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1FZD

STRUCTURE OF RECOMBINANT ALPHAEC DOMAIN FROM HUMAN FIBRINOGEN-420

PDB DOI: https://doi.org/10.2210/pdb1FZD/pdb

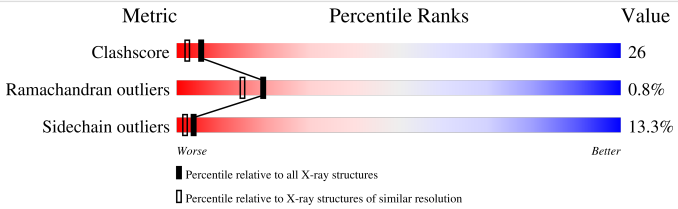
Classification: BLOOD COAGULATION
Organism(s): Homo sapiens
Expression System: Komagataella pastoris
Mutation(s): No

Deposited: 1998-06-22 **Released:** 1998-08-19
Deposition Author(s): Spraggon, G., Applegate, D., Everse, S.J., Zhang, J.-Z., Veerapandian, L., Redman, C., Doolittle, R.F., Grieninger, G.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.10 Å
R-Value Free: 0.255
R-Value Work: 0.195
R-Value Observed: 0.199

wwPDB Validation 3D Report | Full Report



This is version 2.1 of the entry. See complete history.

Literature

Crystal structure of a recombinant alphaEC domain from human fibrinogen-420.

Spraggon, G., **Applegate, D.**, **Everse, S.J.**, **Zhang, J.Z.**, **Veerapandian, L.**, **Redman, C.**, **Doolittle, R.F.**, **Grieninger, G.**
(1998) Proc Natl Acad Sci U S A **95**: 9099-9104

PubMed: **9689040**
DOI: https://doi.org/10.1073/pnas.95.16.9099
Primary Citation of Related Structures:
1FZD

PubMed Abstract:
The crystal structure of a recombinant alphaEC domain from human fibrinogen-420 has been determined at a resolution of 2.1 A. The protein, which corresponds to the carboxyl domain of the alphaE chain, was expressed in and purified from Pichia pastoris cells. Felicitously, during crystallization an amino-terminal segment was removed, apparently by a contaminating protease, allowing the 201-residue remaining parent body to crystallize. An x-ray structure was determined by molecular…

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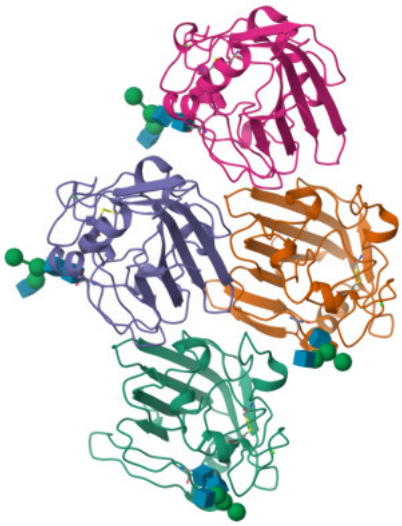
Organizational Affiliation:
Center for Molecular Genetics, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0634, USA.

Biological Assembly 1



Explore in 3D: Structure | Sequence Annotations | Validation Report | Ligand Interaction (NAG)

Global Symmetry: Helical - H (Explore in 3D)
Global Stoichiometry: Homo 4-mer - A4

Find Similar Assemblies

Biological assembly 1 assigned by authors.

Macromolecules

Find similar proteins by: Sequence (by identity cutoff) | 3D Structure

Entity ID: 1

Molecule	Chains	Sequence Length	Organism	Details	Image
FIBRINOGEN-420	A, B, C, D, E	201	Homo sapiens	**Mutation(s)**: 0	

