



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:38 am 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

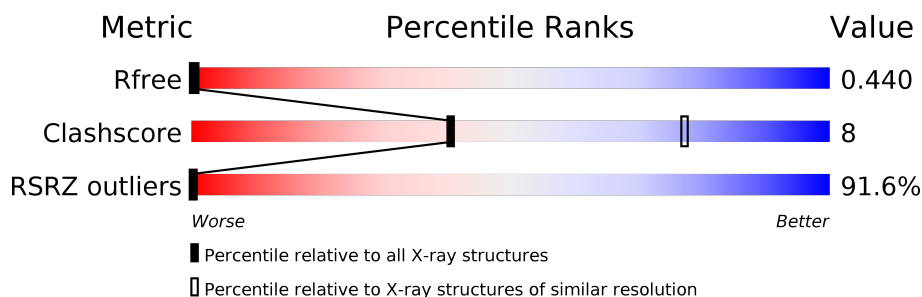
1 Overall quality at a glance

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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
RSRZ outliers	101464	1226 (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 ≥ 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>43%</div> <div>45%</div> <div>54%</div> </div>
1	D	390	<div> <div>45%</div> <div>44%</div> <div>54%</div> </div>
1	N	390	<div> <div>43%</div> <div>46%</div> <div>54%</div> </div>
1	Q	390	<div> <div>46%</div> <div>44%</div> <div>54%</div> </div>
2	B	408	<div> <div>81%</div> <div>93%</div> <div>7%</div> </div>
2	E	408	<div> <div>87%</div> <div>93%</div> <div>7%</div> </div>
2	O	408	<div> <div>79%</div> <div>93%</div> <div>7%</div> </div>
2	R	408	<div> <div>89%</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>82%</div><div></div><div>90%</div><div></div><div>10%</div></div>
3	F	411	<div><div></div><div>78%</div><div></div><div>89%</div><div></div><div>10%</div></div>
3	P	411	<div><div></div><div>83%</div><div></div><div>90%</div><div></div><div>10%</div></div>
3	S	411	<div><div></div><div>86%</div><div></div><div>90%</div><div></div><div>10%</div></div>
4	M	90	<div><div></div><div>87%</div><div></div><div></div><div></div><div>13%</div></div>
4	Z	90	<div><div></div><div>87%</div><div></div><div></div><div></div><div>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

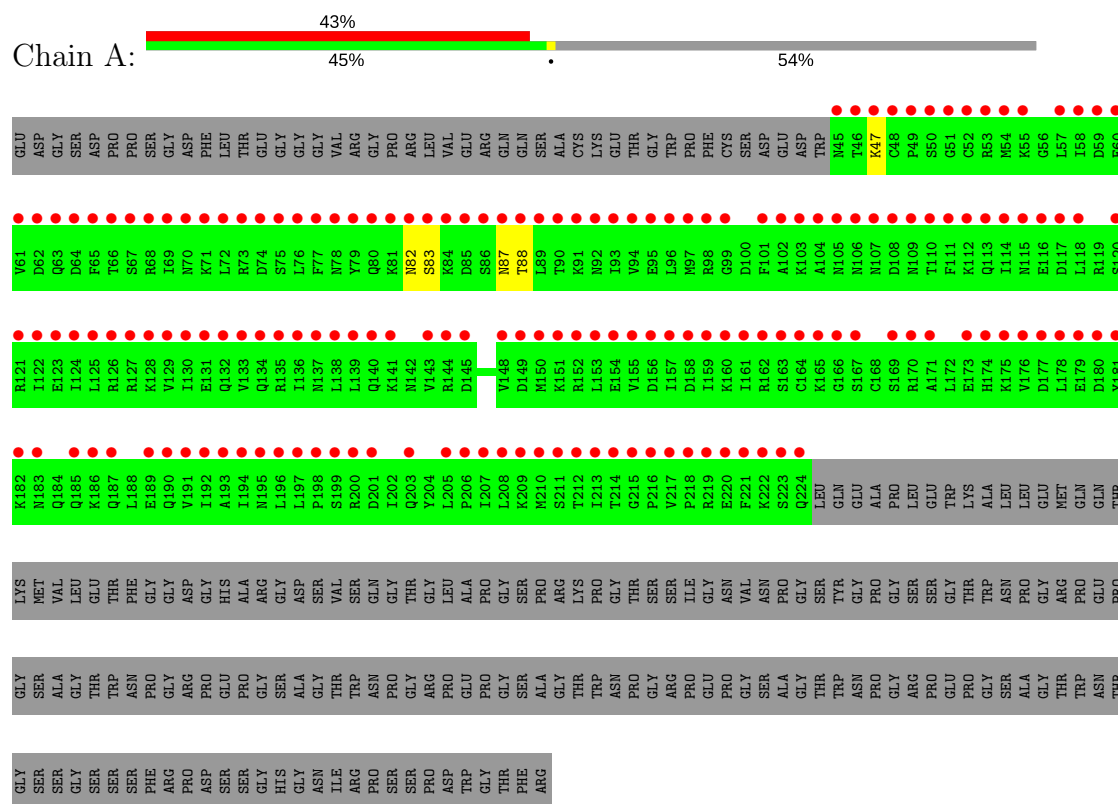
- Molecule 4 is a protein called FIBRINOGEN.

