



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 08:38 PM EDT

PDB ID : 5BT1  
Title : histone chaperone Hif1 playing with histone H2A-H2B dimer  
Authors : Liu, H.; Zhang, M.; Gao, Y.; Teng, M.; Niu, L.  
Deposited on : unknown  
Resolution : 2.62 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345

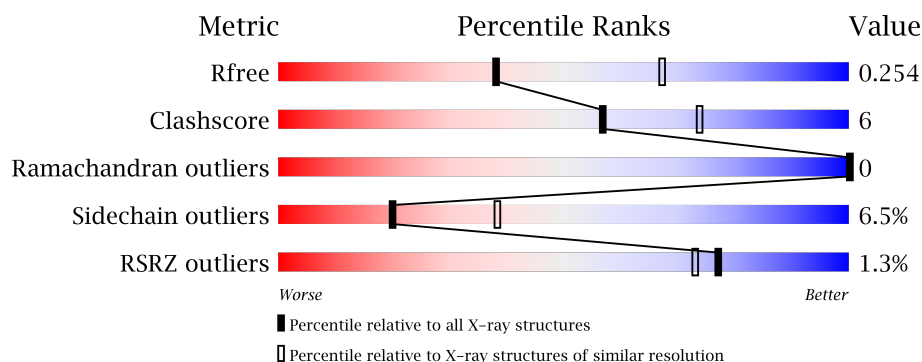
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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))
$R_{free}$	100719	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (2.64-2.60)

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	393	<div> <div> <div></div> <div>51%</div> <div>10%</div> <div>•</div> <div>38%</div> </div> </div>
1	B	393	<div> <div> <div></div> <div>52%</div> <div>11%</div> <div>•</div> <div>37%</div> </div> </div>
2	C	143	<div> <div> <div></div> <div>52%</div> <div>7%</div> <div>•</div> <div>41%</div> </div> </div>
3	D	142	<div> <div> <div></div> <div>53%</div> <div>10%</div> <div>•</div> <div>37%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5317 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 HAT1-interacting factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1932	1219	334	371	8			
1	B	249	Total	C	N	O	S	0	0	0
			1990	1256	346	380	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	expression tag	UNP Q12373
A	387	GLU	-	expression tag	UNP Q12373
A	388	HIS	-	expression tag	UNP Q12373
A	389	HIS	-	expression tag	UNP Q12373
A	390	HIS	-	expression tag	UNP Q12373
A	391	HIS	-	expression tag	UNP Q12373
A	392	HIS	-	expression tag	UNP Q12373
A	393	HIS	-	expression tag	UNP Q12373
B	386	LEU	-	expression tag	UNP Q12373
B	387	GLU	-	expression tag	UNP Q12373
B	388	HIS	-	expression tag	UNP Q12373
B	389	HIS	-	expression tag	UNP Q12373
B	390	HIS	-	expression tag	UNP Q12373
B	391	HIS	-	expression tag	UNP Q12373
B	392	HIS	-	expression tag	UNP Q12373
B	393	HIS	-	expression tag	UNP Q12373

- Molecule 2 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	85	Total	C	N	O	0	0	0
			650	407	128	115			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	MET	-	initiating methionine	UNP P04911
C	-10	GLY	-	expression tag	UNP P04911
C	-9	HIS	-	expression tag	UNP P04911
C	-8	HIS	-	expression tag	UNP P04911
C	-7	HIS	-	expression tag	UNP P04911
C	-6	HIS	-	expression tag	UNP P04911
C	-5	HIS	-	expression tag	UNP P04911
C	-4	HIS	-	expression tag	UNP P04911
C	-3	GLY	-	expression tag	UNP P04911
C	-2	SER	-	expression tag	UNP P04911
C	-1	HIS	-	expression tag	UNP P04911

- Molecule 3 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	90	Total	C	N	O	S	0	0	0
			698	440	120	137	1			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	initiating methionine	UNP P02293
D	-10	GLY	-	expression tag	UNP P02293
D	-9	HIS	-	expression tag	UNP P02293
D	-8	HIS	-	expression tag	UNP P02293
D	-7	HIS	-	expression tag	UNP P02293
D	-6	HIS	-	expression tag	UNP P02293
D	-5	HIS	-	expression tag	UNP P02293
D	-4	HIS	-	expression tag	UNP P02293
D	-3	GLY	-	expression tag	UNP P02293
D	-2	SER	-	expression tag	UNP P02293
D	-1	HIS	-	expression tag	UNP P02293

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	15	Total	O	0	0
			15	15		
4	C	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	8	Total	O	0	0
			8	8		



