

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

Oct 26, 2023 – 05:07 PM EDT

PDB ID : 3I2A

Title: Crystal structure of a chimeric trypsin inhibitor protein STI(L)-WCI(S)

Authors : Sen, U.; Khamrui, S.

Deposited on : 2009-06-29

Resolution : 2.30 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \end{array}$ 

EDS: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

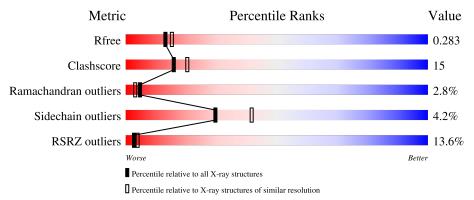
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.30 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of 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	A	187	71%	23%	<del>.</del> .		
1	В	187	66%	28%			



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2970 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 Chymotrypsin inhibitor 3.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	180	Total	С	N	О	S	0	0	0
1	11	100	1408	892	248	263	5	0	U	U
1	D	180	Total	С	N	Ο	S	0	0	0
1	Б	100	1399	887	246	261	5	0	U	U

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P10822
A	1	SER	-	expression tag	UNP P10822
A	2	HIS	-	expression tag	UNP P10822
A	3	MET	-	expression tag	UNP P10822
A	66	PRO	GLN	engineered mutation	UNP P10822
A	67	TYR	PHE	engineered mutation	UNP P10822
A	68	ARG	LEU	engineered mutation	UNP P10822
A	69	ILE	SER	engineered mutation	UNP P10822
A	70	ARG	LEU	engineered mutation	UNP P10822
В	200	GLY	-	expression tag	UNP P10822
В	201	SER	-	expression tag	UNP P10822
В	202	HIS	-	expression tag	UNP P10822
В	203	MET	-	expression tag	UNP P10822
В	266	PRO	GLN	engineered mutation	UNP P10822
В	267	TYR	PHE	engineered mutation	UNP P10822
В	268	ARG	LEU	engineered mutation	UNP P10822
В	269	ILE	SER	engineered mutation	UNP P10822
В	270	ARG	LEU	engineered mutation	UNP P10822

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Cl 1 1	0	0

#### • Molecule 3 is water.

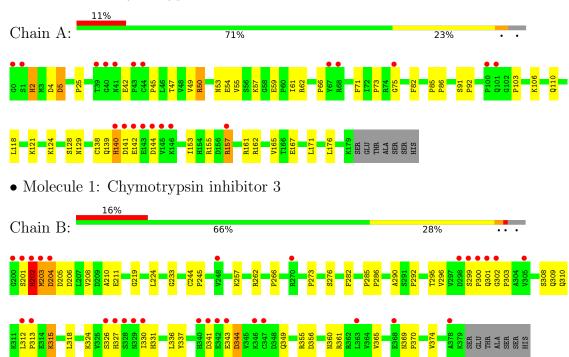
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	81	Total O 81 81	0	0
3	В	80	Total O 80 80	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Chymotrypsin inhibitor 3





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	I 4	Depositor	
Cell constants	141.38Å 141.38Å 46.72Å	Donositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	19.96 - 2.30	Depositor	
Resolution (A)	19.96 - 2.25	EDS	
% Data completeness	96.7 (19.96-2.30)	Depositor	
(in resolution range)	96.1 (19.96-2.25)	EDS	
$R_{merge}$	0.04	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	3.21 (at 2.26Å)	Xtriage	
Refinement program	CNS 1.2	Depositor	
$R, R_{free}$	0.234 , $0.289$	Depositor	
it, it <sub>free</sub>	0.229 , $0.283$	DCC	
$R_{free}$ test set	1093  reflections  (5.10%)	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage	
Anisotropy	0.140	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32, 48.5	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.51, < L^2> = 0.34$	Xtriage	
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage	
$F_o, F_c$ correlation	0.94	EDS	
Total number of atoms	2970	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  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)

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

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		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.35	0/1444	0.71	0/1966	
1	В	0.35	0/1434	0.76	1/1953 (0.1%)	
All	All	0.35	0/2878	0.73	1/3919 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	В	206	ASP	N-CA-C	-5.72	95.56	111.00

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	A	1408	0	1382	34	0
1	В	1399	0	1370	47	0
2	A	1	0	0	1	0
2	В	1	0	0	0	0
3	A	81	0	0	3	0
3	В	80	0	0	6	0
All	All	2970	0	2752	81	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 15.

The worst 5 of 81 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\mbox{\normalfont\AA}) \end{aligned}$
1:B:203:MET:O	1:B:205:ASP:N	1.90	1.04
1:A:157:ARG:H	1:A:157:ARG:HD2	1.23	1.00
1:B:201:SER:O	1:B:202:HIS:HB2	1.66	0.93
1:B:303:PRO:HG2	1:B:365:VAL:HB	1.51	0.92
1:B:295:THR:HG21	1:B:312:LEU:HG	1.57	0.86

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	178/187 (95%)	159 (89%)	15 (8%)	4 (2%)	6 5
1	В	178/187 (95%)	162 (91%)	10 (6%)	6 (3%)	3 2
All	All	356/374~(95%)	321 (90%)	25 (7%)	10 (3%)	5 3

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	В	202	HIS
1	В	203	MET
1	В	204	ASP
1	В	326	SER



#### 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	Percei	ntiles
1	A	155/163 (95%)	145 (94%)	10 (6%)	17	23
1	В	153/163 (94%)	150 (98%)	3 (2%)	55	72
All	All	308/326 (94%)	295 (96%)	13 (4%)	30	42

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	ARG
1	A	157	ARG
1	В	344	ASP
1	В	202	HIS
1	В	315	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	В	301	GLN
1	В	358	ASN
1	A	129	ASN
1	A	110	GLN

#### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	180/187 (96%)	0.68	20 (11%) 5 7	16, 35, 101, 154	0
1	В	180/187 (96%)	0.88	29 (16%) 1 2	21, 41, 116, 146	0
All	All	360/374~(96%)	0.78	49 (13%) 3 4	16, 39, 111, 154	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	A	142	GLU	12.1
1	В	202	HIS	11.3
1	В	201	SER	10.2
1	A	140	HIS	10.0
1	В	300	PRO	9.0

## 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
2	CL	A	402	1/1	0.96	0.17	36,36,36,36	0
2	CL	В	401	1/1	0.97	0.08	32,32,32,32	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

