



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:48 PM GMT

PDB ID : 1M1J
Title : Crystal structure of native chicken fibrinogen with two different bound ligands
Authors : Yang, Z.; Kollman, J.M.; Pandi, L.; Doolittle, R.F.
Deposited on : 2002-06-19
Resolution : 2.70 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

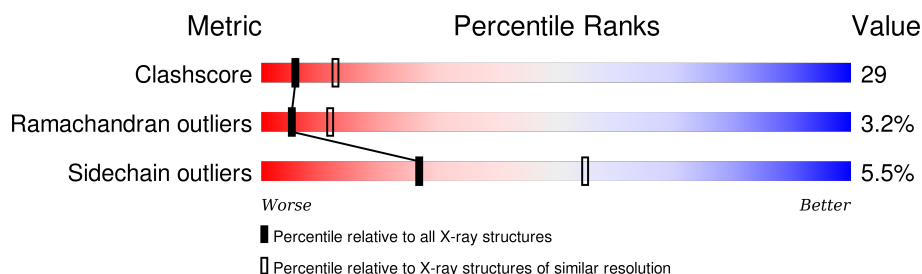
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)




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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	
1	D	491	
2	B	464	
2	E	464	
3	C	409	
3	F	409	
4	G	4	

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Mol	Chain	Length	Quality of chain
4	H	4	
5	I	4	
5	J	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NDG	B	470	-	-	X	-
6	NDG	C	420	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16117 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 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1544	947	282	305	10			
1	D	194	Total	C	N	O	S	0	0	0
			1565	962	286	307	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLY	CYS	SEE REMARK 999	UNP P14448
D	49	GLY	CYS	SEE REMARK 999	UNP P14448

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3225	2023	554	623	25			
2	E	401	Total	C	N	O	S	0	0	0
			3216	2019	553	619	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLN	-	SEE REMARK 999	UNP Q02020
E	1	GLN	-	SEE REMARK 999	UNP Q02020

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	390	Total	C	N	O	S	0	0	0
			3162	1987	539	620	16			
3	F	389	Total	C	N	O	S	0	0	0
			3155	1983	538	618	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	286	ALA	ARG	SEE REMARK 999	UNP O93568
F	286	ALA	ARG	SEE REMARK 999	UNP O93568

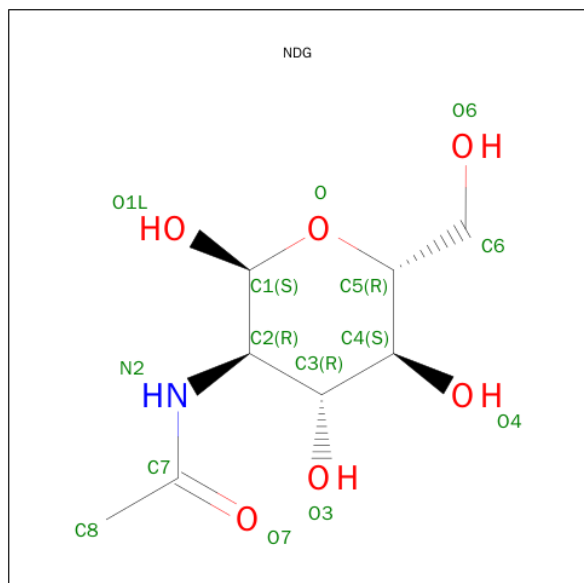
- Molecule 4 is a protein called GLY-PRO-ARG-PRO peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	H	4	Total	C	N	O	0	0	0
			30	18	7	5			

- Molecule 5 is a protein called GLY-HIS-ARG-PRO peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	J	4	Total	C	N	O	0	0	0
			33	19	9	5			

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



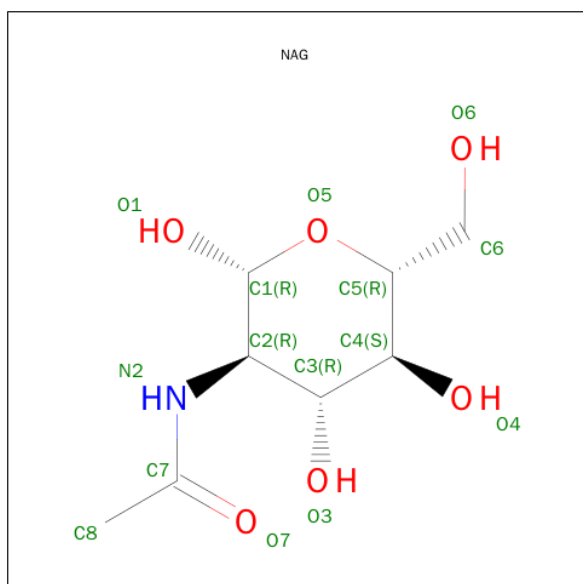
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			15	8	1	6		
6	J	1	Total	C	N	O	0	0
			15	8	1	6		
6	C	1	Total	C	N	O	0	0
			15	8	1	6		
6	F	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	I	1	Total	C	N	O	0	0
			15	8	1	6		
7	C	1	Total	C	N	O	0	0
			15	8	1	6		
7	F	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		

