wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:32 PM GMT

PDB ID : 1FZF
Title : CRYSTAL STRUCTURE OF FRAGMENT DOUBLE-D FROM HUMAN FIBRIN WITH THE PEPTIDE LIGAND GLY-HIS-ARG-PRO-AMIDE
Authors : Everse, S.J.; Spraggon, G.; Veerapandian, L.; Doolittle, R.F.
Deposited on : 1998-12-28
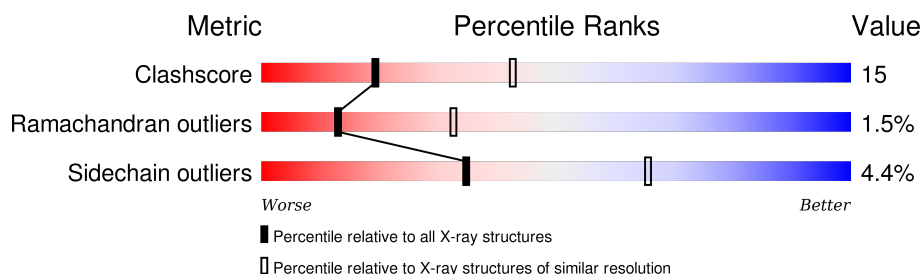Resolution : 2.70 Å(reported)

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Clashscore		15
Ramachandran outliers		1.5%
Sidechain outliers		4.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 <=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	87	47% 26% • 23%
1	D	87	43% 18% • 38%
2	B	328	68% 20% • • 8%
2	E	328	64% 23% • 10%
3	C	319	64% 26% • 8%
3	F	319	62% 24% • 11%
4	M	4	75% 25%

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Mol	Chain	Length	Quality of chain
4	N	4	50% 25% 25%
4	S	4	75% 25%
4	T	4	75% 25%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10581 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			547	337	103	104	3			
1	D	54	Total	C	N	O	S	0	0	0
			441	269	84	85	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2428	1515	429	462	22			
2	E	296	Total	C	N	O	S	0	0	0
			2377	1484	420	451	22			

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	0	0
			2343	1485	396	451	11			
3	F	285	Total	C	N	O	S	0	0	0
			2287	1453	384	439	11			

- Molecule 4 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	S	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	T	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	M	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	N	4	Total	C	N	O	0	0	0
			31	19	9	3			

- 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 14	C 8	N 1	O 5	0	0
5	E	1	Total 14	C 8	N 1	O 5	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Ca 1	0	0
6	C	2	Total 2	Ca 2	0	0
6	F	1	Total 1	Ca 1	0	0
6	E	2	Total 2	Ca 2	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: FIBRINOGEN

Chain A:

- Molecule 1: FIBRINOGEN

Chain D:

- Molecule 2: FIBRINOGEN

Chain B:

- Molecule 2: FIBRINOGEN

Chain E:

I215 M224 Y225 L226 D230 V233 R237 D241 W249 Q253 Q256 W266 D267 P268 Y269 K270 T280 D281 G282 K283 W293 L294 G295 N296 I299 E309 E315 G319 H325 N333 K337 Y345 R346 G350 N351 M354 M361
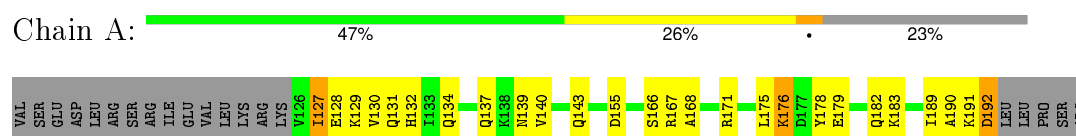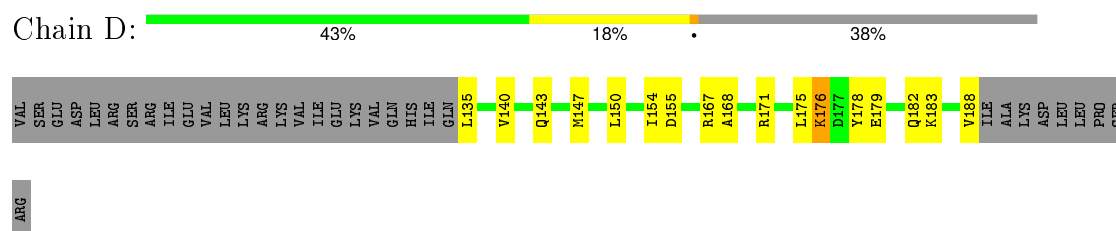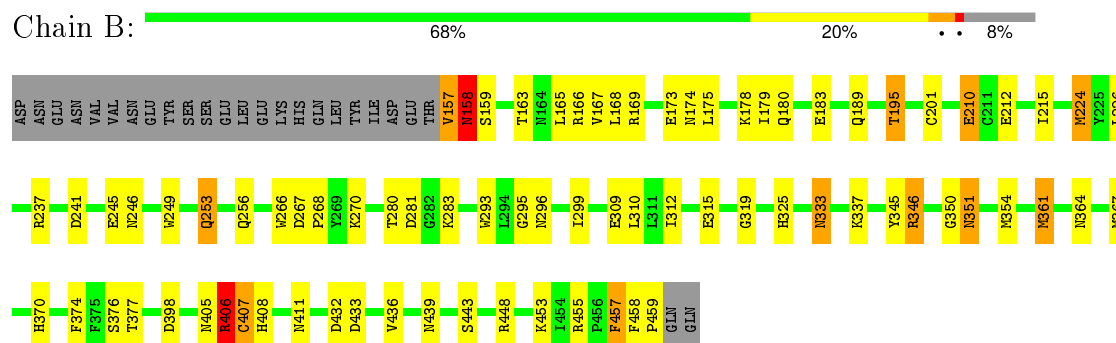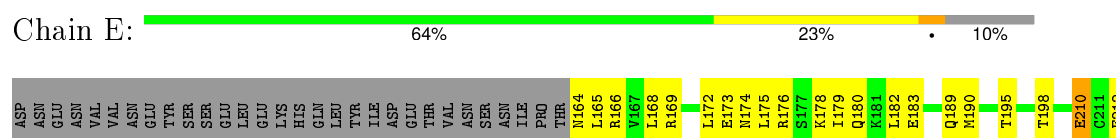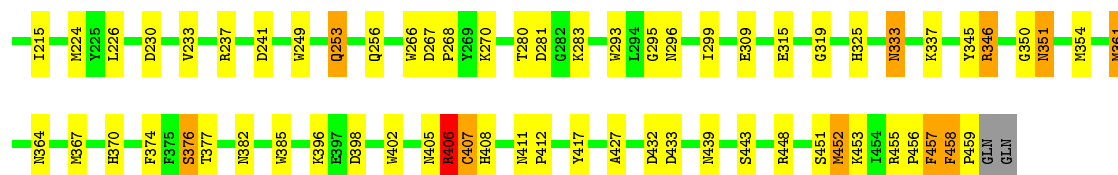
N364 M367 H370 F374 F375 S376 T377 N382 W385 K396 E397 D398 W402 N405 R406 C407 H408 N411 P412 Y417 A427 D432 D433 N439 S443 R448 S451 M452 K453 I454 R455 P456 F457 F458 P459 GLN GLN

• Molecule 3: FIBRINOGEN

Chain C: 64% 26% • 8%

LYS MET LEU GLU GLU ILE MET LYS TYR GLU ALA SER ILE LEU T102 H103 D104 S105 S106 I107 R108 Y109 E112 I113 Y114 N115 S116 N117 N118 V122 E126 V143 T149 G150 I156 A161 L166 P171 L172 L179 E183 I184 D185 N189 G190 W191 Q195

K196 R197 D203 K206 N207 W208 I209 Q210 S219 T224 W227 L228 G229 N230 E231 K232 I233 H234 L235 I236 Q239 S240 A241 I242 P243 Y244 M264 F265 K266 V267 G268 Y274 T277 Y278 D288 D291 D297 P298 P299 S300 H307 M310 T314 N317

F322 E323 G324 N325 C326 W335 M336 N337 K338 C339 H340 A341 G342 H343 G352 P360 N361 I367 S378 T382 T383 M384 F389 N390 R391 L392 T393 ILE GLY GLU GLY GLN GLN HIS HIS LEU GLY GLY ALA LYS

• Molecule 3: FIBRINOGEN

Chain F: 62% 24% • 11%

LYS MET LEU GLU GLU ILE MET LYS TYR GLU ALA SER ILE LEU THR HIS ASP SER SER ILE ARG Y109 L110 Q111 E112 I113 Y114 N115 S116 M117 N118 Q119 K120 I121 V122 N123 L124 K125 E126 L131 Q134 K140 T149 G150 C153 I156 A161 L166 L172 L179

E183 I184 D185 N189 G190 W191 T192 Q195 K196 R197 L198 N207 W208 I209 Q210 S219 T224 W227 L228 G229 N230 E231 K232 I233 H234 L235 I236 Q239 S240 A241 I242 P243 Y244 D261 M264 F265 K266 V267 G268 Y274 Y278 A282 D298 P299 H307

M310 T314 N317 F322 E323 G324 N325 C326 Q329 W334 W335 M336 N337 K338 C339 H340 A341 G342 H343 L344 G352 P360 N361 S378 T382 T383 M384 F389 T393 ILE GLY GLU GLY GLN GLN HIS HIS LEU GLY GLY ALA LYS