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

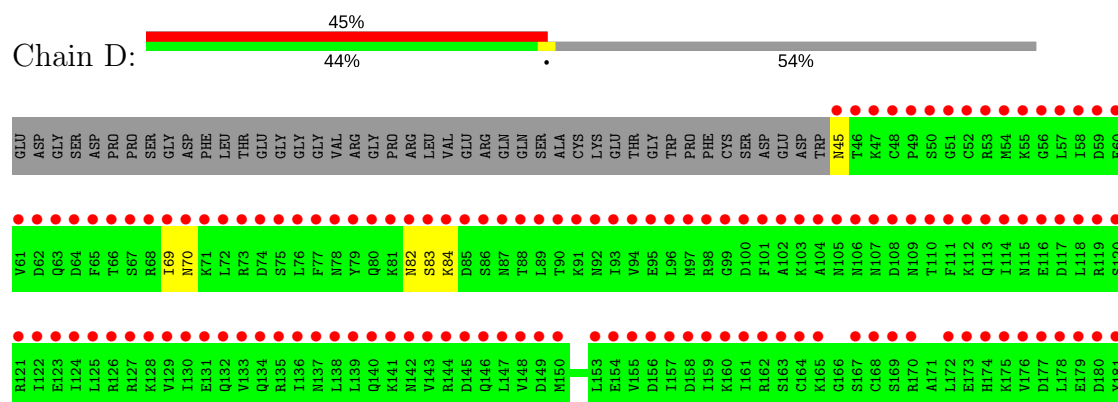
3 Residue-property plots

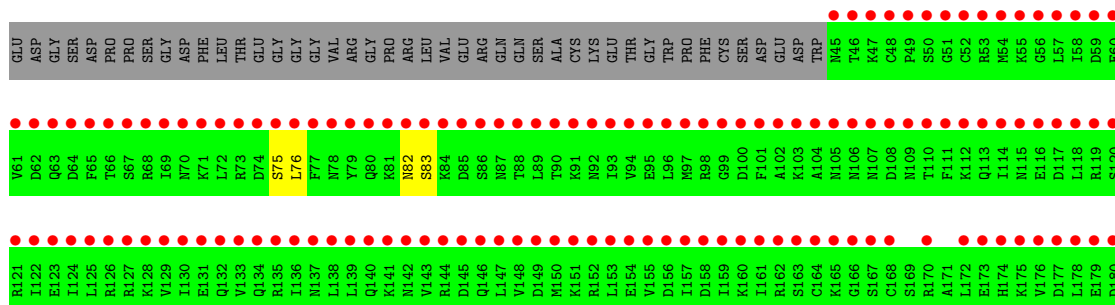
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

