



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:08 pm BST

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 Full wwPDB X-ray Structure Validation 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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

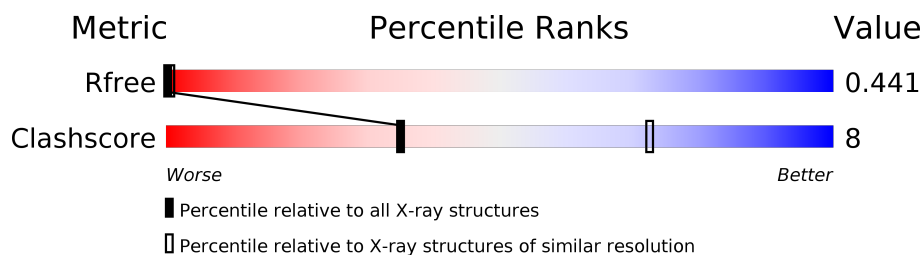
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)

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 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	390	45% 54%
1	D	390	44% 54%
1	N	390	46% 54%
1	Q	390	44% 54%
2	B	408	93% 7%
2	E	408	93% 7%
2	O	408	93% 7%
2	R	408	93% 7%
3	C	411	90% 10%

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Mol	Chain	Length	Quality of chain
3	F	411	 89%10%
3	P	411	 90%10%
3	S	411	 90%10%
4	M	90	 87%13%
4	Z	90	 87%13%

## 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

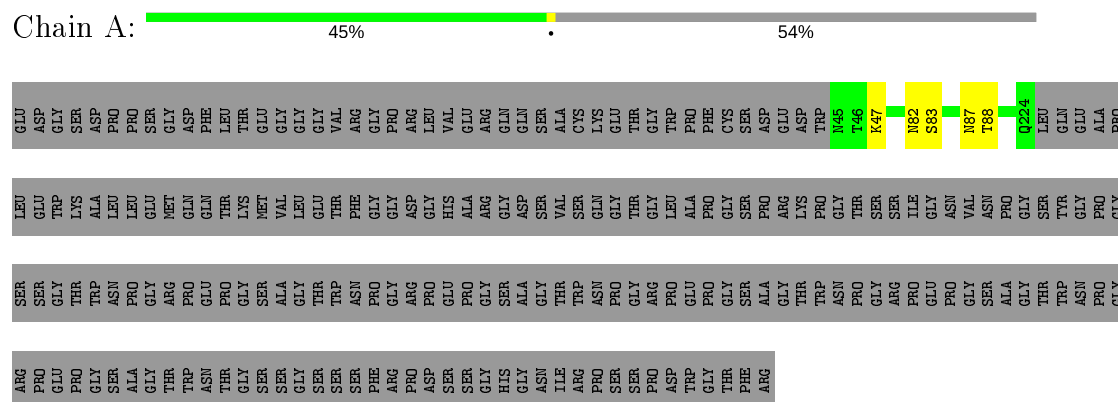
- Molecule 4 is a protein called FIBRINOGEN.

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

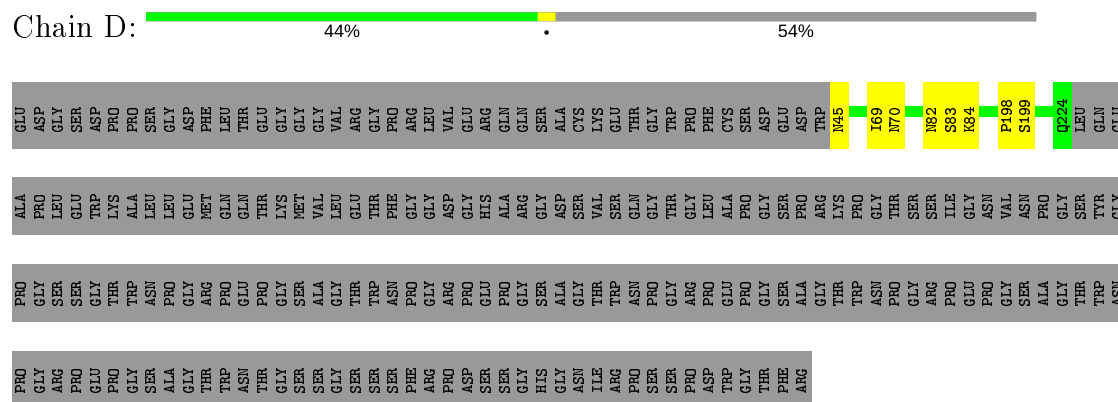
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

