



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 30, 2020 – 04:10 am BST

PDB ID : 3I3J  
Title : Crystal Structure of the Bromodomain of Human EP300  
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Deposited on : 2009-06-30  
Resolution : 2.33 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

PERCENTILES INFOmissingINFO

# 1 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11399 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 Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			932	609	145	173	5			
1	B	114	Total	C	N	O	S	0	0	0
			913	598	139	171	5			
1	C	114	Total	C	N	O	S	0	0	0
			944	612	152	175	5			
1	D	113	Total	C	N	O	S	0	0	0
			920	604	139	172	5			
1	E	115	Total	C	N	O	S	0	0	0
			948	616	149	178	5			
1	F	111	Total	C	N	O	S	0	0	0
			890	580	139	166	5			
1	G	113	Total	C	N	O	S	0	0	0
			918	599	143	171	5			
1	H	113	Total	C	N	O	S	0	1	0
			922	602	145	170	5			
1	I	115	Total	C	N	O	S	0	0	0
			944	615	148	176	5			
1	J	113	Total	C	N	O	S	0	0	0
			925	605	142	173	5			
1	K	114	Total	C	N	O	S	0	1	0
			934	609	151	169	5			
1	L	113	Total	C	N	O	S	0	0	0
			906	590	146	165	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1038	SER	-	EXPRESSION TAG	UNP Q09472
A	1039	MET	-	EXPRESSION TAG	UNP Q09472
B	1038	SER	-	EXPRESSION TAG	UNP Q09472
B	1039	MET	-	EXPRESSION TAG	UNP Q09472
C	1038	SER	-	EXPRESSION TAG	UNP Q09472

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1039	MET	-	EXPRESSION TAG	UNP Q09472
D	1038	SER	-	EXPRESSION TAG	UNP Q09472
D	1039	MET	-	EXPRESSION TAG	UNP Q09472
E	1038	SER	-	EXPRESSION TAG	UNP Q09472
E	1039	MET	-	EXPRESSION TAG	UNP Q09472
F	1038	SER	-	EXPRESSION TAG	UNP Q09472
F	1039	MET	-	EXPRESSION TAG	UNP Q09472
G	1038	SER	-	EXPRESSION TAG	UNP Q09472
G	1039	MET	-	EXPRESSION TAG	UNP Q09472
H	1038	SER	-	EXPRESSION TAG	UNP Q09472
H	1039	MET	-	EXPRESSION TAG	UNP Q09472
I	1038	SER	-	EXPRESSION TAG	UNP Q09472
I	1039	MET	-	EXPRESSION TAG	UNP Q09472
J	1038	SER	-	EXPRESSION TAG	UNP Q09472
J	1039	MET	-	EXPRESSION TAG	UNP Q09472
K	1038	SER	-	EXPRESSION TAG	UNP Q09472
K	1039	MET	-	EXPRESSION TAG	UNP Q09472
L	1038	SER	-	EXPRESSION TAG	UNP Q09472
L	1039	MET	-	EXPRESSION TAG	UNP Q09472

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total 39	O 39	0	0
5	B	14	Total 14	O 14	0	0
5	C	31	Total 31	O 31	0	0
5	D	20	Total 20	O 20	0	0
5	E	32	Total 32	O 32	0	0
5	F	1	Total 1	O 1	0	0
5	G	38	Total 38	O 38	0	0
5	H	15	Total 15	O 15	0	0
5	I	24	Total 24	O 24	0	0
5	J	23	Total 23	O 23	0	0
5	K	28	Total 28	O 28	0	0
5	L	12	Total 12	O 12	0	0

SEQUENCE-PLOTS INFOmissingINFO

## 2 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.90 Å 86.19 Å 149.90 Å 90.00° 96.98° 90.00°	Depositor
Resolution (Å)	32.30 – 2.33 32.30 – 2.33	Depositor EDS
% Data completeness (in resolution range)	91.8 (32.30-2.33) 99.1 (32.30-2.33)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.34 Å)	Xtriage
Refinement program	PHENIX ?	Depositor
R, $R_{free}$	0.229 , 0.275 0.228 , 0.221	Depositor DCC
$R_{free}$ test set	1984 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.96% 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.