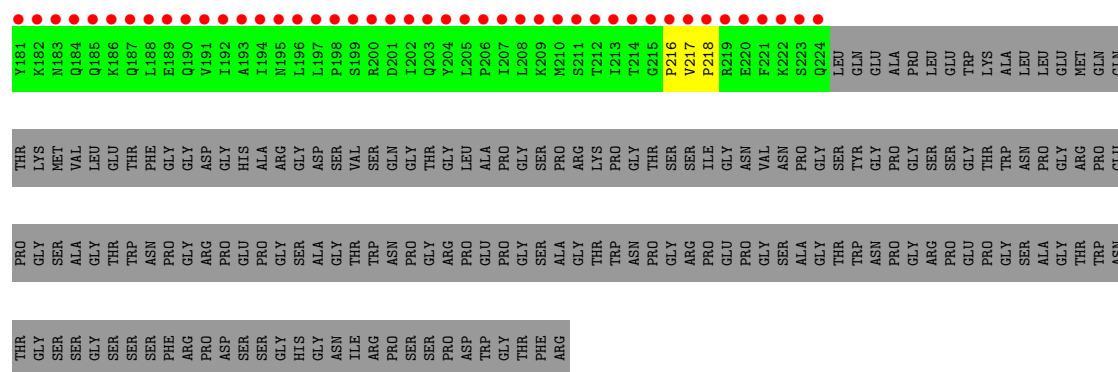
• Molecule 1: FIBRINOGEN (ALPHA CHAIN)



• Molecule 1: FIBRINOGEN (ALPHA CHAIN)



