WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:33 PM GMT

PDB ID	:	1BBR
Title	:	THE STRUCTURE OF RESIDUES 7-16 OF THE A ALPHA CHAIN OF HUMAN FIBRINOGEN BOUND TO BOVINE THROMBIN AT 2.3 ANGSTROMS RESOLUTION
Authors	:	Martin, P.; Edwards, B.
Deposited on	:	1992-04-27
Resolution	:	2.30 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 (i) symbol.

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

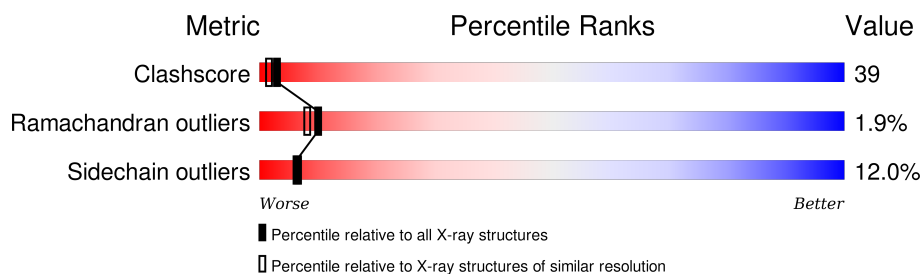|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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		39
Ramachandran outliers		1.9%
Sidechain outliers		12.0%

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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	J	49	24% 39% 8% • 27%
1	L	49	35% 31% 8% 27%
1	M	49	24% 39% 10% 27%
2	H	150	46% 39% 13% •
3	E	109	51% 34% 13% •
4	F	11	27% 55% 18%
4	G	11	64% 18% 18%

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Mol	Chain	Length	Quality of chain
4	I	11	36% 55% 9%
5	K	259	44% 37% 14% •
5	N	259	42% 45% 10% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8084 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
1	L	36	Total 290	C 181	N 48	O 60	S 1	0	0	0
1	J	36	Total 290	C 181	N 48	O 60	S 1	0	0	0
1	M	36	Total 290	C 181	N 48	O 60	S 1	0	0	0

- Molecule 2 is a protein called EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	150	Total 1235	C 793	N 222	O 215	S 5	0	0	0

- Molecule 3 is a protein called EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	109	Total 860	C 544	N 154	O 155	S 7	0	0	0

- Molecule 4 is a protein called FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	11	Total 75	C 46	N 13	O 16	0	0	0
4	G	11	Total 75	C 46	N 13	O 16	0	0	0
4	I	11	Total 75	C 46	N 13	O 16	0	0	0

- Molecule 5 is a protein called EPSILON-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	259	Total 2094	C 1337	N 376	O 369	S 12	0	0	0
5	N	259	Total 2094	C 1337	N 376	O 369	S 12	0	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	69	Total 69	O 69	0	0
6	F	10	Total 10	O 10	0	0
6	G	11	Total 11	O 11	0	0
6	H	126	Total 126	O 126	0	0
6	I	9	Total 9	O 9	0	0
6	J	23	Total 23	O 23	0	0
6	K	213	Total 213	O 213	0	0
6	L	31	Total 31	O 31	0	0
6	M	26	Total 26	O 26	0	0
6	N	188	Total 188	O 188	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.
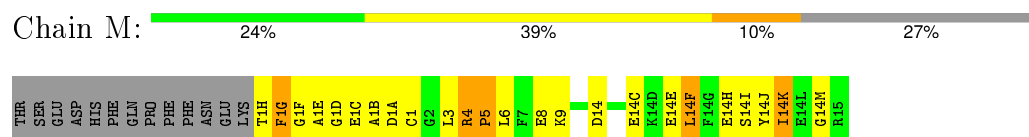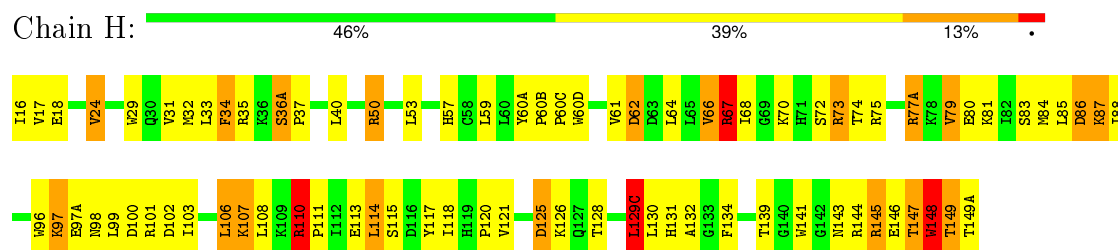
Note EDS was not executed.