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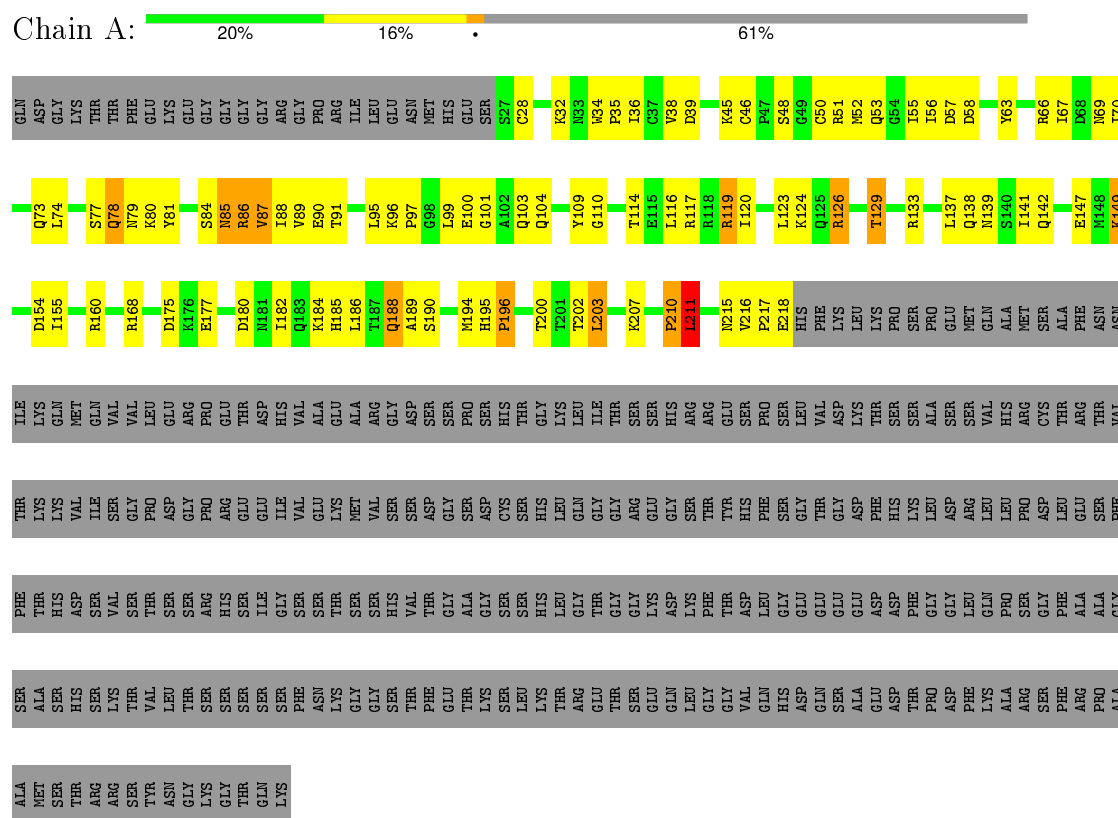
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	1	Total 1	Ca 1	0	0
8	E	1	Total 1	Ca 1	0	0

3 Residue-property plots

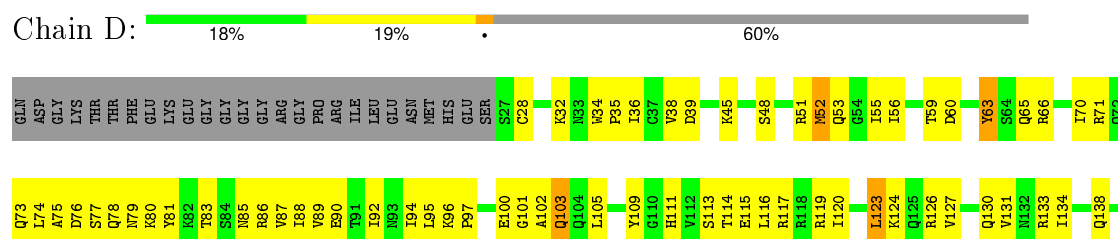
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: Fibrinogen alpha subunit



- Molecule 1: Fibrinogen alpha subunit



SER	GLU	GLY	ASP	PHE	THR	GLY	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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• Molecule 2: Fibrinogen beta chain

