



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:09 PM UTC

PDB ID : 5DSE / pdb\_00005dse  
Title : Crystal Structure of the TTC7B/Hyccin Complex  
Authors : Wu, X.; Baskin, J.M.; Reinisch, K.M.; De Camilli, P.  
Deposited on : 2015-09-17  
Resolution : 2.90 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>.

---

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

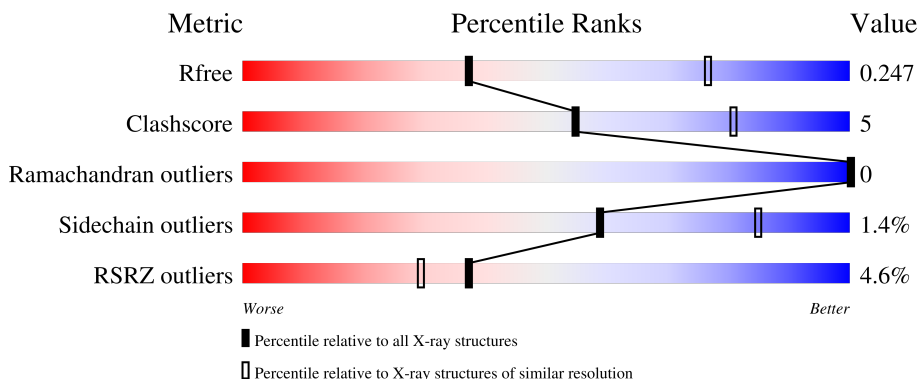
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	837	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 57%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">4%      57%      7%      36%</p>
1	C	837	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">2%      75%      10%      15%</p>
2	B	312	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">6%      62%      12%      26%</p>
2	D	312	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">4%      69%      16%      15%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13875 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 Tetratricopeptide repeat protein 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	4242	2714	730	771	27	0	0	0
1	C	712	5647	3591	982	1042	32	0	0	0

- Molecule 2 is a protein called Hyccin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	231	1844	1205	293	334	12	0	0	0
2	D	264	2091	1357	338	383	13	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q9BYI3
B	-2	PRO	-	expression tag	UNP Q9BYI3
B	-1	LEU	-	expression tag	UNP Q9BYI3
B	0	GLY	-	expression tag	UNP Q9BYI3
B	1	SER	-	expression tag	UNP Q9BYI3
D	-3	GLY	-	expression tag	UNP Q9BYI3
D	-2	PRO	-	expression tag	UNP Q9BYI3
D	-1	LEU	-	expression tag	UNP Q9BYI3
D	0	GLY	-	expression tag	UNP Q9BYI3
D	1	SER	-	expression tag	UNP Q9BYI3

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		

*Continued on next page...*

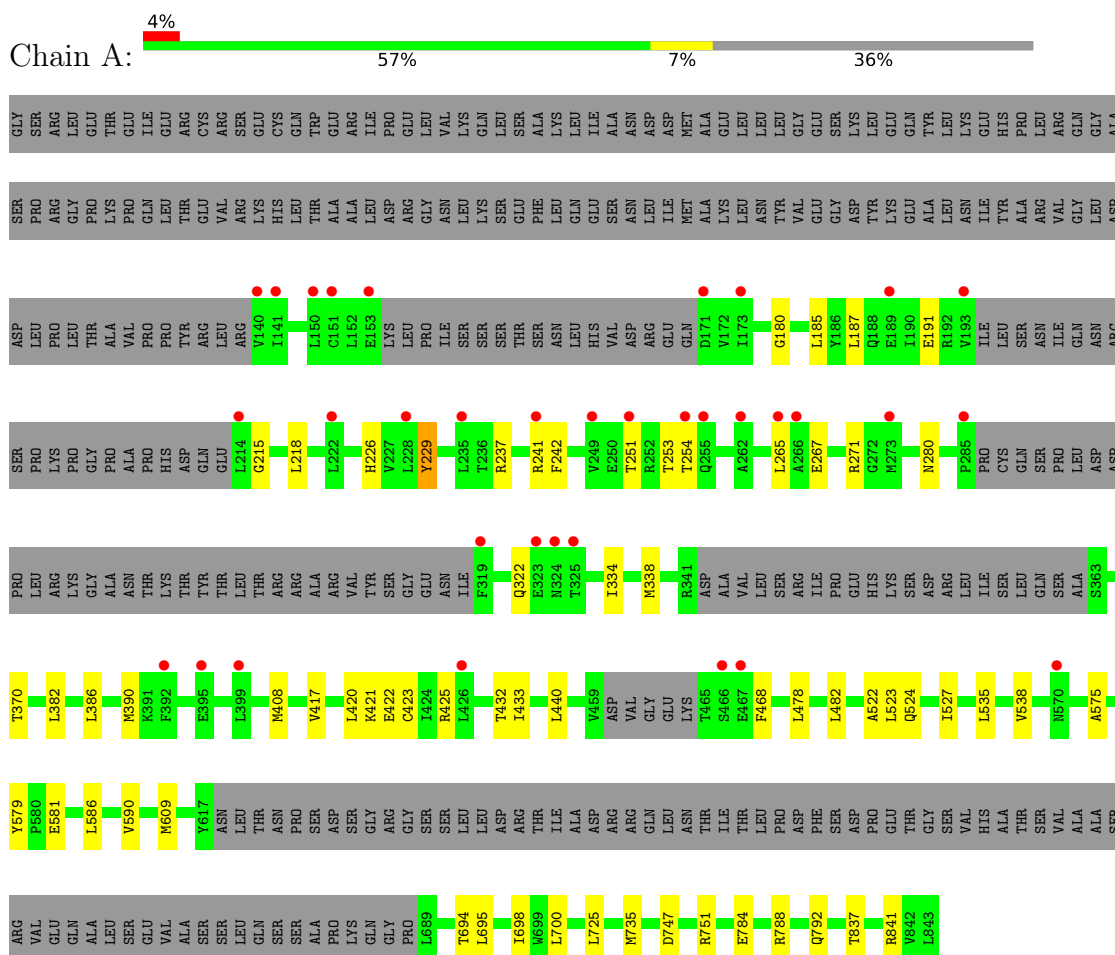
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	C	32	Total	O	0	0
			32	32		
3	D	2	Total	O	0	0
			2	2		