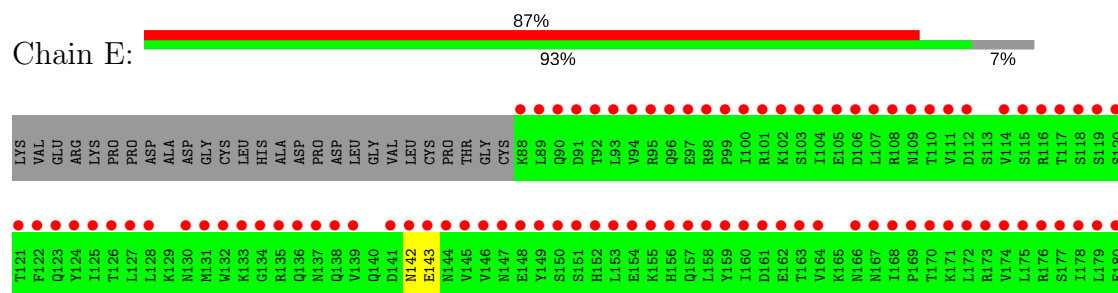


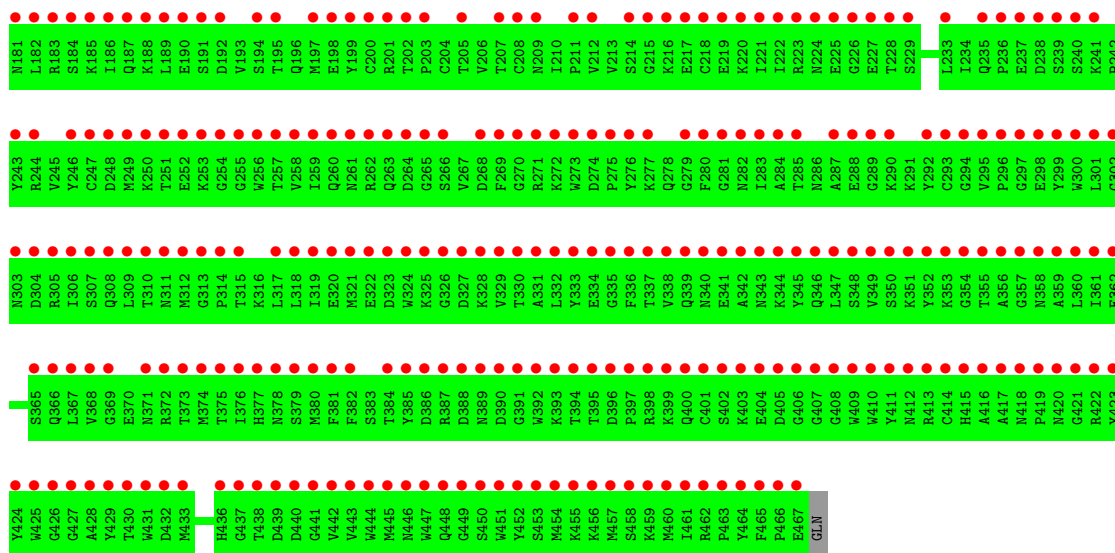


• Molecule 2: FIBRINOGEN (BETA CHAIN)

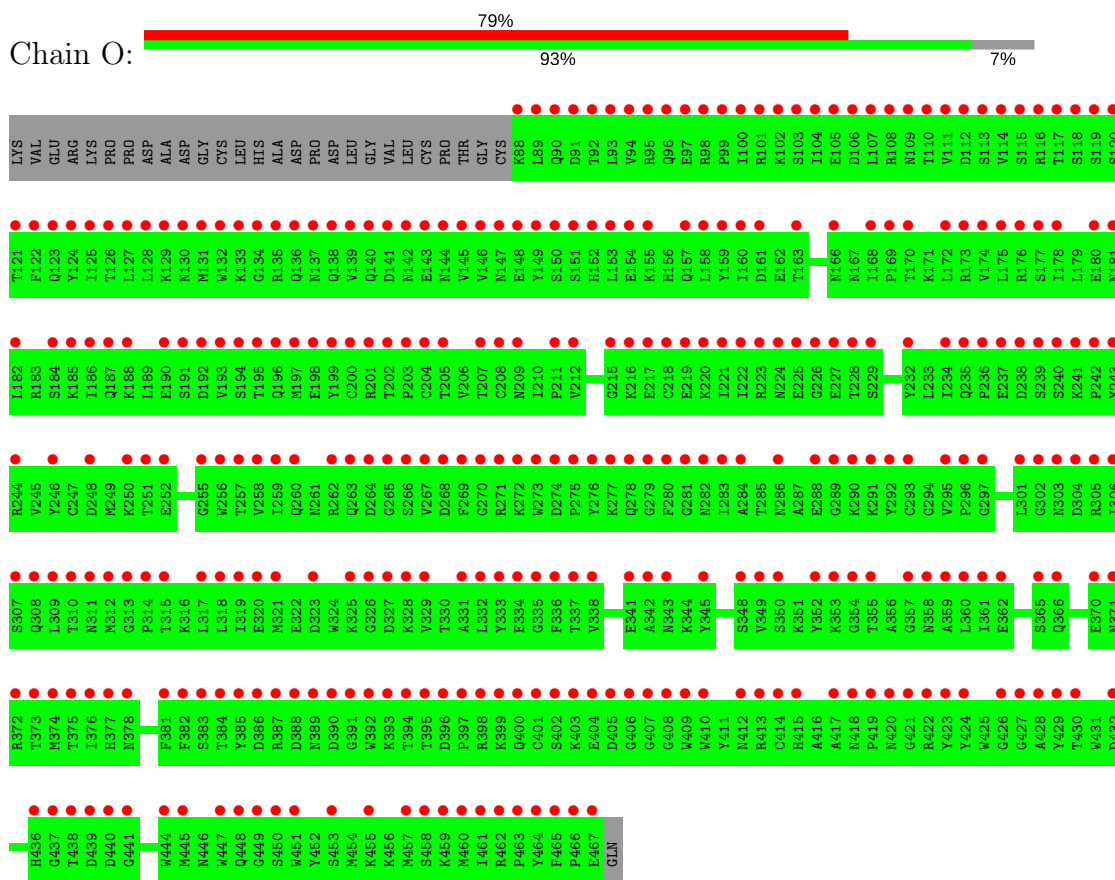


• Molecule 2: FIBRINOGEN (BETA CHAIN)

