



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 04:06 am GMT

PDB ID : 1X7A
Title : Porcine Factor IXa Complexed to 1-{3-[amino(imino)methyl]phenyl}-N-[4-(1H-benzimidazol-1-yl)-2-fluorophenyl]-3-(trifluoromethyl)-1H-pyrazole-5-carboxamide
Authors : Alexander, R.S.; Smallwood, A.M.; Smallheer, J.M.; Wang, J.; Wang, S.; Nakajima, S.; Rossi, K.A.; Barbera, F.; Burdick, D.; Luetttgen, J.M.
Deposited on : 2004-08-13
Resolution : 2.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

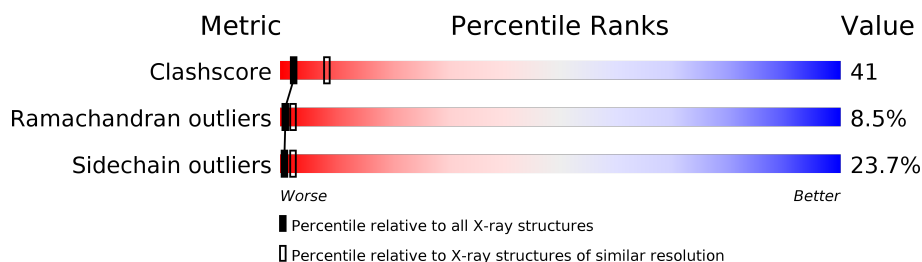
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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 $\leq 5\%$. 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	C	235	
2	L	146	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2595 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 Coagulation Factor IXa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	235	Total	C	N	O	S	28	0	0
			1833	1170	312	343	8			

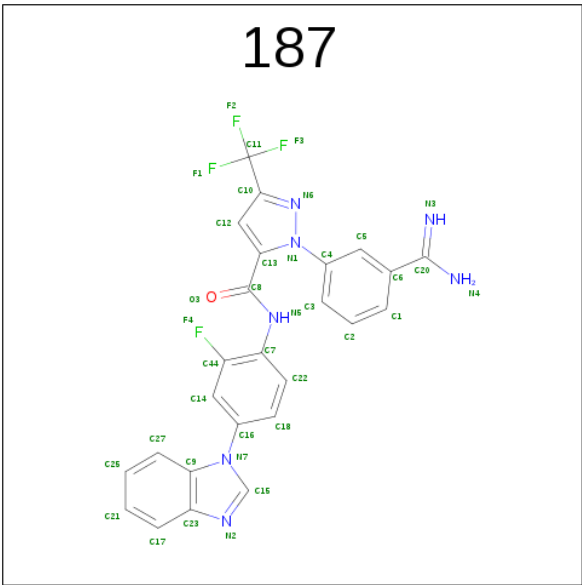
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	174	PHE	VAL	SEE REMARK 999	UNP P16293
C	192	GLN	LEU	SEE REMARK 999	UNP P16293
C	238	ILE	-	SEE REMARK 999	UNP P16293
C	239	LYS	-	SEE REMARK 999	UNP P16293
C	240	GLU	-	SEE REMARK 999	UNP P16293
C	241	LYS	-	SEE REMARK 999	UNP P16293
C	242	THR	-	SEE REMARK 999	UNP P16293
C	243	LYS	-	SEE REMARK 999	UNP P16293
C	244	LEU	-	SEE REMARK 999	UNP P16293
C	245	THR	-	SEE REMARK 999	UNP P16293

- Molecule 2 is a protein called Coagulation Factor IX, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	97	Total	C	N	O	S	82	0	0
			725	442	130	140	13			

- Molecule 3 is 1-{3-[AMINO(IMINO)METHYL]PHENYL}-N-[4-(1H-BENZIMIDAZOL-1-YL)-2-FLUOROPHENYL]-3-(TRIFLUOROMETHYL)-1H-PYRAZOLE-5-CARBOXAMIDE (three-letter code: 187) (formula: C₂₅H₁₇F₄N₇O).



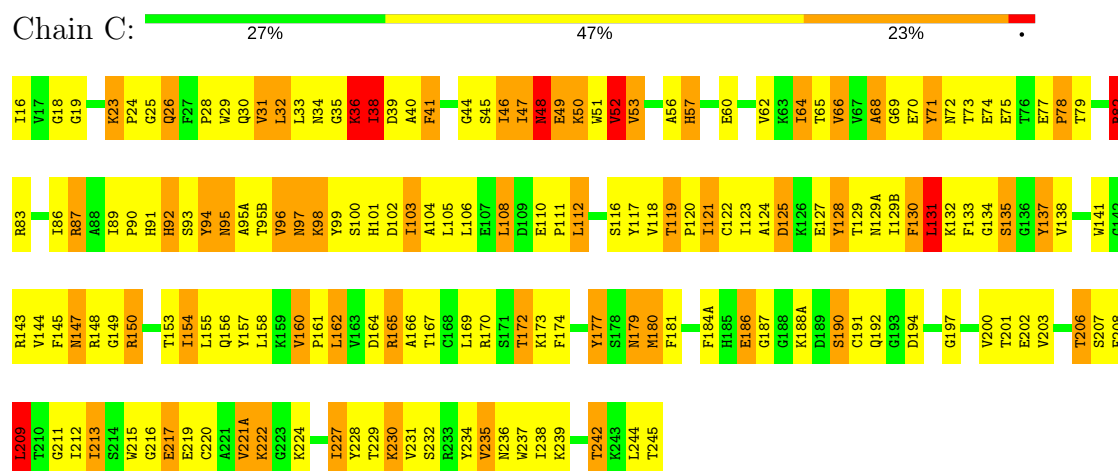
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	F	N	O	0	0
			37	25	4	7	1		