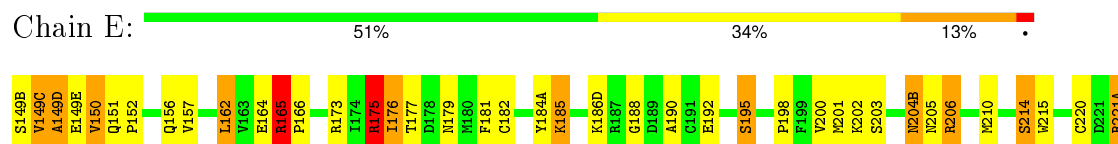- Molecule 1: EPSILON-THROMBIN
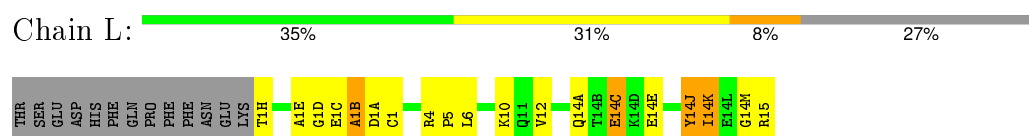
- Molecule 1: EPSILON-THROMBIN
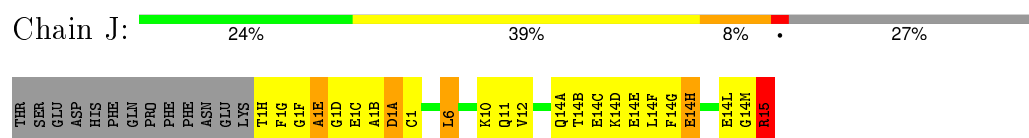
- Molecule 1: EPSILON-THROMBIN

- Molecule 2: EPSILON-THROMBIN

- Molecule 3: EPSILON-THROMBIN

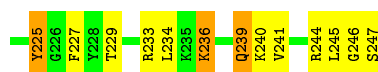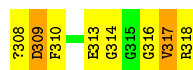Y225 G226 F227 Y228 T229 R233 L234 K235 K236 Q239 K240 V241 R244 L245 G246 S247

• Molecule 4: FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR

Chain F: 27%   55%   18%

?308 D309 F310 E313 G314 G315 G316 V317 R318

• Molecule 4: FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR

Chain G: 64%   18%   18%

?308 L311 G314 V317 R318

• Molecule 4: FIBRINOGEN ALPHA/ALPHA-E CHAIN PRECURSOR

Chain I: 36%   55%   9%

?308 D309 F310 L311 A312 E313 G316 V317 R318

• Molecule 5: EPSILON-THROMBIN

Chain K: 44%   37%   14%   •

I16 V17 E18 G19 A22 S27 L33 F34 R35 K36 S36A P37 Q38 E39 L40 L41 C42 G43 A44 S45 L46 I47 S48 D49 R50 W51 V52 H57 Y60A P60B P60C W60D D60E K60F N60G F60H T60I V61 D62 D63 L64 L65 V66 R67 H71 S72 R73 T74 R75 Y76 E77 R77A K78 V79

E80 K81 M84 L85 D86 K87 I88 Y89 I90 H91 P92 R93 Y94 N95 W96 K97 E97A N98 L99 D100 R101 A104 L105 L106 K107 L108 K109 R110 P111 I112 E113 I118 H119 P120 L123 P124 D125 K126 Q127 T128 K129B L129C F134 T139 G140 W141 G142 N143 R144 R145 E146 I147 W148

T149 T149A S149B V149C A149D E149E V150 Q151 P152 S153 V154 V157 V158 N159 L160 P161 L162 V163 E164 R165 P166 V167 C168 E169 K169 R173 I174 R175 I176 T177 D178 G184 Y184A K185 E186B G188 D189 A190 C191 E192 S195 K202 S203 P204 Y204A N204B N205 R206 W207 Y208 Q209 M210 G211 I212

D221 R221A K224 Y225 Y228 T229 R233 L234 K235 I238 Q239 K240 V241 R244 L245 G246 S247

• Molecule 5: EPSILON-THROMBIN

Chain N: 42%   45%   10%   •

I16 V17 D21 A22 E23 V24 G25 L26 S27 P28 W29 M32 L33 F34 R35 K36 S36A P37 Q38 E39 L40 S45 L46 I47 S48 D49 R50 L53 H57 C58 L59 P60B P60C W60D D60E K60F T60I L64 L65 V66 R67 I68 G69 K70 H71 S72 R73 T74 R75 Y76 E77 R77A

K78 V79 E80 K81 I82 S83 M84 L85 D86 K87 H91 P92 R93 Y94 N95 W96 K97 L99 D100 R101 D102 I103 L106 K109 R110 P111 I112 E113 L114 S115 D116 Y117 I118 H119 D125 K126 Q127 T128 K129B L129C L130 H131 F134 K135 G136 R137 V138 T139 N143 R144 T147

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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.02Å 89.41Å 99.30Å 90.00° 106.64° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8084	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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: ACE

