



# wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 02:06 AM GMT

PDB ID : 3BEF  
Title : Crystal structure of thrombin bound to the extracellular fragment of PAR1  
Authors : Gandhi, P.S.; Bah, A.; Chen, Z.; Mathews, F.S.; Di Cera, E.  
Deposited on : 2007-11-17  
Resolution : 2.20 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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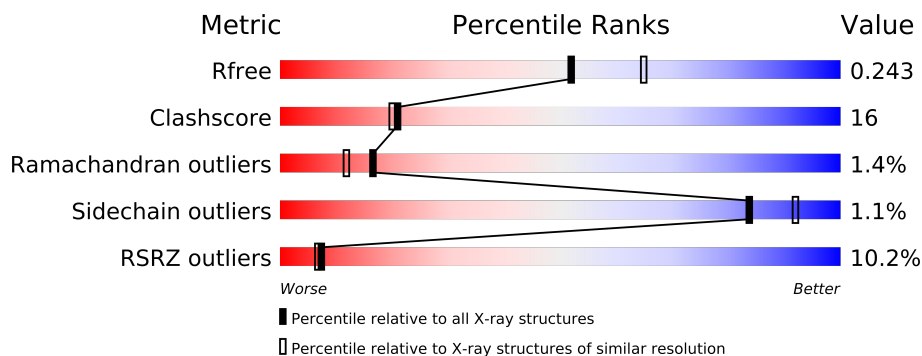
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	46	
1	D	46	
2	B	259	
2	E	259	
3	C	9	
3	F	9	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5186 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	44	Total	C	N	O	S	0	0	0
			357	226	58	72	1			
1	D	42	Total	C	N	O	S	0	0	0
			347	220	56	70	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1R	SER	-	EXPRESSION TAG	UNP P00734
A	1Q	GLU	-	EXPRESSION TAG	UNP P00734
D	1R	SER	-	EXPRESSION TAG	UNP P00734
D	1Q	GLU	-	EXPRESSION TAG	UNP P00734

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	251	Total	C	N	O	S	0	0	0
			2034	1298	361	361	14			
2	E	251	Total	C	N	O	S	0	0	0
			2034	1298	361	361	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	102	ASN	ASP	ENGINEERED	UNP P00734
E	102	ASN	ASP	ENGINEERED	UNP P00734

- Molecule 3 is a protein called Proteinase-activated receptor 1.

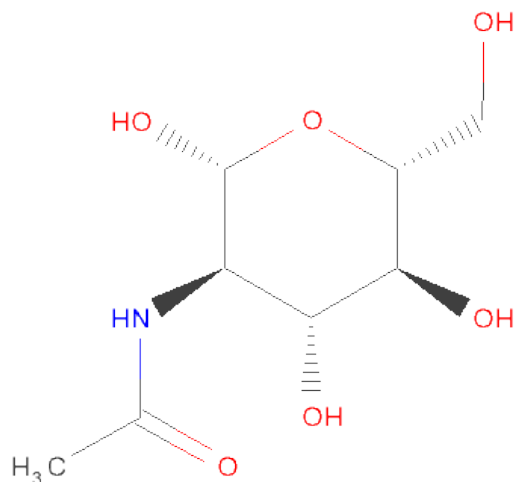
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			87	58	12	17			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	0	0	0
			70	49	9	12			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	102	Total	O	0	0
			102	102		
5	C	5	Total	O	0	0
			5	5		
5	D	18	Total	O	0	0
			18	18		
5	E	79	Total	O	0	0
			79	79		
5	F	1	Total	O	0	0
			1	1		





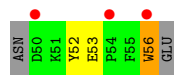
- Molecule 3: Proteinase-activated receptor 1

Chain C: 



