



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:00 PM GMT

PDB ID : 1DEQ  
Title : THE CRYSTAL STRUCTURE OF MODIFIED BOVINE FIBRINOGEN (AT 4 ANGSTROM RESOLUTION)  
Authors : Brown, J.H.; Volkmann, N.; Jun, G.; Henschen-Edman, A.H.; Cohen, C.  
Deposited on : 1999-11-15  
Resolution : 3.50 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)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

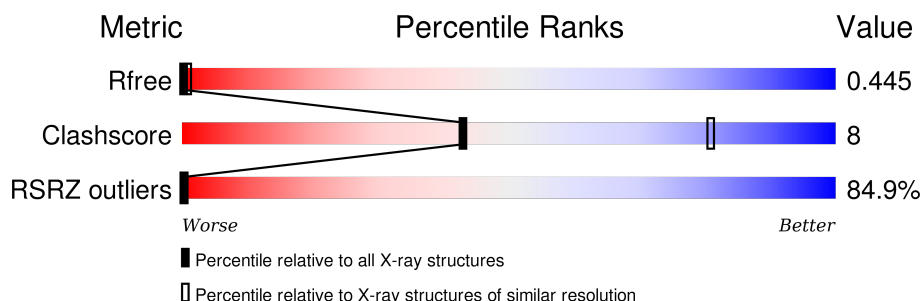
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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.

Mol	Chain	Length	Quality of chain
1	A	390	<div> <div>39%</div> <div>45%</div> <div>54%</div> </div>
1	D	390	<div> <div>43%</div> <div>44%</div> <div>54%</div> </div>
1	N	390	<div> <div>38%</div> <div>46%</div> <div>54%</div> </div>
1	Q	390	<div> <div>44%</div> <div>44%</div> <div>54%</div> </div>
2	B	408	<div> <div>74%</div> <div>93%</div> <div>7%</div> </div>
2	E	408	<div> <div>80%</div> <div>93%</div> <div>7%</div> </div>
2	O	408	<div> <div>72%</div> <div>93%</div> <div>7%</div> </div>
2	R	408	<div> <div>86%</div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	411	<div><div></div><div>74%90%10%</div></div>
3	F	411	<div><div></div><div>70%89%10%</div></div>
3	P	411	<div><div></div><div>76%90%10%</div></div>
3	S	411	<div><div></div><div>83%90%10%</div></div>
4	M	90	<div><div></div><div>87%13%</div></div>
4	Z	90	<div><div></div><div>87%13%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3900 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 FIBRINOGEN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	180	Total C 180 180	0	0	180
1	D	180	Total C 180 180	0	0	180
1	N	180	Total C 180 180	0	0	180
1	Q	180	Total C 180 180	0	0	180

- Molecule 2 is a protein called FIBRINOGEN (BETA CHAIN).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	380	Total C 380 380	0	0	380
2	E	380	Total C 380 380	0	0	380
2	O	380	Total C 380 380	0	0	380
2	R	380	Total C 380 380	0	0	380

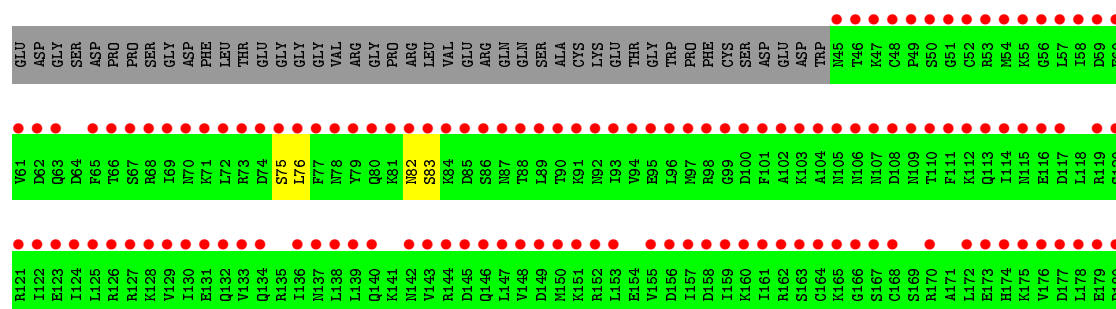
- Molecule 3 is a protein called FIBRINOGEN (GAMMA CHAIN).

