

wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 07:38 PM EDT

PDB ID : 2B2Y

Title: Tandem chromodomains of human CHD1

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Deposited on : 2005-09-19

Resolution : 2.35 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467 Xtriage (Phenix): 1.13

EDS: 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

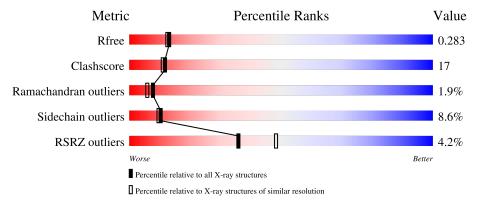
Validation Pipeline (wwPDB-VP) : 2.35

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 2.35 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 >=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 <=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					
			4%					
1	A	187	68%	20%	5% 6%			
	_		2%					
1	В	187	60%	26%	5% 10%			
			5%					
2	$^{\circ}$	115	48% 19%	6% •	25%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3707 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 Chromodomain-helicase-DNA-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	175	Total	С	N	О	S	0	0	0
1 A	170	1438	906	247	278	7	U	U	0	
1	B	169	Total	С	N	O	S	0	0	0
I D	Б 109	1383	871	234	271	7	0	U	U	

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP O14646
A	2	LYS	-	cloning artifact	UNP O14646
A	3	LYS	-	cloning artifact	UNP O14646
A	4	HIS	-	expression tag	UNP O14646
A	5	HIS	-	expression tag	UNP O14646
A	6	HIS	-	expression tag	UNP O14646
A	7	HIS	-	expression tag	UNP O14646
A	8	HIS	-	expression tag	UNP O14646
A	9	HIS	-	expression tag	UNP O14646
A	186	LYS	-	cloning artifact	UNP O14646
A	187	LYS	-	cloning artifact	UNP O14646
В	1	MET	-	cloning artifact	UNP O14646
В	2	LYS	-	cloning artifact	UNP O14646
В	3	LYS	-	cloning artifact	UNP O14646
В	4	HIS	-	expression tag	UNP O14646
В	5	HIS	-	expression tag	UNP O14646
В	6	HIS	-	expression tag	UNP O14646
В	7	HIS	-	expression tag	UNP O14646
В	8	HIS	-	expression tag	UNP O14646
В	9	HIS	-	expression tag	UNP O14646
В	186	LYS	-	cloning artifact	UNP O14646
В	187	LYS	-	cloning artifact	UNP O14646

• Molecule 2 is a protein called Chromodomain-helicase-DNA-binding protein 1.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	86	Total	С	N	О	S	0	0	0
		00	689	433	120	133	3	U	0	U

There are 9 discrepancies between the modelled and reference sequences: $\frac{1}{2}$

Chain	Residue	Modelled	Actual	Comment	Reference
С	1	MET	-	cloning artifact	UNP O14646
С	2	LYS	-	cloning artifact	UNP O14646
С	3	LYS	-	cloning artifact	UNP O14646
С	4	HIS	-	expression tag	UNP O14646
С	5	HIS	-	expression tag	UNP O14646
С	6	HIS	-	expression tag	UNP O14646
С	7	HIS	-	expression tag	UNP O14646
С	8	HIS	-	expression tag	UNP O14646
С	9	HIS	-	expression tag	UNP O14646

• Molecule 3 is water.

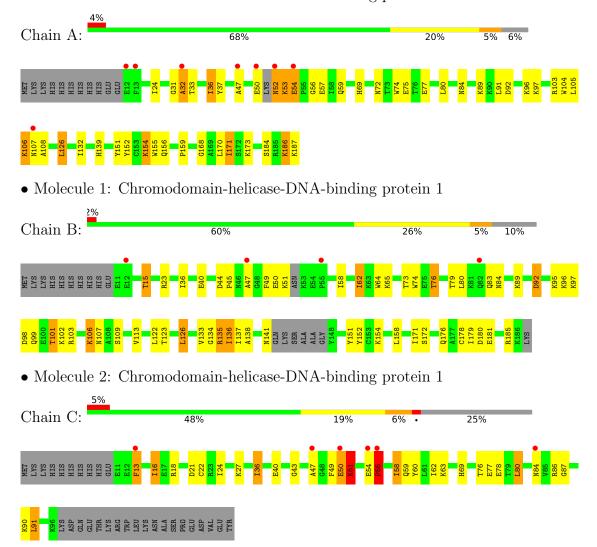
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0
3	В	67	Total O 67 67	0	0
3	С	30	Total O 30 30	0	0



