



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:44 PM UTC

PDB ID : 2YYN / pdb\_00002yyn  
Title : Crystal structure of human bromodomain protein  
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Deposited on : 2007-04-30  
Resolution : 2.50 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

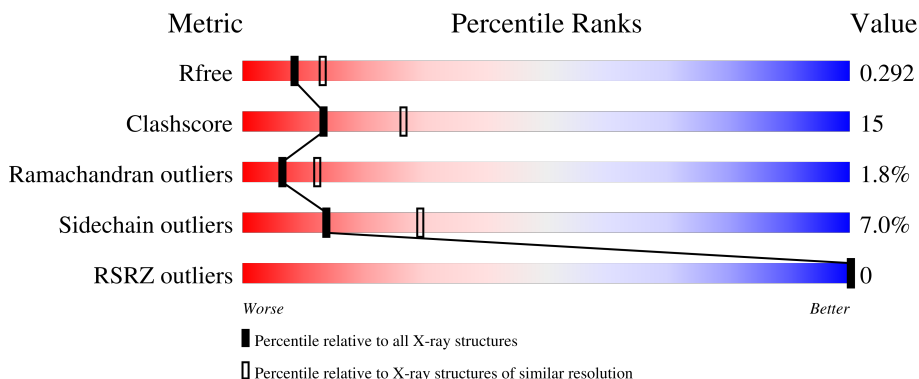
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 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	135	 64% 19% • 16%
1	B	135	 47% 27% 8% • 16%
1	C	135	 57% 21% 6% 16%
1	D	135	 64% 18% • 16%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3896 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 Transcription intermediary factor 1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	113	947	616	150	175	6	0	0	0
1	B	114	956	622	152	176	6	0	0	0
1	C	113	947	616	150	175	6	0	0	0
1	D	113	947	616	150	175	6	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O15164
A	2	SER	-	expression tag	UNP O15164
A	3	SER	-	expression tag	UNP O15164
A	4	GLY	-	expression tag	UNP O15164
A	5	SER	-	expression tag	UNP O15164
A	6	SER	-	expression tag	UNP O15164
A	7	GLY	-	expression tag	UNP O15164
A	130	SER	-	expression tag	UNP O15164
A	131	GLY	-	expression tag	UNP O15164
A	132	PRO	-	expression tag	UNP O15164
A	133	SER	-	expression tag	UNP O15164
A	134	SER	-	expression tag	UNP O15164
A	135	GLY	-	expression tag	UNP O15164
B	1	GLY	-	expression tag	UNP O15164
B	2	SER	-	expression tag	UNP O15164
B	3	SER	-	expression tag	UNP O15164
B	4	GLY	-	expression tag	UNP O15164
B	5	SER	-	expression tag	UNP O15164
B	6	SER	-	expression tag	UNP O15164
B	7	GLY	-	expression tag	UNP O15164
B	130	SER	-	expression tag	UNP O15164

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Chain	Residue	Modelled	Actual	Comment	Reference
B	131	GLY	-	expression tag	UNP O15164
B	132	PRO	-	expression tag	UNP O15164
B	133	SER	-	expression tag	UNP O15164
B	134	SER	-	expression tag	UNP O15164
B	135	GLY	-	expression tag	UNP O15164
C	1	GLY	-	expression tag	UNP O15164
C	2	SER	-	expression tag	UNP O15164
C	3	SER	-	expression tag	UNP O15164
C	4	GLY	-	expression tag	UNP O15164
C	5	SER	-	expression tag	UNP O15164
C	6	SER	-	expression tag	UNP O15164
C	7	GLY	-	expression tag	UNP O15164
C	130	SER	-	expression tag	UNP O15164
C	131	GLY	-	expression tag	UNP O15164
C	132	PRO	-	expression tag	UNP O15164
C	133	SER	-	expression tag	UNP O15164
C	134	SER	-	expression tag	UNP O15164
C	135	GLY	-	expression tag	UNP O15164
D	1	GLY	-	expression tag	UNP O15164
D	2	SER	-	expression tag	UNP O15164
D	3	SER	-	expression tag	UNP O15164
D	4	GLY	-	expression tag	UNP O15164
D	5	SER	-	expression tag	UNP O15164
D	6	SER	-	expression tag	UNP O15164
D	7	GLY	-	expression tag	UNP O15164
D	130	SER	-	expression tag	UNP O15164
D	131	GLY	-	expression tag	UNP O15164
D	132	PRO	-	expression tag	UNP O15164
D	133	SER	-	expression tag	UNP O15164
D	134	SER	-	expression tag	UNP O15164
D	135	GLY	-	expression tag	UNP O15164

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	40	Total O 40 40	0	0
2	B	23	Total O 23 23	0	0
2	C	18	Total O 18 18	0	0
2	D	18	Total O 18 18	0	0

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

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.