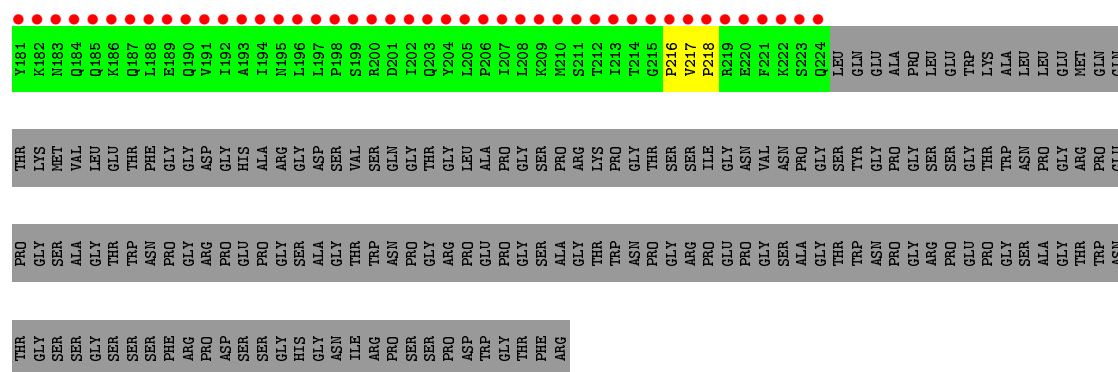
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	370	Total C 370 370	0	0	370
3	F	370	Total C 370 370	0	0	370
3	P	370	Total C 370 370	0	0	370
3	S	370	Total C 370 370	0	0	370

- Molecule 4 is a protein called FIBRINOGEN.

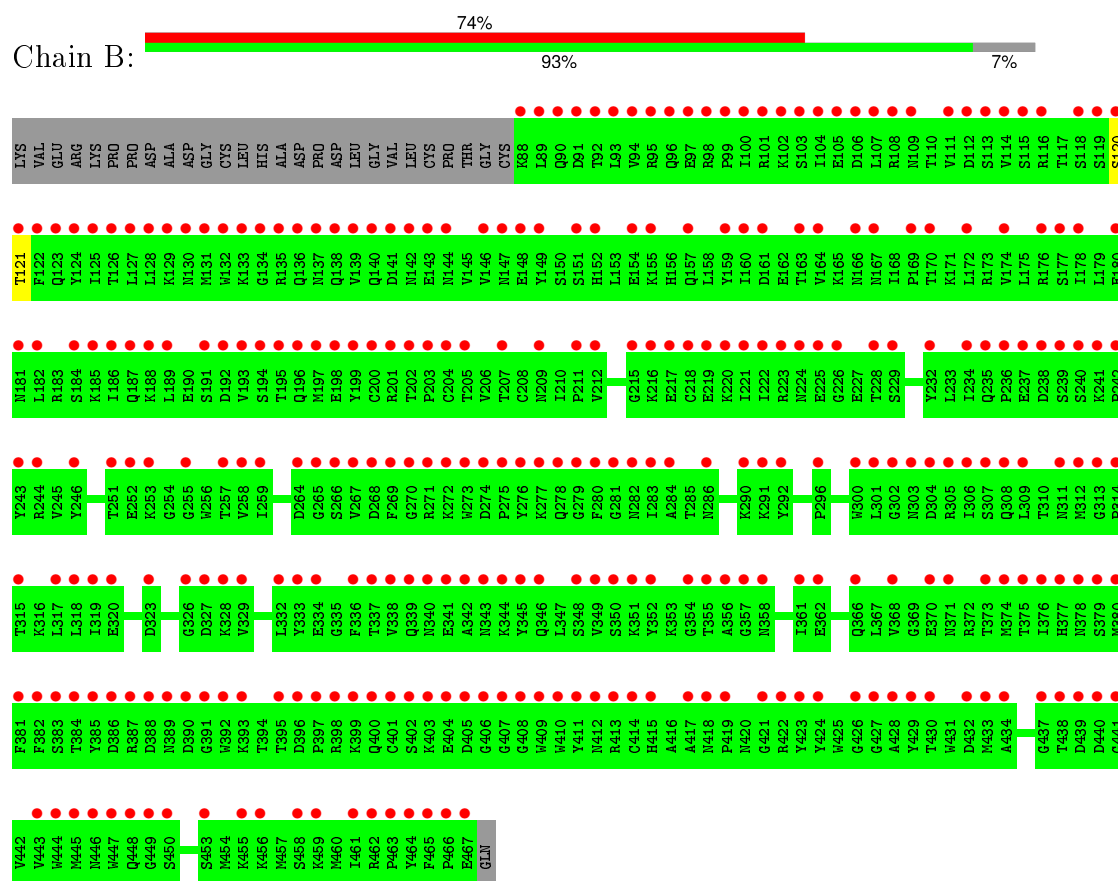
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	M	90	Total C 90 90	0	0	90
4	Z	90	Total C 90 90	0	0	90



