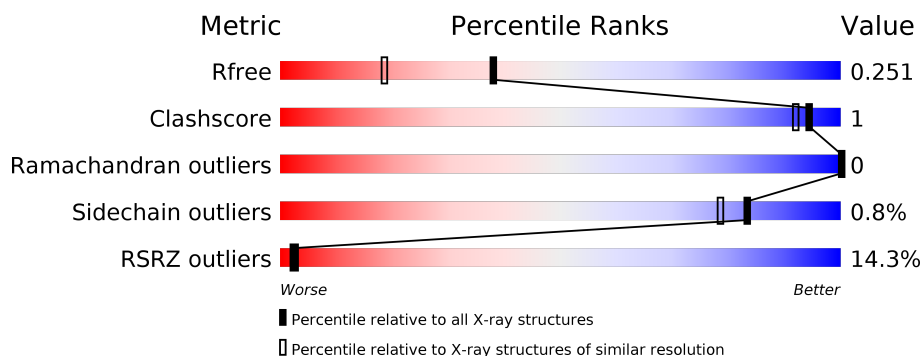
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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))
$R_{free}$	111664	2111 (1.86-1.86)
Clashscore	122126	2258 (1.86-1.86)
Ramachandran outliers	120053	2234 (1.86-1.86)
Sidechain outliers	120020	2234 (1.86-1.86)
RSRZ outliers	108989	2075 (1.86-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	168	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>••</div> <div>17%</div> </div> </div>
1	B	168	<div> <div>13%</div> <div> <div></div> <div>82%</div> <div>•</div> <div>17%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HG	B	901	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2347 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 CST complex subunit CTC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1096	707	188	195	6			
1	B	140	Total	C	N	O	S	0	0	0
			1098	708	188	196	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	713	SER	-	expression tag	UNP Q2NKJ3
A	714	ASN	-	expression tag	UNP Q2NKJ3
A	715	ALA	-	expression tag	UNP Q2NKJ3
B	713	SER	-	expression tag	UNP Q2NKJ3
B	714	ASN	-	expression tag	UNP Q2NKJ3
B	715	ALA	-	expression tag	UNP Q2NKJ3

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Hg	0	0
			3	3		
2	A	3	Total	Hg	0	0
			3	3		

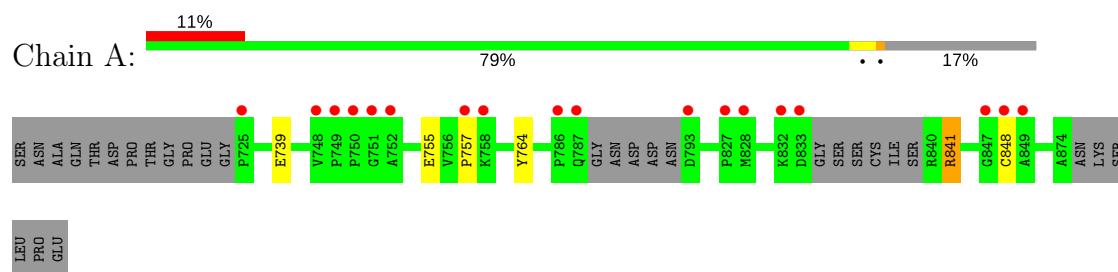
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	73	Total	O	0	0
			73	73		

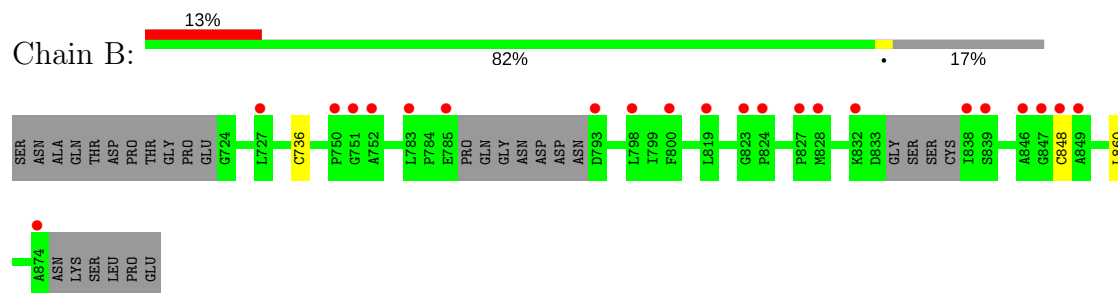
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: CST complex subunit CTC1



