

# Full wwPDB X-ray Structure Validation Report (i)

#### May 16, 2020 – 12:45 pm BST

PDB ID : 2ACT

Title : CRYSTALLOGRAPHIC REFINEMENT OF THE STRUCTURE OF AC-

TINIDIN AT 1.7 ANGSTROMS RESOLUTION BY FAST FOURIER

LEAST-SQUARES METHODS

Authors : Baker, E.N. Deposited on : 1979-11-27

Resolution : 1.70 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
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

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

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

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

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

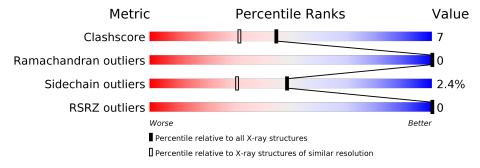
Validation Pipeline (wwPDB-VP) : 2.11

## 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 1.70 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
Metric	$(\# \mathrm{Entries})$	$\mid \; (\#  ext{Entries},   ext{resolution range}( ext{Å})) \; \mid \;$
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 >=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	220	80%	14%	5% •



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1931 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 ACTINIDIN PRECURSOR.

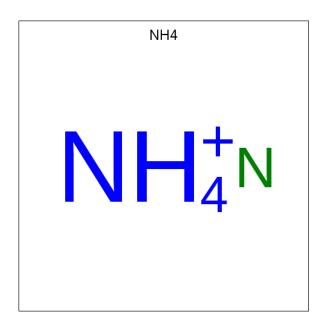
$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	218	Total 1658	C 1039	N 270	O 340	S 9	0	5	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	THR	VAL	CONFLICT	UNP P00785
A	42	SER	THR	CONFLICT	UNP P00785
A	44	SER	VAL	CONFLICT	UNP P00785
A	66	ASP	ASN	CONFLICT	UNP P00785
A	80	ASP	ASN	CONFLICT	UNP P00785
A	97	ASP	GLU	CONFLICT	UNP P00785
A	99	ASP	ASN	CONFLICT	UNP P00785
A	100	VAL	LEU	CONFLICT	UNP P00785
A	101	ALA	ASP	CONFLICT	UNP P00785
A	104	ASP	ASN	CONFLICT	UNP P00785
A	105	GLN	GLU	CONFLICT	UNP P00785
A	146	GLN	HIS	CONFLICT	UNP P00785
A	148	ALA	SER	CONFLICT	UNP P00785
A	160	VAL	ILE	CONFLICT	UNP P00785
A	164	ILE	VAL	CONFLICT	UNP P00785
A	165	VAL	THR	CONFLICT	UNP P00785
A	175	VAL	ILE	CONFLICT	UNP P00785

• Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).





Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
2	A	1	Total N 1 1	0	0

• Molecule 3 is water.

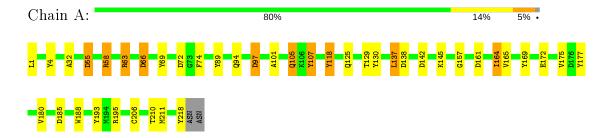
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	272	Total O 272 272	0	0



## 3 Residue-property plots (i)

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.

#### • Molecule 1: ACTINIDIN PRECURSOR





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	78.20Å 81.80Å 33.03Å	Donogiton
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	10.00 - 1.70	Depositor
Resolution (A)	40.90 - 1.70	EDS
% Data completeness	(Not available) (10.00-1.70)	Depositor
(in resolution range)	100.0 (40.90-1.70)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.30 (at 1.70Å)	Xtriage
Refinement program	FAST-FOURIER LEAST-SQUARES REFINEMENT	Depositor
D D.	0.171 , (Not available)	Depositor
$R, R_{free}$	0.160 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.6	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.30 , 45.6	EDS
L-test for twinning <sup>2</sup>	$< L >=0.46, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	1931	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.01% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, NH4

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	Bond	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.86	0/1713	1.90	47/2338 (2.0%)	

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	Α	58[A]	ARG	NE-CZ-NH1	-13.88	113.36	120.30
1	A	58[B]	ARG	NE-CZ-NH1	-13.88	113.36	120.30
1	A	63	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	A	97	ASP	CB-CG-OD2	-11.99	107.50	118.30
1	A	58[A]	ARG	CD-NE-CZ	-10.98	108.23	123.60
1	A	58[B]	ARG	CD-NE-CZ	-10.98	108.23	123.60
1	A	58[A]	ARG	NE-CZ-NH2	10.69	125.65	120.30
1	A	58[B]	ARG	NE-CZ-NH2	10.69	125.65	120.30
1	A	130	TYR	CB-CG-CD1	-10.36	114.78	121.00
1	A	185	ASP	CB-CG-OD1	-9.53	109.73	118.30
1	A	169	TYR	CB-CG-CD1	-9.24	115.46	121.00
1	A	97	ASP	CA-CB-CG	-9.02	93.56	113.40
1	A	107	TYR	CB-CG-CD1	-8.69	115.79	121.00
1	A	195	ARG	NE-CZ-NH1	-8.36	116.12	120.30
1	A	4	TYR	CB-CG-CD2	-8.24	116.05	121.00
1	A	4	TYR	CB-CG-CD1	8.01	125.80	121.00
1	A	218	TYR	CZ-CE2-CD2	-7.76	112.81	119.80
1	A	172	GLU	N-CA-CB	-7.68	96.78	110.60
1	Α	185	ASP	CB-CG-OD2	7.11	124.69	118.30
1	A	177	TYR	CG-CD1-CE1	-7.09	115.63	121.30
1	A	69	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	A	107	TYR	CA-CB-CG	-6.87	100.36	113.40
1	A	218	TYR	CG-CD1-CE1	-6.72	115.92	121.30
1	Α	66	ASP	CA-CB-CG	-6.69	98.67	113.40

