



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID : 1N73  
Title : Fibrin D-Dimer, Lamprey complexed with the PEPTIDE LIGAND: GLY-HI  
S-ARG-PRO-AMIDE  
Authors : Yang, Z.; Pandi, L.; Doolittle, R.F.  
Deposited on : 2002-11-12  
Resolution : 2.90 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)  
Xtrriage (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

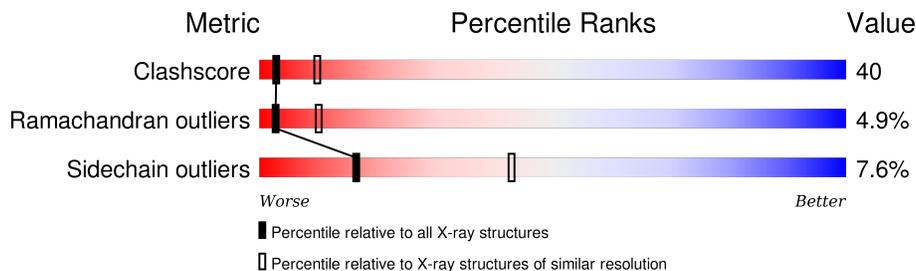
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	
1	D	119	
2	B	323	
2	E	323	
3	C	330	
3	F	330	
4	G	4	

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Mol	Chain	Length	Quality of chain
4	H	4	 25% 75%
4	I	4	 25% 50% 25%
4	J	4	 25% 50% 25%

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
5	NAG	C	480	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12039 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 Fibrin alpha-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	91	763	480	143	137	3	0	0	0
1	D	90	758	477	142	136	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	THR	SEE REMARK 999	UNP P02674
D	153	ALA	THR	SEE REMARK 999	UNP P02674

- Molecule 2 is a protein called Fibrin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	315	2535	1579	453	482	21	0	0	0
2	E	315	2535	1579	453	482	21	0	0	0

- Molecule 3 is a protein called Fibrin gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	322	2630	1658	457	502	13	0	0	0
3	F	322	2630	1658	457	502	13	0	0	0

- Molecule 4 is a protein called peptide ligand: Gly-his-Arg-Pro-amide.

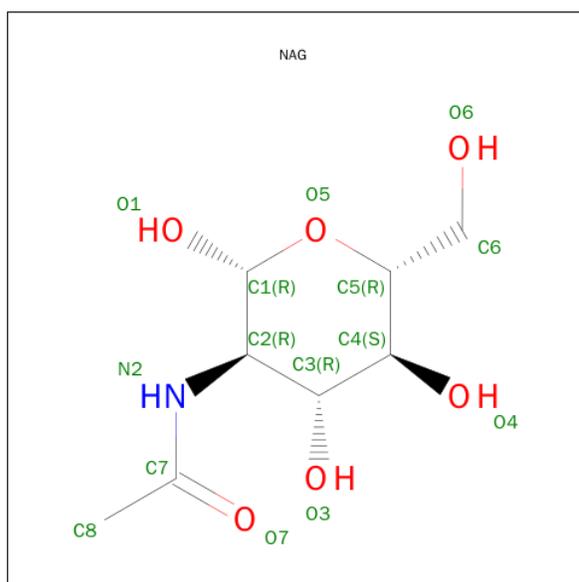
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	4	32	19	9	4	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			32	19	9	4			
4	I	4	Total	C	N	O	0	0	0
			32	19	9	4			
4	J	4	Total	C	N	O	0	0	0
			32	19	9	4			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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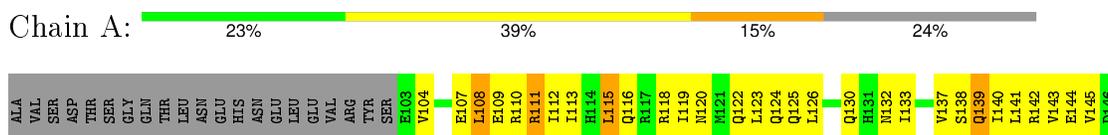
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	F	1	Total 1	Ca 1	0	0
6	E	1	Total 1	Ca 1	0	0

### 3 Residue-property plots [i](#)

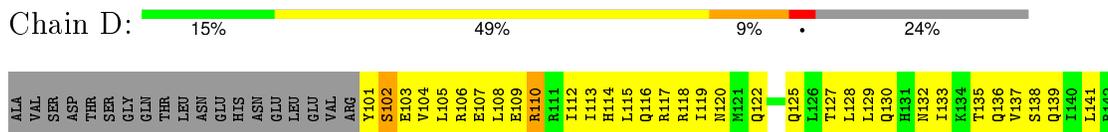
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

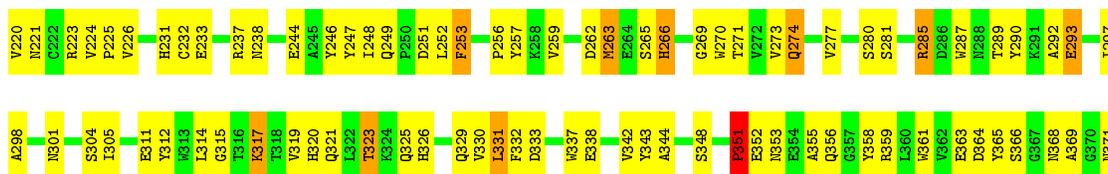
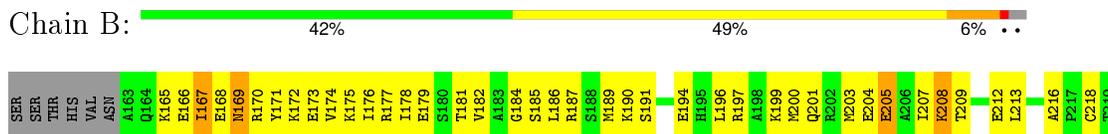
- Molecule 1: Fibrin alpha-1 chain