PRO
ASN
ILE
HIS
GLN
ASN
LEU
LEU
PRO
LYS
LYS
SER
ALA
LYS
ALA
THR
LYS
ALA
SER
GLN
GLU
LEU

● Molecule 3: Histone H2B.1



MET	GLY	HIS	HIS	HIS	HIS	HIS	GLY	SER	HIS	MET	SER	ALA	LYS	ALA	GLU	LYS	LYS	PRO	ALA	SER	LYS	ALA	PRO	ALA	GLU	LYS	LYS	PRO	ALA	ALA	LYS	THR	SER	THR	SER	THR	ASP	GLY	LYS	LYS	ARG	SER	LYS	ALA	ALA	ARG	K37	Y43	I57	S61	I65	D71
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E79	R95	E96	R102	L103	I104	L105	A110	S115	E116	S126	SER	THR	GLN	ALA
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.67Å 48.36Å 160.71Å 90.00° 107.05° 90.00°	Depositor
Resolution (Å)	43.38 – 2.62 43.38 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.1 (43.38-2.62) 98.0 (43.38-2.62)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.207 , 0.262 0.203 , 0.254	Depositor DCC
$R_{free}$ test set	1162 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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	0.44	0/1962	0.58	1/2649 (0.0%)
1	B	0.41	0/2022	0.56	0/2729
2	C	0.36	0/658	0.51	0/889
3	D	0.41	0/708	0.52	0/955
All	All	0.42	0/5350	0.55	1/7222 (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	325	LEU	CA-CB-CG	5.41	127.75	115.30

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	1932	0	1892	20	0
1	B	1990	0	1954	29	0
2	C	650	0	670	8	0
3	D	698	0	712	8	0
4	A	20	0	0	0	0
4	B	15	0	0	0	0
4	C	4	0	0	0	0
4	D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5317	0	5228	60	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 6.

All (60) 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)
3:D:102:ARG:HH11	3:D:102:ARG:HG2	1.49	0.76
1:B:227:LEU:H	1:B:227:LEU:HD12	1.53	0.73
1:A:296:VAL:HG13	1:A:301:LYS:HE3	1.73	0.70
1:B:291:ARG:HG2	1:B:292:TRP:CD1	2.26	0.70
1:B:326:GLN:HE22	1:B:329:ARG:HH11	1.39	0.69
1:B:320:PRO:HB2	1:B:322:ASP:OD1	1.94	0.68
1:B:326:GLN:NE2	1:B:329:ARG:HH11	1.93	0.66
3:D:102:ARG:NH1	3:D:102:ARG:HG2	2.11	0.65
1:B:326:GLN:HE22	1:B:329:ARG:NH1	1.94	0.65
1:B:332:GLN:OE1	3:D:37:LYS:HG3	1.95	0.65
1:A:190:ARG:H	1:A:212:GLN:NE2	1.94	0.65
1:A:190:ARG:HB3	1:A:212:GLN:HE22	1.62	0.62
3:D:79:GLU:HB2	3:D:104:ILE:HD11	1.81	0.62
1:A:190:ARG:H	1:A:212:GLN:HE21	1.48	0.62
1:B:182:GLU:OE2	1:B:258:HIS:NE2	2.32	0.60
1:B:190:ARG:H	1:B:212:GLN:NE2	2.00	0.60
1:A:256:ILE:HD11	1:A:290:LEU:HA	1.83	0.60
1:B:190:ARG:HB3	1:B:212:GLN:HE22	1.67	0.59
1:A:69:GLN:HG3	1:A:241:LEU:HD21	1.85	0.58
1:B:62:GLU:HG3	1:B:234:ARG:HH21	1.69	0.57
1:A:316:MET:HE2	1:A:326:GLN:HB3	1.87	0.57
1:A:336:ASP:O	1:A:340:VAL:HG12	2.05	0.56
1:B:341:GLN:HA	1:B:344:GLN:HG2	1.86	0.56
1:B:189:LEU:HD12	1:B:212:GLN:HE21	1.70	0.56
1:A:170:LEU:HD22	1:A:173:PHE:HB2	1.89	0.55
1:A:283:GLU:OE1	1:A:304:ARG:NH2	2.39	0.54
2:C:92:ASP:OD1	2:C:92:ASP:N	2.41	0.54
1:B:82:LEU:HD13	2:C:81:PRO:HB2	1.90	0.53
1:A:316:MET:HE3	1:A:327:GLN:HG3	1.89	0.53
1:A:180:ASP:OD1	1:A:261:LYS:NZ	2.39	0.51
1:B:83:PHE:H	2:C:85:GLN:HE22	1.59	0.49
2:C:18:ARG:NH2	2:C:32:HIS:ND1	2.48	0.49
1:A:72:TYR:CD1	1:A:245:ILE:HG12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:O	1:A:67:PHE:HB2	2.13	0.48
3:D:79:GLU:CB	3:D:104:ILE:HD11	2.42	0.48
1:B:20:ILE:HD11	1:B:51:SER:OG	2.13	0.48
1:B:264:GLY:O	1:B:268:THR:HG23	2.15	0.47
1:B:69:GLN:HG2	1:B:241:LEU:HD21	1.96	0.46
2:C:84:LEU:O	2:C:88:ILE:HG12	2.16	0.46
3:D:105:LEU:HB2	3:D:110:ALA:HB2	1.98	0.45
1:B:210:LEU:HD21	1:B:241:LEU:HD23	1.99	0.45
1:B:339:GLU:OE2	3:D:43:TYR:OH	2.33	0.45
1:B:274:GLN:O	1:B:278:LYS:HG2	2.17	0.44
1:A:173:PHE:CE2	1:A:175:PRO:HD3	2.52	0.44
1:B:227:LEU:H	1:B:227:LEU:CD1	2.26	0.44
1:A:324:GLU:CD	1:A:324:GLU:H	2.20	0.44
2:C:45:GLY:O	2:C:49:PRO:HD3	2.17	0.44
1:B:227:LEU:HD12	1:B:227:LEU:N	2.28	0.43
1:B:342:GLU:OE1	2:C:18:ARG:NH1	2.51	0.43
1:B:177:ASN:H	1:B:177:ASN:HD22	1.66	0.43
1:B:75:GLU:HB2	1:B:202:LEU:HD12	2.00	0.43
1:B:62:GLU:HG3	1:B:234:ARG:NH2	2.33	0.43
1:A:186:VAL:HG11	1:A:219:ARG:HD2	1.99	0.43
1:B:291:ARG:NH1	1:B:336:ASP:OD1	2.52	0.42
1:A:316:MET:HE1	1:A:323:SER:O	2.20	0.41
2:C:38:GLY:HA3	2:C:40:TYR:CE2	2.55	0.41
3:D:57:ILE:HG13	3:D:61:SER:OG	2.21	0.40
1:A:316:MET:CE	1:A:327:GLN:HG3	2.52	0.40
1:A:22:MET:HE3	1:A:60:ASP:HB2	2.04	0.40
1:B:60:ASP:HA	1:B:61:PRO:HD2	1.93	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	240/393 (61%)	229 (95%)	11 (5%)	0	100	100
1	B	245/393 (62%)	242 (99%)	3 (1%)	0	100	100
2	C	83/143 (58%)	82 (99%)	1 (1%)	0	100	100
3	D	88/142 (62%)	85 (97%)	3 (3%)	0	100	100
All	All	656/1071 (61%)	638 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	202/341 (59%)	187 (93%)	15 (7%)	16	31
1	B	209/341 (61%)	196 (94%)	13 (6%)	21	41
2	C	64/108 (59%)	63 (98%)	1 (2%)	68	86
3	D	77/118 (65%)	70 (91%)	7 (9%)	11	20
All	All	552/908 (61%)	516 (94%)	36 (6%)	20	38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	22	MET
1	A	23	GLU
1	A	46	GLN
1	A	62	GLU
1	A	67	PHE
1	A	78	ASN
1	A	169	GLU
1	A	177	ASN
1	A	263	LEU
1	A	273	GLU
1	A	274	GLN
1	A	291	ARG

