



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:32 PM GMT

PDB ID : 1BA7  
Title : SOYBEAN TRYPSIN INHIBITOR  
Authors : De Meester, P.; Brick, P.; Lloyd, L.F.; Blow, D.M.; Onesti, S.  
Deposited on : 1998-04-22  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

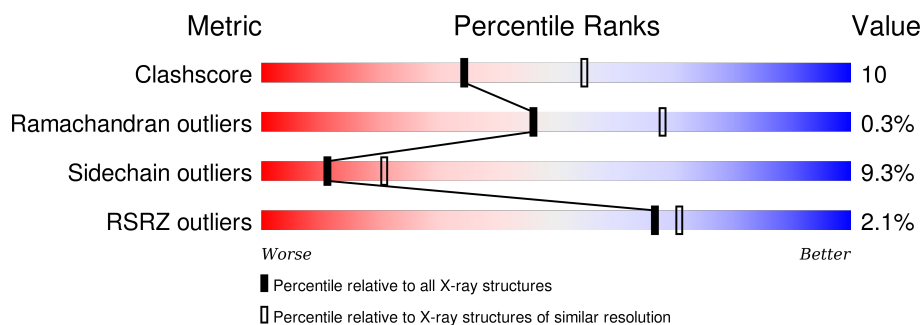
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	181	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	181	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>•</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2653 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 TRYPSIN INHIBITOR (KUNITZ).

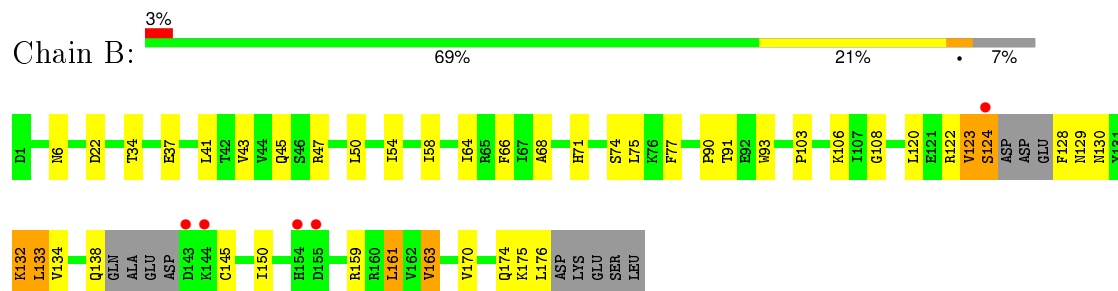
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1238	794	210	228	6			
1	B	169	Total	C	N	O	S	0	0	0
			1258	806	213	233	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	93	Total	O	0	0
			93	93		



- Molecule 1: TRYPSIN INHIBITOR (KUNITZ)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.11Å 53.87Å 58.20Å 71.75° 90.00° 82.98°	Depositor
Resolution (Å)	15.00 – 2.50 14.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (15.00-2.50) 85.6 (14.91-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.03 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.160 , 0.223 0.168 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 71.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 16384 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	A	0.41	1/1263 (0.1%)	0.64	0/1716
1	B	0.40	0/1283	0.66	0/1744
All	All	0.40	1/2546 (0.0%)	0.65	0/3460

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	1	0
1	B	1	0
All	All	2	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	GLU	CB-CG	-5.01	1.42	1.52

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	23	ILE	CB
1	B	23	ILE	CB

There are no planarity outliers.

## 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	1238	0	1196	22	0
1	B	1258	0	1206	28	0
2	A	64	0	0	1	0
2	B	93	0	0	2	0
All	All	2653	0	2402	49	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 10.