- Molecule 1: Fibrin alpha-1 chain



- Molecule 2: Fibrin beta chain







- Molecule 4: peptide ligand: Gly-his-Arg-Pro-amide



- Molecule 4: peptide ligand: Gly-his-Arg-Pro-amide



- Molecule 4: peptide ligand: Gly-his-Arg-Pro-amide



- Molecule 4: peptide ligand: Gly-his-Arg-Pro-amide



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.73 Å 99.30 Å 120.73 Å 99.58° 101.46° 92.36°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	81.7 (20.00-2.90)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.258 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	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

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	0.41	0/769	0.71	0/1030
1	D	0.36	0/765	0.63	0/1024
2	B	0.41	0/2602	0.65	0/3517
2	E	0.41	0/2602	0.65	0/3517
3	C	0.44	0/2701	0.69	1/3653 (0.0%)
3	F	0.43	0/2701	0.67	1/3653 (0.0%)
4	G	0.41	0/33	0.66	0/43
4	H	0.42	0/33	0.55	0/43
4	I	0.42	0/33	0.45	0/43
4	J	0.46	0/33	0.59	0/43
All	All	0.42	0/12272	0.67	2/16566 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	336	ARG	N-CA-C	-5.23	96.88	111.00
3	F	336	ARG	N-CA-C	-5.17	97.05	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	763	0	799	89	0
1	D	758	0	789	113	0
2	B	2535	0	2363	221	0
2	E	2535	0	2363	218	0
3	C	2630	0	2455	176	0
3	F	2630	0	2453	191	0
4	G	32	0	32	13	0
4	H	32	0	32	6	0
4	I	32	0	32	3	0
4	J	32	0	32	8	0
5	B	14	0	13	3	0
5	C	14	0	13	2	0
5	E	14	0	13	4	0
5	F	14	0	13	2	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	12039	0	11402	925	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 40.

The worst 5 of 925 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)
3:C:203:ASN:HD21	5:C:480:NAG:C1	1.30	1.40
2:E:381:MET:HB2	5:E:480:NAG:C8	1.67	1.22
2:B:381:MET:HB2	5:B:480:NAG:C8	1.73	1.18
1:D:168:LYS:HD2	1:D:169:GLU:H	0.97	1.10
2:E:381:MET:HB2	5:E:480:NAG:H82	1.33	1.09

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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	89/119 (75%)	62 (70%)	16 (18%)	11 (12%)	0	1
1	D	88/119 (74%)	58 (66%)	20 (23%)	10 (11%)	0	1
2	B	313/323 (97%)	261 (83%)	41 (13%)	11 (4%)	4	18
2	E	313/323 (97%)	259 (83%)	43 (14%)	11 (4%)	4	18
3	C	320/330 (97%)	268 (84%)	36 (11%)	16 (5%)	3	9
3	F	320/330 (97%)	264 (82%)	44 (14%)	12 (4%)	4	16
4	G	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	H	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	I	2/4 (50%)	2 (100%)	0	0	100	100
4	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1451/1560 (93%)	1178 (81%)	202 (14%)	71 (5%)	3	10

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	SER
1	A	182	ALA
1	A	186	PHE
2	B	455	VAL
3	C	337	CYS

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

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	84/110 (76%)	73 (87%)	11 (13%)	5	15
1	D	83/110 (76%)	73 (88%)	10 (12%)	6	18
2	B	266/274 (97%)	247 (93%)	19 (7%)	18	47
2	E	266/274 (97%)	249 (94%)	17 (6%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	280/286 (98%)	259 (92%)	21 (8%)	17	44
3	F	280/286 (98%)	265 (95%)	15 (5%)	27	62
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	1
4	H	3/3 (100%)	3 (100%)	0	100	100
4	I	3/3 (100%)	2 (67%)	1 (33%)	0	1
4	J	3/3 (100%)	2 (67%)	1 (33%)	0	1
All	All	1271/1352 (94%)	1175 (92%)	96 (8%)	16	43

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

Mol	Chain	Res	Type
3	C	304	THR
1	D	165	ARG
3	F	372	ASP
3	C	336	ARG
3	C	384	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	253	ASN
1	D	132	ASN
3	F	253	ASN
3	C	262	HIS
3	C	398	GLN

### 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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
5	NAG	B	480	2	14,14,15	0.74	0	15,19,21	0.65	0
5	NAG	C	480	3	14,14,15	0.47	0	15,19,21	1.01	1 (6%)
5	NAG	E	480	2	14,14,15	0.73	0	15,19,21	0.65	0
5	NAG	F	480	3	14,14,15	0.55	0	15,19,21	0.72	1 (6%)

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
5	NAG	B	480	2	-	0/6/23/26	0/1/1/1
5	NAG	C	480	3	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	480	2	-	0/6/23/26	0/1/1/1
5	NAG	F	480	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	480	NAG	C2-N2-C7	-2.87	119.35	123.04
5	F	480	NAG	C2-N2-C7	-2.00	120.47	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	480	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	480	NAG	3	0
5	C	480	NAG	2	0
5	E	480	NAG	4	0
5	F	480	NAG	2	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.