#### • Molecule 1: CST complex subunit CTC1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.54Å 50.78Å 144.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 1.86 19.86 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.86-1.86) 100.0 (19.86-1.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.209 , 0.249 0.212 , 0.251	Depositor DCC
$R_{free}$ test set	1549 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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: HG

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	0.46	0/1128	0.52	0/1530
1	B	0.49	0/1129	0.54	0/1531
All	All	0.48	0/2257	0.53	0/3061

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	1096	0	1076	3	0
1	B	1098	0	1080	3	0
2	A	3	0	0	0	0
2	B	3	0	0	3	0
3	A	74	0	0	0	0
3	B	73	0	0	0	0
All	All	2347	0	2156	6	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 1.

All (6) 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:848:CYS:SG	2:B:901:HG:HG	1.99	0.80
1:B:736:CYS:SG	2:B:902:HG:HG	2.01	0.79
1:B:848:CYS:HG	2:B:901:HG:HG	1.45	0.58
1:A:739:GLU:HG3	1:A:764:TYR:CZ	2.52	0.44
1:A:841:ARG:NH2	1:A:848:CYS:O	2.54	0.40
1:A:755:GLU:O	1:A:757:PRO:HD3	2.22	0.40

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	133/168 (79%)	128 (96%)	5 (4%)	0	100	100
1	B	134/168 (80%)	132 (98%)	2 (2%)	0	100	100
All	All	267/336 (80%)	260 (97%)	7 (3%)	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	119/143 (83%)	118 (99%)	1 (1%)	83	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	119/143 (83%)	118 (99%)	1 (1%)	83	78
All	All	238/286 (83%)	236 (99%)	2 (1%)	83	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	841	ARG
1	B	860	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	139/168 (82%)	0.70	18 (12%) <b>3</b> <b>3</b>	25, 36, 77, 97	0
1	B	140/168 (83%)	0.59	22 (15%) <b>2</b> <b>2</b>	25, 36, 68, 83	0
All	All	279/336 (83%)	0.64	40 (14%) <b>2</b> <b>3</b>	25, 36, 73, 97	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	PRO	8.1
1	A	748	VAL	7.8
1	B	838	ILE	6.3
1	A	786	PRO	5.3
1	A	847	GLY	4.8
1	B	828	MET	4.6
1	B	793	ASP	4.2
1	B	848	CYS	3.8
1	A	793	ASP	3.7
1	A	749	PRO	3.6
1	A	751	GLY	3.6
1	A	833	ASP	3.5
1	B	874	ALA	3.4
1	B	839	SER	3.3
1	A	828	MET	3.2
1	B	824	PRO	3.2
1	B	849	ALA	3.2
1	B	752	ALA	3.0
1	B	832	LYS	2.9
1	A	848	CYS	2.9
1	A	757	PRO	2.8
1	A	849	ALA	2.7
1	A	832	LYS	2.6
1	B	827	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	847	GLY	2.6
1	B	785	GLU	2.5
1	B	783	LEU	2.5
1	B	846	ALA	2.4
1	A	758	LYS	2.3
1	B	800	PHE	2.3
1	B	751	GLY	2.3
1	A	787	GLN	2.2
1	B	823	GLY	2.2
1	B	750	PRO	2.2
1	B	727	LEU	2.1
1	A	827	PRO	2.1
1	A	725	PRO	2.1
1	A	752	ALA	2.1
1	B	798	LEU	2.0
1	B	819	LEU	2.0

## 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 carbohydrates 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(Å <sup>2</sup> )	Q<0.9
2	HG	A	901	1/1	0.57	0.10	158,158,158,158	1
2	HG	B	901	1/1	0.94	0.20	57,57,57,57	1
2	HG	B	902	1/1	0.99	0.18	358,358,358,358	1
2	HG	A	903	1/1	0.99	0.04	30,30,30,30	1
2	HG	B	903	1/1	0.99	0.03	27,27,27,27	1
2	HG	A	902	1/1	0.99	0.19	45,45,45,45	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.