All (49) 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:B:41:LEU:O	1:B:106:LYS:HG3	1.90	0.71
1:B:45:GLN:NE2	1:B:159:ARG:HE	1.88	0.71
1:B:123:VAL:O	1:B:124:SER:HB2	1.93	0.68
1:A:130:ASN:HD22	1:A:172:GLN:HG2	1.60	0.66
1:B:45:GLN:HE21	1:B:159:ARG:HE	1.44	0.66
1:B:103:PRO:HB2	1:B:163:VAL:CG1	2.26	0.65
1:B:6:ASN:HD21	1:B:174:GLN:HE21	1.41	0.64
1:A:103:PRO:HB2	1:A:163:VAL:HG13	1.79	0.64
1:A:56:THR:HG21	1:A:75:LEU:HD12	1.79	0.64
1:A:84:MET:H	1:B:174:GLN:HE22	1.45	0.63
1:A:147:ASP:HB3	1:A:168:PRO:HB3	1.81	0.61
1:A:49:GLU:HG3	1:A:50:LEU:HD22	1.84	0.58
1:A:134:VAL:HG13	1:A:145:CYS:HB3	1.86	0.57
1:A:130:ASN:ND2	1:A:172:GLN:HG2	2.19	0.57
1:B:130:ASN:HB3	1:B:170:VAL:CG1	2.35	0.56
1:A:18:TYR:CE2	1:A:176:LEU:HD13	2.42	0.55
1:B:43:VAL:HG12	1:B:161:LEU:HG	1.87	0.55
1:A:99:LEU:HD13	1:A:101:GLU:OE2	2.08	0.54
1:B:68:ALA:H	1:B:71:HIS:CD2	2.26	0.53
1:B:90:PRO:HD2	1:B:108:GLY:HA2	1.90	0.53
1:A:103:PRO:HB2	1:A:163:VAL:CG1	2.39	0.52
1:B:134:VAL:CG1	1:B:145:CYS:HB3	2.39	0.52
1:B:123:VAL:O	1:B:124:SER:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:PHE:HB2	1:B:91:THR:HB	1.92	0.52
1:A:135:PHE:O	1:A:145:CYS:HA	2.10	0.51
1:A:106:LYS:NZ	2:A:239:HOH:O	2.43	0.51
1:B:45:GLN:HE22	1:B:159:ARG:HH21	1.58	0.51
1:A:37:GLU:HG2	1:A:41:LEU:HD12	1.93	0.50
1:B:45:GLN:HG3	2:B:301:HOH:O	2.13	0.49
1:B:75:LEU:HD12	1:B:93:TRP:CE3	2.48	0.49
1:B:120:LEU:CD2	1:B:133:LEU:HD13	2.43	0.47
1:A:41:LEU:O	1:A:106:LYS:HG3	2.14	0.47
1:A:130:ASN:HB3	1:A:170:VAL:CG1	2.45	0.47
1:B:128:PHE:O	1:B:129:ASN:HB2	2.15	0.47
1:A:34:THR:O	1:A:37:GLU:HB2	2.15	0.47
1:A:21:SER:HB2	1:A:45:GLN:NE2	2.30	0.47
1:B:120:LEU:HD23	1:B:133:LEU:HD13	1.97	0.46
1:B:54:ILE:HD11	2:B:353:HOH:O	2.15	0.46
1:B:103:PRO:HB2	1:B:163:VAL:HG13	1.98	0.45
1:B:58:ILE:HG12	1:B:75:LEU:HD22	1.98	0.45
1:B:134:VAL:HG13	1:B:145:CYS:HB3	2.01	0.42
1:A:156:ASP:C	1:A:158:THR:H	2.23	0.42
1:B:150:ILE:HD13	1:B:161:LEU:HD22	2.01	0.42
1:A:77:PHE:HB2	1:A:91:THR:HB	2.03	0.41
1:A:99:LEU:HD22	1:A:100:PRO:HD2	2.03	0.41
1:B:123:VAL:HG23	1:B:132:LYS:HB3	2.02	0.41
1:A:111:LYS:C	1:A:113:ALA:H	2.24	0.41
1:B:34:THR:O	1:B:37:GLU:HB2	2.21	0.40
1:B:64:ILE:HD13	1:B:66:PHE:O	2.22	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	159/181 (88%)	150 (94%)	8 (5%)	1 (1%)	30	50
1	B	163/181 (90%)	156 (96%)	7 (4%)	0	100	100
All	All	322/362 (89%)	306 (95%)	15 (5%)	1 (0%)	46	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	GLU

### 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	A	128/157 (82%)	118 (92%)	10 (8%)	16	29
1	B	129/157 (82%)	115 (89%)	14 (11%)	8	15
All	All	257/314 (82%)	233 (91%)	24 (9%)	11	21

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	52	LYS
1	A	64	ILE
1	A	65	ARG
1	A	74	SER
1	A	92	GLU
1	A	134	VAL
1	A	163	VAL
1	A	175	LYS
1	A	176	LEU
1	B	22	ASP
1	B	47	ARG
1	B	50	LEU
1	B	74	SER
1	B	122	ARG

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Mol	Chain	Res	Type
1	B	123	VAL
1	B	124	SER
1	B	132	LYS
1	B	133	LEU
1	B	138	GLN
1	B	161	LEU
1	B	163	VAL
1	B	175	LYS
1	B	176	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	71	HIS
1	A	129	ASN
1	A	130	ASN
1	A	172	GLN
1	A	174	GLN
1	B	45	GLN
1	B	48	ASN
1	B	71	HIS
1	B	130	ASN
1	B	174	GLN

### 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 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 [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	165/181 (91%)	-0.58	2 (1%) 81 83	17, 33, 69, 95	0
1	B	169/181 (93%)	-0.64	5 (2%) 54 59	18, 31, 66, 94	0
All	All	334/362 (92%)	-0.61	7 (2%) 67 71	17, 32, 69, 95	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	SER	4.7
1	B	143	ASP	3.3
1	B	154	HIS	3.2
1	A	166	ASN	2.8
1	B	155	ASP	2.5
1	A	98	ASP	2.1
1	B	144	LYS	2.0

### 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 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.