



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:39 AM GMT

PDB ID : 1BR8  
Title : IMPLICATIONS FOR FUNCTION AND THERAPY OF A 2.9A STRUCTURE OF BINARY-COMPLEXED ANTITHROMBIN  
Authors : Skinner, R.; Chang, W.S.W.; Jin, L.; Pei, X.Y.; Huntington, J.A.; Abrahams, J.P.; Carrell, R.W.; Lomas, D.A.  
Deposited on : 1998-08-26  
Resolution : 2.90 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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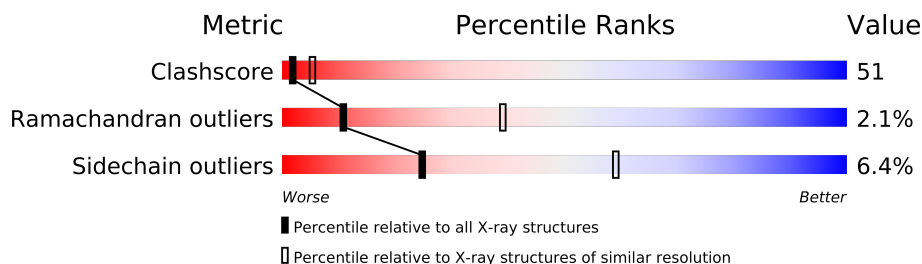
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.90 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))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	432	
1	L	432	
2	P	12	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6526 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 PROTEIN (ANTITHROMBIN-III).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	398	Total	C	N	O	S	0	0	0
			3182	2028	536	600	18			
1	I	404	Total	C	N	O	S	0	0	0
			3245	2071	548	608	18			

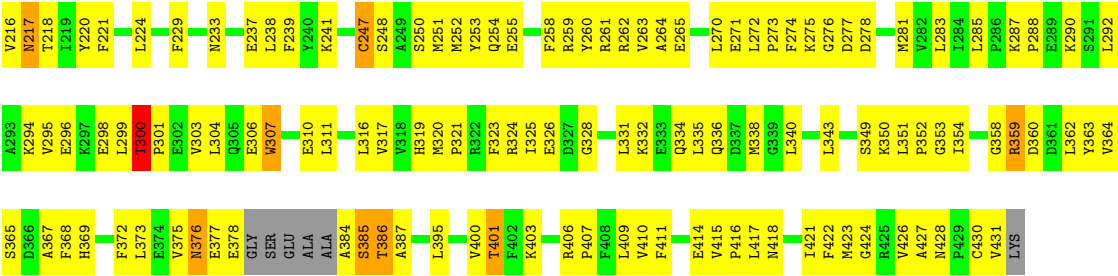
- Molecule 2 is a protein called PROTEIN (PEPTIDE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	12	Total	C	N	O	0	0	0
			76	46	12	18			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	18	Total	O	0	0
			18	18		
3	L	5	Total	O	0	0
			5	5		





• Molecule 2: PROTEIN (PEPTIDE)

Chain P:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.12Å 101.69Å 87.02Å 90.00° 104.36° 90.00°	Depositor
Resolution (Å)	6.00 – 2.90	Depositor
% Data completeness (in resolution range)	87.8 (6.00-2.90)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT V. 5.0	Depositor
R, $R_{free}$	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	I	0.48	0/3309	0.63	1/4465 (0.0%)
1	L	0.45	0/3243	0.66	2/4374 (0.0%)
2	P	0.50	0/75	0.48	0/101
All	All	0.47	0/6627	0.64	3/8940 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	406	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	I	247	CYS	CA-CB-SG	-5.40	104.28	114.00
1	L	407	PRO	O-C-N	5.08	130.83	122.70

There are no chirality outliers.

There are no planarity outliers.

### 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	I	3245	0	3252	311	1
1	L	3182	0	3182	357	0
2	P	76	0	79	12	0
3	I	18	0	0	1	0
3	L	5	0	0	0	0
All	All	6526	0	6513	666	1

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 51.

The worst 5 of 666 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:7:ILE:HD13	1:I:8:CYS:H	1.04	1.11
1:L:60:THR:HG21	1:L:301:PRO:HD3	1.32	1.08
1:L:257:LYS:HE2	1:L:313:GLU:HB3	1.37	1.06
1:I:263:VAL:HG11	1:I:307:TRP:CZ3	1.92	1.03
1:L:111:ILE:HG22	1:L:112:SER:H	1.18	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:160:ASP:OD1	1:I:262:ARG:NH2[2.657]	2.08	0.12

## 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	I	398/432 (92%)	344 (86%)	46 (12%)	8 (2%)	11	40
1	L	392/432 (91%)	345 (88%)	38 (10%)	9 (2%)	10	36
2	P	10/12 (83%)	10 (100%)	0	0	100	100
All	All	800/876 (91%)	699 (87%)	84 (10%)	17 (2%)	11	39

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	11	LYS
1	L	115	THR
1	L	137	SER
1	I	207	ILE
1	I	359	ARG



### 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	I	362/383 (94%)	347 (96%)	15 (4%)	41	80
1	L	353/383 (92%)	322 (91%)	31 (9%)	14	40
2	P	7/7 (100%)	7 (100%)	0	100	100
All	All	722/773 (93%)	676 (94%)	46 (6%)	25	59

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	316	LEU
1	L	357	GLU
1	I	300	THR
1	L	324	ARG
1	L	340	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	100	GLN
1	I	120	HIS
1	I	217	ASN
1	L	428	ASN
1	I	254	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 ⓘ

There are no ligands in this entry.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.