3 Residue-property plots

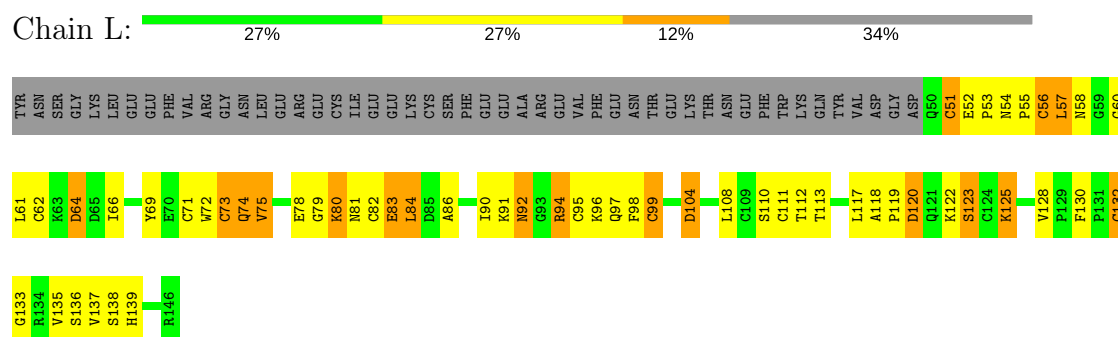
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Coagulation Factor IXa



• Molecule 2: Coagulation Factor IX, light chain



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.00Å 129.00Å 71.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2595	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
187

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	C	0.67	1/1877 (0.1%)	0.94	9/2547 (0.4%)
2	L	0.88	5/739 (0.7%)	1.09	9/999 (0.9%)
All	All	0.74	6/2616 (0.2%)	0.99	18/3546 (0.5%)

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	C	0	7
2	L	0	3
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	56	CYS	CB-SG	-6.57	1.71	1.82
2	L	95	CYS	CB-SG	-6.27	1.71	1.82
2	L	128	VAL	C-N	-5.59	1.23	1.34
2	L	62	CYS	CB-SG	5.54	1.91	1.82
1	C	119	THR	C-N	-5.19	1.24	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	71	CYS	CA-CB-SG	-11.43	93.42	114.00
2	L	75	VAL	CG1-CB-CG2	-9.14	96.27	110.90
1	C	147	ASN	CA-CB-CG	-8.32	95.10	113.40
1	C	66	VAL	CG1-CB-CG2	-8.29	97.63	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	51	CYS	CA-CB-SG	-7.65	100.22	114.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	128	TYR	Sidechain
1	C	130	PHE	Sidechain
1	C	36	LYS	Mainchain
1	C	71	TYR	Sidechain
1	C	82	ARG	Mainchain

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	C	1833	0	1802	172	0
2	L	725	0	692	33	0
3	C	37	0	16	3	0
All	All	2595	0	2510	200	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 41.

The worst 5 of 200 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)
1:C:122:CYS:SG	2:L:132:CYS:HB2	1.89	1.11
1:C:33:LEU:HD21	1:C:106:LEU:HD11	1.40	1.00
2:L:51:CYS:SG	2:L:64:ASP:HB3	2.02	0.99
1:C:19:GLY:HA2	1:C:158:LEU:HD13	1.56	0.88
1:C:187:GLY:HA3	1:C:222:LYS:HA	1.57	0.86

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	C	233/235 (99%)	179 (77%)	35 (15%)	19 (8%)	1	2
2	L	95/146 (65%)	70 (74%)	16 (17%)	9 (10%)	1	1
All	All	328/381 (86%)	249 (76%)	51 (16%)	28 (8%)	1	2

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	36	LYS
1	C	38	ILE
1	C	68	ALA
1	C	217	GLU
2	L	66	ILE

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	C	198/198 (100%)	147 (74%)	51 (26%)	0	2
2	L	85/130 (65%)	69 (81%)	16 (19%)	2	5
All	All	283/328 (86%)	216 (76%)	67 (24%)	1	2

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	157	TYR

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Mol	Chain	Res	Type
1	C	180	MET
2	L	120	ASP
1	C	162	LEU
1	C	169	LEU

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

Mol	Chain	Res	Type
1	C	91	HIS
1	C	156	GLN
1	C	179	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](#)

1 ligand is 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	$\# Z > 2$
3	187	C	298	-	39,41,41	2.41	15 (38%)	48,61,61	2.36	17 (35%)

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
3	187	C	298	-	-	0/23/26/26	0/5/5/5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	298	187	C16-N7	-8.40	1.33	1.44
3	C	298	187	C8-N5	-2.73	1.28	1.35
3	C	298	187	N6-N1	-2.36	1.35	1.39
3	C	298	187	C13-C8	-2.30	1.36	1.50
3	C	298	187	F2-C11	-2.11	1.25	1.32

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	298	187	C3-C4-C5	-6.12	115.48	121.55
3	C	298	187	F2-C11-C10	-3.94	105.81	112.46
3	C	298	187	C14-C44-C7	-3.76	119.67	123.44
3	C	298	187	C15-N7-C16	-3.65	119.04	125.23
3	C	298	187	C12-C10-N6	-3.54	106.35	111.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	298	187	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.