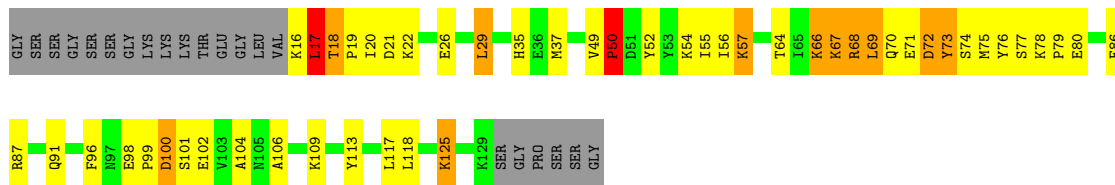
- Molecule 1: Transcription intermediary factor 1-alpha

Chain A: 



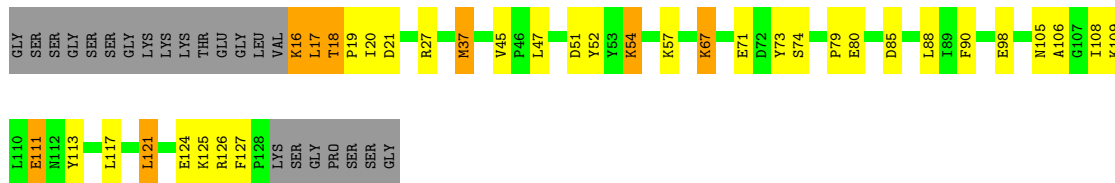
- Molecule 1: Transcription intermediary factor 1-alpha

Chain B: 



- Molecule 1: Transcription intermediary factor 1-alpha

Chain C: 



- Molecule 1: Transcription intermediary factor 1-alpha

Chain D: 



F127
P128
LYS
SER
GLY
PRO
SER
SER
GLY

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.86Å 76.16Å 107.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.08 – 2.50 48.08 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.08-2.50) 95.4 (48.08-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.42Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.285 0.246 , 0.292	Depositor DCC
$R_{free}$ test set	2017 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtrriage
Anisotropy	0.161	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 20.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.470 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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	0.46	0/971	0.90	1/1311 (0.1%)
1	B	0.46	0/980	0.98	6/1322 (0.5%)
1	C	0.46	1/971 (0.1%)	0.88	2/1311 (0.2%)
1	D	0.46	0/971	0.92	2/1311 (0.2%)
All	All	0.46	1/3893 (0.0%)	0.92	11/5255 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	MET	SD-CE	-5.44	1.66	1.79

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ARG	N-CA-C	-8.37	102.52	112.89
1	B	66	LYS	N-CA-C	-8.11	100.43	110.41
1	D	48	THR	N-CA-C	6.80	121.41	113.18
1	C	57	LYS	N-CA-C	6.27	118.19	111.36
1	A	48	THR	N-CA-C	5.88	120.46	113.28

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	947	0	942	20	0
1	B	956	0	954	37	0
1	C	947	0	941	34	0
1	D	947	0	942	23	0
2	A	40	0	0	1	0
2	B	23	0	0	1	0
2	C	18	0	0	0	0
2	D	18	0	0	0	0
All	All	3896	0	3779	112	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 15.

The worst 5 of 112 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:C:37:MET:HE3	1:C:106:ALA:HA	1.36	1.03
1:A:49:VAL:HG23	1:A:52:TYR:HB2	1.41	1.01
1:B:37:MET:HE3	1:B:106:ALA:HA	1.44	0.94
1:B:56:ILE:HD11	1:B:96:PHE:HB2	1.49	0.93
1:D:49:VAL:HG23	1:D:52:TYR:HB2	1.52	0.88

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	111/135 (82%)	103 (93%)	7 (6%)	1 (1%)	14 27
1	B	112/135 (83%)	99 (88%)	8 (7%)	5 (4%)	2 2
1	C	111/135 (82%)	103 (93%)	6 (5%)	2 (2%)	6 12
1	D	111/135 (82%)	107 (96%)	4 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	445/540 (82%)	412 (93%)	25 (6%)	8 (2%)	6	12

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	50	PRO
1	B	72	ASP
1	C	17	LEU
1	B	18	THR
1	B	101	SER

### 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	107/123 (87%)	102 (95%)	5 (5%)	23	47
1	B	108/123 (88%)	98 (91%)	10 (9%)	8	18
1	C	107/123 (87%)	101 (94%)	6 (6%)	19	39
1	D	107/123 (87%)	98 (92%)	9 (8%)	10	22
All	All	429/492 (87%)	399 (93%)	30 (7%)	14	29

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	LYS
1	D	102	GLU
1	C	54	LYS
1	D	118	LEU
1	D	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	70	GLN
1	C	120	ASN
1	D	112	ASN
1	D	70	GLN
1	B	42	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 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	113/135 (83%)	-1.19	0 100 100	22, 36, 51, 60	0
1	B	114/135 (84%)	-0.94	0 100 100	22, 41, 67, 83	0
1	C	113/135 (83%)	-0.99	0 100 100	22, 41, 73, 83	0
1	D	113/135 (83%)	-1.18	0 100 100	20, 36, 52, 58	0
All	All	453/540 (83%)	-1.08	0 100 100	20, 39, 66, 83	0

There are no RSRZ outliers to report.

### 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.