

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 04:06 PM EDT

PDB ID : 1CPJ

Title : CRYSTAL STRUCTURES OF RECOMBINANT RAT CATHEPSIN B

AND A CATHEPSIN B-INHIBITOR COMPLEX: IMPLICATIONS FOR

STRUCTURE-BASED INHIBITOR DESIGN

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Deposited on : 1995-07-17

Resolution : 2.20 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:

MolProbity: 4.02b-467 Xtriage (Phenix): 1.13

EDS : 2.23.2

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

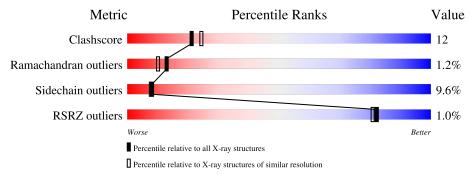
Validation Pipeline (wwPDB-VP) : 2.23.2

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 2.20 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	Similar resolution
Wiedlie	(# Entries)	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	260	66%	26%	5% •		
1	В	260	65%	29%			



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4058 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 CATHEPSIN B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	253	Total 1934	C 1210	N 332	O 374	S 18	17	0	0
1	В	253	Total 1934	C 1210	N 332	O 374	S 18	20	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	ALA	SER	engineered mutation	UNP P00787
A	223	ALA	VAL	cloning artifact	UNP P00787
В	115	ALA	SER	engineered mutation	UNP P00787
В	223	ALA	VAL	cloning artifact	UNP P00787

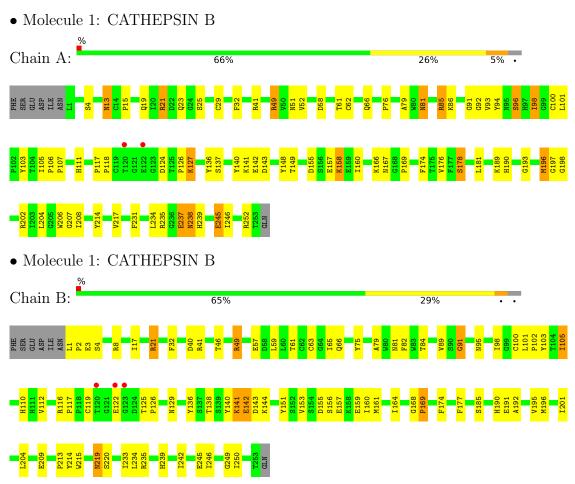
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	96	Total O 96 96	0	0
2	В	94	Total O 94 94	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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	47.09Å 90.25Å 62.10Å	Depositor
a, b, c, α , β , γ	90.00° 97.29° 90.00°	Depositor
Resolution (Å)	8.00 - 2.20	Depositor
Resolution (A)	7.99 - 2.20	EDS
% Data completeness	93.9 (8.00-2.20)	Depositor
(in resolution range)	91.1 (7.99-2.20)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
It, It free	0.173 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.23, 82.1	EDS
L-test for twinning ¹	$ < L >=0.33, < L^2>=0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4058	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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).

Mal	Chain	Bo	nd lengths	Bo	ond angles
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.86	3/1989 (0.2%)	0.81	3/2701 (0.1%)
1	В	0.65	1/1989 (0.1%)	0.67	0/2701
All	All	0.76	4/3978 (0.1%)	0.74	3/5402 (0.1%)

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	В	0	4
All	All	0	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$Ideal(\AA)$
1	A	127	LYS	CB-CG	-26.36	0.81	1.52
1	В	122	GLU	CD-OE2	7.61	1.34	1.25
1	A	127	LYS	CD-CE	5.16	1.64	1.51
1	A	158	LYS	CD-CE	5.16	1.64	1.51

All (3) bond angle outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	127	LYS	CA-CB-CG	15.93	148.45	113.40
1	A	142	GLU	OE1-CD-OE2	-12.89	107.83	123.30
1	A	142	GLU	CG-CD-OE2	7.47	133.24	118.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	103	TYR	Sidechain
1	A	32	PHE	Sidechain
1	A	85	ARG	Sidechain
1	A	94	TYR	Sidechain
1	A	96	SER	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	1934	0	1783	39	0
1	В	1934	0	1783	50	0
2	A	96	0	0	6	0
2	В	94	0	0	3	0
All	All	4058	0	3566	89	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 12.

The worst 5 of 89 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:49:ARG:H	1:A:49:ARG:HD2	1.31	0.95
1:A:49:ARG:HD2	1:A:49:ARG:N	1.90	0.82
1:A:176:VAL:HG12	1:A:196:MET:HG3	1.61	0.81
1:A:4:SER:HB3	1:A:207:GLY:HA2	1.73	0.71
1:A:100:CYS:HB2	1:A:143:ASP:OD2	1.95	0.66

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	251/260 (96%)	211 (84%)	36 (14%)	4 (2%)	9 7
1	В	251/260~(96%)	226 (90%)	23 (9%)	2 (1%)	19 19
All	All	502/520~(96%)	437 (87%)	59 (12%)	6 (1%)	13 10

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
1	A	238	ASN
1	В	155	ASP
1	A	178	SER
1	В	169	PRO

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	204/211 (97%)	184 (90%)	20 (10%)	8 7
1	В	204/211 (97%)	185 (91%)	19 (9%)	9 8
All	All	408/422 (97%)	369 (90%)	39 (10%)	8 8

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	112	VAL
1	В	196	MET
1	В	129	ASN
1	В	174	PHE
1	В	209	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:



Mol	Chain	Res	Type
1	В	45	HIS
1	В	129	ASN
1	В	239	HIS
1	В	219	ASN
1	В	238	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 monosaccharides 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^{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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	253/260 (97%)	-0.26	2 (0%) 86 85	2, 18, 44, 75	4 (1%)
1	В	253/260 (97%)	-0.19	3 (1%) 79 77	2, 20, 44, 68	5 (1%)
All	All	506/520 (97%)	-0.22	5 (0%) 82 81	2, 19, 44, 75	9 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	THR	3.2
1	В	123	GLY	3.1
1	В	122	GLU	2.9
1	A	122	GLU	2.3
1	В	120	THR	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 monosaccharides 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.

