



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:58 PM BST

PDB ID : 5F8Z  
Title : The crystal structure of human Plasma Kallikrein in complex with its peptide inhibitor pkalin-1  
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Deposited on : 2015-12-09  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

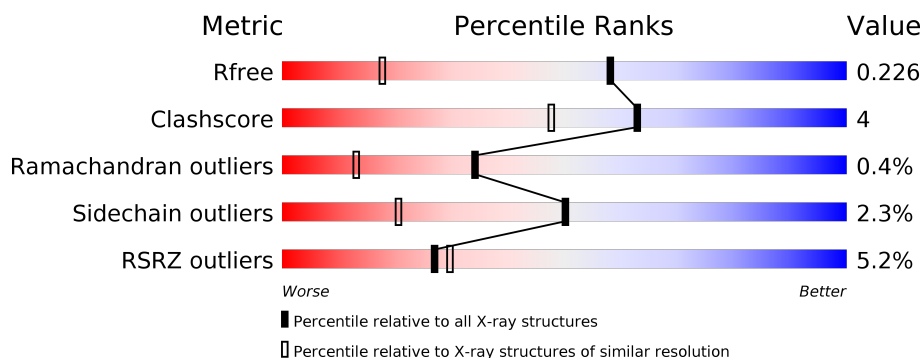
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	239	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div></div> </div> </div>
2	B	10	<div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2207 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 Plasma kallikrein LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	1891	1201	326	353	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	SER	CYS	engineered mutation	UNP P03952

- Molecule 2 is a protein called CYS-PRO-ALA-ARG-PHE-M70-ALA-LEU-PHE-CYS.

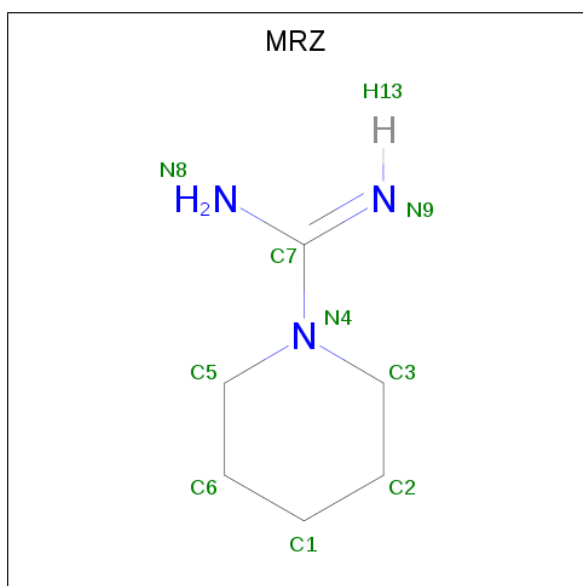
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	10	81	53	14	11	3	0	1	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is piperidine-1-carboximidamide (three-letter code: MRZ) (formula: C<sub>6</sub>H<sub>13</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N 9 6 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	197	Total O 197 197	0	0
5	B	4	Total O 4 4	0	0



● Molecule 1: Plasma kallikrein LIGHT CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.28 Å 90.28 Å 57.62 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.50 32.35 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-1.50) 99.1 (32.35-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.50 Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.179 , 0.217 0.185 , 0.226	Depositor DCC
$R_{free}$ test set	2132 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MRZ

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	0.76	4/1938 (0.2%)	0.77	2/2628 (0.1%)
2	B	0.52	0/82	0.77	0/108
All	All	0.75	4/2020 (0.2%)	0.77	2/2736 (0.1%)

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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186(C)	LYS	C-N	8.90	1.54	1.34
1	A	148	GLY	C-N	6.31	1.48	1.34
1	A	60(C)	PRO	C-N	-5.54	1.21	1.34
1	A	146	GLU	CD-OE2	-5.49	1.19	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	THR	C-N-CA	6.82	138.76	121.70
1	A	143	PHE	CB-CG-CD1	5.12	124.38	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	THR	Peptide

## 5.2 Too-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 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	A	1891	0	1849	17	0
2	B	81	0	78	0	0
3	A	25	0	0	2	0
4	B	9	0	11	0	0
5	A	197	0	0	0	0
5	B	4	0	0	0	0
All	All	2207	0	1938	17	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 4.

