

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 22, 2020 – 12:25 pm BST

PDB ID	:	4KEL
$\operatorname{Title}$	:	Atomic resolution crystal structure of Kallikrein-Related Peptidase 4 com-
		plexed with a modified SFTI inhibitor $FCQR(N)$
Authors	:	Ilyichova, O.V.; Swedberg, J.E.; de Veer, S.J.; Sit, K.C.; Harris, J.M.; Buckle,
		A.M.
Deposited on		
Resolution	:	1.15 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

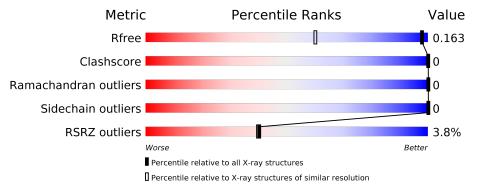
Percentile statistics : 20191225.v01 (using entries in the PDB archive Refmac : 5.8.0158 CCP4 : 7.0.044 (Gargrove) Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996) Validation Pipeline (wwPDB-VP) : 2.11	OB archive December 25th 2019)
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# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.15 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1492(1.18-1.10)
Clashscore	141614	1537(1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)
RSRZ outliers	127900	1464 (1.18-1.10)

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 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 <=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	А	223	3%
2	В	14	14%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2084 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 Kallikrein-4.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	223	Total 1766	C 1103	N 303	O 342	S 18	0	17	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	186A	GLN	HIS	SEE REMARK 999	UNP Q9Y5K2

• Molecule 2 is a protein called Trypsin inhibitor 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	14	Total 109	C 71	N 19	0 17	S 2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	2	PHE	ARG	ENGINEERED MUTATION	UNP Q4GWU5
В	4	GLN	THR	ENGINEERED MUTATION	UNP Q4GWU5
В	5	ARG	LYS	ENGINEERED MUTATION	UNP Q4GWU5
В	14	ASN	ASP	ENGINEERED MUTATION	UNP Q4GWU5

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	201	Total         O           201         201	0	0
3	В	8	Total O 8 8	0	0



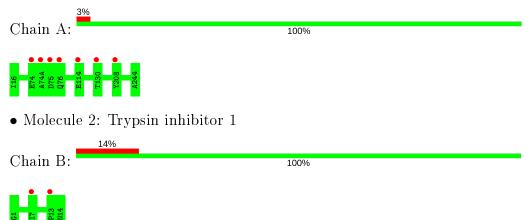
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# 3 Residue-property plots (i)

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.

• Molecule 1: Kallikrein-4





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	39.84Å $63.33$ Å $41.19$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $115.58^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	37.15 - 1.15	Depositor
Resolution (A)	37.15 - 1.15	EDS
% Data completeness	98.7 (37.15 - 1.15)	Depositor
(in resolution range)	98.7 (37.15 - 1.15)	EDS
R <sub>merge</sub>	0.08	Depositor
$R_{sym}$	0.08	Depositor
$< I/\sigma(I) > 1$	$4.25 (at 1.15 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
$R, R_{free}$	0.137 , $0.163$	Depositor
n, n <i>free</i>	0.137 , $0.163$	DCC
$R_{free}$ test set	3300 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	8.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , $44.0$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2084	wwPDB-VP
Average B, all atoms $(Å^2)$	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.34% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

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	А	0.31	0/1803	0.56	0/2453
2	В	0.36	0/113	0.61	0/153
All	All	0.31	0/1916	0.56	0/2606

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	А	1766	0	1675	0	0
2	В	109	0	104	0	0
3	А	201	0	0	0	1
3	В	8	0	0	0	0
All	All	2084	0	1779	0	1

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 0.

There are no clashes within the asymmetric unit.

All (1) 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	${f Interatomic} \ {f distance} \ ({ m \AA})$	Clash overlap (Å)
3:A:367:HOH:O	3:A:467:HOH:O[1_656]	2.12	0.08

### 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	Perce	entiles
1	А	238/223~(107%)	234~(98%)	4 (2%)	0	100	100
2	В	12/14~(86%)	$11 \ (92\%)$	1 (8%)	0	100	100
All	All	250/237~(106%)	245~(98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	А	195/189~(103%)	195~(100%)	0	100 100	
2	В	13/13~(100%)	13~(100%)	0	100 100	
All	All	208/202~(103%)	208~(100%)	0	100 100	

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



#### 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)

There are no ligands in this entry.

### 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 (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 $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	223/223~(100%)	0.38	7 (3%) 49 48	5, 10, 20, 39	4 (1%)
2	В	14/14~(100%)	0.88	2 (14%) 2 4	9, 14, 24, 26	0
All	All	237/237~(100%)	0.41	9 (3%) 40 40	5, 10, 21, 39	4 (1%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	75	ASP	4.8
1	А	76	GLN	4.6
2	В	13	PRO	3.8
1	А	74(A)	ALA	3.7
2	В	7	ILE	2.9

## 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 carbohydrates in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.

