



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2017 – 02:17 PM EST

PDB ID : 1BBS  
Title : X-RAY ANALYSES OF PEPTIDE INHIBITOR COMPLEXES DEFINE  
THE STRUCTURAL BASIS OF SPECIFICITY FOR HUMAN AND MOUSE  
RENINS  
Authors : Dhanaraj, V.; Blundell, T.L.  
Deposited on : unknown  
Resolution : 2.80 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](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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

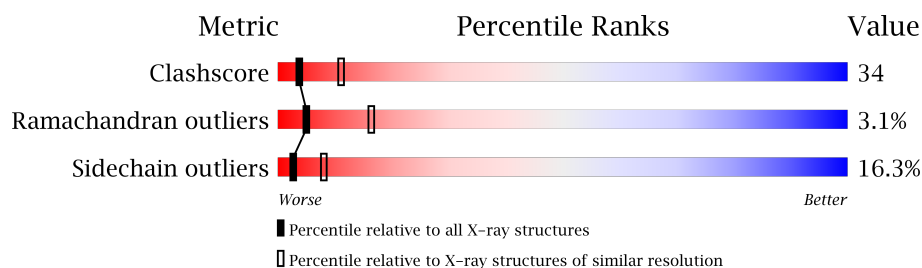
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	340	
1	B	340	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5018 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 RENIN.

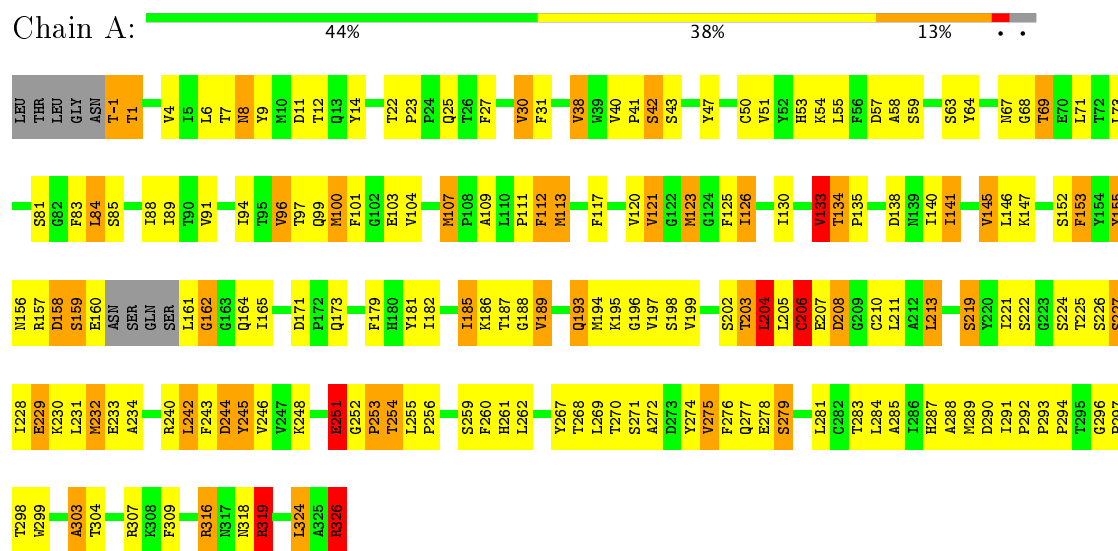
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2509	1609	398	488	14			
1	B	331	Total	C	N	O	S	0	0	0
			2509	1609	398	488	14			