## 3 Model quality ⓘ

### 3.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4, CL

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	0.40	0/959	0.57	1/1307 (0.1%)
1	B	0.34	0/940	0.50	0/1284
1	C	0.37	0/971	1.00	3/1322 (0.2%)
1	D	0.36	0/947	0.55	0/1291
1	E	0.38	0/975	0.55	1/1326 (0.1%)
1	F	0.36	0/917	0.51	1/1254 (0.1%)
1	G	0.39	0/945	0.54	0/1290
1	H	0.32	0/949	0.51	0/1296
1	I	0.41	0/971	1.05	3/1322 (0.2%)
1	J	0.34	0/952	0.52	0/1299
1	K	0.34	0/961	0.51	1/1310 (0.1%)
1	L	0.33	0/933	0.55	2/1274 (0.2%)
All	All	0.36	0/11420	0.64	12/15575 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1137	ARG	NE-CZ-NH1	-21.85	109.37	120.30
1	C	1137	ARG	NE-CZ-NH1	-21.78	109.41	120.30
1	I	1137	ARG	NE-CZ-NH2	20.72	130.66	120.30
1	C	1137	ARG	NE-CZ-NH2	20.01	130.31	120.30
1	I	1137	ARG	CD-NE-CZ	10.35	138.09	123.60

There are no chirality outliers.

There are no planarity outliers.



### 3.2 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	932	0	889	28	0
1	B	913	0	856	16	0
1	C	944	0	910	16	0
1	D	920	0	874	23	0
1	E	948	0	914	23	0
1	F	890	0	828	16	0
1	G	918	0	871	11	0
1	H	922	0	867	19	0
1	I	944	0	907	19	0
1	J	925	0	881	17	0
1	K	934	0	892	28	0
1	L	906	0	849	5	0
2	A	1	0	0	1	0
2	E	1	0	0	1	0
3	A	7	0	10	1	0
3	E	7	0	10	0	0
4	E	5	0	0	0	0
4	L	5	0	0	1	0
5	A	39	0	0	1	0
5	B	14	0	0	0	0
5	C	31	0	0	1	0
5	D	20	0	0	0	0
5	E	32	0	0	0	0
5	F	1	0	0	0	0
5	G	38	0	0	0	0
5	H	15	0	0	0	0
5	I	24	0	0	0	0
5	J	23	0	0	1	0
5	K	28	0	0	0	0
5	L	12	0	0	0	0
All	All	11399	0	10558	166	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.

The worst 5 of 166 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:1150:GLU:OE2	1:E:1140:LYS:HG2	1.17	1.28
1:A:1150:GLU:OE2	1:E:1140:LYS:CG	2.06	1.02
1:B:1115:TRP:HZ2	1:I:1135:THR:O	1.46	0.97
1:A:1150:GLU:OE1	1:E:1140:LYS:NZ	1.98	0.96
1:D:1134:LYS:HE2	1:K:1092:ILE:CD1	2.01	0.89

There are no symmetry-related clashes.

### 3.3 Torsion angles [i](#)

#### 3.3.1 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	112/124 (90%)	112 (100%)	0	0	100	100
1	B	112/124 (90%)	112 (100%)	0	0	100	100
1	C	112/124 (90%)	112 (100%)	0	0	100	100
1	D	111/124 (90%)	110 (99%)	1 (1%)	0	100	100
1	E	113/124 (91%)	113 (100%)	0	0	100	100
1	F	109/124 (88%)	109 (100%)	0	0	100	100
1	G	111/124 (90%)	111 (100%)	0	0	100	100
1	H	112/124 (90%)	112 (100%)	0	0	100	100
1	I	113/124 (91%)	113 (100%)	0	0	100	100
1	J	111/124 (90%)	111 (100%)	0	0	100	100
1	K	113/124 (91%)	113 (100%)	0	0	100	100
1	L	111/124 (90%)	111 (100%)	0	0	100	100
All	All	1340/1488 (90%)	1339 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 3.3.2 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	100/116 (86%)	100 (100%)	0	100	100
1	B	96/116 (83%)	95 (99%)	1 (1%)	76	85
1	C	104/116 (90%)	102 (98%)	2 (2%)	57	68
1	D	98/116 (84%)	96 (98%)	2 (2%)	55	66
1	E	104/116 (90%)	103 (99%)	1 (1%)	76	85
1	F	94/116 (81%)	93 (99%)	1 (1%)	73	83
1	G	99/116 (85%)	99 (100%)	0	100	100
1	H	97/116 (84%)	96 (99%)	1 (1%)	76	85
1	I	102/116 (88%)	99 (97%)	3 (3%)	42	52
1	J	100/116 (86%)	100 (100%)	0	100	100
1	K	99/116 (85%)	97 (98%)	2 (2%)	55	66
1	L	94/116 (81%)	93 (99%)	1 (1%)	73	83
All	All	1187/1392 (85%)	1173 (99%)	14 (1%)	71	82

