wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 04:15 PM EDT

PDB ID	:	1YCP
Title	:	THE CRYSTAL STRUCTURE OF FIBRINOGEN-AA PEPTIDE 1-23 (F8Y) BOUND TO BOVINE THROMBIN EXPLAINS WHY THE MUTATION OF PHE-8 TO TYROSINE STRONGLY INHIBITS NORMAL CLEAVAGE AT ARGININE-16
Authors	:	Malkowski, M.G.; Edwards, B.F.P.
Deposited on	:	1997-05-01
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

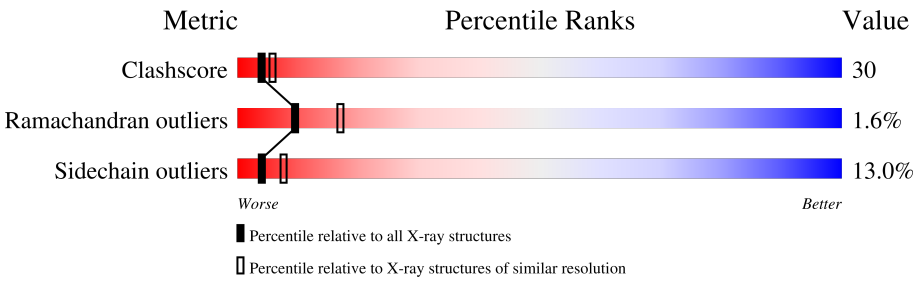
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	J	49	22% 37% 41%
1	L	49	37% 20% • 41%
2	H	259	41% 44% 10% 5%
3	F	23	• 17% • 74%
3	N	23	• 22% 74%
4	K	150	43% 46% 9% •
5	M	109	47% 39% 6% • 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4846 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 EPSILON THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	29	238	150	38	49	1	0	0	0
1	J	29	238	150	38	49	1	0	0	0

- Molecule 2 is a protein called ALPHA THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	247	2002	1281	360	349	12	0	0	0

- Molecule 3 is a protein called FIBRINOPEPTIDE A-ALPHA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	6	45	29	9	7	0	0	0
3	N	6	45	29	9	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	308	TYR	PHE	engineered mutation	UNP P02671
N	308	TYR	PHE	engineered mutation	UNP P02671

- Molecule 4 is a protein called EPSILON THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	K	146	1199	770	217	207	5	0	0	0

- Molecule 5 is a protein called EPSILON THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	M	101	803	511	143	142	7	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	L	27	27	27	0	0
6	H	148	Total 148	O 148	0	0
6	F	6	Total 6	O 6	0	0
6	J	11	Total 11	O 11	0	0
6	K	61	Total 61	O 61	0	0
6	M	23	Total 23	O 23	0	0

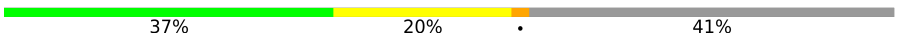
3 Residue-property plots (i)

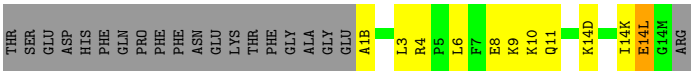
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

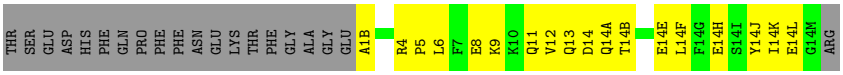
Chain L:





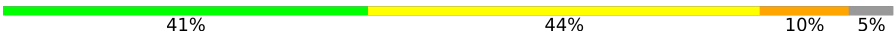
• Molecule 1: EPSILON THROMBIN

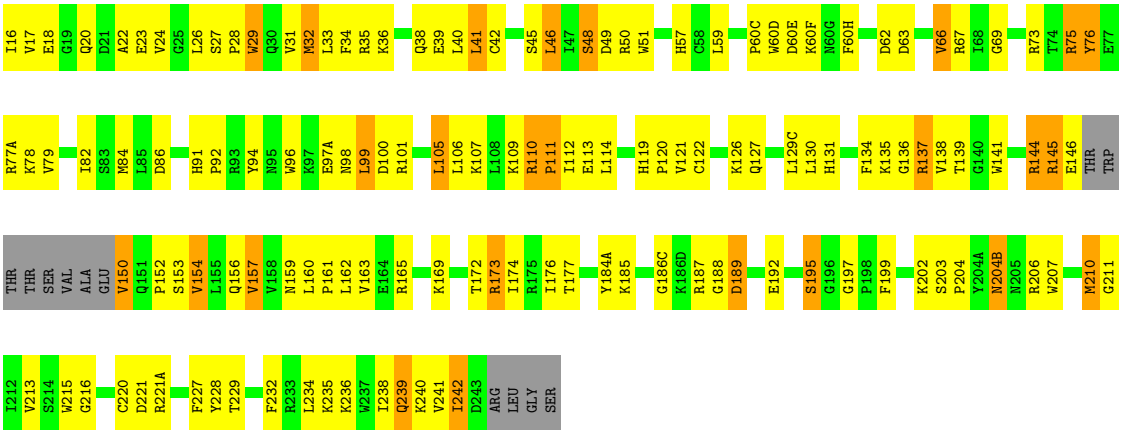
Chain J:



• Molecule 2: ALPHA THROMBIN

Chain H:





• Molecule 3: FIBRINOPEPTIDE A-ALPHA

Chain F:

• Molecule 3: FIBRINOPEPTIDE A-ALPHA

Chain N: • 22% 74%

ALA ASP SER GLY GLU GLY ASP Y308 LEU ALA GLU GLY GLY G314 V315 R316 G317 P318 ARG VAL VAL GLU ARG

- Molecule 4: EPSILON THROMBIN

Chain K: 43% 46% 9% •

I16 V17 E18 E23 V24 G25 L26 S27 P28 W29 M32 L33 F34 R35 K36 Q38 E39 L40 L41 S45 L46 I47 S48 D49 R50 W51 A55 A56 H57 C58 Y60A P60B P60C W60D D60E K60F D62 D63 L64 L65 V66 R67 I68 G69 K70 H71 T74 R75 Y76 E77 R77A

E80 K81 I82 S83 M84 L85 D86 K87 I88 Y89 I90 H91 P92 R93 R101 D102 I103 A104 L105 L106 K107 L108 K109 R110 P111 I112 E113 L114 S115 D116 Y117 D125 K126 Q127 K129B L129C L130 H131 F134 K135 T139 R145 E146 THR TRP THR THR

- Molecule 5: EPSILON THROMBIN

Chain M: 47% 39% 6% • 7%

SER VAL ALA GLU V150 S153 V154 V157 V158 N159 L160 P161 E164 R165 P166 V167 C168 K169 A170 S171 D178 N179 M180 F181 C182 P186 G186C K186D R187 G188 D189 A190 C191 E192 G193 D194 S195 F199 V200 S203 P204 Y204A N204B N205 R206 W207 Y208 Q209 V213 S214 W215

G216 D221 R221A D222 Y225 G226 F227 Y228 R233 K236 W237 I238 Q239 K240 V241 I242 D243 ARG LEU GLY SER

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.27Å 88.27Å 195.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4846	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	J	0.49	0/241	0.73	0/321
1	L	0.57	0/241	0.78	0/321
2	H	0.58	0/2053	0.93	2/2774 (0.1%)
3	F	0.58	0/45	0.97	0/58
3	N	0.51	0/45	0.79	0/58
4	K	0.50	0/1229	0.91	2/1663 (0.1%)
5	M	0.58	0/824	0.91	2/1111 (0.2%)
All	All	0.56	0/4678	0.90	6/6306 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	199	PHE	N-CA-C	-6.57	93.27	111.00
5	M	182	CYS	CA-CB-SG	6.20	125.15	114.00
2	H	189	ASP	CB-CG-OD1	5.72	123.45	118.30
4	K	41	LEU	CA-CB-CG	5.50	127.95	115.30
2	H	41	LEU	CA-CB-CG	5.28	127.44	115.30

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	J	238	0	230	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	238	0	230	20	0
2	H	2002	0	2008	139	3
3	F	45	0	42	12	0
3	N	45	0	42	7	1
4	K	1199	0	1221	76	1
5	M	803	0	787	48	1
6	F	6	0	0	2	0
6	H	148	0	0	18	0
6	J	11	0	0	2	0
6	K	61	0	0	9	0
6	L	27	0	0	1	0
6	M	23	0	0	2	0
All	All	4846	0	4560	276	3

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 30.

The worst 5 of 276 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:H:192:GLU:HB3	3:F:318:PRO:HA	1.46	0.97
3:F:308:TYR:HH	3:F:314:GLY:N	1.64	0.94
4:K:66:VAL:HG21	4:K:85:LEU:HD21	1.51	0.93
2:H:76:TYR:HB3	6:H:575:HOH:O	1.69	0.93
5:M:213:VAL:HG22	5:M:228:TYR:HE1	1.34	0.91

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:186(C):GLY:O	4:K:145:ARG:NH1[1_545]	1.97	0.23
2:H:145:ARG:NE	5:M:186(C):GLY:O[1_545]	2.05	0.15
2:H:60(D):TRP:NE1	3:N:308:TYR:N[8_655]	2.06	0.14

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	J	27/49 (55%)	22 (82%)	4 (15%)	1 (4%)	3 4
1	L	27/49 (55%)	20 (74%)	7 (26%)	0	100 100
2	H	243/259 (94%)	213 (88%)	26 (11%)	4 (2%)	9 17
3	F	3/23 (13%)	1 (33%)	1 (33%)	1 (33%)	0 0
3	N	3/23 (13%)	1 (33%)	2 (67%)	0	100 100
4	K	144/150 (96%)	126 (88%)	16 (11%)	2 (1%)	11 20
5	M	99/109 (91%)	86 (87%)	12 (12%)	1 (1%)	15 28
All	All	546/662 (82%)	469 (86%)	68 (12%)	9 (2%)	9 17

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	111	PRO
5	M	205	ASN
2	H	79	VAL
3	F	316	ARG
4	K	77(A)	ARG

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	J	26/43 (60%)	24 (92%)	2 (8%)	13 25
1	L	26/43 (60%)	25 (96%)	1 (4%)	33 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	216/226 (96%)	181 (84%)	35 (16%)	2 4
3	F	4/15 (27%)	4 (100%)	0	100 100
3	N	4/15 (27%)	4 (100%)	0	100 100
4	K	130/134 (97%)	114 (88%)	16 (12%)	4 9
5	M	86/92 (94%)	76 (88%)	10 (12%)	5 10
All	All	492/568 (87%)	428 (87%)	64 (13%)	4 7

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	M	182	CYS
5	M	187	ARG
2	H	145	ARG
2	H	144	ARG
5	M	233	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	20	GLN
5	M	204(B)	ASN
4	K	38	GLN
5	M	239	GLN
5	M	156	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.