



wwPDB X-ray Structure Validation Summary Report i

Apr 10, 2014 – 06:49 PM EDT

PDB ID : 4IBL
Title : Rubidium Sites in Blood Coagulation Factor VIIa
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Deposited on : 2012-12-08
Resolution : 1.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

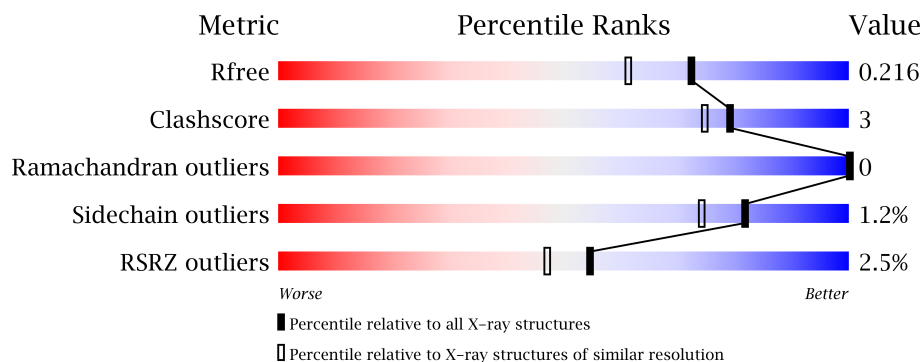
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
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)	:	stable22978

1 Overall quality at a glance




The reported resolution of this entry is 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. 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	L	152	
2	H	254	
3	T	219	

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 5267 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 Coagulation factor VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	140	Total	C	N	O	S	0	0	0
			1121	676	186	244	15			

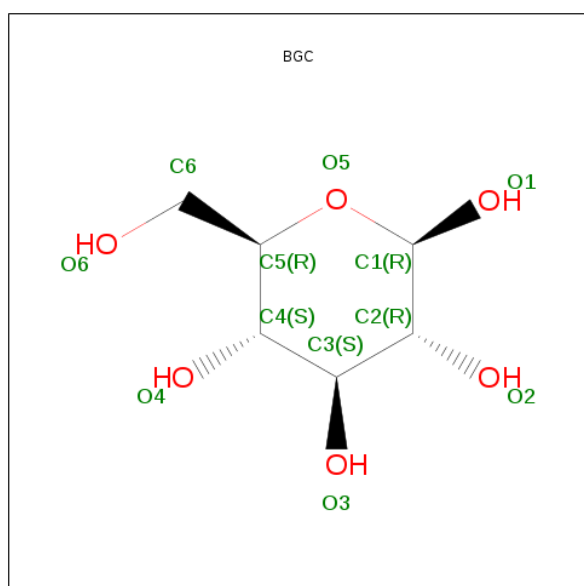
- Molecule 2 is a protein called Coagulation factor VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	254	Total	C	N	O	S	0	0	0
			1974	1253	351	357	13			

- Molecule 3 is a protein called Tissue factor.

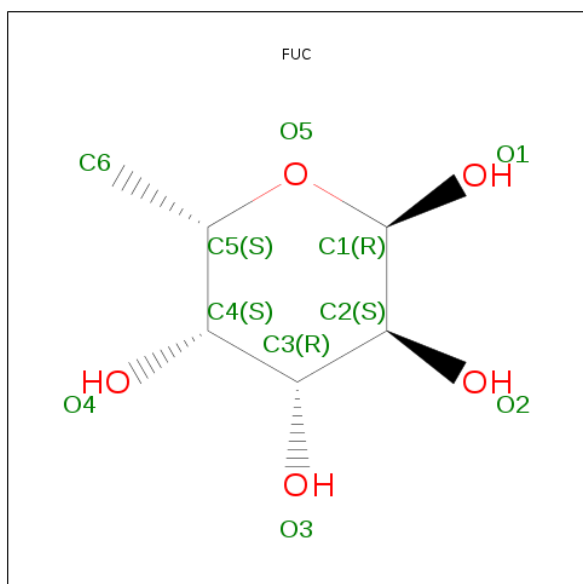
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	198	Total	C	N	O	S	0	0	0
			1596	1013	259	319	5			

- Molecule 4 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	3	Total	Mg	0	0
			3	3		