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: Chromodomain-helicase-DNA-binding protein 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	112.27Å 55.03Å 101.55Å	Depositor
a, b, c, α , β , γ	90.00° 112.42° 90.00°	Depositor
Resolution (Å)	15.00 - 2.35	Depositor
Resolution (A)	31.29 - 2.35	EDS
% Data completeness	75.8 (15.00-2.35)	Depositor
(in resolution range)	90.7 (31.29-2.35)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	3.95 (at 2.36Å)	Xtriage
Refinement program	CNS	Depositor
P. P.	0.215 , 0.264	Depositor
R, R_{free}	0.235 , 0.283	DCC
R_{free} test set	1507 reflections (6.88%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 50.9	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3707	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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	Bo	nd lengths	Bond angles		
Woi Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.44	0/1473	1.00	17/1983~(0.9%)	
1	В	0.40	1/1416 (0.1%)	0.65	3/1911 (0.2%)	
2	С	0.44	0/704	0.72	1/948 (0.1%)	
All	All	0.42	1/3593 (0.0%)	0.82	21/4842 (0.4%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mo	l Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
1	В	180	ASP	C-N	7.03	1.50	1.34

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	186	LYS	CB-CA-C	-12.90	84.59	110.40
1	A	47	ALA	CB-CA-C	-12.29	91.66	110.10
1	A	32	ALA	CB-CA-C	-11.52	92.83	110.10
1	A	47	ALA	N-CA-C	8.78	134.71	111.00
1	A	53	LYS	CB-CA-C	-8.49	93.42	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	LYS	Mainchain



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	1438	0	1359	31	0
1	В	1383	0	1279	56	0
2	С	689	0	649	37	0
3	A	100	0	0	1	0
3	В	67	0	0	3	0
3	С	30	0	0	3	0
All	All	3707	0	3287	118	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 17.

The worst 5 of 118 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:137:ILE:HD11	1:B:152:TYR:HD2	1.09	1.15
1:B:103:ARG:O	1:B:106:LYS:HD2	1.56	1.02
1:A:132:ILE:HG13	1:A:156:GLN:HG3	1.40	1.00
1:B:137:ILE:HD11	1:B:152:TYR:CD2	1.98	0.98
1:B:76:THR:HG23	1:B:79:THR:H	1.35	0.91

There are no symmetry-related clashes.

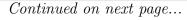
5.3 Torsion angles (i)

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.

\mathbf{Mol}	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	171/187 (91%)	159 (93%)	9 (5%)	3 (2%)	8 6





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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	В	163/187 (87%)	151 (93%)	11 (7%)	1 (1%)	25 27
2	С	84/115 (73%)	72 (86%)	8 (10%)	4 (5%)	2 0
All	All	418/489 (86%)	382 (91%)	28 (7%)	8 (2%)	8 6

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLY
1	A	32	ALA
1	В	47	ALA
2	С	47	ALA
2	С	55	PRO

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	150/164 (92%)	139 (93%)	11 (7%)	14 14
1	В	143/164 (87%)	132 (92%)	11 (8%)	13 12
2	С	69/101 (68%)	60 (87%)	9 (13%)	4 4
All	All	362/429 (84%)	331 (91%)	31 (9%)	10 9

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	62	ILE
2	С	55	PRO
1	В	89	LYS
2	С	80	LEU
2	С	21	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	142	GLN
1	A	176	GLN
1	В	176	GLN
2	С	69	HIS

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 monosaccharides 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^{th} 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>	#RS	$\mathrm{SRZ}{>}2$	$ \mathbf{OWAB}(\mathbf{\mathring{A}}^2) $	Q < 0.9
1	A	175/187 (93%)	0.28	8 (4%)	32 45	20, 39, 64, 81	0
1	В	169/187 (90%)	0.27	4 (2%)	59 68	28, 51, 66, 78	0
2	С	86/115 (74%)	0.32	6 (6%)	16 24	28, 43, 81, 88	0
All	All	430/489 (87%)	0.28	18 (4%)	36 48	20, 44, 68, 88	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	С	55	PRO	5.4
1	A	52	ASN	3.9
1	A	13	PHE	3.1
2	С	13	PHE	3.0
2	С	54	GLU	2.9

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 monosaccharides 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.