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	Α	138	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	A	72	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	172	GLU	CB-CG-CD	6.57	131.93	114.20
1	A	94	GLN	CB-CA-C	-6.52	97.37	110.40
1	Α	193	TYR	CB-CG-CD1	-6.31	117.21	121.00
1	A	94	GLN	CA-CB-CG	6.19	127.02	113.40
1	A	118	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	A	145	LYS	CA-CB-CG	-6.08	100.02	113.40
1	Α	177	TYR	CD1-CE1-CZ	6.04	125.24	119.80
1	A	63	ARG	CD-NE-CZ	6.03	132.04	123.60
1	A	66	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	Α	55	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	A	218	TYR	CG-CD2-CE2	5.57	125.75	121.30
1	Α	161	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	175	VAL	CA-CB-CG1	-5.51	102.63	110.90
1	A	74	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	A	211	MET	CG-SD-CE	5.30	108.68	100.20
1	A	193	TYR	CG-CD2-CE2	-5.23	117.12	121.30
1	A	130	TYR	CB-CA-C	-5.21	99.99	110.40
1	A	69	TYR	CD1-CG-CD2	5.19	123.61	117.90
1	A	188	TRP	CB-CG-CD2	-5.14	119.92	126.60
1	A	142	ASP	CA-CB-CG	-5.12	102.13	113.40
1	A	105	GLN	N-CA-CB	-5.07	101.47	110.60

There are no chirality outliers.

There are no planarity outliers.

## 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	1658	0	1548	21	0
2	A	1	0	0	0	0
3	A	272	0	0	6	2
All	All	1931	0	1548	21	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 7.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + a ma 1	A 4 a res - O	Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	overlap (Å)
1:A:101:ALA:HB2	3:A:313:HOH:O	1.16	1.29
1:A:58[B]:ARG:CZ	3:A:413:HOH:O	2.20	0.89
1:A:32:ALA:HB3	1:A:165:VAL:HG21	1.55	0.89
1:A:164:ILE:HG13	1:A:180:VAL:HG13	1.55	0.86
1:A:55:ASP:HA	1:A:58[B]:ARG:HH12	1.49	0.77
1:A:58[B]:ARG:NH1	3:A:413:HOH:O	2.21	0.72
1:A:164:ILE:HG13	1:A:180:VAL:CG1	2.21	0.71
1:A:125:GLN:O	1:A:129[B]:THR:HG23	1.94	0.68
1:A:55:ASP:HA	1:A:58[B]:ARG:NH1	2.14	0.61
1:A:58[B]:ARG:NH1	3:A:412:HOH:O	2.35	0.59
1:A:118:TYR:HB2	1:A:210:THR:O	2.04	0.57
1:A:32:ALA:CB	1:A:165:VAL:HG21	2.31	0.57
1:A:137:LEU:HG	1:A:164:ILE:CD1	2.41	0.51
1:A:58[A]:ARG:CG	1:A:58[A]:ARG:NH1	2.71	0.51
1:A:97:ASP:N	1:A:97:ASP:OD2	2.48	0.46
1:A:1:LEU:HD22	1:A:129[B]:THR:HG21	1.98	0.45
1:A:101:ALA:CB	3:A:313:HOH:O	2.03	0.44
1:A:105:GLN:HG2	1:A:107:TYR:CE2	2.53	0.43
1:A:157:GLY:O	1:A:206:CYS:HA	2.20	0.42
1:A:137:LEU:HD21	1:A:164:ILE:HD12	2.02	0.41
1:A:63:ARG:HB2	3:A:446:HOH:O	2.20	0.41

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	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
3:A:425:HOH:O	3:A:493:HOH:O[2_655]	0.85	1.35
3:A:338:HOH:O	3:A:465:HOH:O[2_655]	2.18	0.02

## 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	rsed Favoured Allowed		Outliers	Percentiles	
1	A	$220/220 \ (100\%)$	214 (97%)	6 (3%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	Analysed Rotameric		Percentiles	
1	A	175/173 (101%)	171 (98%)	4 (2%)	50 33	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	${ m Res}$	$\mathbf{Type}$
1	A	66	ASP
1	A	89	TYR
1	A	137	LEU
1	A	164	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	${f Res}$	$\mathbf{Type}$
1	A	75	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul



statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type	Chain	Chain	Chain	Chain	Chain	Type Chain	Chain	Res	Link	В	ond leng	$\operatorname{gths}$	E	Bond an	gles
	Type		Ites	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2					
1	CSD	A	25	1	3,7,8	0.69	0	1,8,10	7.22	1 (100%)					

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	${f Res}$	Link	Chirals	Torsions	Rings
1	CSD	A	25	1	-	0/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$ \operatorname{Ideal}({}^o) $
1	A	25	CSD	OD1-SG-CB	-7.22	91.79	105.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	<RSRZ $>$	# RSRZ > 2		$\#RSRZ>2 \mid OWAB(A^2)$	
1	A	217/220 (98%)	-0.52	0 100	100	5, 9, 23, 33	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q<0.9
1	CSD	Α	25	8/9	0.97	0.09	5,7,15,22	2

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q < 0.9
2	NH4	A	221	1/1	0.99	0.22	8,8,8,8	0



# 6.5 Other polymers (i)

There are no such residues in this entry.

