



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:24 PM GMT

PDB ID : 1ANT  
Title : BIOLOGICAL IMPLICATIONS OF A 3 ANGSTROMS STRUCTURE OF DIMERIC ANTITHROMBIN  
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Deposited on : 1994-02-28  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

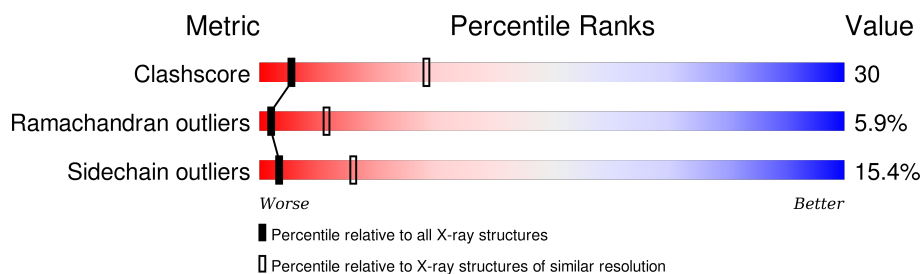
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	432	
1	L	432	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6371 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 ANTITHROMBIN.

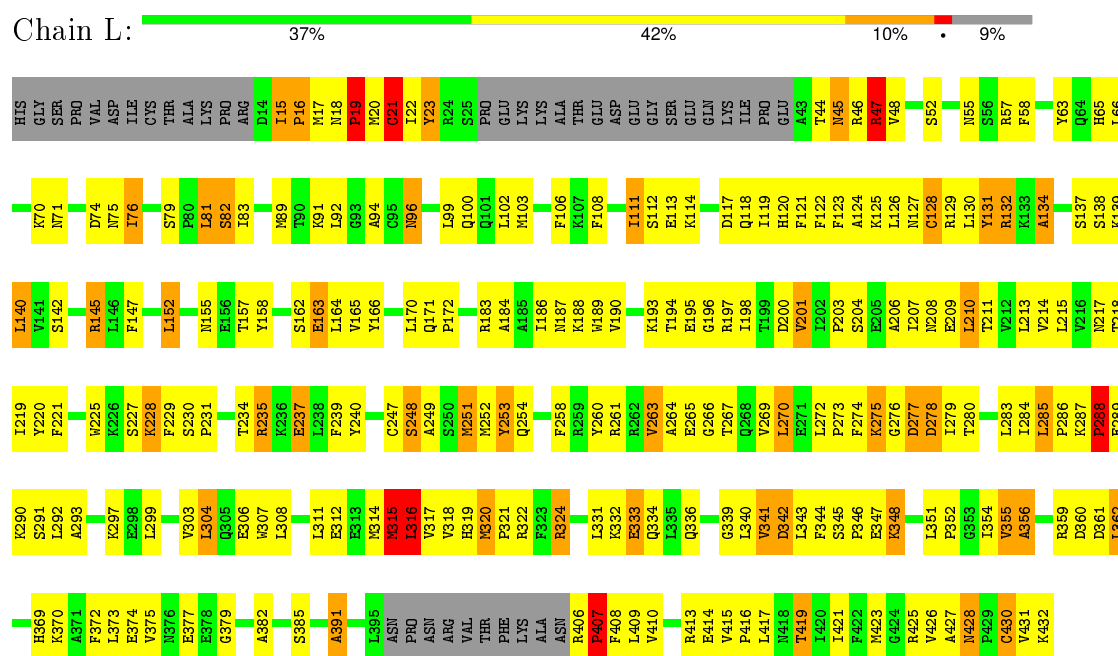
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	392	Total	C	N	O	S	0	0	0
			3139	2003	526	593	17			
1	I	402	Total	C	N	O	S	0	0	0
			3232	2063	548	604	17			