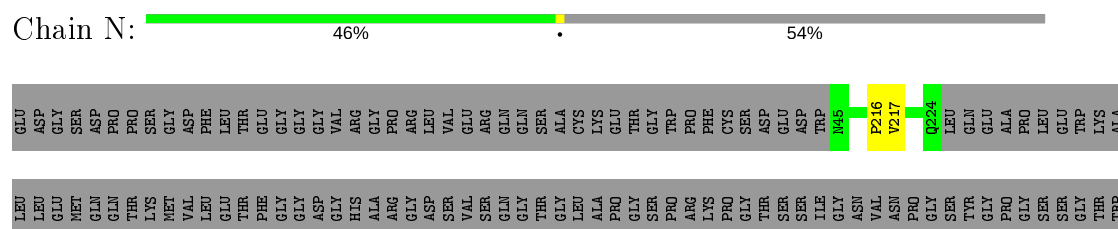
- Molecule 1: FIBRINOGEN (ALPHA CHAIN)



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ASN	PRO	GLY	ALA	GLY	THR	ARG	PRO	PRO	GLU	PRO	GLY	SER	SER	ALA	GLY	THR	THR	ASN	ASN	PHE	PRO	GLY	ARG	PRO	ASP	PRO	GLU	SER	GLY	THR	ILE	ARG	TRP	ASN	PRO	GLY	SER	GLY	ALA	GLY	THR	THR	ASN	PRO	GLY	ASP	TRP	GLY	THR	PHE	ARG
SER	ALA	GLY	THR	ARG	TRP	PRO	ASN	THR	GLY	SER	SER	ALA	GLY	THR	THR	SER	SER	ASN	PHE	PRO	GLY	ARG	PRO	ASP	PRO	GLU	SER	GLY	THR	ILE	ARG	TRP	ASN	PRO	GLY	SER	GLY	ALA	GLY	THR	THR	ASN	PRO	GLY	ASP	TRP	GLY	THR	PHE	ARG	

• Molecule 1: FIBRINOGEN (ALPHA CHAIN)

Chain Q:  44% 54%

GLU	ASP	GLY	SER	ASP	PRO	PRO	SER	GLY	ASP	PHE	LEU	THR	GLU	GLY	VAL	ARG	GLY	PRO	GLY	LEU	VAL	GLY	ARG	GLN	SER	ALA	CYS	LYS	GLY	THR	TRP	PRO	PHE	CYS	ASP	GLU	ASP	TRP	N45	S75	L76	N82	S83	P216	V217	P218	Q224	PRO	GLU	LEU	GLN	GLY		
ALA	PRO	GLU	GLY	TRP	LYS	ALA	LEU	GLY	GLY	MET	GLN	THR	THR	GLY	VAL	LEU	THR	PHE	PRO	GLY	LEU	VAL	ARG	GLN	SER	ALA	ASP	SER	VAL	SER	GLY	THR	TRP	PRO	ARG	GLY	THR	LYS	PRO	GLY	THR	SER	ARG	PRO	ILE	GLY	VAL	ASN	ASN	PRO	GLY	THR	TYR	GLY
PRO	GLY	SER	PRO	GLY	THR	TRP	ASN	PRO	GLY	ARG	PRO	GLU	PRO	GLY	ALA	THR	THR	TRP	ASN	PRO	GLY	ARG	GLY	GLY	SER	ALA	GLY	THR	GLY	THR	PRO	ARG	PRO	GLY	THR	ALA	GLY	THR	ASN	PRO	GLY	THR	ARG	PRO	GLU	GLY	THR	SER	ALA	GLY	THR	TYR	GLY	
PRO	GLY	ARG	PRO	GLU	PRO	GLY	SER	ALA	ALA	THR	ASN	THR	THR	GLY	SER	GLY	SER	THR	TRP	ASN	PRO	GLY	ARG	GLY	GLY	SER	ALA	GLY	THR	GLY	THR	PRO	ARG	PRO	GLY	THR	ALA	GLY	THR	ASN	PRO	GLY	THR	ARG	PRO	GLU	GLY	THR	SER	ALA	GLY	THR	TYR	GLY

• Molecule 2: FIBRINOGEN (BETA CHAIN)

Chain B:  93% 7%

LYS	VAL	GLU	ARG	PRO	GLY	PRO	ASP	ALA	GLY	THR	ASN	THR	GLY	ASP	ASP	PRO	ASP	LEU	GLY	VAL	CYS	PRO	GLY	THR	GLY	K88	S120	T121	E467	GLN
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• Molecule 2: FIBRINOGEN (BETA CHAIN)

Chain E:  93% 7%

LYS	VAL	GLU	ARG	PRO	PRO	ASP	ALA	GLY	GLY	CYS	HIS	ALA	ALA	ASP	PRO	ASP	LEU	GLY	VAL	CYS	PRO	GLY	THR	CYS	K88	N142	E143	E467	GLN
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• Molecule 2: FIBRINOGEN (BETA CHAIN)