UniProt & NIH Common Fund Data Resources

Find proteins for **P02671** *(Homo sapiens)*
Explore P02671

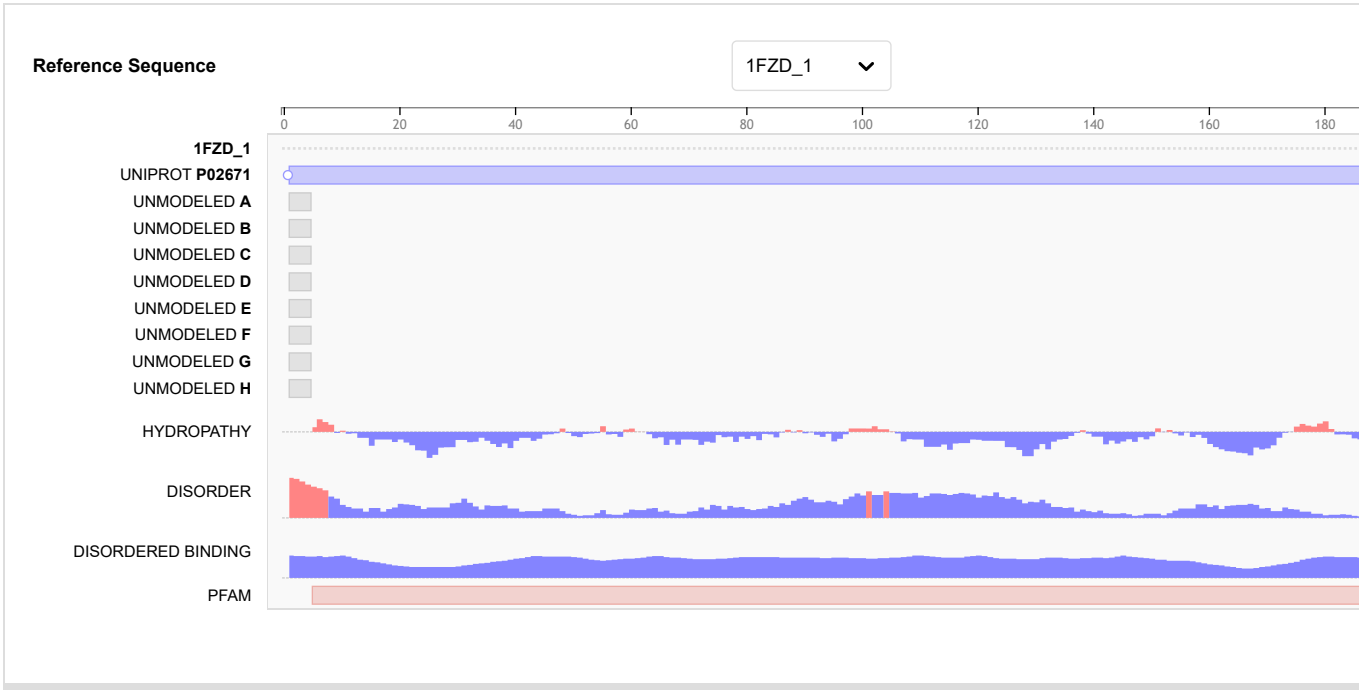
Go to UniProt

PHAROS: P02671
GTEx: ENSG00000171560

Entity Groups

Sequence Clusters	30% Identity 50% Identity 70% Identity 90% Identity 95% Identity 100% Identity
UniProt Group	P02671

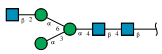
Sequence Annotations



Oligosaccharides

Help

Entity ID: 2

Molecule	Chains	Length	2D Diagram	Glycosylation	3D Interactions
2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	I, K, L	6		N-Glycosylation	Interactions

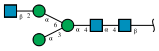
Glycosylation Resources

GlyTouCan: G73276UD

GlyCosmos: G73276UD

GlyGen: G73276UD

Entity ID: 3

Molecule	Chains	Length	2D Diagram	Glycosylation	3D Interactions
2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	J	6		N-Glycosylation	Interactions

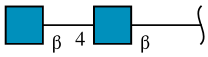
Glycosylation Resources

GlyTouCan: G47074NJ

GlyCosmos: G47074NJ

GlyGen: G47074NJ

Entity ID: 4

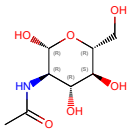
Molecule	Chains	Length	2D Diagram	Glycosylation	3D Interactions
2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose	M, N	2		N-Glycosylation	Interactions

Glycosylation Resources

GlyTouCan: G42666HT GlyCosmos: G42666HT GlyGen: G42666HT

Small Molecules

Ligands 2 Unique

ID	Chains	Name / Formula / InChI Key	2D Diagram	3D Interactions
NAG	U [auth G], V [auth G], X [auth H], Y [auth H]	**2-acetamido-2-deoxy-beta-D-glucopyranose** $C_8 H_{15} N O_6$ OVRNDRQMDRJTHS-FMDGEEDCSA-N		Interactions
Download Instance Coordinates				
CA		**CALCIUM ION** Ca BHPQYMZQTOCNFJ-UHFFFAOYSA-N	Ca^{+2}	Interactions
Download Instance Coordinates				

Experimental Data & Validation

Experimental Data

Method: X-RAY DIFFRACTION
Resolution: 2.10 Å
R-Value Free: 0.255
R-Value Work: 0.195
R-Value Observed: 0.199
Space Group: P 1

Unit Cell:

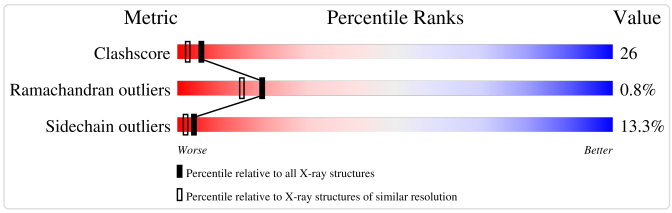
Length (Å)	Angle (°)
a = 71.25	α = 104.6
b = 105.18	β = 108.95
c = 71.14	γ = 71.47

Software Package:

Software Name	Purpose
SCALEPACK	data scaling
X-PLOR	model building
REFMAC	refinement
X-PLOR	refinement
X-PLOR	phasing

Structure Validation

View Full Validation Report



Entry History

Deposition Data

Released Date: 1998-08-19
Deposition Author(s): Spraggon, G., Applegate, D., Everse, S.J., Zhang, J.-Z., Veerapandian, L., Redman, C., Doolittle, R.F., Grieninger, G.

Revision History (Full details and data files)

- **Version 1.0: 1998-08-19**
  Type: Initial release
- **Version 1.1: 2008-03-21**
  Changes: Version format compliance
- **Version 1.2: 2011-07-13**
  Changes: Non-polymer description, Version format compliance
- **Version 2.0: 2020-07-29**
  Type: Remediation
  Reason: Carbohydrate remediation
  Changes: Advisory, Atomic model, Data collection, Derived calculations, Structure summary
- **Version 2.1: 2023-08-09**
  Changes: Advisory, Database references, Refinement description, Structure summary

RCSB PDB Core Operations are funded by the National Science Foundation (DBI-1832184), the US Department of Energy (DE-SC0019749), and the National Cancer Institute, National Institute of Allergy and Infectious Diseases, and National Institute of General Medical Sciences of the National Institutes of Health under grant R01GM133198.