### 3 Residue-property plots

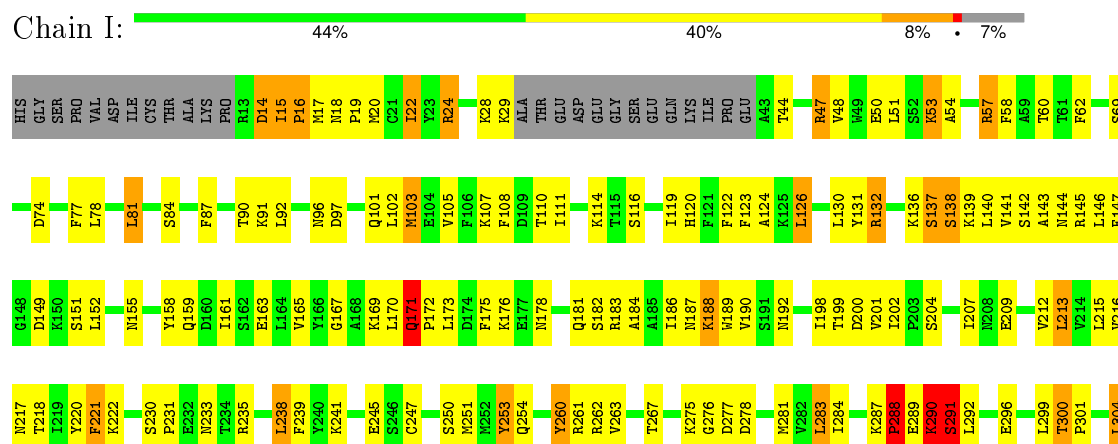
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: ANTITHROMBIN



#### • Molecule 1: ANTITHROMBIN



E377	E306	E307	E310	E314	E315	E316	E317	E318	E319	E320	E321	E322	E323	E324	E325	E326	E327	E328	E329	E332	E335	E336	E337	E338	E339	E340	E341	E342	E343	E346	E349	E350	E351	E352	E353	E354	E355	E356	E359	E360	E361	E362	E363	E364	E367	E368	E369	E370	E374
GLU	GLY	GLY	SER	GLU	ALA	A383	A384	S385	T386	A387	V388	V389	I390	A391	G392	R393	S394	L395	N396	P397	N398	R399	V400	T401	F402	K403	R406	L409	R413	E414	V415	P416	L417	N418	T419	F422	R425	N428	P429	C430	V431	K432							

## 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, $\alpha$ , $\beta$ , $\gamma$	70.06Å 101.52Å 90.45Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	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	0.64	0/3295	0.90	4/4441 (0.1%)
1	L	0.62	0/3199	0.91	6/4312 (0.1%)
All	All	0.63	0/6494	0.90	10/8753 (0.1%)

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	I	0	2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	I	283	LEU	CA-CB-CG	8.26	134.30	115.30
1	I	138	SER	N-CA-C	-6.85	92.51	111.00
1	L	210	LEU	CA-CB-CG	6.46	130.15	115.30
1	I	316	LEU	CA-CB-CG	6.04	129.19	115.30
1	L	316	LEU	CA-CB-CG	5.71	128.43	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	253	TYR	Sidechain
1	I	260	TYR	Sidechain

## 5.2 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	I	3232	0	3249	175	0
1	L	3139	0	3141	211	0
All	All	6371	0	6390	380	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 30.

The worst 5 of 380 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:I:198:ILE:HG23	1:I:370:LYS:HD3	1.41	1.00
1:L:190:VAL:HG21	1:L:201:VAL:HG21	1.46	0.96
1:I:108:PHE:HB3	1:I:119:ILE:HD12	1.47	0.94
1:I:132:ARG:HH11	1:I:132:ARG:HB3	1.36	0.90
1:L:406:ARG:CG	1:L:407:PRO:HD2	2.02	0.89

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	I	396/432 (92%)	313 (79%)	59 (15%)	24 (6%)	<b>2</b>	<b>11</b>
1	L	386/432 (89%)	305 (79%)	59 (15%)	22 (6%)	<b>2</b>	<b>12</b>
All	All	782/864 (90%)	618 (79%)	118 (15%)	46 (6%)	<b>2</b>	<b>11</b>



5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	21	CYS
1	L	47	ARG
1	L	132	ARG
1	L	195	GLU
1	L	277	ASP

### 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	359/383 (94%)	306 (85%)	53 (15%)	4	17
1	L	348/383 (91%)	292 (84%)	56 (16%)	3	14
All	All	707/766 (92%)	598 (85%)	109 (15%)	3	16

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	348	LYS
1	I	53	LYS
1	I	343	LEU
1	L	359	ARG
1	L	430	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	217	ASN
1	L	254	GLN
1	I	96	ASN
1	L	159	GLN
1	I	64	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 carbohydrates 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](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

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

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