• Molecule 4: FIBRINOGEN

Chain S: 75% 25%

G1 H2 R3 P4

• Molecule 4: FIBRINOGEN

Chain T: 75% 25%

G1 H2 R3 P4

• Molecule 4: FIBRINOGEN

Chain M: 75% 25%

G1 P4

• Molecule 4: FIBRINOGEN

Chain N:

50%   25%   25%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.80Å 149.40Å 234.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	88.5 (30.00-2.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.233 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10581	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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	0.53	1/548 (0.2%)	0.71	1/731 (0.1%)
1	D	0.33	0/441	0.57	0/587
2	B	0.39	0/2490	0.72	5/3364 (0.1%)
2	E	0.38	0/2438	0.67	3/3291 (0.1%)
3	C	0.40	0/2408	0.62	0/3257
3	F	0.42	0/2351	0.64	0/3180
4	M	0.57	0/32	0.44	0/42
4	N	0.45	0/32	0.47	0/42
4	S	0.36	0/32	0.72	0/42
4	T	0.47	0/32	0.47	0/42
All	All	0.40	1/10804 (0.0%)	0.66	9/14578 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	ASP	C-O	-9.73	1.04	1.23

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	157	VAL	N-CA-C	13.26	146.79	111.00
1	A	192	ASP	CA-C-O	-12.26	94.35	120.10
2	B	406	ARG	NE-CZ-NH2	-7.01	116.79	120.30
2	B	157	VAL	CB-CA-C	-6.77	98.54	111.40
2	E	406	ARG	NE-CZ-NH2	-6.42	117.09	120.30

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	547	0	573	24	0
1	D	441	0	458	18	0
2	B	2428	0	2296	62	0
2	E	2377	0	2245	86	0
3	C	2343	0	2188	68	0
3	F	2287	0	2136	82	0
4	M	31	0	32	1	0
4	N	31	0	32	2	0
4	S	31	0	32	1	0
4	T	31	0	32	1	0
5	B	14	0	13	6	0
5	E	14	0	13	3	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
All	All	10581	0	10050	312	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 15.

The worst 5 of 312 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:176:ARG:HA	3:F:117:ASN:HB3	1.30	1.06
3:C:310:MET:SD	3:C:337:ASN:HB2	2.16	0.85
3:C:107:ILE:H	3:C:107:ILE:HD12	1.42	0.85
3:F:310:MET:SD	3:F:337:ASN:HB2	2.18	0.84
5:B:470:NAG:H2	5:B:470:NAG:H62	1.61	0.82

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	65/87 (75%)	58 (89%)	3 (5%)	4 (6%)	2	2
1	D	52/87 (60%)	50 (96%)	2 (4%)	0	100	100
2	B	301/328 (92%)	271 (90%)	25 (8%)	5 (2%)	11	29
2	E	294/328 (90%)	267 (91%)	23 (8%)	4 (1%)	14	35
3	C	290/319 (91%)	265 (91%)	22 (8%)	3 (1%)	19	45
3	F	283/319 (89%)	257 (91%)	23 (8%)	3 (1%)	17	42
4	M	2/4 (50%)	2 (100%)	0	0	100	100
4	N	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	S	2/4 (50%)	2 (100%)	0	0	100	100
4	T	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1293/1484 (87%)	1175 (91%)	99 (8%)	19 (2%)	13	32

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LYS
2	B	407	CYS
3	C	339	CYS
2	E	407	CYS
3	F	110	LEU

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	62/82 (76%)	58 (94%)	4 (6%)	21	46
1	D	50/82 (61%)	47 (94%)	3 (6%)	24	50
2	B	261/286 (91%)	249 (95%)	12 (5%)	33	64
2	E	254/286 (89%)	243 (96%)	11 (4%)	35	66
3	C	246/267 (92%)	237 (96%)	9 (4%)	41	72
3	F	239/267 (90%)	231 (97%)	8 (3%)	45	76
4	M	3/3 (100%)	3 (100%)	0	100	100
4	N	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	S	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	T	3/3 (100%)	3 (100%)	0	100	100
All	All	1124/1282 (88%)	1075 (96%)	49 (4%)	35	65

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	325	ASN
1	D	176	LYS
3	F	382	THR
3	C	389	PHE
2	E	164	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	239	GLN
2	E	164	ASN
3	F	307	HIS
3	C	307	HIS
3	C	319	ASN

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, 6 are monoatomic - leaving 2 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	470	-	14,14,15	0.50	0	15,19,21	0.89	1 (6%)
5	NAG	E	470	-	14,14,15	0.48	0	15,19,21	0.71	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
5	NAG	B	470	-	-	0/6/23/26	0/1/1/1
5	NAG	E	470	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	470	NAG	C2-N2-C7	-2.37	119.99	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	470	NAG	6	0
5	E	470	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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