



# Full wwPDB X-ray Structure Validation Report i

Oct 23, 2021 – 08:30 AM EDT

PDB ID : 1PCI  
Title : PROCARICAIN  
Authors : Groves, M.R.; Taylor, M.A.J.; Scott, M.; Cummings, N.J.; Pickersgill, R.W.; Jenkins, J.A.  
Deposited on : 1996-06-28  
Resolution : 3.20 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  
<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 : 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

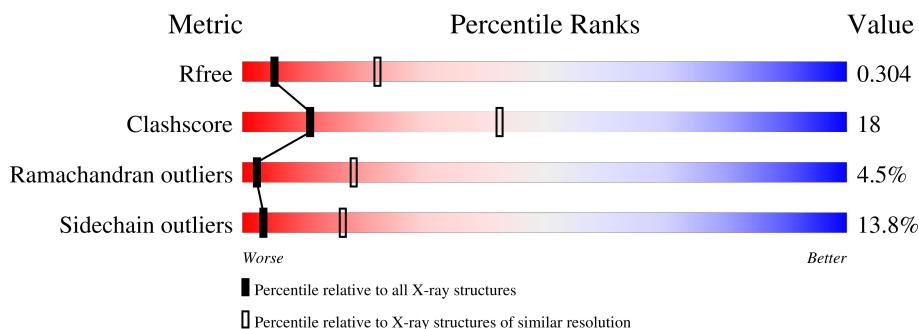
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

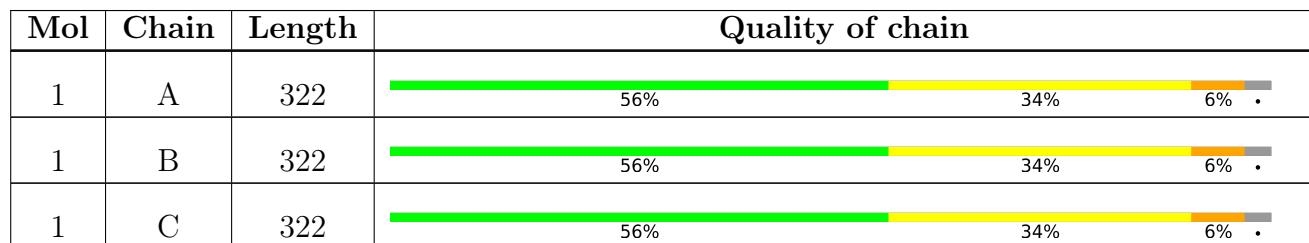
The reported resolution of this entry is 3.20 Å.

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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  $\geq 3$ , 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  $\leq 5\%$ .



## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7341 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.

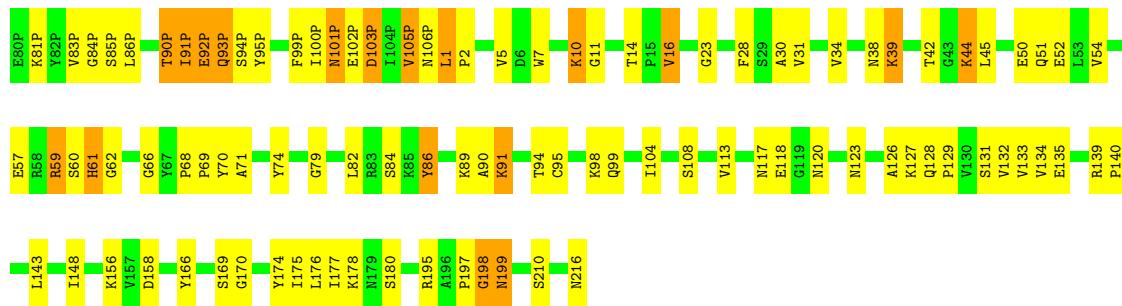
- Molecule 1 is a protein called PROCARICAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2447	1550	425	464	8			
1	B	311	Total	C	N	O	S	0	0	0
			2447	1550	425	464	8			
1	C	311	Total	C	N	O	S	0	0	0
			2447	1550	425	464	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ILE	THR	conflict	UNP P10056
A	159	GLY	HIS	engineered mutation	UNP P10056
B	104	ILE	THR	conflict	UNP P10056
B	159	GLY	HIS	engineered mutation	UNP P10056
C	104	ILE	THR	conflict	UNP P10056
C	159	GLY	HIS	engineered mutation	UNP P10056