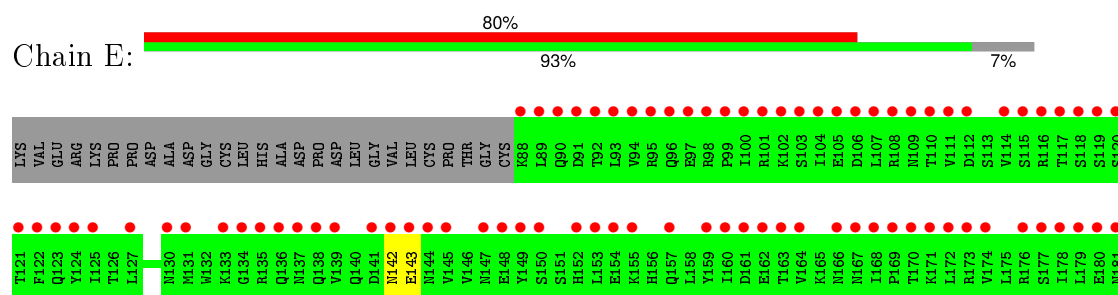




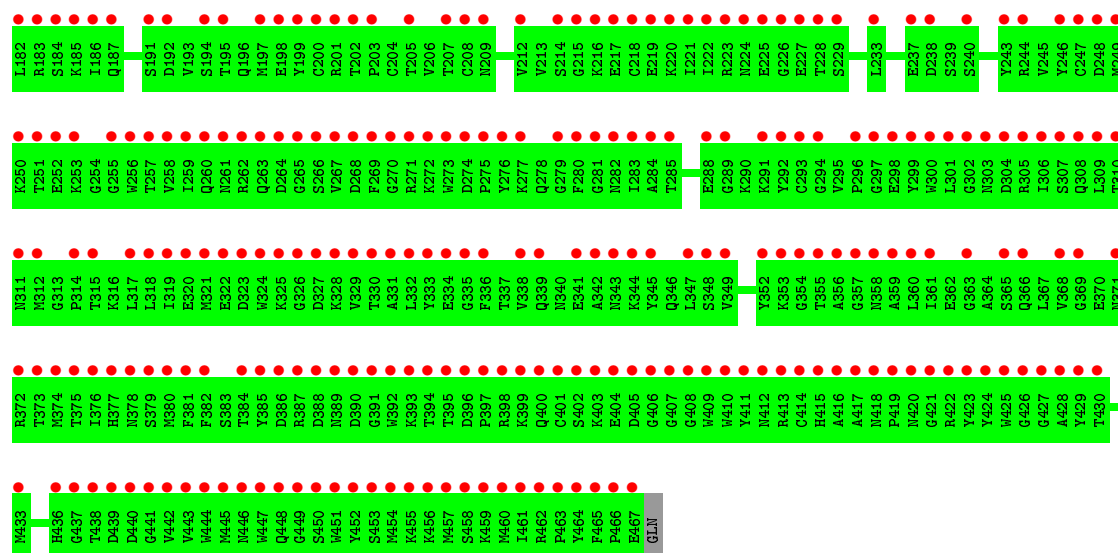
- Molecule 2: FIBRINOGEN (BETA CHAIN)