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1134	LYS
1	H	1083	LEU
1	K	1134	LYS
1	E	1053	GLU
1	I	1106	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1112	GLN
1	K	1126	ASN
1	G	1082	GLN
1	C	1082	GLN

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Mol	Chain	Res	Type
1	K	1082	GLN

### 3.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 3.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 3.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	PEG	E	1162	-	6,6,6	0.48	0	5,5,5	1.52	0
4	SO4	E	1	-	4,4,4	0.19	0	6,6,6	0.18	0
3	PEG	A	1	-	6,6,6	0.59	0	5,5,5	2.10	3 (60%)
4	SO4	L	2	-	4,4,4	0.16	0	6,6,6	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	E	1162	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	1	-	-	4/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	PEG	O2-C3-C4	2.76	122.21	110.07
3	A	1	PEG	C3-O2-C2	2.39	123.64	113.29
3	A	1	PEG	O2-C2-C1	2.36	120.43	110.07

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	PEG	C1-C2-O2-C3
3	E	1162	PEG	O1-C1-C2-O2
3	A	1	PEG	C4-C3-O2-C2
3	E	1162	PEG	O2-C3-C4-O4
3	A	1	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	PEG	1	0
4	L	2	SO4	1	0

### 3.7 Other polymers [i](#)

There are no such residues in this entry.

### 3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 4 Fit of model and data [i](#)

### 4.1 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	114/124 (91%)	0.56	8 (7%) 16 24	23, 41, 90, 121	0
1	B	114/124 (91%)	0.40	8 (7%) 16 24	40, 61, 101, 120	0
1	C	114/124 (91%)	0.32	7 (6%) 21 30	25, 45, 88, 108	0
1	D	113/124 (91%)	0.37	7 (6%) 20 28	30, 51, 95, 114	0
1	E	115/124 (92%)	0.23	4 (3%) 44 54	23, 44, 86, 102	0
1	F	111/124 (89%)	1.39	30 (27%) 0 0	49, 88, 135, 178	0
1	G	113/124 (91%)	0.47	9 (7%) 12 18	24, 45, 92, 102	0
1	H	113/124 (91%)	0.59	8 (7%) 16 23	36, 64, 96, 111	0
1	I	115/124 (92%)	0.34	9 (7%) 13 19	22, 44, 81, 112	0
1	J	113/124 (91%)	0.45	11 (9%) 7 12	36, 52, 95, 100	0
1	K	114/124 (91%)	0.22	6 (5%) 26 37	29, 55, 101, 144	0
1	L	113/124 (91%)	0.78	12 (10%) 6 10	39, 70, 116, 145	0
All	All	1362/1488 (91%)	0.51	119 (8%) 10 15	22, 55, 102, 178	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1160	LEU	11.7
1	J	1048	ILE	6.9
1	B	1161	GLY	6.6
1	C	1048	ILE	6.1
1	D	1160	LEU	6.0

### 4.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 4.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 4.4 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( $\text{\AA}^2$ )	Q<0.9
3	PEG	A	1	7/7	0.72	0.40	48,48,48,48	0
3	PEG	E	1162	7/7	0.86	0.24	66,66,66,66	0
4	SO4	E	1	5/5	0.91	0.12	42,49,65,96	0
2	CL	E	2	1/1	0.92	0.13	67,67,67,67	0
4	SO4	L	2	5/5	0.95	0.18	52,57,109,127	0
2	CL	A	3	1/1	0.97	0.27	61,61,61,61	0

### 4.5 Other polymers [i](#)

There are no such residues in this entry.