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.00 Å    205.40 Å    192.20 Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	90.60 – 3.20 90.58 – 2.62	Depositor EDS
% Data completeness (in resolution range)	(Not available) (90.60-3.20) 96.3 (90.58-2.62)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.01 (at 2.62 Å)	Xtriage
Refinement program	X-PLOR	Depositor
$R$ , $R_{free}$	0.226 , 0.286 0.270 , 0.304	Depositor DCC
$R_{free}$ test set	1451 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.8	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.48$ , $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7341	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.















*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ASN:HB3	1:B:120:ASN:OD1	2.21	0.41
1:A:5:VAL:CG2	1:A:166:TYR:CE2	3.04	0.40
1:A:74:TYR:CD1	1:A:74:TYR:C	2.94	0.40
1:B:21(P):LEU:HD12	1:B:21(P):LEU:C	2.42	0.40
1:B:31(P):LYS:C	1:B:32(P):PHE:HD1	2.24	0.40
1:B:53(P):ILE:HD12	1:B:67(P):LEU:HD12	2.03	0.40
1:B:3:GLU:HB3	1:B:4:ASN:HD22	1.86	0.40
1:B:28:PHE:HA	1:B:50:GLU:HG2	2.02	0.40
1:C:31(P):LYS:HD3	1:C:31(P):LYS:HA	1.77	0.40
1:C:79(P):ASN:OD1	1:C:83(P):VAL:HG11	2.22	0.40
1:C:74:TYR:CD1	1:C:74:TYR:C	2.94	0.40
1:C:99:GLN:NE2	1:C:99:GLN:H	2.18	0.40
1:A:31(P):LYS:C	1:A:32(P):PHE:HD1	2.24	0.40
1:A:53(P):ILE:C	1:A:56(P):THR:HG22	2.41	0.40
1:C:20(P):GLN:O	1:C:23(P):ASN:HB2	2.21	0.40
1:C:21(P):LEU:HD12	1:C:21(P):LEU:C	2.42	0.40
1:A:79(P):ASN:OD1	1:A:83(P):VAL:HG11	2.22	0.40
1:A:117:ASN:HB3	1:A:120:ASN:OD1	2.20	0.40
1:B:20(P):GLN:O	1:B:23(P):ASN:HB2	2.21	0.40
1:B:91:LYS:HE2	1:B:91:LYS:HB2	1.37	0.40
1:C:51:GLN:HA	1:C:54:VAL:HG12	2.03	0.40
1:A:15(P):THR:CG2	1:C:41(P):TYR:HD1	2.33	0.40
1:C:5:VAL:CG2	1:C:166:TYR:CE2	3.04	0.40
1:C:10:LYS:H	1:C:10:LYS:HG2	1.56	0.40

All (1) 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:101(P):ASN:O	1:B:99:GLN:CA[8_566]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	309/322 (96%)	269 (87%)	26 (8%)	14 (4%)	2 18
1	B	309/322 (96%)	269 (87%)	26 (8%)	14 (4%)	2 18
1	C	309/322 (96%)	269 (87%)	26 (8%)	14 (4%)	2 18
All	All	927/966 (96%)	807 (87%)	78 (8%)	42 (4%)	2 18

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92(P)	GLU
1	A	100(P)	ILE
1	A	105(P)	VAL
1	B	92(P)	GLU
1	B	100(P)	ILE
1	B	105(P)	VAL
1	C	92(P)	GLU
1	C	100(P)	ILE
1	C	105(P)	VAL
1	A	103(P)	ASP
1	A	95	CYS
1	A	170	GLY
1	A	198	GLY
1	B	103(P)	ASP
1	B	95	CYS
1	B	170	GLY
1	B	198	GLY
1	C	103(P)	ASP
1	C	95	CYS
1	C	170	GLY
1	C	198	GLY
1	A	93(P)	GLN
1	A	101(P)	ASN
1	B	93(P)	GLN
1	B	101(P)	ASN
1	C	93(P)	GLN
1	C	101(P)	ASN
1	A	7	TRP
1	A	10	LYS
1	B	7	TRP
1	B	10	LYS
1	C	7	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	10	LYS
1	A	94(P)	SER
1	B	94(P)	SER
1	C	94(P)	SER
1	A	91(P)	ILE
1	A	2	PRO
1	B	91(P)	ILE
1	B	2	PRO
1	C	91(P)	ILE
1	C	2	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	261/271 (96%)	225 (86%)	36 (14%)	3   16
1	B	261/271 (96%)	225 (86%)	36 (14%)	3   16
1	C	261/271 (96%)	225 (86%)	36 (14%)	3   16
All	All	783/813 (96%)	675 (86%)	108 (14%)	3   16