- Molecule 3: Proteinase-activated receptor 1

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.06Å 50.34Å 85.08Å 76.89° 84.30° 73.69°	Depositor
Resolution (Å)	28.00 – 2.20 28.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.8 (28.00-2.20) 91.9 (28.00-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.248 0.206 , 0.243	Depositor DCC
$R_{free}$ test set	1658 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 34055 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/364	0.60	0/488
1	D	0.38	0/354	0.60	0/474
2	B	0.34	0/2086	0.64	1/2817 (0.0%)
2	E	0.33	0/2086	0.60	0/2817
3	C	0.37	0/91	0.61	0/123
3	F	0.39	0/74	0.48	0/100
All	All	0.34	0/5055	0.61	1/6819 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	PHE	N-CA-C	-5.32	96.63	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	357	0	334	7	0
1	D	347	0	330	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2034	0	2014	73	0
2	E	2034	0	2014	76	0
3	C	87	0	69	8	0
3	F	70	0	57	3	0
4	B	14	0	13	0	0
4	E	14	0	13	1	0
5	A	24	0	0	0	0
5	B	102	0	0	2	0
5	C	5	0	0	0	0
5	D	18	0	0	0	0
5	E	79	0	0	2	0
5	F	1	0	0	0	0
All	All	5186	0	4844	152	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 152 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:127:GLU:HG2	3:C:57:GLU:HA	1.38	1.05
2:B:186(B):GLU:HB3	2:E:173:ARG:HH22	1.46	0.77
2:B:127:GLU:CG	3:C:57:GLU:HA	2.15	0.75
2:B:35:ARG:O	2:B:38:GLN:HA	1.91	0.70
2:E:127:GLU:OE1	3:F:56:TRP:HB3	1.92	0.69

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	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
1	D	40/46 (87%)	38 (95%)	2 (5%)	0	100	100
2	B	247/259 (95%)	235 (95%)	11 (4%)	1 (0%)	43	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	247/259 (95%)	221 (90%)	21 (8%)	5 (2%)	11	6
3	C	7/9 (78%)	5 (71%)	0	2 (29%)	0	0
3	F	5/9 (56%)	3 (60%)	2 (40%)	0	100	100
All	All	588/628 (94%)	543 (92%)	37 (6%)	8 (1%)	16	12

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	61	GLU
2	B	244	GLN
3	C	56	TRP
2	E	243	ASP
2	E	244	GLN

### 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	38/41 (93%)	36 (95%)	2 (5%)	32	36
1	D	38/41 (93%)	38 (100%)	0	100	100
2	B	220/225 (98%)	219 (100%)	1 (0%)	94	98
2	E	220/225 (98%)	219 (100%)	1 (0%)	94	98
3	C	9/9 (100%)	8 (89%)	1 (11%)	9	7
3	F	7/9 (78%)	6 (86%)	1 (14%)	5	4
All	All	532/550 (97%)	526 (99%)	6 (1%)	84	92

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	204(B)	ASN
3	F	56	TRP
3	C	56	TRP
1	A	14(L)	ASP
2	E	204(B)	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	239	GLN
2	E	209	GLN
2	E	131	GLN
2	B	204(B)	ASN
2	E	71	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	$\# Z  > 2$
4	NAG	B	301	2	12,14,15	1.42	3 (25%)	15,19,21	1.62	3 (20%)
4	NAG	E	302	2	12,14,15	1.50	3 (25%)	15,19,21	1.55	3 (20%)

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
4	NAG	B	301	2	-	0/6/23/26	0/1/1/1
4	NAG	E	302	2	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	302	NAG	C3-C2	3.13	1.59	1.52
4	B	301	NAG	C3-C2	2.83	1.58	1.52
4	E	302	NAG	C2-N2	2.58	1.49	1.46
4	B	301	NAG	C4-C5	2.24	1.58	1.53
4	B	301	NAG	C2-N2	2.22	1.48	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	NAG	C6-C5-C4	3.50	121.45	113.00
4	E	302	NAG	C6-C5-C4	3.46	121.37	113.00
4	B	301	NAG	O5-C5-C4	-3.21	106.58	110.65
4	E	302	NAG	O5-C5-C4	-3.09	106.73	110.65
4	B	301	NAG	C3-C2-N2	2.69	115.85	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	44/46 (95%)	-0.10	2 (4%) 32 32	16, 28, 49, 78	0
1	D	42/46 (91%)	0.12	5 (11%) 5 5	21, 33, 53, 79	0
2	B	251/259 (96%)	0.22	15 (5%) 21 21	10, 27, 55, 86	0
2	E	251/259 (96%)	0.72	34 (13%) 4 4	16, 39, 74, 89	0
3	C	9/9 (100%)	1.83	3 (33%) 1 1	30, 42, 85, 91	0
3	F	7/9 (77%)	2.06	3 (42%) 1 0	59, 68, 77, 87	0
All	All	604/628 (96%)	0.44	62 (10%) 7 6	10, 32, 70, 91	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	149(E)	LYS	7.7
2	E	149(E)	LYS	7.2
3	C	56	TRP	6.1
2	E	147	THR	5.8
2	E	60(D)	TRP	5.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	301	14/15	0.30	-	73,78,82,83	0
4	NAG	E	302	14/15	0.32	-	78,83,86,86	0

## 6.5 Other polymers

There are no such residues in this entry.