wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 03:11 PM EDT

PDB ID	:	1ATT
Title	:	CRYSTAL STRUCTURE OF CLEAVED BOVINE ANTITHROMBIN III AT 3.2 ANGSTROMS RESOLUTION
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Deposited on	:	1993-03-29
Resolution	:	3.20 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:

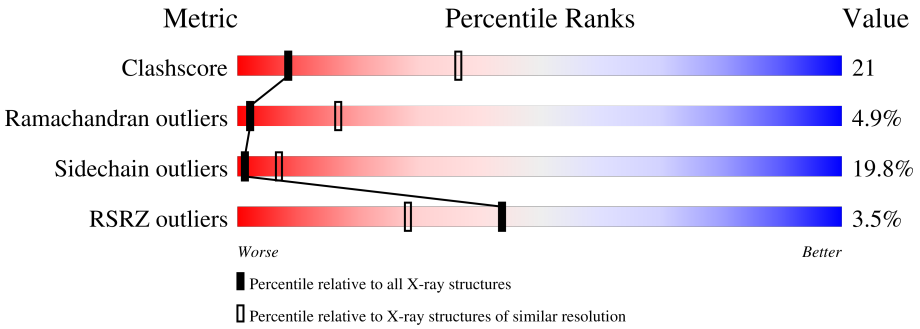
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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
1	A	429	4% 51% 32% 12%
1	B	429	3% 44% 36% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6640 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 III.

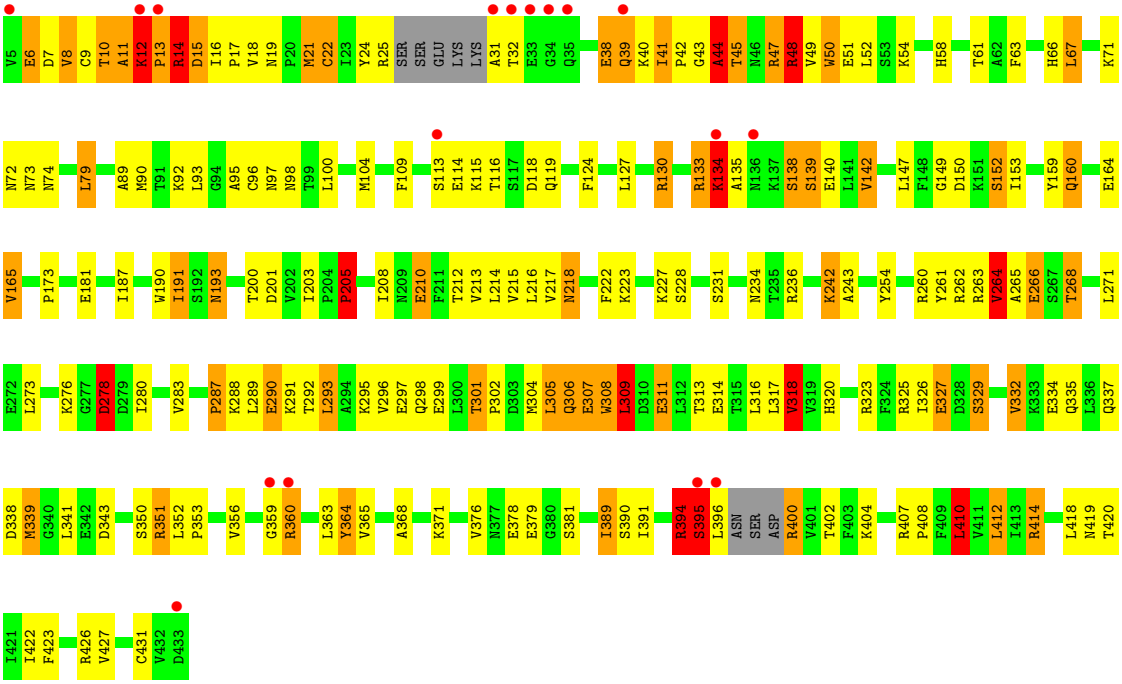
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	1
			3354	2131	568	639	16			
1	B	411	Total	C	N	O	S	0	0	1
			3286	2090	558	623	15			

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.