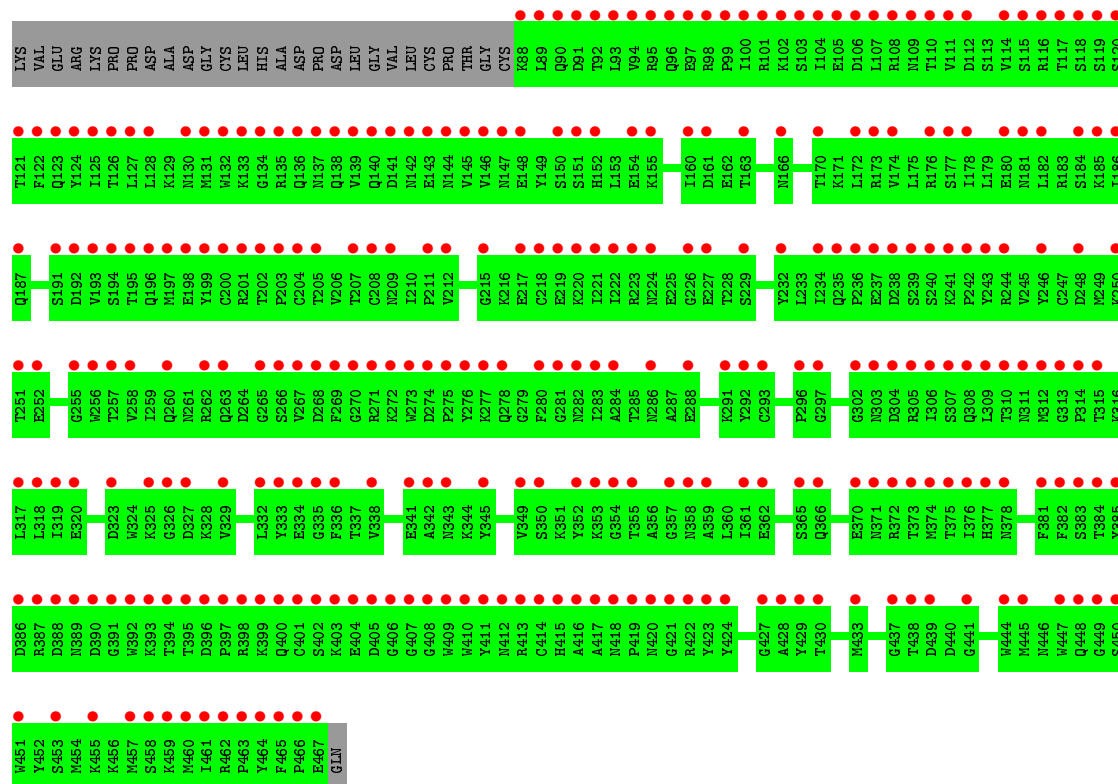
- Molecule 2: FIBRINOGEN (BETA CHAIN)



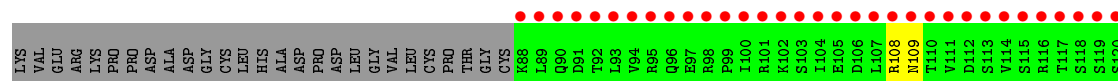
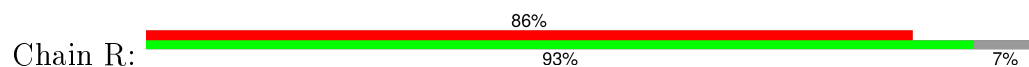


