



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1BBS / pdb_00001bbs
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 : 1992-05-21
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

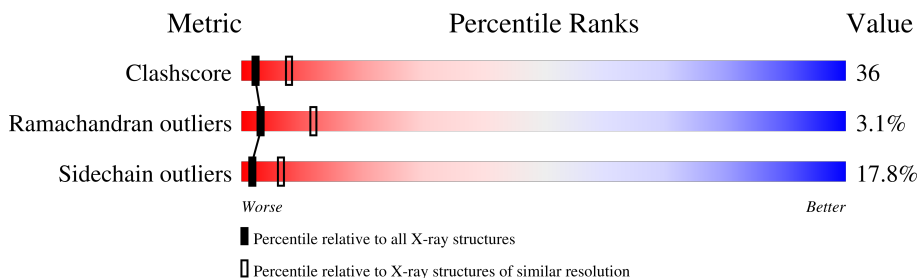
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	340	 34% 42% 17% . .
1	B	340	 33% 42% 18% . .

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
			Total	C	N	O	S			
1	A	331	2509	1609	398	488	14	0	0	0
1	B	331	2509	1609	398	488	14	0	0	0

T268	L269	T270	S271	A272	D273	Y274	Y276	F276	Q277	E278	S279	Y279A	K280	L281	C282	T283	L284	A285	T286	H287	A288	H289	D290	L291	P292	P293	P294	T295	G296	P297	T298	W299	A300	A303	T304	R307	Y310	R316	N317	N318	R319	I320	A323	L324	A325	R326
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4 Data and refinement statistics

Xtrriage (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, α , β , γ	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.	Xtrriage
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å ²)	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	1.33	26/2568 (1.0%)	2.15	123/3493 (3.5%)
1	B	1.33	26/2568 (1.0%)	2.15	124/3493 (3.5%)
All	All	1.33	52/5136 (1.0%)	2.15	247/6986 (3.5%)

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

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	TYR	C-N	12.76	1.50	1.33
1	B	245	TYR	C-N	12.69	1.50	1.33
1	B	204	LEU	C-N	9.12	1.45	1.33
1	A	204	LEU	C-N	9.10	1.45	1.33
1	B	206	CYS	CA-C	-8.82	1.41	1.52

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	PHE	CA-C-N	13.53	144.09	122.17
1	A	31	PHE	C-N-CA	13.53	144.09	122.17
1	B	31	PHE	CA-C-N	13.53	144.09	122.17
1	B	31	PHE	C-N-CA	13.53	144.09	122.17
1	B	162	GLY	O-C-N	-12.48	110.20	122.18

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 [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	2509	0	2398	175	1
1	B	2509	0	2398	176	2
All	All	5018	0	4796	351	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 36.

The worst 5 of 351 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:196:GLY:HA2	1:A:206:CYS:CB	1.77	1.15
1:B:196:GLY:HA2	1:B: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%)	3	12
1	B	327/340 (96%)	290 (89%)	27 (8%)	10 (3%)	3	12
All	All	654/680 (96%)	580 (89%)	54 (8%)	20 (3%)	3	12

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%)	222 (82%)	48 (18%)	2	6
1	B	270/290 (93%)	222 (82%)	48 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	540/580 (93%)	444 (82%)	96 (18%)	2 6

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	69	THR
1	B	164	GLN
1	B	84	LEU
1	B	134	THR
1	B	193	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	174	HIS
1	B	261	HIS
1	B	191	GLN
1	A	261	HIS
1	B	156	ASN

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 oligosaccharides 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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.