Chain O:  93% 7%


LYS	VAL	GLU	ARG	PRO	PRO	ASP	ALA	GLY	GLY	CYS	HIS	ALA	ALA	ASP	PRO	ASP	LEU	GLY	VAL	CYS	PRO	GLY	THR	CYS	K88	E467	GLN
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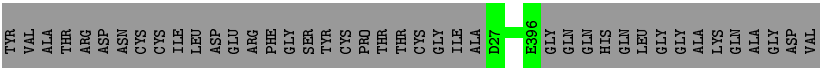
• Molecule 2: FIBRINOGEN (BETA CHAIN)

Chain R:  93% 7%


LYS	VAL	GLU	ARG	PRO	PRO	ASP	ALA	GLY	GLY	CYS	HIS	ALA	ALA	ASP	PRO	ASP	LEU	GLY	VAL	CYS	PRO	GLY	THR	CYS	K88	R108	N109	E467	GLN
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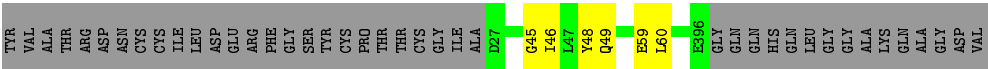
• Molecule 3: FIBRINOGEN (GAMMA CHAIN)

Chain C:  90% 10%



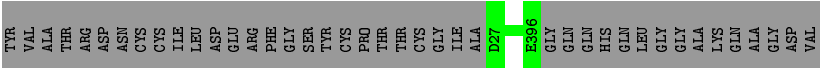
• Molecule 3: FIBRINOGEN (GAMMA CHAIN)

Chain F:  89% 10%




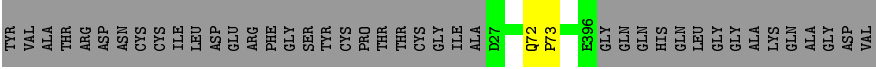
• Molecule 3: FIBRINOGEN (GAMMA CHAIN)

Chain P:  90% 10%




• Molecule 3: FIBRINOGEN (GAMMA CHAIN)

Chain S:  90% 10%




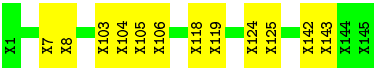
• Molecule 4: FIBRINOGEN

Chain M:  87% 13%



• Molecule 4: FIBRINOGEN

Chain Z:  87% 13%





## 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 0.441 , 0.441	Depositor DCC
$R_{free}$ test set	3953 reflections (4.98%)	wwPDB-VP
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 , 152.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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).

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

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.

All (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
4:Z:124:UNK:CA	4:Z:125:UNK:CA	2.33	1.05
1:Q:216:PRO:CA	1:Q:217:VAL:CA	2.44	0.96
1:D:83:SER:CA	1:D:84:LYS:CA	2.47	0.92
3:F:48:TYR:CA	3:F:49:GLN:CA	2.50	0.89
3:S:72:GLN:CA	3:S:73:PRO:CA	2.54	0.86
4:Z:142:UNK:CA	4:Z:143:UNK:CA	2.56	0.83
4:M:142:UNK:CA	4:M:143:UNK:CA	2.56	0.83
4:M:42:UNK:CA	4:M:43:UNK:CA	2.56	0.82
3:F:59:GLU:CA	3:F:60:LEU:CA	2.60	0.80
1:D:45:ASN:CA	4:M:114:UNK:CA	2.59	0.80
4:M:133:UNK:CA	4:M:134:UNK:CA	2.64	0.76
3:F:45:GLY:CA	3:F:46:ILE:CA	2.64	0.74
1:N:216:PRO:CA	1:N:217:VAL:CA	2.68	0.71
1:D:82:ASN:CA	1:D:83:SER:CA	2.73	0.66
1:A:82:ASN:CA	1:A:83:SER:CA	2.74	0.65
2:B:120:SER:CA	2:B:121:THR:CA	2.77	0.62
4:Z:7:UNK:CA	4:Z:8:UNK:CA	2.81	0.58
1:D:198:PRO:CA	1:D:199:SER:CA	2.82	0.57
4:Z:118:UNK:CA	4:Z:119:UNK:CA	2.83	0.56
1:A:47:LYS:CA	4:M:118:UNK:CA	2.83	0.56
1:A:87:ASN:CA	1:A:88:THR:CA	2.85	0.54
4:Z:103:UNK:CA	4:Z:104:UNK:CA	2.93	0.46
2:R:108:ARG:CA	2:R:109:ASN:CA	2.95	0.45
4:Z:105:UNK:CA	4:Z:106:UNK:CA	2.96	0.44
1:D:69:ILE:CA	1:D:70:ASN:CA	2.97	0.42
1:Q:75:SER:CA	1:Q:76:LEU:CA	2.98	0.42
1:Q:217:VAL:CA	1:Q:218:PRO:CA	2.98	0.41

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.