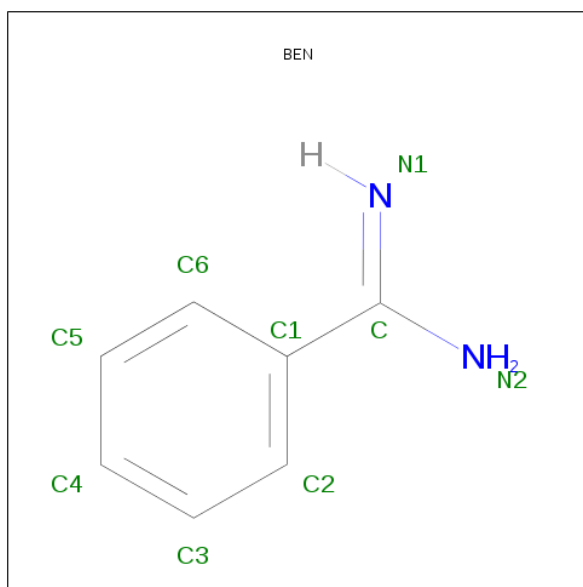
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Ca	0	0
			1	1		
7	L	3	Total	Ca	0	0
			3	3		

- Molecule 8 is RUBIDIUM ION (three-letter code: RB) (formula: Rb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	2	Total	Rb	0	0
			2	2		
8	L	4	Total	Rb	0	0
			4	4		

- Molecule 9 is BENZAMIDINE (three-letter code: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	N	0	0
			9	7	2		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	3	Total	Cl	0	0
			3	3		
10	T	1	Total	Cl	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	133	Total	O	0	0
			133	133		
11	H	248	Total	O	0	0
			248	248		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	T	148	Total 148	O 148	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.

- Molecule 1: Coagulation factor VII

Chain L: 



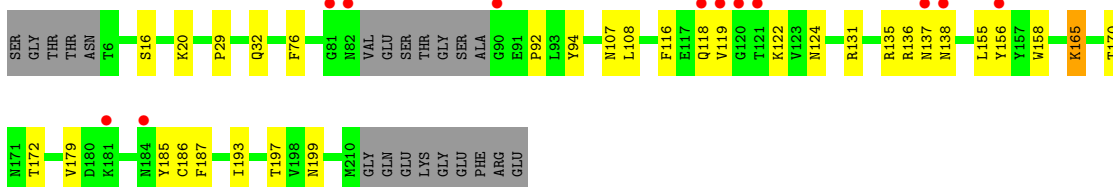
- Molecule 2: Coagulation factor VII

Chain H: 



- Molecule 3: Tissue factor

Chain T: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.90Å 81.06Å 126.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.24 – 1.80 68.24 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.24-1.80) 100.0 (68.24-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.215 0.179 , 0.216	Depositor DCC
R_{free} test set	6702 reflections (11.11%)	DCC
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67021 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5267	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: MG, BGC, BEN, CL, CA, FUC, RB, CGU

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	L	1.02	0/1015	0.90	0/1356
2	H	1.17	4/2024 (0.2%)	1.01	1/2755 (0.0%)
3	T	1.12	0/1631	0.97	0/2218
All	All	1.12	4/4670 (0.1%)	0.97	1/6329 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	214	SER	CB-OG	5.92	1.50	1.42
2	H	215	TRP	CE3-CZ3	5.51	1.47	1.38
2	H	236	GLU	CG-CD	5.41	1.60	1.51
2	H	135	PHE	CE1-CZ	5.04	1.47	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	188	LYS	CD-CE-NZ	5.86	125.17	111.70

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	L	1121	0	973	4	0
2	H	1974	0	1950	6	0
3	T	1596	0	1551	23	0
4	L	11	0	10	0	0
5	L	10	0	10	0	0
6	L	3	0	0	0	0
7	H	1	0	0	0	0
7	L	3	0	0	0	0
8	H	2	0	0	0	0
8	L	4	0	0	0	0
9	H	9	0	7	0	0
10	H	3	0	0	1	0
10	T	1	0	0	0	0
11	H	248	0	0	4	0
11	L	133	0	0	1	0
11	T	148	0	0	4	0
All	All	5267	0	4501	32	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 3.