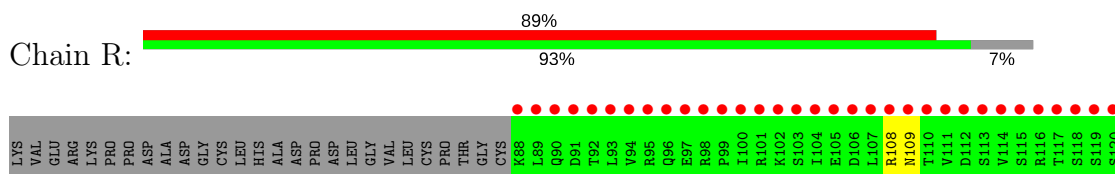


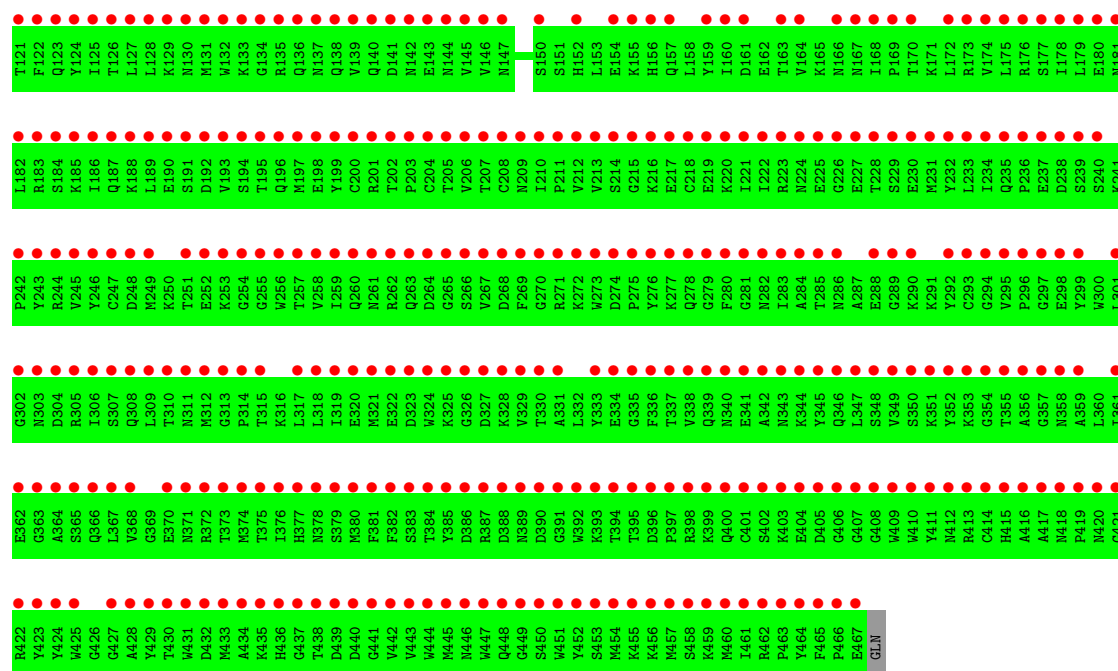


- Molecule 2: FIBRINOGEN (BETA CHAIN)