Chain B:  53% 31% 13%

GLN	ALA	SER	VAL	GLU	TYR	ASP	ASN	GLU	GLU	ASP	SER	PRO	GLN	ILE	ASP	ALA	ARG	ALA	ALA	HIS	ARG	THR	GLN	GLY	ALA	ALA	PRO	THR	LEU	ARG	PRO	VAL	VAL	ALA	ALA	PRO	PRO	PRO	ILE	GLY	THR	GLY	TYR	GLN	PRO	ARG	PRO	PRO	LYS	GLN	ASP	LYS	GLN	ALA	MET	LYS	LYS	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
PRO	ILE	I63	Y64	P65	D66	A67	G68	G69	C70	K71	H72	P73	L74	D75	E76	L77	L80	C81	P82	T83	G84	C85	Q88	T89	N90	L91	L92	K93	Q94	V98	K99	P100	V101	L102	L105	K106	F112	T115	S116	M119	Y120	M125	L126	D127	N128	K129	L130	V131	K132	T133	P134																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
Q136	R137	K138	D139	N140	D141	I142	I143	I144	S145	E146	Y147	N148	T149	D150	M151	E152	L153	H154	Y157	I158	K159	D160	H161	L162	N165	I166	P167	L170	L173	V176	N177	D178	L187	I191	T195	R199	V203	A204	S205	C206	N207	L208	E215	C216	M229	K230	P234																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
D235	T238	T239	D246	W254	T255	Q258	N259	K260	Q261	D262	G263	N266	P267	G268	W271	K275	R276	K288	T290	W297	N300	D301	K302	L303	Q304	L306	T307	K308	I316	E317	K318	G332	F333	T334	I335	H336	K341	Y342	Q343	L344	S345	V346	S347	N348	Y349	K350																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
K355	M358	E359	G360	A361	Q362	Q363	N368	K371	T372	M377	Y378	T381	K384	T391	T392	D393	P394	Q397	K400	E401	P402	G403	W406	W407	Y408	N409	R410	O411	G418	G424	T425	Y426	D429	K432	K443	W448	Y449	S450	M451	M456	K457																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
I458	P463	D464																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																

• Molecule 2: Fibrinogen beta chain

Chain E:  50% 33% 14%

K129	L130	V131	K132	T133	K135			M140		I143	E146		T149	E150	M151	E152	H153	H154	V155	N156	V157	I158	K159	D160	M161		M164	M165	I166	P167	S168	S169	L170	K171	V172		V176		S179	L180		I184	D196	F197	G198	R199		V203	A204		I208	F209		E215	C216	E217					
PRO	ILE	I63	Y64	P65	D66	A67	G68	G69	C70	K71	H72	P73	L74	D75	E76	L77	L80	T83	G84	C85	E86	L87	Q88	T89	T90	L91	L92	K93	Q94	E95		V98	K99	P100		R103	D104	L105	K106		V109	K111	F112	S113		T118	M119	Y120	Q121	Y122	V123	M124	M125	I126	D127	M128					
GLN	ALA	SER	VAL	GLU	TYR	ASP	ASN	GLU	GLU	ASP	SER	PRO	GLN	ILE	ASP	ALA	ARG	ALA	HIS	ARG	PRO	LEU	ASP	LYS	ARG	GLN	GLU	ALA	ALA	PRO	THR	THR	LEU	ARG	PRO	VAL	ALA	PRO	PRO	ILE	SER	ILE	GLY	THR	GLY	TYR	GLN	PRO	ARG	PRO	PRO	LYS	GLN	ASP	LYS	GLN	ALA	MET	LYS	LYS	GLY



- Molecule 4: GLY-PRO-ARG-PRO peptide



- Molecule 5: GLY-HIS-ARG-PRO peptide



- Molecule 5: GLY-HIS-ARG-PRO peptide



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.09Å 100.02Å 200.09Å 90.00° 105.79° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	93.1 (20.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16117	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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: CA, NAG, NDG

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	A	0.33	0/1564	0.57	0/2108
1	D	0.30	0/1587	0.58	0/2139
2	B	0.39	0/3304	0.63	1/4467 (0.0%)
2	E	0.34	0/3295	0.61	1/4456 (0.0%)
3	C	0.42	0/3236	0.65	1/4374 (0.0%)
3	F	0.39	0/3229	0.65	1/4364 (0.0%)
4	G	0.62	0/31	0.80	0/40
4	H	0.60	0/31	0.69	0/40
5	I	0.55	0/34	0.69	0/43
5	J	0.46	0/34	0.52	0/43
All	All	0.37	0/16345	0.63	4/22074 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	338	ARG	N-CA-C	-6.79	92.66	111.00
3	C	338	ARG	N-CA-C	-6.79	92.67	111.00
2	B	403	GLY	N-CA-C	5.09	125.82	113.10
2	E	410	ARG	N-CA-C	-5.09	97.26	111.00