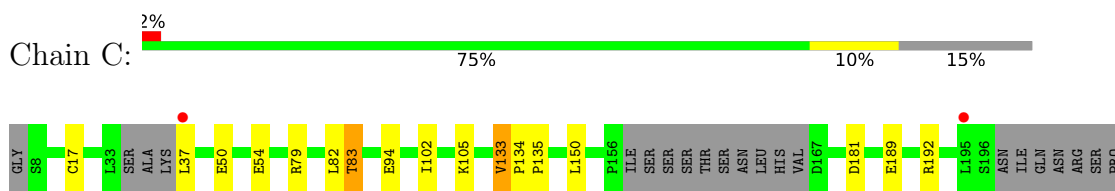
### 3 Residue-property plots

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: Tetratricopeptide repeat protein 7B



- Molecule 1: Tetratricopeptide repeat protein 7B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.78Å 168.07Å 239.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.90 29.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.96-2.90) 96.2 (29.96-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.32 (at 2.90Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1630)	Depositor
R, $R_{free}$	0.212 , 0.242 0.217 , 0.247	Depositor DCC
$R_{free}$ test set	2000 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.1	Xtrriage
Anisotropy	0.249	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.29	0/4319	0.69	0/5839
1	C	0.30	0/5747	0.72	4/7771 (0.1%)
2	B	0.29	0/1887	0.74	0/2560
2	D	0.31	0/2140	0.74	0/2903
All	All	0.30	0/14093	0.72	4/19073 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	VAL	CA-C-N	7.05	124.81	119.66
1	C	133	VAL	C-N-CA	7.05	124.81	119.66
1	C	284	ASP	CA-C-N	6.01	124.05	119.66
1	C	284	ASP	C-N-CA	6.01	124.05	119.66

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	4242	0	4292	39	0
1	C	5647	0	5715	48	0
2	B	1844	0	1847	22	0
2	D	2091	0	2096	32	0
3	A	17	0	0	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	32	0	0	0	0
3	D	2	0	0	0	0
All	All	13875	0	13950	134	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 5.

The worst 5 of 134 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)
2:D:274:GLU:HG2	2:D:275:PRO:HD3	1.58	0.85
2:B:274:GLU:HG2	2:B:275:PRO:HD3	1.61	0.83
1:C:482:LEU:HD23	1:C:841:ARG:HH11	1.55	0.72
1:A:187:LEU:HD21	1:A:253:THR:HB	1.73	0.70
1:A:180:GLY:HA3	1:A:241:ARG:HH22	1.55	0.70

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	523/837 (62%)	514 (98%)	9 (2%)	0	100	100
1	C	696/837 (83%)	687 (99%)	9 (1%)	0	100	100
2	B	217/312 (70%)	213 (98%)	4 (2%)	0	100	100
2	D	254/312 (81%)	247 (97%)	7 (3%)	0	100	100
All	All	1690/2298 (74%)	1661 (98%)	29 (2%)	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	445/708 (63%)	440 (99%)	5 (1%)	65 88
1	C	601/708 (85%)	590 (98%)	11 (2%)	51 80
2	B	207/279 (74%)	205 (99%)	2 (1%)	68 89
2	D	236/279 (85%)	233 (99%)	3 (1%)	61 86
All	All	1489/1974 (75%)	1468 (99%)	21 (1%)	59 85

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	302	LYS
1	C	736	ARG
2	D	274	GLU
2	D	102	GLU
1	C	435	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	792	GLN
1	C	811	GLN
2	D	154	GLN
1	C	32	GLN
1	C	280	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](#)

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 [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	537/837 (64%)	0.17	34 (6%) 26 20	43, 78, 176, 226	0
1	C	712/837 (85%)	-0.15	13 (1%) 67 59	43, 67, 136, 211	0
2	B	231/312 (74%)	0.56	20 (8%) 16 13	65, 113, 191, 233	0
2	D	264/312 (84%)	0.23	13 (4%) 35 27	51, 85, 156, 191	0
All	All	1744/2298 (75%)	0.10	80 (4%) 37 29	43, 77, 169, 233	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	114	VAL	6.0
2	D	8	VAL	5.1
1	A	140	VAL	4.7
2	D	34	LYS	4.3
1	A	235	LEU	4.0

### 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 oligosaccharides 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.