### 3 Residue-property plots

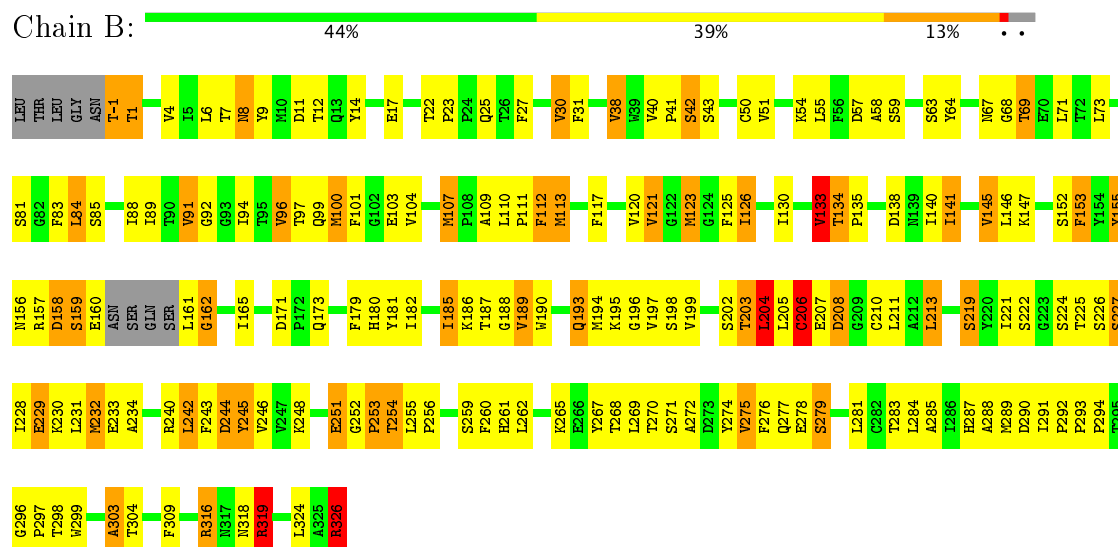
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: RENIN



#### • Molecule 1: RENIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.10Å 143.10Å 143.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 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	0.94	1/2568 (0.0%)	1.57	40/3493 (1.1%)
1	B	0.94	2/2568 (0.1%)	1.57	36/3493 (1.0%)
All	All	0.94	3/5136 (0.1%)	1.57	76/6986 (1.1%)

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	1	4
1	B	1	4
All	All	2	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	TYR	C-N	7.05	1.50	1.34
1	B	245	TYR	C-N	7.01	1.50	1.34
1	B	190	TRP	NE1-CE2	-5.00	1.31	1.37

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	ARG	NE-CZ-NH2	9.01	124.80	120.30
1	A	31	PHE	C-N-CA	8.96	144.09	121.70
1	B	31	PHE	C-N-CA	8.96	144.09	121.70
1	A	319	ARG	NE-CZ-NH2	8.95	124.77	120.30
1	B	96	VAL	CA-CB-CG2	8.72	123.98	110.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	303	ALA	CA
1	B	303	ALA	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLY	Mainchain
1	A	195	LYS	Mainchain
1	A	316	ARG	Sidechain
1	A	326	ARG	Sidechain
1	B	162	GLY	Mainchain

## 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	2509	0	2397	167	1
1	B	2509	0	2397	167	2
All	All	5018	0	4794	334	2

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 34.

The worst 5 of 334 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:196:GLY:HA2	1:B:206:CYS:CB	1.77	1.15
1:A:196:GLY:HA2	1:A:206:CYS:CB	1.77	1.15
1:B:196:GLY:CA	1:B:206:CYS:HB3	1.76	1.15
1:A:196:GLY:CA	1:A:206:CYS:HB3	1.76	1.13
1:B:199:VAL:HG21	1:B:204:LEU:HD21	1.28	1.08

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:CD2	1:B:254:THR:CG2[5_555]	1.86	0.34
1:A:270:THR:OG1	1:B:17:GLU:OE2[5_555]	1.93	0.27

### 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	327/340 (96%)	290 (89%)	27 (8%)	10 (3%)	5	16
1	B	327/340 (96%)	290 (89%)	27 (8%)	10 (3%)	5	16
All	All	654/680 (96%)	580 (89%)	54 (8%)	20 (3%)	5	16

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	206	CYS
1	B	158	ASP
1	B	206	CYS
1	A	242	LEU

#### 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	270/290 (93%)	226 (84%)	44 (16%)	3	8
1	B	270/290 (93%)	226 (84%)	44 (16%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	540/580 (93%)	452 (84%)	88 (16%)	<b>3</b> <b>8</b>

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	ARG
1	B	59	SER
1	B	277	GLN
1	A	318	ASN
1	B	-1	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	B	25	GLN
1	B	261	HIS
1	B	8	ASN
1	B	99	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 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.