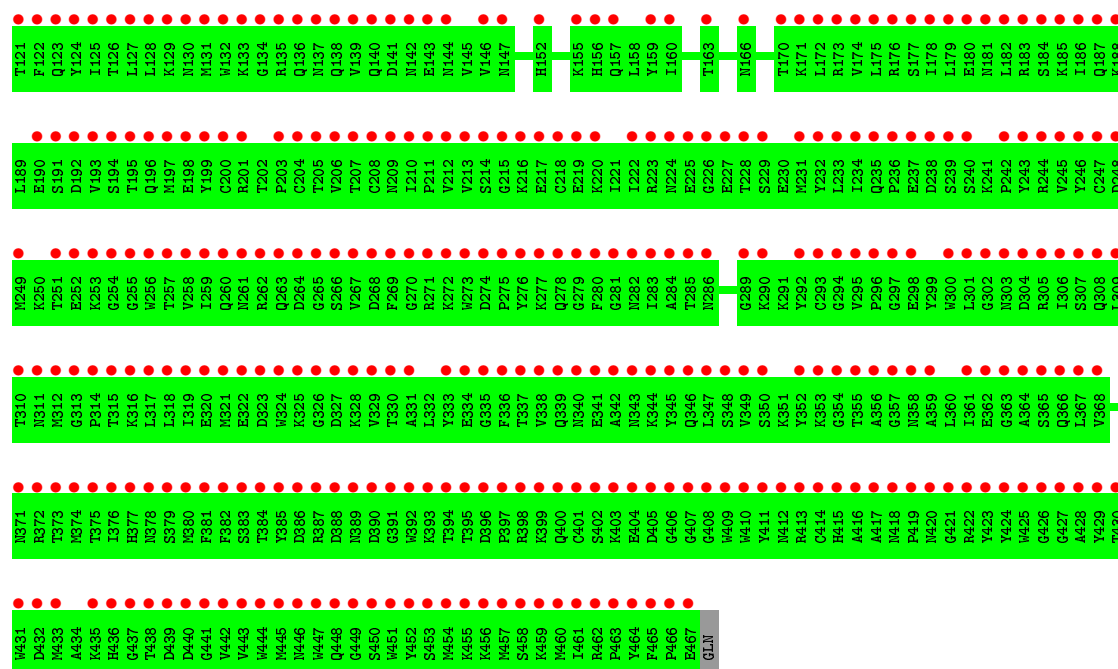


### • Molecule 2: FIBRINOGEN (BETA CHAIN)



### • Molecule 2: FIBRINOGEN (BETA CHAIN)



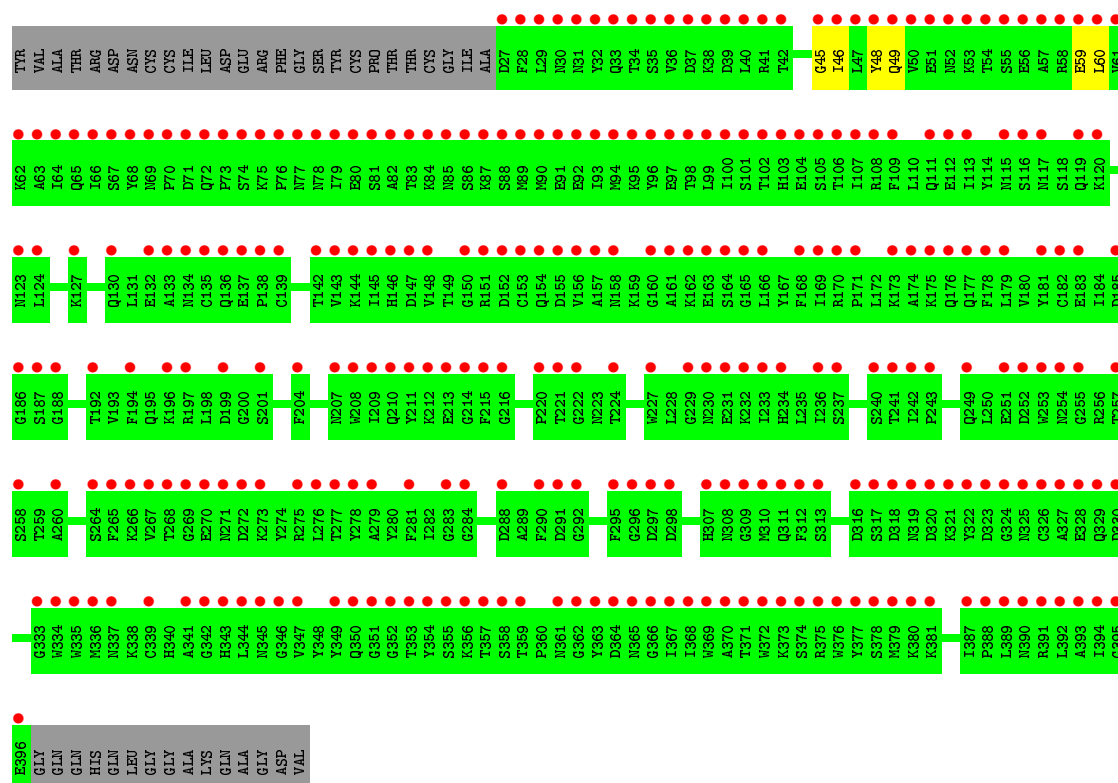