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Mol	Chain	Res	Type
1	A	312	LEU
1	A	325	LEU
1	B	67	PHE
1	B	77	GLN
1	B	82	LEU
1	B	172	ASN
1	B	178	GLU
1	B	199	GLU
1	B	223	ASP
1	B	227	LEU
1	B	280	ILE
1	B	291	ARG
1	B	294	ASP
1	B	311	LEU
1	B	321	LYS
2	C	92	ASP
3	D	65	LEU
3	D	71	ASP
3	D	95	ARG
3	D	96	GLU
3	D	102	ARG
3	D	115	SER
3	D	116	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	177	ASN
1	A	212	GLN
1	A	343	ASN
1	B	47	GLN
1	B	78	ASN
1	B	177	ASN
1	B	212	GLN
1	B	315	HIS
1	B	326	GLN
2	C	85	GLN
2	C	90	ASN
3	D	98	GLN

### 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 [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	244/393 (62%)	0.12	4 (1%) 72 67	26, 42, 73, 89	0
1	B	249/393 (63%)	0.18	4 (1%) 72 67	25, 42, 69, 92	0
2	C	85/143 (59%)	0.06	1 (1%) 79 75	28, 53, 75, 83	0
3	D	90/142 (63%)	0.08	0 100 100	31, 48, 61, 69	0
All	All	668/1071 (62%)	0.13	9 (1%) 77 73	25, 44, 71, 92	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	PHE	4.8
1	A	15	ARG	4.3
1	A	16	HIS	3.7
1	B	175	PRO	3.6
2	C	16	GLN	2.8
1	B	223	ASP	2.5
1	B	176	ALA	2.5
1	A	79	SER	2.5
1	A	345	GLN	2.2

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.