



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:00 PM GMT

PDB ID : 1DM4  
Title : SER195ALA MUTANT OF HUMAN THROMBIN COMPLEXED WITH  
FIBRINOPEPTIDE A (7-16)  
Authors : Krishnan, R.; Sadler, E.J.; Tulinsky, A.  
Deposited on : 1999-12-13  
Resolution : 2.50 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)  
Xtrriage (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

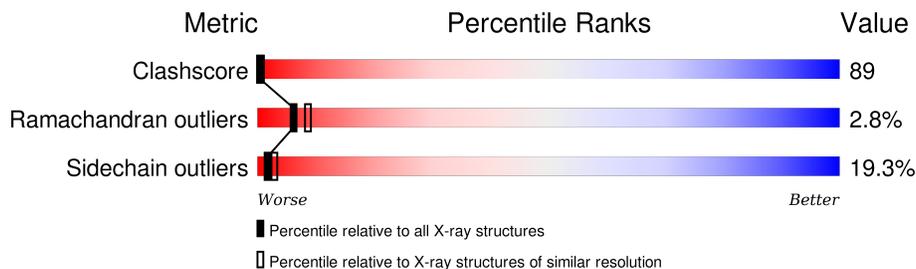
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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	A	35	
2	B	260	
3	C	11	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2525 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 PROTEIN (ALPHA THROMBIN:LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	33	263	165	42	55	1	0	0	0

- Molecule 2 is a protein called PROTEIN (MUTANT ALPHA THROMBIN:HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	2038	1299	360	365	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	ALA	SER	MUTATION	UNP P00734

- Molecule 3 is a protein called PROTEIN (FIBRINOPEPTIDE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	11	75	46	13	16	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total 15	O 15	0	0
4	B	127	Total 127	O 127	0	0
4	C	7	Total 7	O 7	0	0

### 3 Residue-property plots [i](#)

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.

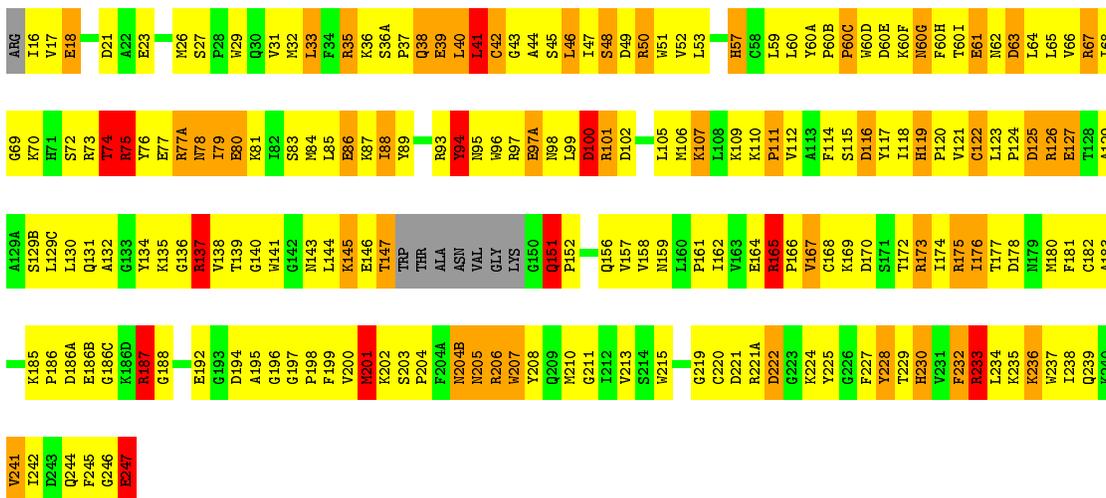
- Molecule 1: PROTEIN (ALPHA THROMBIN:LIGHT CHAIN)

Chain A: 



- Molecule 2: PROTEIN (MUTANT ALPHA THROMBIN:HEAVY CHAIN)

Chain B: 



- Molecule 3: PROTEIN (FIBRINOPEPTIDE)

Chain C: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.10Å 135.10Å 135.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2525	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.07	0/266	2.06	11/354 (3.1%)
2	B	0.99	0/2090	2.05	72/2822 (2.6%)
3	C	1.09	0/73	2.51	5/95 (5.3%)
All	All	1.00	0/2429	2.07	88/3271 (2.7%)

There are no bond length outliers.

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	126	ARG	CD-NE-CZ	20.03	151.65	123.60
2	B	75	ARG	NE-CZ-NH1	12.93	126.76	120.30
2	B	35	ARG	NE-CZ-NH2	-12.56	114.02	120.30
3	C	309	ASP	CB-CG-OD2	-12.55	107.00	118.30
2	B	165	ARG	NE-CZ-NH2	-12.33	114.14	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	263	0	258	105	0
2	B	2038	0	2010	345	0
3	C	75	0	69	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	15	0	0	8	0
4	B	127	0	0	51	0
4	C	7	0	0	0	0
All	All	2525	0	2337	420	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 89.

The worst 5 of 420 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:1(F):GLY:HA2	2:B:235:LYS:CE	1.54	1.35
1:A:1(F):GLY:HA2	2:B:235:LYS:NZ	1.46	1.28
1:A:1(G):PHE:CD1	1:A:1(F):GLY:N	2.12	1.17
2:B:89:TYR:HE2	4:B:433:HOH:O	1.29	1.16
1:A:1(C):GLU:HB2	1:A:1:CYS:HB3	1.28	1.10

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	31/35 (89%)	22 (71%)	7 (23%)	2 (6%)	<b>1</b> <b>1</b>
2	B	248/260 (95%)	215 (87%)	28 (11%)	5 (2%)	<b>9</b> <b>15</b>
3	C	9/11 (82%)	6 (67%)	2 (22%)	1 (11%)	<b>0</b> <b>0</b>
All	All	288/306 (94%)	243 (84%)	37 (13%)	8 (3%)	<b>6</b> <b>9</b>

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1(F)	GLY
3	C	309	ASP
1	A	1(B)	ALA
2	B	61	GLU
2	B	77(A)	ARG

### 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	29/30 (97%)	18 (62%)	11 (38%)	0	0
2	B	219/225 (97%)	182 (83%)	37 (17%)	2	4
3	C	6/6 (100%)	5 (83%)	1 (17%)	3	5
All	All	254/261 (97%)	205 (81%)	49 (19%)	2	3

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	75	ARG
2	B	94	TYR
2	B	236	LYS
2	B	83	SER
2	B	100	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	38	GLN
2	B	78	ASN
2	B	151	GLN
2	B	204(B)	ASN
2	B	244	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

### 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.