All (17) 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:A:69:GLY:HA3	3:A:303:SO4:O2	1.87	0.74
1:A:131:THR:O	1:A:132:ILE:HG13	1.99	0.63
1:A:129:THR:O	1:A:132:ILE:HD11	1.98	0.62
1:A:130:SER:HA	1:A:131:THR:C	2.26	0.56
1:A:126:LYS:HD2	1:A:236:ASP:OD1	2.05	0.56
1:A:71:LEU:HB2	3:A:302:SO4:O3	2.06	0.56
1:A:35:VAL:HB	1:A:65(C):VAL:HG22	1.89	0.55
1:A:37:LEU:CD1	1:A:65(C):VAL:HG21	2.37	0.55
1:A:130:SER:HA	1:A:131:THR:O	2.10	0.51
1:A:36:LYS:O	1:A:65(C):VAL:HG23	2.11	0.50
1:A:114:TYR:CE1	1:A:120:PRO:HD3	2.47	0.50
1:A:128:ASP:OD2	1:A:129:THR:N	2.45	0.49
1:A:37:LEU:HD12	1:A:65(C):VAL:HG21	1.95	0.48
1:A:37:LEU:HD12	1:A:65(C):VAL:CG2	2.44	0.47
1:A:203:HIS:CE1	1:A:204:ASN:OD1	2.70	0.45
1:A:37:LEU:HD11	1:A:65(C):VAL:HG21	2.00	0.44
1:A:130:SER:CA	1:A:131:THR:O	2.69	0.40



There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	237/239 (99%)	230 (97%)	6 (2%)	1 (0%)	34	13
2	B	8/10 (80%)	8 (100%)	0	0	100	100
All	All	245/249 (98%)	238 (97%)	6 (2%)	1 (0%)	34	13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ILE

### 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	A	206/206 (100%)	201 (98%)	5 (2%)	49	19
2	B	8/7 (114%)	8 (100%)	0	100	100
All	All	214/213 (100%)	209 (98%)	5 (2%)	50	20

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	129	THR

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Mol	Chain	Res	Type
1	A	131	THR
1	A	173	GLN
1	A	208(B)	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38(B)	GLN
1	A	203	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 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	$\# Z  > 2$
3	SO4	A	303	-	4,4,4	0.16	0	6,6,6	0.78	0
3	SO4	A	304	-	4,4,4	0.28	0	6,6,6	0.47	0
3	SO4	A	301	-	4,4,4	0.35	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MRZ	B	100	2	9,9,9	1.12	1 (11%)	10,11,11	1.28	1 (10%)
3	SO4	A	302	-	4,4,4	0.58	0	6,6,6	0.54	0
3	SO4	A	305	-	4,4,4	0.35	0	6,6,6	0.13	0

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	MRZ	B	100	2	-	0/4/12/12	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	100	MRZ	C7-N8	-2.67	1.27	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	100	MRZ	N8-C7-N9	-2.07	113.98	120.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	SO4	1	0
3	A	302	SO4	1	0

## 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](#)

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	239/239 (100%)	0.35	13 (5%) 25 28	11, 16, 31, 52	21 (8%)
2	B	10/10 (100%)	0.47	0 100 100	16, 22, 27, 28	0
All	All	249/249 (100%)	0.36	13 (5%) 27 30	11, 17, 30, 52	21 (8%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	GLY	24.0
1	A	132	ILE	7.4
1	A	126	LYS	6.2
1	A	130	SER	5.9
1	A	128	ASP	5.3
1	A	129	THR	5.2
1	A	131	THR	4.4
1	A	125	SER	3.9
1	A	245	SER	3.9
1	A	173	GLN	3.1
1	A	222	ARG	2.6
1	A	244	SER	2.3
1	A	246	ASP	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	305	5/5	0.66	0.24	79,82,89,96	0
3	SO4	A	304	5/5	0.86	0.20	46,54,56,61	0
3	SO4	A	302	5/5	0.88	0.22	29,32,41,42	0
3	SO4	A	303	5/5	0.95	0.20	27,29,42,42	0
4	MRZ	B	100	9/9	0.95	0.07	15,15,16,18	0
3	SO4	A	301	5/5	0.99	0.08	24,25,27,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.