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	1544	0	1532	133	0
1	D	1565	0	1548	161	0
2	B	3225	0	3081	182	0
2	E	3216	0	3077	233	0
3	C	3162	0	2992	189	0
3	F	3155	0	2985	190	0
4	G	30	0	32	1	0
4	H	30	0	32	2	0
5	I	33	0	32	1	0
5	J	33	0	32	4	0
6	B	15	0	15	11	0
6	C	15	0	15	10	0
6	E	15	0	15	4	0
6	F	15	0	15	3	0
6	J	15	0	15	0	0
7	C	15	0	15	1	0
7	F	15	0	15	0	0
7	I	15	0	15	3	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
All	All	16117	0	15463	916	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 29.

The worst 5 of 916 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)
1:A:216:VAL:HG22	2:B:129:LYS:HE3	1.24	1.15
3:F:52:ASN:HD21	6:F:520:NDG:H8C3	1.01	1.13
2:E:443:ASN:H	2:E:443:ASN:HD22	1.05	1.01
2:E:371:MET:HB2	2:E:410:ARG:CB	1.92	0.99
3:F:356:ARG:HB3	3:F:356:ARG:NH1	1.79	0.97

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	190/491 (39%)	159 (84%)	24 (13%)	7 (4%)	4	9
1	D	192/491 (39%)	147 (77%)	32 (17%)	13 (7%)	1	2
2	B	400/464 (86%)	353 (88%)	39 (10%)	8 (2%)	9	24
2	E	399/464 (86%)	335 (84%)	52 (13%)	12 (3%)	5	13
3	C	388/409 (95%)	350 (90%)	27 (7%)	11 (3%)	6	15
3	F	387/409 (95%)	342 (88%)	34 (9%)	11 (3%)	6	15
4	G	2/4 (50%)	2 (100%)	0	0	100	100
4	H	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
5	I	2/4 (50%)	2 (100%)	0	0	100	100
5	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1964/2744 (72%)	1693 (86%)	209 (11%)	62 (3%)	5	12

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	LEU
1	A	210	PRO
1	A	211	LEU
2	B	65	PRO
2	B	411	CYS

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	A	177/430 (41%)	164 (93%)	13 (7%)	17	39
1	D	179/430 (42%)	167 (93%)	12 (7%)	20	44
2	B	350/402 (87%)	335 (96%)	15 (4%)	35	66
2	E	349/402 (87%)	335 (96%)	14 (4%)	38	69
3	C	341/355 (96%)	317 (93%)	24 (7%)	19	42
3	F	340/355 (96%)	322 (95%)	18 (5%)	28	57
4	G	3/3 (100%)	3 (100%)	0	100	100
4	H	3/3 (100%)	3 (100%)	0	100	100
5	I	3/3 (100%)	3 (100%)	0	100	100
5	J	3/3 (100%)	3 (100%)	0	100	100
All	All	1748/2386 (73%)	1652 (94%)	96 (6%)	27	55

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	317	ASN
1	D	63	TYR
3	F	325	ASN
3	C	325	ASN
3	C	356	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	319	ASN
1	D	103	GLN
3	F	239	GLN
3	C	325	ASN
1	D	33	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NDG	B	470	-	15,15,15	0.49	0	17,21,21	0.71	0
6	NDG	C	420	-	15,15,15	0.41	0	17,21,21	0.53	0
7	NAG	C	421	-	15,15,15	0.47	0	17,21,21	0.56	0
6	NDG	E	570	-	15,15,15	0.44	0	17,21,21	0.59	0
6	NDG	F	520	-	15,15,15	0.44	0	17,21,21	0.52	0
7	NAG	F	521	-	15,15,15	0.42	0	17,21,21	0.53	0
7	NAG	I	471	-	15,15,15	0.47	0	17,21,21	0.53	0
6	NDG	J	571	-	15,15,15	0.54	0	17,21,21	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NDG	B	470	-	-	0/6/26/26	0/1/1/1
6	NDG	C	420	-	-	0/6/26/26	0/1/1/1
7	NAG	C	421	-	-	0/6/26/26	0/1/1/1
6	NDG	E	570	-	-	0/6/26/26	0/1/1/1
6	NDG	F	520	-	-	0/6/26/26	0/1/1/1
7	NAG	F	521	-	-	0/6/26/26	0/1/1/1
7	NAG	I	471	-	-	1/6/26/26	0/1/1/1
6	NDG	J	571	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	471	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	470	NDG	11	0
6	C	420	NDG	10	0
7	C	421	NAG	1	0
6	E	570	NDG	4	0
6	F	520	NDG	3	0
7	I	471	NAG	3	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.