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	1.18	0/294	1.86	7/390 (1.8%)
1	L	1.07	0/294	1.64	1/390 (0.3%)
1	M	1.18	2/294 (0.7%)	1.87	5/390 (1.3%)
2	H	1.09	0/1267	1.71	17/1716 (1.0%)
3	E	1.14	0/881	1.77	16/1186 (1.3%)
4	F	1.18	0/73	2.25	3/95 (3.2%)
4	G	1.21	0/73	1.60	1/95 (1.1%)
4	I	1.24	0/73	1.95	1/95 (1.1%)
5	K	1.27	2/2148 (0.1%)	2.05	69/2905 (2.4%)
5	N	1.08	3/2148 (0.1%)	1.76	46/2905 (1.6%)
All	All	1.16	7/7545 (0.1%)	1.85	166/10167 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
2	H	0	2
3	E	0	2
4	G	0	1
5	K	0	6
5	N	0	5
All	All	0	17

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	19	GLY	N-CA	5.75	1.54	1.46
5	K	80	GLU	CB-CG	-5.57	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	33	LEU	N-CA	5.54	1.57	1.46
1	M	14(H)	GLU	CD-OE2	-5.48	1.19	1.25
1	M	14(M)	GLY	N-CA	-5.42	1.38	1.46

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	225	TYR	CB-CG-CD1	16.06	130.63	121.00
5	K	225	TYR	CB-CG-CD2	-15.70	111.58	121.00
5	K	175	ARG	NE-CZ-NH2	-13.93	113.34	120.30
5	N	75	ARG	CD-NE-CZ	12.89	141.65	123.60
5	K	60(F)	LYS	CA-CB-CG	12.84	141.65	113.40

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	165	ARG	Sidechain
3	E	175	ARG	Sidechain
2	H	110	ARG	Sidechain
2	H	67	ARG	Sidechain
1	J	15	ARG	Sidechain

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	290	0	276	37	0
1	L	290	0	276	30	0
1	M	290	0	276	47	0
2	H	1235	0	1252	101	0
3	E	860	0	844	87	0
4	F	75	0	69	8	0
4	G	75	0	69	6	0
4	I	75	0	69	8	0
5	K	2094	0	2097	156	0
5	N	2094	0	2097	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	69	0	0	15	0
6	F	10	0	0	0	0
6	G	11	0	0	1	0
6	H	126	0	0	24	0
6	I	9	0	0	6	0
6	J	23	0	0	9	0
6	K	213	0	0	53	0
6	L	31	0	0	6	0
6	M	26	0	0	18	0
6	N	188	0	0	51	0
All	All	8084	0	7325	573	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 39.

The worst 5 of 573 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)
5:K:60(F):LYS:HB2	6:K:422:HOH:O	1.17	1.28
5:K:176:ILE:HG21	6:K:407:HOH:O	1.27	1.25
1:J:14(G):PHE:HB3	6:J:616:HOH:O	1.30	1.24
5:K:52:VAL:HG22	6:K:432:HOH:O	1.39	1.23
5:N:204:PRO:HB3	6:N:396:HOH:O	1.40	1.21

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	J	34/49 (69%)	28 (82%)	5 (15%)	1 (3%)	6 3
1	L	34/49 (69%)	27 (79%)	4 (12%)	3 (9%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	34/49 (69%)	26 (76%)	6 (18%)	2 (6%)	2	1
2	H	148/150 (99%)	135 (91%)	13 (9%)	0	100	100
3	E	107/109 (98%)	97 (91%)	7 (6%)	3 (3%)	6	4
4	F	9/11 (82%)	8 (89%)	0	1 (11%)	0	0
4	G	9/11 (82%)	9 (100%)	0	0	100	100
4	I	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
5	K	257/259 (99%)	235 (91%)	19 (7%)	3 (1%)	16	16
5	N	257/259 (99%)	229 (89%)	24 (9%)	4 (2%)	12	11
All	All	898/957 (94%)	802 (89%)	79 (9%)	17 (2%)	10	8

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(B)	ALA
1	L	14(K)	ILE
3	E	149(C)	VAL
3	E	150	VAL
4	F	309	ASP

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	30/43 (70%)	24 (80%)	6 (20%)	1	1
1	L	30/43 (70%)	29 (97%)	1 (3%)	45	61
1	M	30/43 (70%)	28 (93%)	2 (7%)	20	26
2	H	134/134 (100%)	119 (89%)	15 (11%)	7	8
3	E	92/92 (100%)	82 (89%)	10 (11%)	8	9
4	F	6/6 (100%)	4 (67%)	2 (33%)	0	0
4	G	6/6 (100%)	5 (83%)	1 (17%)	3	2
4	I	6/6 (100%)	5 (83%)	1 (17%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	K	226/226 (100%)	195 (86%)	31 (14%)	4	4
5	N	226/226 (100%)	201 (89%)	25 (11%)	8	8
All	All	786/825 (95%)	692 (88%)	94 (12%)	6	6

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	63	ASP
5	K	149	THR
5	N	157	VAL
5	K	64	LEU
5	K	110	ARG

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

Mol	Chain	Res	Type
5	K	71	HIS
5	K	204(B)	ASN
5	N	204(B)	ASN
1	J	14(A)	GLN
5	N	131	HIS

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)

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.