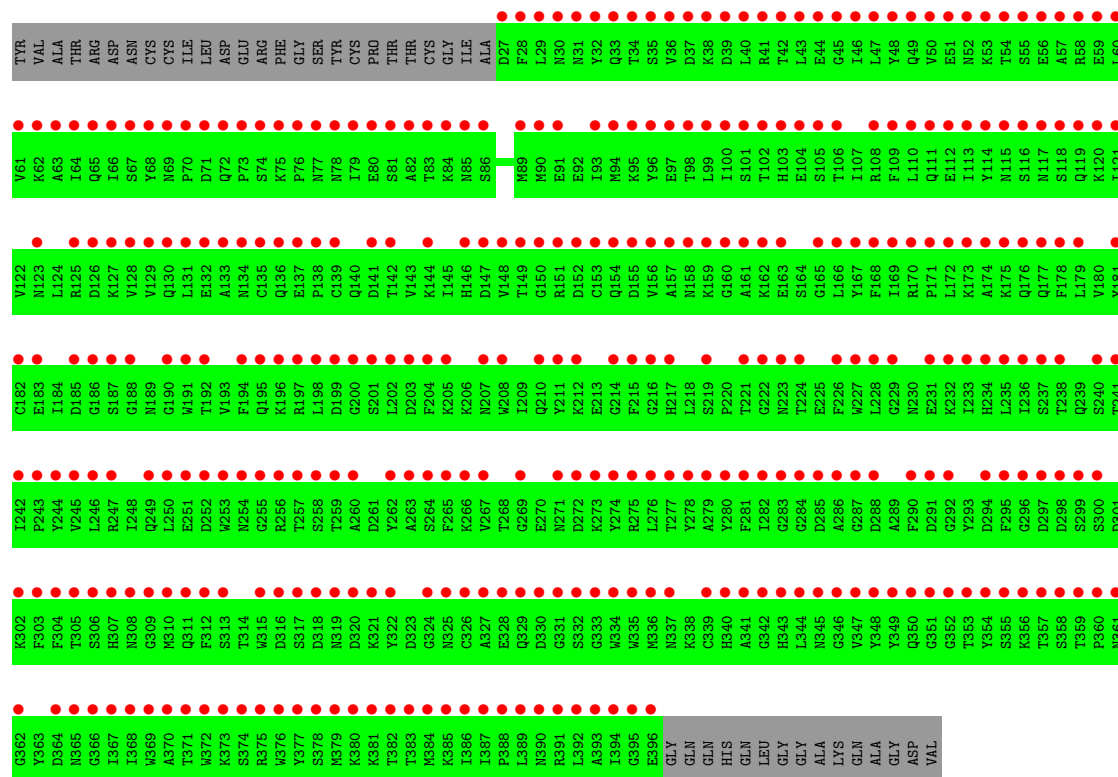
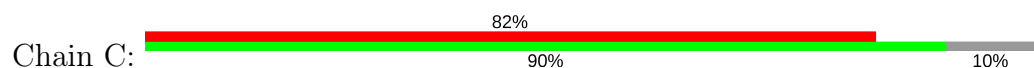


- Molecule 2: FIBRINOGEN (BETA CHAIN)

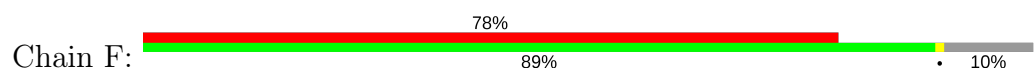




● Molecule 3: FIBRINOGEN (GAMMA CHAIN)

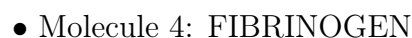


● Molecule 3: FIBRINOGEN (GAMMA CHAIN)



