



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2016 – 03:15 PM EDT

PDB ID : 5IC9  
Title : Structure of the CTD complex of Utp12 and Utp13  
Authors : Zhang, C.; Ye, K.  
Deposited on : 2016-02-23  
Resolution : 3.70 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

<http://wwpdb.org/validation/2016/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  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

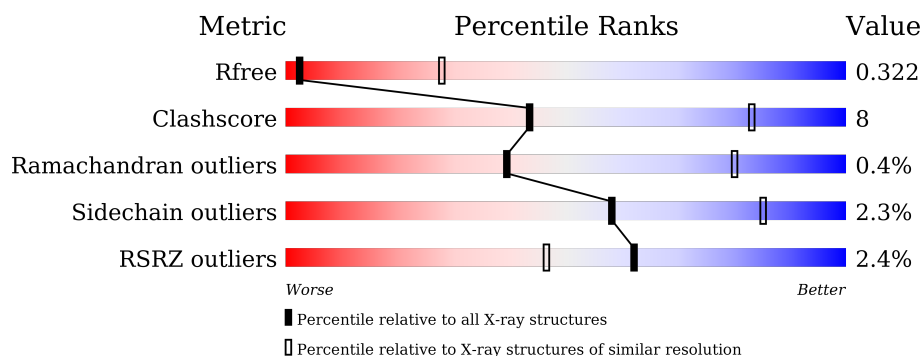
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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))
$R_{free}$	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	209	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>14%</div> <div>38%</div> </div> </div>
1	C	209	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>14%</div> <div>36%</div> </div> </div>
2	B	175	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>14%</div> <div>25%</div> </div> </div>
2	D	175	<div> <div>%</div> <div> <div></div> <div>43%</div> <div>15%</div> <div>41%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4015 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 Putative uncharacterized protein.

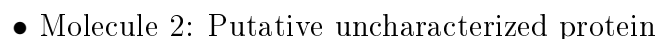
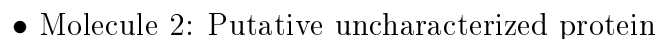
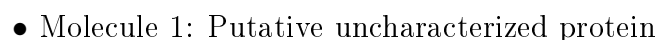
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1025	655	183	181	6			
1	C	134	Total	C	N	O	S	0	0	0
			1072	685	191	190	6			

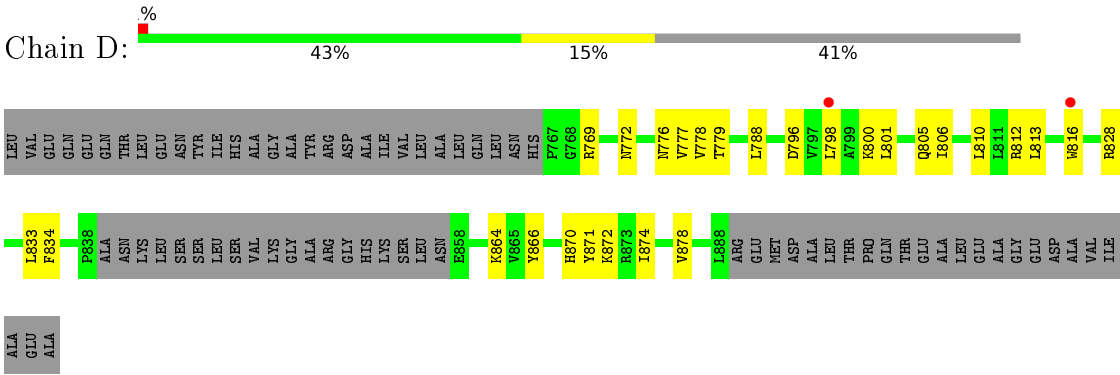
- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	0	0	0
			1074	685	188	201			
2	D	103	Total	C	N	O	0	0	0
			844	541	146	157			



- Molecule 1: Putative uncharacterized protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.31Å 160.31Å 134.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.90 – 3.70 38.51 – 3.69	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.90-3.70) 90.6 (38.51-3.69)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 3.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.275 , 0.299 0.296 , 0.322	Depositor DCC
$R_{free}$ test set	1088 reflections (10.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	123.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 87.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	4015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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

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	0.28	0/1036	0.51	1/1396 (0.1%)
1	C	0.27	0/1087	0.50	0/1467
2	B	0.28	0/1094	0.47	0/1491
2	D	0.28	0/860	0.47	0/1170
All	All	0.28	0/4077	0.49	1/5524 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	842	LEU	CA-CB-CG	5.03	126.87	115.30

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	1025	0	1092	19	0
1	C	1072	0	1125	23	0
2	B	1074	0	1076	15	0
2	D	844	0	855	16	0
All	All	4015	0	4148	66	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 8.