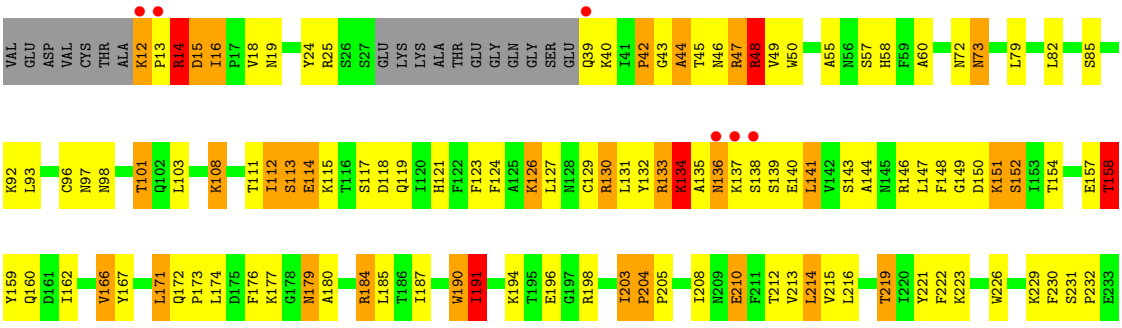
• Molecule 1: ANTITHROMBIN III

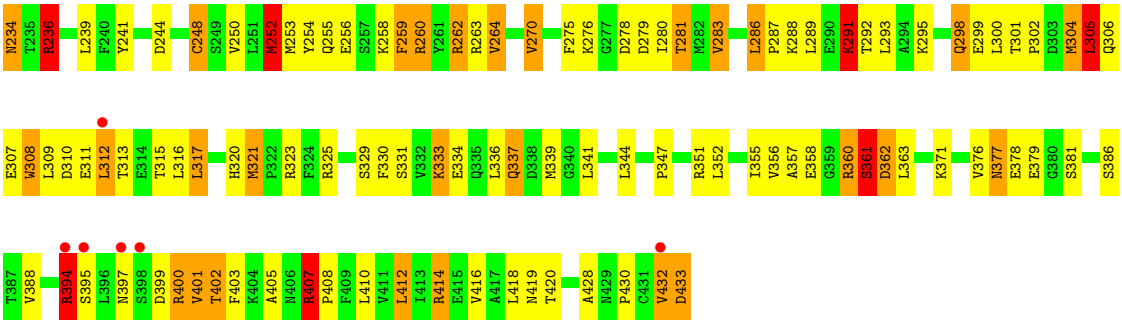
Chain A:



• Molecule 1: ANTITHROMBIN III

Chain B:




N234 T235 R236 L239 F240 Y241 D244 C248 S249 V250 L251 M252 M253 Y254 Q255 E256 S257 K258 F259 R260 Y261 R262 R263 V264 V270 F275 K276 G277 D278 D279 I280 T281 M282 V283 L286 P287 K288 L289 E290 K291 T292 L293 A294 K295 Q298 E299 L300 T301 P302 D303 M304 L305 Q306
E307 W308 L309 D310 E311 L312 T313 E314 T315 L316 L317 H320 M321 P322 R323 F324 R325 S329 F330 S331 V332 K333 E334 Q335 L336 Q337 D338 M339 G340 L341 L344 P347 R351 L352 I355 V356 A357 E358 G359 R360 S361 D362 L363 K371 V376 N377 E378 E379 G380 S381 S386
T387 V388 R394 S395 L396 N397 S398 D399 R400 V401 T402 F403 K404 A405 N406 R407 P408 F409 L410 V411 L412 I413 R414 E415 V416 A417 L418 N419 T420 A428 N429 P430 C431 V432 D433

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	91.30Å 91.30Å 383.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 41.75 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.20) 79.8 (41.75-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.51 (at 3.19Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , (Not available) 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 98.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6640	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

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	A	0.91	5/3417 (0.1%)	1.73	61/4616 (1.3%)
1	B	0.88	2/3349 (0.1%)	1.74	76/4523 (1.7%)
All	All	0.89	7/6766 (0.1%)	1.74	137/9139 (1.5%)

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	1
1	B	0	3
All	All	0	4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	LYS	C-N	-6.00	1.22	1.33
1	A	231	SER	CA-CB	-5.56	1.44	1.52
1	A	50	TRP	CG-CD2	-5.37	1.34	1.43
1	B	134	LYS	C-N	5.16	1.46	1.34
1	B	126	LYS	C-N	-5.16	1.22	1.34

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	A	260	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	B	263	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	B	133	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	B	48	ARG	NE-CZ-NH2	-10.42	115.09	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	ALA	Mainchain
1	B	134	LYS	Mainchain
1	B	167	TYR	Sidechain
1	B	18	VAL	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	3354	0	3345	142	0
1	B	3286	0	3281	134	0
All	All	6640	0	6626	276	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 21.

The worst 5 of 276 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:A:41:ILE:N	1:A:42:PRO:HD3	1.53	1.16
1:A:11:ALA:HB1	1:A:12:LYS:HE2	1.37	1.05
1:A:41:ILE:N	1:A:42:PRO:CD	2.28	0.97
1:A:153:ILE:HD13	1:A:213:VAL:HG13	1.51	0.93
1:B:317:LEU:HD13	1:B:401:VAL:HG23	1.50	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.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	415/429 (97%)	348 (84%)	52 (12%)	15 (4%)	3 23
1	B	405/429 (94%)	334 (82%)	46 (11%)	25 (6%)	1 11
All	All	820/858 (96%)	682 (83%)	98 (12%)	40 (5%)	2 17

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	12	LYS
1	A	278	ASP
1	A	395	SER
1	B	44	ALA

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	374/383 (98%)	295 (79%)	79 (21%)	1 6
1	B	368/383 (96%)	300 (82%)	68 (18%)	1 8
All	All	742/766 (97%)	595 (80%)	147 (20%)	1 7

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	223	LYS
1	B	412	LEU
1	B	248	CYS
1	B	323	ARG
1	A	293	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	A	193	ASN
1	A	218	ASN
1	B	429	ASN
1	B	97	ASN
1	A	66	HIS

5.3.3 RNA

There are no RNA molecules 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 monosaccharides 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

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>2			OWAB(Å^2)	Q<0.9
1	A	421/429 (98%)	-0.27	17 (4%)	38	25	2, 13, 54, 66	0
1	B	411/429 (95%)	-0.28	12 (2%)	51	36	3, 23, 50, 69	0
All	All	832/858 (96%)	-0.28	29 (3%)	44	28	2, 20, 52, 69	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	GLY	5.4
1	B	312	LEU	4.4
1	A	5	VAL	4.4
1	B	136	ASN	4.2
1	A	433	ASP	4.2

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.