● Molecule 3: FIBRINOGEN (GAMMA CHAIN)

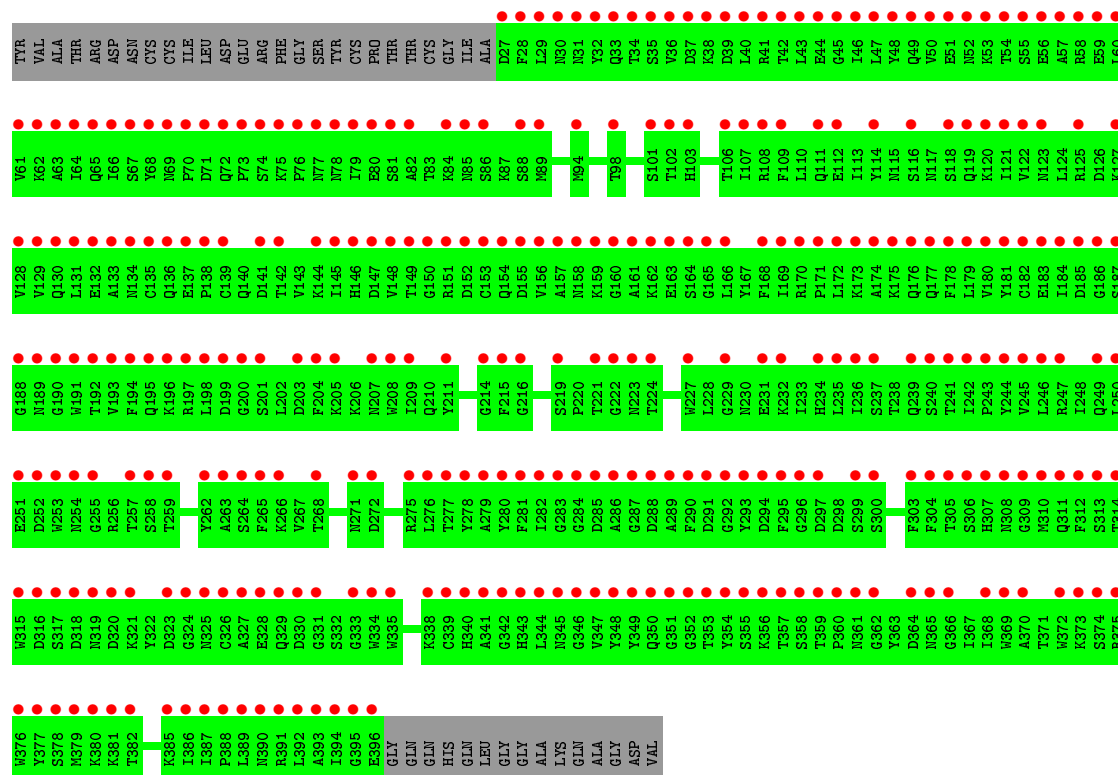
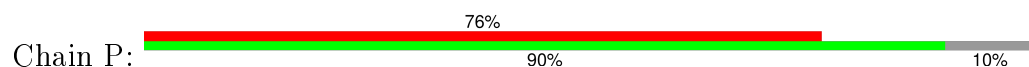


● Molecule 3: FIBRINOGEN (GAMMA CHAIN)