All (66) 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:854:ILE:HG13	1:A:855:PRO:HD3	1.58	0.84
1:C:871:VAL:HG23	1:C:872:PRO:HD3	1.78	0.64
1:C:861:LEU:HD22	1:C:874:THR:HG23	1.78	0.64
1:C:815:ASN:HB3	1:C:816:PRO:HD3	1.79	0.64
1:C:921:ILE:HG22	1:C:925:LYS:HE2	1.80	0.62
2:D:801:LEU:HB2	2:D:806:ILE:HG13	1.81	0.62
1:A:868:GLU:OE2	2:B:828:ARG:NH2	2.26	0.62
1:A:920:ASN:HD21	2:B:831:TRP:HB2	1.63	0.61
2:B:869:ARG:HH21	2:B:873:ARG:HH21	1.47	0.61
1:C:814:ARG:NH1	1:C:816:PRO:O	2.34	0.61
1:A:776:LEU:HD23	1:A:848:VAL:HG11	1.86	0.58
2:B:801:LEU:HG	2:B:805:GLN:HB2	1.85	0.58
1:C:868:GLU:HG3	1:C:912:ARG:HH12	1.70	0.57
1:C:833:THR:HA	1:C:836:LYS:HE2	1.87	0.56
2:D:810:LEU:HA	2:D:813:LEU:HB2	1.87	0.55
1:C:871:VAL:HG21	1:C:913:GLN:OE1	2.07	0.55
2:B:831:TRP:CZ2	2:B:835:LYS:HD2	2.42	0.55
2:D:769:ARG:HD3	2:D:772:ASN:HB2	1.89	0.55
1:A:830:VAL:HG11	1:A:860:PHE:CD1	2.43	0.53
1:C:909:ALA:O	1:C:913:GLN:HG2	2.09	0.53
2:D:801:LEU:HD23	2:D:805:GLN:HB3	1.91	0.52
1:C:914:LYS:NZ	2:D:871:TYR:OH	2.43	0.52
1:A:838:LYS:HD2	1:A:839:PRO:HD2	1.92	0.52
1:A:852:SER:O	1:A:855:PRO:HD2	2.10	0.52
1:A:927:VAL:HA	1:A:930:GLN:HG2	1.92	0.51
1:A:772:THR:O	1:A:775:THR:OG1	2.24	0.49
1:A:849:LEU:HD12	1:A:850:PRO:HD2	1.95	0.48
2:B:788:LEU:HD23	2:B:832:ALA:HA	1.95	0.48
1:C:814:ARG:NH1	1:C:816:PRO:HD2	2.28	0.48
1:C:912:ARG:HH21	2:D:828:ARG:HH21	1.61	0.48
1:C:873:LEU:O	1:C:877:ILE:HG13	2.13	0.47
1:A:779:GLY:O	1:A:782:ILE:HG12	2.15	0.47
2:D:874:ILE:O	2:D:878:VAL:HG23	2.14	0.47
2:D:776:ASN:HA	2:D:779:THR:HG22	1.96	0.46
1:C:832:ASN:O	1:C:836:LYS:HG3	2.15	0.46
1:A:861:LEU:HD21	1:A:877:ILE:HG22	1.97	0.46
2:B:749:ILE:HG21	2:B:756:ASP:HB2	1.99	0.45
1:A:914:LYS:HB2	2:B:874:ILE:HG21	1.98	0.45
1:C:862:ASN:HB2	1:C:902:VAL:HG22	1.99	0.45
1:C:799:TRP:CG	1:C:812:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:747:ASN:O	2:B:750:HIS:HB3	2.16	0.45
2:B:814:ARG:NH1	2:B:859:VAL:HG12	2.32	0.45
1:C:912:ARG:NH2	2:D:828:ARG:HH21	2.15	0.44
2:D:812:ARG:HB3	2:D:816:TRP:CZ2	2.52	0.44
1:A:792:ASP:O	1:A:796:ILE:HG13	2.17	0.44
2:B:762:LEU:HD13	2:B:805:GLN:HB3	1.99	0.44
1:C:825:PRO:HA	1:C:826:ALA:HA	1.55	0.43
2:D:796:ASP:O	2:D:800:LYS:HG2	2.18	0.43
2:D:798:LEU:HA	2:D:801:LEU:HD11	1.99	0.43
1:C:861:LEU:HD11	1:C:877:ILE:HG22	1.99	0.43
2:D:872:LYS:HA	2:D:872:LYS:HD2	1.85	0.43
2:B:761:ALA:HB3	2:B:770:LEU:HD13	2.01	0.42
1:A:899:LEU:HA	1:A:902:VAL:HG12	2.01	0.42
1:C:868:GLU:CD	1:C:912:ARG:HH22	2.23	0.42
2:D:777:VAL:HG23	2:D:778:VAL:HG13	2.02	0.42
2:D:866:TYR:O	2:D:870:HIS:ND1	2.52	0.42
1:A:878:LEU:HD22	1:A:906:LEU:HD12	2.02	0.41
2:B:819:ASN:HB3	2:B:822:THR:OG1	2.20	0.41
1:A:930:GLN:NE2	2:B:839:ALA:O	2.44	0.41
1:A:839:PRO:O	1:A:842:LEU:HD12	2.20	0.41
2:B:837:HIS:HA	2:B:838:PRO:HD3	1.87	0.41
1:C:900:GLU:CD	1:C:903:ARG:HH12	2.23	0.41
1:C:777:MET:HG2	1:C:777:MET:H	1.55	0.40
1:C:830:VAL:HG12	1:C:834:LEU:HD23	2.03	0.40
1:A:911:ARG:HD3	1:A:911:ARG:HA	1.87	0.40
2:D:864:LYS:HB2	2:D:864:LYS:HE3	1.90	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	123/209 (59%)	121 (98%)	2 (2%)	0	100	100
1	C	126/209 (60%)	123 (98%)	3 (2%)	0	100	100
2	B	128/175 (73%)	125 (98%)	2 (2%)	1 (1%)	24	70
2	D	99/175 (57%)	96 (97%)	2 (2%)	1 (1%)	19	66
All	All	476/768 (62%)	465 (98%)	9 (2%)	2 (0%)	39	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	839	ALA
2	D	788	LEU

