



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:50 AM GMT

PDB ID : 1B47  
Title : STRUCTURE OF THE N-TERMINAL DOMAIN OF CBL IN COMPLEX  
WITH ITS BINDING SITE IN ZAP-70  
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Deposited on : 1999-01-06  
Resolution : 2.20 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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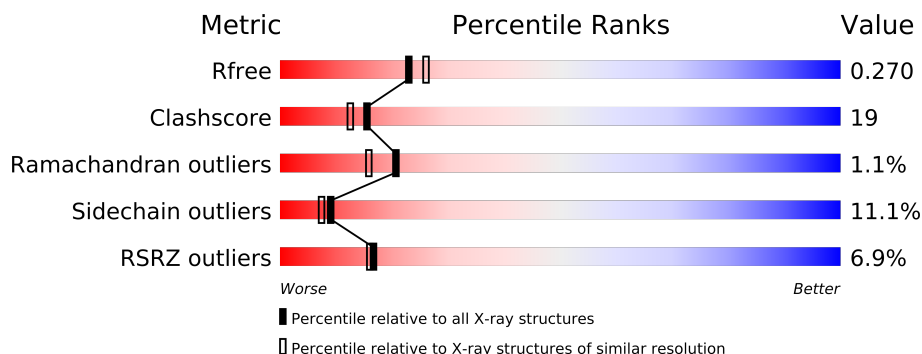
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	304	
1	B	304	
1	C	304	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	351	-	X
2	CA	B	351	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8092 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CBL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2475	1604	423	435	13			
1	B	304	Total	C	N	O	S	0	0	0
			2472	1603	422	434	13			
1	C	304	Total	C	N	O	S	0	0	0
			2476	1605	422	436	13			

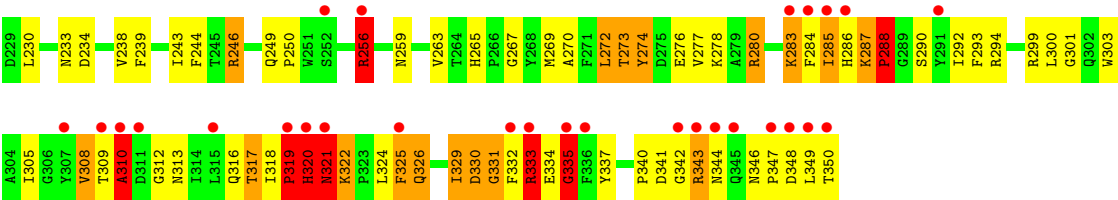
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total	O	0	0
			221	221		
3	B	261	Total	O	0	0
			261	261		
3	C	184	Total	O	0	0
			184	184		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.96Å 105.48Å 84.92Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.20) 99.3 (19.98-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.19Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.218 , 0.266 0.224 , 0.270	Depositor DCC
$R_{free}$ test set	3595 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.7	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 70917 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.91	0/2541	1.47	30/3433 (0.9%)
1	B	0.95	3/2538 (0.1%)	1.48	26/3429 (0.8%)
1	C	0.81	0/2542	1.33	27/3434 (0.8%)
All	All	0.89	3/7621 (0.0%)	1.43	83/10296 (0.8%)

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
1	B	0	14
1	C	0	12
All	All	0	42

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	343	ARG	NE-CZ	-5.89	1.25	1.33
1	B	343	ARG	CD-NE	-5.48	1.37	1.46
1	B	82	PRO	N-CD	5.33	1.55	1.47

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ARG	CD-NE-CZ	38.05	176.88	123.60
1	A	139	ARG	CD-NE-CZ	16.03	146.05	123.60
1	A	101	ARG	CD-NE-CZ	15.05	144.66	123.60
1	B	206	ARG	NE-CZ-NH1	13.41	127.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	ARG	NE-CZ-NH2	-10.48	115.06	120.30

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	SER	Mainchain
1	A	170	PRO	Mainchain
1	A	213	HIS	Mainchain
1	A	48	PRO	Mainchain
1	A	80	SER	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2475	0	2474	78	0
1	B	2472	0	2469	76	0
1	C	2476	0	2474	128	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	221	0	0	16	0
3	B	261	0	0	8	0
3	C	184	0	0	17	0
All	All	8092	0	7417	278	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 278 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:256:ARG:HH11	1:C:256:ARG:HG2	1.16	1.07
1:A:319:PRO:HA	3:A:474:HOH:O	1.61	0.99
1:B:265:HIS:HD2	1:B:267:GLY:H	1.12	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:82:PRO:HG3	1:C:156:LEU:HD22	1.49	0.95
1:C:265:HIS:HD2	1:C:267:GLY:H	1.12	0.94

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	302/304 (99%)	284 (94%)	16 (5%)	2 (1%)	30	28
1	B	302/304 (99%)	292 (97%)	10 (3%)	0	100	100
1	C	302/304 (99%)	273 (90%)	21 (7%)	8 (3%)	8	4
All	All	906/912 (99%)	849 (94%)	47 (5%)	10 (1%)	21	16

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	PRO
1	C	310	ALA
1	C	319	PRO
1	C	329	ILE
1	C	288	PRO

### 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	267/272 (98%)	237 (89%)	30 (11%)	9	7
1	B	266/272 (98%)	242 (91%)	24 (9%)	14	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	267/272 (98%)	232 (87%)	35 (13%)	6	4
All	All	800/816 (98%)	711 (89%)	89 (11%)	9	7

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	138	GLU
1	B	316	GLN
1	C	317	THR
1	B	139	ARG
1	B	224	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	HIS
1	B	313	ASN
1	C	321	ASN
1	B	265	HIS
1	B	302	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	304/304 (100%)	0.22	16 (5%) 25 25	27, 42, 68, 74	0
1	B	304/304 (100%)	0.05	9 (2%) 48 48	24, 36, 59, 68	0
1	C	304/304 (100%)	0.56	36 (11%) 5 5	30, 50, 75, 84	0
All	All	912/912 (100%)	0.28	61 (6%) 17 17	24, 43, 70, 84	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	HIS	9.2
1	C	319	PRO	5.8
1	C	336	PHE	5.6
1	C	345	GLN	5.3
1	C	342	GLY	5.2

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	351	1/1	0.32	7.77	28,28,28,28	0
2	CA	B	351	1/1	0.37	6.93	19,19,19,19	0
2	CA	C	351	1/1	0.21	1.69	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.