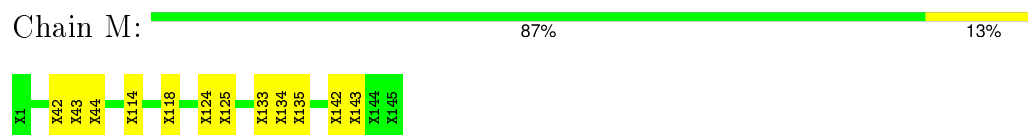
• Molecule 3: FIBRINOGEN (GAMMA CHAIN)



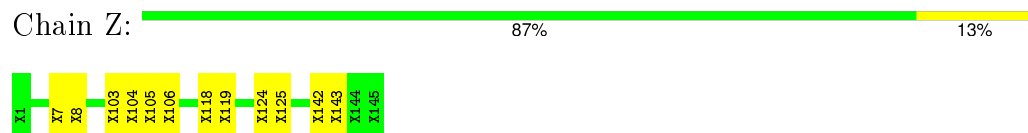
- Molecule 3: FIBRINOGEN (GAMMA CHAIN)



- Molecule 4: FIBRINOGEN



- Molecule 4: FIBRINOGEN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.01Å 94.94Å 209.81Å 90.00° 94.41° 90.00°	Depositor
Resolution (Å)	10.00 – 3.50 209.18 – 3.34	Depositor EDS
% Data completeness (in resolution range)	86.9 (10.00-3.50) 78.8 (209.18-3.34)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 3.33Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.257 , 0.370 0.438 , 0.445	Depositor DCC
$R_{free}$ test set	3661 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	91.6	Xtriage
Anisotropy	0.887	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 153.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 79450 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.72	EDS
Total number of atoms	3900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	225.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	180	0	0	3	0
1	D	180	0	0	5	0
1	N	180	0	0	1	0
1	Q	180	0	0	4	0
2	B	380	0	0	1	0
2	E	380	0	0	1	0
2	O	380	0	0	0	0
2	R	380	0	0	1	0
3	C	370	0	0	0	0
3	F	370	0	0	3	0
3	P	370	0	0	0	0
3	S	370	0	0	1	0
4	M	90	0	0	8	0
4	Z	90	0	0	6	0
All	All	3900	0	0	32	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 8.

The worst 5 of 32 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)
2:E:142:ASN:CA	2:E:143:GLU:CA	2.09	1.29
4:M:134:UNK:CA	4:M:135:UNK:CA	2.16	1.22
4:M:43:UNK:CA	4:M:44:UNK:CA	2.18	1.21
1:Q:82:ASN:CA	1:Q:83:SER:CA	2.22	1.17
4:M:124:UNK:CA	4:M:125:UNK:CA	2.27	1.12

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	180/390 (46%)	8.27	153 (85%)  	4, 93, 999, 999	0
1	D	180/390 (46%)	10.44	167 (92%)  	25, 131, 999, 999	0
1	N	180/390 (46%)	8.61	148 (82%)  	2, 88, 999, 999	0
1	Q	180/390 (46%)	10.21	173 (96%)  	2, 151, 999, 999	0
2	B	380/408 (93%)	9.88	302 (79%)  	2, 62, 214, 999	0
2	E	380/408 (93%)	11.69	326 (85%)  	2, 81, 999, 999	0
2	O	380/408 (93%)	9.80	292 (76%)  	2, 63, 191, 359	0
2	R	380/408 (93%)	15.79	349 (91%)  	2, 130, 358, 999	0
3	C	370/411 (90%)	9.27	303 (81%)  	2, 58, 999, 999	0
3	F	370/411 (90%)	9.38	288 (77%)  	2, 68, 999, 999	0
3	P	370/411 (90%)	13.45	313 (84%)  	2, 96, 386, 999	0
3	S	370/411 (90%)	13.06	343 (92%)  	6, 112, 999, 999	0
4	M	0/90	-	-	-	-
4	Z	0/90	-	-	-	-
All	All	3720/5016 (74%)	11.13	3157 (84%)  	2, 87, 999, 999	0

The worst 5 of 3157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	390	ASP	73.2
2	R	453	SER	62.3
2	R	198	GLU	58.1
2	R	450	SER	57.5
3	C	176	GLN	57.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.