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12(P)	LEU
1	A	24(P)	SER
1	A	27(P)	LEU
1	A	34(P)	GLU
1	A	40(P)	LEU
1	A	60(P)	ASN
1	A	61(P)	ASN
1	A	73(P)	LEU
1	A	81(P)	LYS
1	A	86(P)	LEU
1	A	90(P)	THR
1	A	92(P)	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	103(P)	ASP
1	A	14	THR
1	A	16	VAL
1	A	39	LYS
1	A	44	LYS
1	A	45	LEU
1	A	57	GLU
1	A	59	ARG
1	A	61	HIS
1	A	82	LEU
1	A	84	SER
1	A	86	TYR
1	A	91	LYS
1	A	94	THR
1	A	108	SER
1	A	127	LYS
1	A	131	SER
1	A	158	ASP
1	A	169	SER
1	A	176	LEU
1	A	180	SER
1	A	199	ASN
1	A	210	SER
1	A	216	ASN
1	B	12(P)	LEU
1	B	24(P)	SER
1	B	27(P)	LEU
1	B	34(P)	GLU
1	B	40(P)	LEU
1	B	60(P)	ASN
1	B	61(P)	ASN
1	B	73(P)	LEU
1	B	81(P)	LYS
1	B	86(P)	LEU
1	B	90(P)	THR
1	B	92(P)	GLU
1	B	103(P)	ASP
1	B	14	THR
1	B	16	VAL
1	B	39	LYS
1	B	44	LYS
1	B	45	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	57	GLU
1	B	59	ARG
1	B	61	HIS
1	B	82	LEU
1	B	84	SER
1	B	86	TYR
1	B	91	LYS
1	B	94	THR
1	B	108	SER
1	B	127	LYS
1	B	131	SER
1	B	158	ASP
1	B	169	SER
1	B	176	LEU
1	B	180	SER
1	B	199	ASN
1	B	210	SER
1	B	216	ASN
1	C	12(P)	LEU
1	C	24(P)	SER
1	C	27(P)	LEU
1	C	34(P)	GLU
1	C	40(P)	LEU
1	C	60(P)	ASN
1	C	61(P)	ASN
1	C	73(P)	LEU
1	C	81(P)	LYS
1	C	86(P)	LEU
1	C	90(P)	THR
1	C	92(P)	GLU
1	C	103(P)	ASP
1	C	14	THR
1	C	16	VAL
1	C	39	LYS
1	C	44	LYS
1	C	45	LEU
1	C	57	GLU
1	C	59	ARG
1	C	61	HIS
1	C	82	LEU
1	C	84	SER
1	C	86	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	91	LYS
1	C	94	THR
1	C	108	SER
1	C	127	LYS
1	C	131	SER
1	C	158	ASP
1	C	169	SER
1	C	176	LEU
1	C	180	SER
1	C	199	ASN
1	C	210	SER
1	C	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61(P)	ASN
1	A	4	ASN
1	A	38	ASN
1	A	99	GLN
1	A	116	ASN
1	A	123	ASN
1	A	128	GLN
1	A	199	ASN
1	B	61(P)	ASN
1	B	4	ASN
1	B	38	ASN
1	B	99	GLN
1	B	116	ASN
1	B	123	ASN
1	B	128	GLN
1	B	199	ASN
1	C	61(P)	ASN
1	C	4	ASN
1	C	38	ASN
1	C	99	GLN
1	C	116	ASN
1	C	123	ASN
1	C	128	GLN
1	C	199	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 [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.