



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2024 – 01:38 PM EDT

PDB ID : 1BBR  
Title : THE STRUCTURE OF RESIDUES 7-16 OF THE A ALPHA CHAIN  
OF HUMAN FIBRINOGEN BOUND TO BOVINE THROMBIN AT 2.3  
ANGSTROMS RESOLUTION  
Authors : Martin, P.; Edwards, B.  
Deposited on : 1992-04-27  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

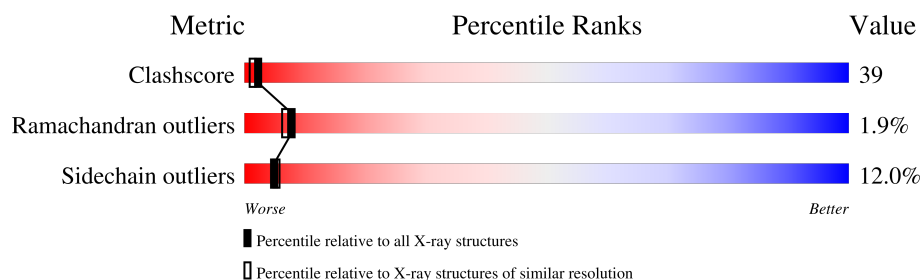
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)



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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	J	49	24% 39% 8% • 27%
1	L	49	35% 31% 8% 27%
1	M	49	24% 39% 10% 27%
2	H	150	46% 39% 13% •
3	E	109	51% 34% 13% •
4	F	11	27% 55% 18%
4	G	11	64% 18% 18%
4	I	11	36% 55% 9%

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Mol	Chain	Length	Quality of chain
5	K	259	 44% 37% 14% •
5	N	259	 42% 45% 10% •

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8084 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 EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			
1	J	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			
1	M	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			

- Molecule 2 is a protein called EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	150	Total	C	N	O	S	0	0	0
			1235	793	222	215	5			

- Molecule 3 is a protein called EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	109	Total	C	N	O	S	0	0	0
			860	544	154	155	7			

- Molecule 4 is a protein called FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	11	Total	C	N	O	0	0	0
			75	46	13	16			
4	G	11	Total	C	N	O	0	0	0
			75	46	13	16			
4	I	11	Total	C	N	O	0	0	0
			75	46	13	16			

- Molecule 5 is a protein called EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	259	Total 2094	C 1337	N 376	O 369	S 12	0	0	0
5	N	259	Total 2094	C 1337	N 376	O 369	S 12	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	31	Total 31	O 31	0	0
6	H	126	Total 126	O 126	0	0
6	E	69	Total 69	O 69	0	0
6	F	10	Total 10	O 10	0	0
6	J	23	Total 23	O 23	0	0
6	K	213	Total 213	O 213	0	0
6	G	11	Total 11	O 11	0	0
6	M	26	Total 26	O 26	0	0
6	N	188	Total 188	O 188	0	0
6	I	9	Total 9	O 9	0	0

### 3 Residue-property plots

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. 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. 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.

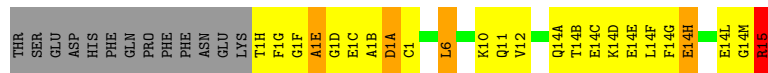
#### • Molecule 1: EPSILON-THROMBIN

Chain L: 

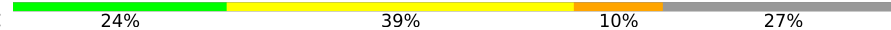


#### • Molecule 1: EPSILON-THROMBIN

Chain J: 



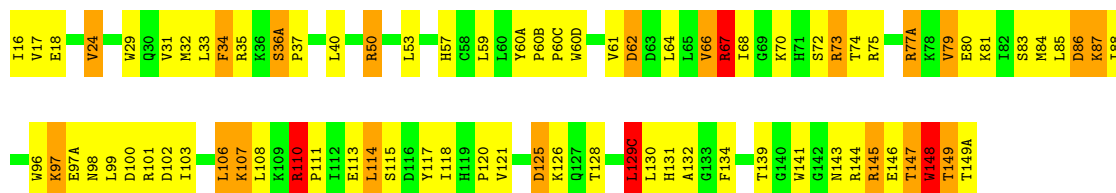
#### • Molecule 1: EPSILON-THROMBIN

Chain M: 



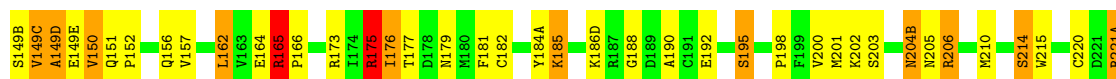
#### • Molecule 2: EPSILON-THROMBIN

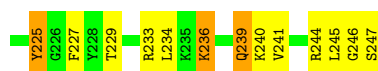
Chain H: 



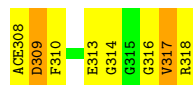
#### • Molecule 3: EPSILON-THROMBIN

Chain E: 

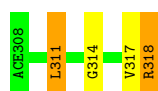




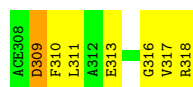
• Molecule 4: FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR



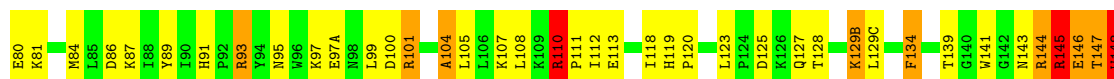
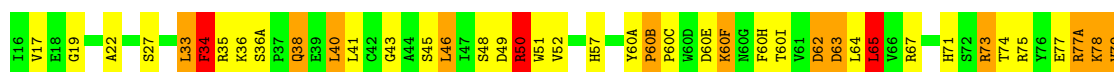
• Molecule 4: FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR



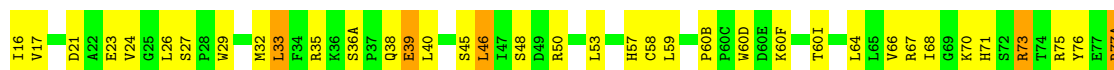
• Molecule 4: FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR



• Molecule 5: EPSILON-THROMBIN



• Molecule 5: EPSILON-THROMBIN







## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.02Å 89.41Å 99.30Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8084	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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	J	1.18	0/294	1.86	7/390 (1.8%)
1	L	1.07	0/294	1.64	1/390 (0.3%)
1	M	1.18	2/294 (0.7%)	1.87	5/390 (1.3%)
2	H	1.09	0/1267	1.71	17/1716 (1.0%)
3	E	1.14	0/881	1.77	16/1186 (1.3%)
4	F	1.18	0/73	2.25	3/95 (3.2%)
4	G	1.21	0/73	1.60	1/95 (1.1%)
4	I	1.24	0/73	1.95	1/95 (1.1%)
5	K	1.27	2/2148 (0.1%)	2.05	69/2905 (2.4%)
5	N	1.08	3/2148 (0.1%)	1.76	46/2905 (1.6%)
All	All	1.16	7/7545 (0.1%)	1.85	166/10167 (1.6%)

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	J	0	1
2	H	0	2
3	E	0	2
4	G	0	1
5	K	0	6
5	N	0	5
All	All	0	17

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	19	GLY	N-CA	5.75	1.54	1.46
5	K	80	GLU	CB-CG	-5.57	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	33	LEU	N-CA	5.54	1.57	1.46
1	M	14(H)	GLU	CD-OE2	-5.48	1.19	1.25
1	M	14(M)	GLY	N-CA	-5.42	1.38	1.46

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	225	TYR	CB-CG-CD1	16.06	130.63	121.00
5	K	225	TYR	CB-CG-CD2	-15.70	111.58	121.00
5	K	175	ARG	NE-CZ-NH2	-13.93	113.34	120.30
5	N	75	ARG	CD-NE-CZ	12.89	141.65	123.60
5	K	60(F)	LYS	CA-CB-CG	12.84	141.65	113.40

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	165	ARG	Sidechain
3	E	175	ARG	Sidechain
2	H	110	ARG	Sidechain
2	H	67	ARG	Sidechain
1	J	15	ARG	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	J	290	0	276	37	0
1	L	290	0	276	30	0
1	M	290	0	276	47	0
2	H	1235	0	1252	101	0
3	E	860	0	844	87	0
4	F	75	0	69	8	0
4	G	75	0	69	6	0
4	I	75	0	69	8	0
5	K	2094	0	2097	156	0
5	N	2094	0	2097	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	69	0	0	15	0
6	F	10	0	0	0	0
6	G	11	0	0	1	0
6	H	126	0	0	24	0
6	I	9	0	0	6	0
6	J	23	0	0	9	0
6	K	213	0	0	53	0
6	L	31	0	0	6	0
6	M	26	0	0	18	0
6	N	188	0	0	51	0
All	All	8084	0	7325	573	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 39.

The worst 5 of 573 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)
5:K:60(F):LYS:HB2	6:K:422:HOH:O	1.17	1.28
5:K:176:ILE:HG21	6:K:407:HOH:O	1.27	1.25
1:J:14(G):PHE:HB3	6:J:616:HOH:O	1.30	1.24
5:K:52:VAL:HG22	6:K:432:HOH:O	1.39	1.23
5:N:204:PRO:HB3	6:N:396:HOH:O	1.40	1.21

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	J	34/49 (69%)	28 (82%)	5 (15%)	1 (3%)	4	3
1	L	34/49 (69%)	27 (79%)	4 (12%)	3 (9%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	34/49 (69%)	26 (76%)	6 (18%)	2 (6%)	1	0
2	H	148/150 (99%)	135 (91%)	13 (9%)	0	100	100
3	E	107/109 (98%)	97 (91%)	7 (6%)	3 (3%)	5	3
4	F	9/11 (82%)	8 (89%)	0	1 (11%)	0	0
4	G	9/11 (82%)	9 (100%)	0	0	100	100
4	I	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
5	K	257/259 (99%)	235 (91%)	19 (7%)	3 (1%)	13	14
5	N	257/259 (99%)	229 (89%)	24 (9%)	4 (2%)	9	9
All	All	898/957 (94%)	802 (89%)	79 (9%)	17 (2%)	8	7

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(B)	ALA
1	L	14(K)	ILE
3	E	149(C)	VAL
3	E	150	VAL
4	F	309	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	J	30/43 (70%)	24 (80%)	6 (20%)	1	1
1	L	30/43 (70%)	29 (97%)	1 (3%)	38	53
1	M	30/43 (70%)	28 (93%)	2 (7%)	16	21
2	H	134/134 (100%)	119 (89%)	15 (11%)	6	6
3	E	92/92 (100%)	82 (89%)	10 (11%)	6	7
4	F	6/6 (100%)	4 (67%)	2 (33%)	0	0
4	G	6/6 (100%)	5 (83%)	1 (17%)	2	2
4	I	6/6 (100%)	5 (83%)	1 (17%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	K	226/226 (100%)	195 (86%)	31 (14%)	3	3
5	N	226/226 (100%)	201 (89%)	25 (11%)	6	7
All	All	786/825 (95%)	692 (88%)	94 (12%)	5	5

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	160	LEU
5	N	40	LEU
5	K	185	LYS
4	G	311	LEU
5	N	93	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
5	K	204(B)	ASN
5	N	205	ASN
1	M	13	GLN
5	N	239	GLN
5	N	131	HIS

### 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 monosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.