### 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	113/183 (62%)	112 (99%)	1 (1%)	84	93
1	C	118/183 (64%)	115 (98%)	3 (2%)	55	84
2	B	117/150 (78%)	113 (97%)	4 (3%)	44	79
2	D	94/150 (63%)	92 (98%)	2 (2%)	61	86
All	All	442/666 (66%)	432 (98%)	10 (2%)	58	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	842	LEU
2	B	791	LEU
2	B	795	ASP
2	B	810	LEU
2	B	828	ARG
1	C	777	MET
1	C	808	ASN
1	C	913	GLN
2	D	833	LEU

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Mol	Chain	Res	Type
2	D	834	PHE

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

### 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 carbohydrates 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 ⓘ

### 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	129/209 (61%)	0.11	5 (3%)	43 29	105, 145, 179, 190	0
1	C	134/209 (64%)	0.02	3 (2%)	65 50	100, 140, 181, 197	0
2	B	132/175 (75%)	-0.00	2 (1%)	76 62	105, 131, 171, 181	0
2	D	103/175 (58%)	0.06	2 (1%)	70 55	100, 127, 168, 194	0
All	All	498/768 (64%)	0.05	12 (2%)	62 46	100, 137, 177, 197	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	858	LEU	3.0
1	C	857	LEU	2.7
1	A	827	GLU	2.5
1	A	774	GLU	2.4
1	A	788	LEU	2.4
1	A	860	PHE	2.3
2	B	782	ASN	2.3
1	C	854	ILE	2.2
2	D	816	TRP	2.1
1	A	928	SER	2.1
2	D	798	LEU	2.1
2	B	746	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.