



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:37 PM GMT

PDB ID : 1C5M  
Title : STRUCTURAL BASIS FOR SELECTIVITY OF A SMALL MOLECULE,  
S1-BINDING, SUB-MICROMOLAR INHIBITOR OF UROKINASE TYPE  
PLASMINOGEN ACTIVATOR  
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Deposited on : 1999-12-22  
Resolution : 1.95 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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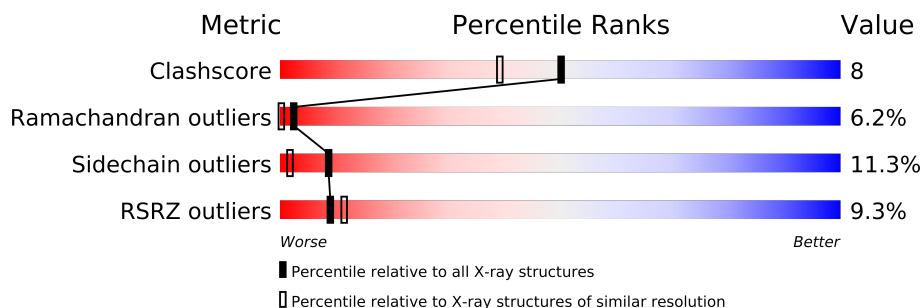
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.95 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	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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	D	255	
2	F	96	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5896 atoms, of which 3142 are hydrogens 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 PROTEIN (COAGULATION FACTOR X).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	241	Total	C	H	N	O	S	68	1	0
			3786	1201	1879	335	357	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	257	VAL	-	INSERTION	UNP P00742

- Molecule 2 is a protein called PROTEIN (COAGULATION FACTOR X).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	52	Total	C	H	N	O	S	26	1	0
			748	235	355	70	81	7			

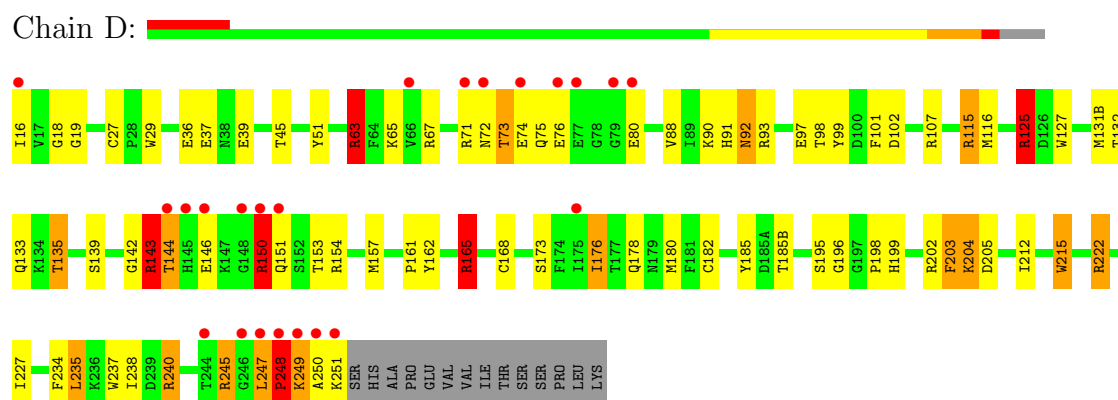
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	354	Total	H	O	0	9
			1062	708	354		
3	F	100	Total	H	O	0	1
			300	200	100		

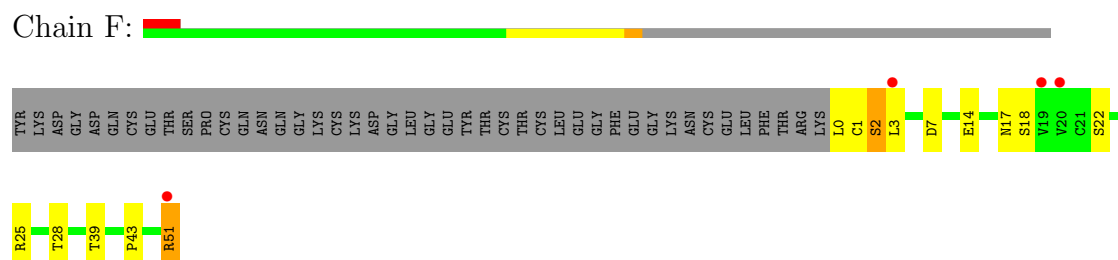
### 3 Residue-property plots

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: PROTEIN (COAGULATION FACTOR X)