The worst 5 of 32 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:27:CYS:HB3	11:H:625:HOH:O	1.47	1.10
10:H:306:CL:CL	11:H:545:HOH:O	2.39	0.76
3:T:156:TYR:CD2	11:T:525:HOH:O	2.40	0.75
3:T:76:PHE:CD1	3:T:92:PRO:HG2	2.22	0.73
3:T:136:ARG:HG2	3:T:136:ARG:HH11	1.57	0.70

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	L	128/152 (84%)	122 (95%)	6 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	252/254 (99%)	247 (98%)	5 (2%)	0	100	100
3	T	194/219 (89%)	191 (98%)	3 (2%)	0	100	100
All	All	574/625 (92%)	560 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	L	113/122 (93%)	111 (98%)	2 (2%)	71	58
2	H	216/216 (100%)	214 (99%)	2 (1%)	87	83
3	T	184/200 (92%)	182 (99%)	2 (1%)	84	77
All	All	513/538 (95%)	507 (99%)	6 (1%)	82	74

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

Mol	Chain	Res	Type
2	H	29	TRP
3	T	197	THR
2	H	245	GLU
1	L	110	ARG
3	T	165	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	105	HIS
2	H	110	GLN
2	H	159	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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, 95th 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 ²)	Q<0.9
1	L	140/152 (92%)	-0.24	2 (1%) 72 68	13, 24, 40, 46	0
2	H	254/254 (100%)	-0.45	1 (0%) 90 89	9, 15, 33, 51	0
3	T	198/219 (90%)	-0.05	12 (6%) 21 15	13, 21, 46, 60	0
All	All	592/625 (94%)	-0.27	15 (2%) 54 47	9, 20, 41, 60	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	82	ASN	6.5
3	T	119	VAL	5.7
3	T	81	GLY	4.2
3	T	121	THR	3.7
3	T	120	GLY	3.6

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

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, 95th 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(Å ²)	Q<0.9
1	CGU	L	19	12/13	0.10	-	38,43,46,46	0
1	CGU	L	7	12/13	0.10	-	25,29,42,44	0
1	CGU	L	25	12/13	0.08	-	24,26,33,35	0
1	CGU	L	6	12/13	0.14	-	24,35,44,45	0
1	CGU	L	14	12/13	0.10	-	30,36,42,44	0
1	CGU	L	26	12/13	0.09	-	21,24,27,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	CGU	L	29	12/13	0.09	-	24,27,28,28	0
1	CGU	L	16	12/13	0.07	-	22,25,29,30	0
1	CGU	L	35	12/13	0.30	-	32,46,55,56	0
1	CGU	L	20	12/13	0.09	-	35,40,43,44	0

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, 95th 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(\AA^2)	Q<0.9
6	MG	L	206	1/1	0.05	-	24,24,24,24	0
7	CA	H	302	1/1	0.04	-	27,27,27,27	0
7	CA	L	204	1/1	0.08	-	60,60,60,60	0
6	MG	L	209	1/1	0.06	-	47,47,47,47	0
8	RB	L	207	1/1	0.05	-	55,55,55,55	1
10	CL	H	306	1/1	0.05	-	21,21,21,21	0
7	CA	L	210	1/1	0.08	-	21,21,21,21	0
10	CL	H	307	1/1	0.05	-	32,32,32,32	0
8	RB	L	212	1/1	0.10	-	45,45,45,45	1
7	CA	L	208	1/1	0.11	-	71,71,71,71	0
10	CL	H	303	1/1	0.07	-	23,23,23,23	0
8	RB	L	211	1/1	0.06	-	31,31,31,31	1
5	FUC	L	202	10/11	0.13	-	29,30,33,37	0
8	RB	H	305	1/1	0.09	-	52,52,52,52	1
8	RB	L	205	1/1	0.07	-	48,48,48,48	1
4	BGC	L	201	11/12	0.10	-	30,36,37,39	0
6	MG	L	203	1/1	0.06	-	32,32,32,32	0
8	RB	H	304	1/1	0.09	-	46,46,46,46	1
9	BEN	H	301	9/9	0.07	-	12,15,16,18	0
10	CL	T	301	1/1	0.08	-	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.