TYR	V61	I121	Y181	R247	D316	Y377	D27	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60
VAL	K62	V122	C162	R247	D316	Y377	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
ALA	A63	I124	E183	Q249	D318	S378	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
THR	I64	I124	E183	Q249	D318	S378	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
ARG	D125	D125	G186	E251	D320	K381	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
ASP	I66	D126	G186	E251	D320	K381	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
ASN	S67	K127	S187	D252	D321	K382	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
CYS	Y68	V128	G188	D253	D322	K383	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
ILE	N69	V129	G189	D254	D323	K384	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
LEU	D71	Q130	G190	D255	D324	K385	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
GLU	Q72	Q131	G191	D256	D325	K386	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
ASP	Q73	E132	T192	D257	D326	K387	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
GLY	P73	E133	T193	D258	D327	K388	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
ARG	S74	N134	F194	D259	D328	K389	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
PHE	K75	Q135	Q195	D260	D329	K390	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
GLY	P76	Q136	Q196	D261	D330	K391	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
SER	N77	E137	R197	D262	D331	K392	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
TYR	N78	E138	R198	D263	D332	K393	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
CYS	I79	E139	D199	D264	D333	K394	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
PRO	E80	Q140	G200	D265	D334	K395	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
THR	S81	Q141	S201	D266	D335	K396	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
THR	A82	Q142	S202	D267	D336	K397	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
CYS	T83	Q143	D203	D271	D337	K398	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
GLY	K84	Q144	D204	D272	D338	K399	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
ILE	N85	Q145	D205	D273	D339	K400	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
ALA	S86	H146	D206	D274	D340	K401	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
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F28	S88	L276	D208	D276	D342	K403	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
L29	S89	L148	D209	D277	D343	K404	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
N30	M90	T149	D210	D278	D344	K405	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
N31	E91	G150	D211	D279	D345	K406	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
Y32	E92	R151	D212	D280	D346	K407	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
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S35	K95	Q154	D215	D283	D349	K410	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
V36	Y96	V156	D216	D284	D350	K411	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
D37	E97	V157	D217	D285	D351	K412	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
K38	T98	N158	D218	D286	D352	K413	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
D39	L99	K159	D219	D287	D353	K414	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
L40	I100	G160	D220	D288	D354	K415	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
R41	S101	A161	D221	D289	D355	K416	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
T42	T102	K162	D222	D290	D356	K417	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38	D39	L40	R41	T42	R43	E44	G45	L46	Y48	Q49	V50	E51	N52	K53	T54	S55	E56	A57	R58	E59	L60	
R43	S102	E163	D223	D291	D357	K418	F28	L29	N30	N31	Y32	Q33	Q34	S35	V36	D37	K38																						

Response	Percentage
Yes	86%
No	10%



Response	Percentage
Doing a good job	87%
Doing a bad job	13%



Category	Percentage
Satisfied	87%
Not Satisfied	13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 3.33Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.257 , 0.370 0.434 , 0.440	Depositor DCC
R_{free} test set	3653 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	91.6	Xtriage
Anisotropy	0.887	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 152.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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, 95th 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	180/390 (46%)	10.57	168 (93%)  	4, 93, 999, 999	0
1	D	180/390 (46%)	13.16	175 (97%)  	25, 131, 999, 999	0
1	N	180/390 (46%)	12.10	169 (93%)  	2, 88, 999, 999	0
1	Q	180/390 (46%)	11.57	178 (98%)  	2, 151, 999, 999	0
2	B	380/408 (93%)	12.77	330 (86%)  	2, 62, 214, 999	0
2	E	380/408 (93%)	14.09	353 (92%)  	2, 81, 999, 999	0
2	O	380/408 (93%)	11.91	321 (84%)  	2, 63, 191, 359	0
2	R	380/408 (93%)	18.33	362 (95%)  	2, 130, 358, 999	0
3	C	370/411 (90%)	11.64	337 (91%)  	2, 58, 999, 999	0
3	F	370/411 (90%)	11.81	319 (86%)  	2, 68, 999, 999	0
3	P	370/411 (90%)	16.37	341 (92%)  	2, 96, 386, 999	0
3	S	370/411 (90%)	15.26	353 (95%)  	6, 112, 999, 999	0
4	M	0/90	-	-	-	-
4	Z	0/90	-	-	-	-
All	All	3720/5016 (74%)	13.60	3406 (91%)  	2, 87, 999, 999	0

The worst 5 of 3406 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	390	ASP	92.0
3	P	285	ASP	79.9
2	R	184	SER	79.0
2	E	115	SER	63.3
2	R	274	ASP	61.2

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.