#### • Molecule 2: PROTEIN (COAGULATION FACTOR X)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.82Å 81.82Å 108.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.50 – 1.95 33.69 – 1.64	Depositor EDS
% Data completeness (in resolution range)	60.4 (7.50-1.95) 41.6 (33.69-1.64)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 1.64Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.218 , 0.307 0.280 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 62.0	EDS
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 21642 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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

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	D	1.42	7/1950 (0.4%)	1.68	38/2625 (1.4%)
2	F	1.36	0/404	1.52	1/545 (0.2%)
All	All	1.41	7/2354 (0.3%)	1.65	39/3170 (1.2%)

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	D	0	14
2	F	0	2
All	All	0	16

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	196	GLY	C-N	-6.38	1.21	1.33
1	D	76	GLU	CD-OE2	6.20	1.32	1.25
1	D	76	GLU	CG-CD	5.72	1.60	1.51
1	D	76	GLU	CD-OE1	-5.43	1.19	1.25
1	D	237	TRP	CG-CD2	-5.39	1.34	1.43

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	GLU	OE1-CD-OE2	17.68	144.52	123.30
1	D	215	TRP	CD1-NE1-CE2	10.29	118.27	109.00
1	D	127	TRP	CD1-NE1-CE2	9.72	117.75	109.00
1	D	237	TRP	CD1-NE1-CE2	9.27	117.34	109.00
1	D	115	ARG	NE-CZ-NH2	-8.99	115.81	120.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	115	ARG	Sidechain
1	D	125	ARG	Sidechain
1	D	63	ARG	Sidechain
1	D	67	ARG	Sidechain
1	D	93	ARG	Sidechain

## 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	D	1907	1879	0	28	1
2	F	393	355	0	0	3
3	D	354	708	0	0	10
3	F	100	200	0	0	5
All	All	2754	3142	0	28	11

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 8.

The worst 5 of 28 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:131(B):MET:HE2	1:D:162:TYR:CE1	2.40	0.57
1:D:215:TRP:CE2	1:D:227:ILE:HG12	2.39	0.56
1:D:16:ILE:N	1:D:142:GLY:O	2.39	0.56
1:D:92:ASN:HD21	1:D:92:ASN:N	2.04	0.55
1:D:90:LYS:O	1:D:248:PRO:HA	2.11	0.50

The worst 5 of 11 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	Distance(Å)	Clash(Å)
3:F:119[C]:HOH:O	3:F:119[C]:HOH:O[5.675]	0.42	1.78
3:D:482:HOH:O	3:F:67:HOH:O[5.675]	1.04	1.16
3:D:375:HOH:O	3:F:140:HOH:O[2.665]	1.19	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:18:SER:OG	3:D:514:HOH:O[5.675]	1.53	0.67
3:D:302:HOH:O	3:D:500:HOH:O[4.566]	1.57	0.63

## 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	D	240/255 (94%)	202 (84%)	25 (10%)	13 (5%)	3	0
2	F	51/96 (53%)	38 (74%)	8 (16%)	5 (10%)	1	0
All	All	291/351 (83%)	240 (82%)	33 (11%)	18 (6%)	2	0

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	36	GLU
1	D	125	ARG
2	F	7	ASP
1	D	18	GLY
1	D	73	THR

### 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	D	205/217 (94%)	182 (89%)	23 (11%)	9	2
2	F	45/82 (55%)	39 (87%)	6 (13%)	6	1
All	All	250/299 (84%)	221 (88%)	29 (12%)	9	1

5 of 29 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	D	144	THR
1	D	173	SER
2	F	28	THR
1	D	150	ARG
1	D	185(B)	THR

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

Mol	Chain	Res	Type
1	D	30	GLN
1	D	38	ASN
1	D	92	ASN

### 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 ⓘ

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

### 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	D	239/255 (93%)	0.21	23 (9%)	8 10	5, 31, 69, 78	29 (12%)
2	F	52/96 (54%)	0.01	4 (7%)	13 17	5, 27, 66, 84	11 (21%)
All	All	291/351 (82%)	0.18	27 (9%)	9 11	5, 30, 69, 84	40 (13%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	GLU	9.5
1	D	151	GLN	8.6
2	F	51	ARG	7.8
1	D	76	GLU	6.8
1	D	150	ARG	6.7

### 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

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.