



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:54 AM UTC

PDB ID : 2ACT / pdb_00002act
Title : CRYSTALLOGRAPHIC REFINEMENT OF THE STRUCTURE OF ACTINIDIN 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 ⓘ 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

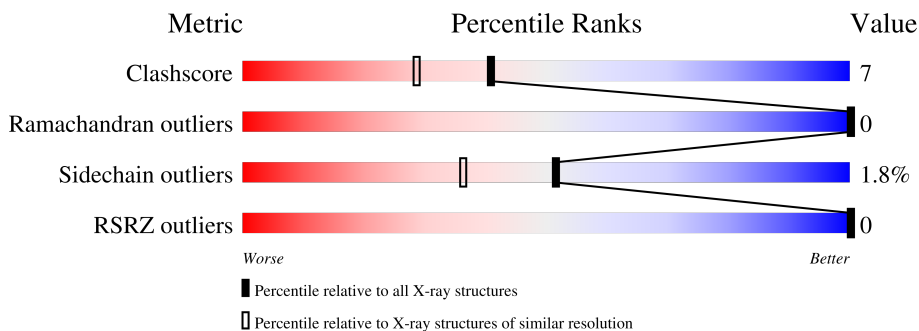
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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 $\leq 5\%$. 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	 76% 19% . .

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.

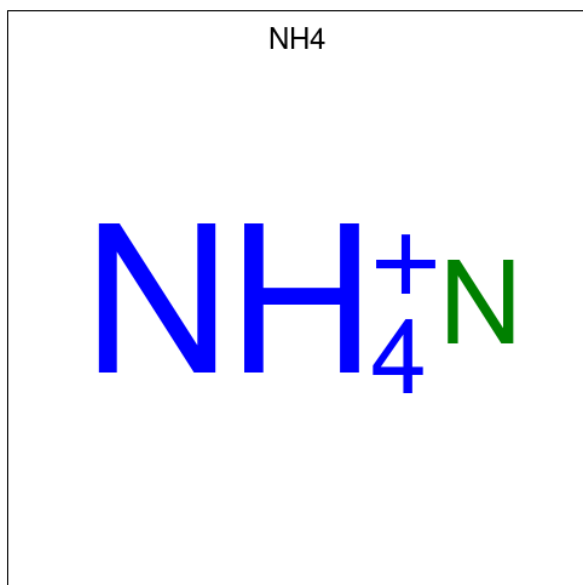
- Molecule 1 is a protein called ACTINIDIN PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1658	1039	270	340	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 (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total N 1 1	0	0

- Molecule 3 is water.

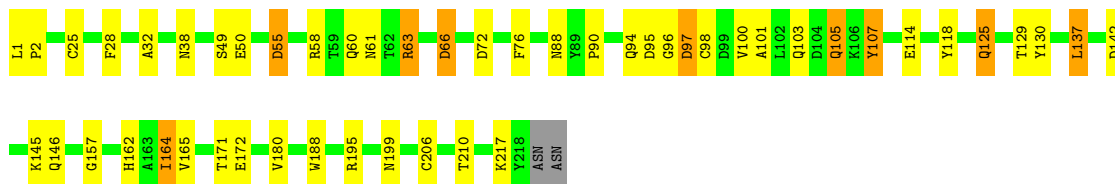
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	272	Total O 272 272	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

- Molecule 1: ACTINIDIN PRECURSOR

Chain A:  76% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.20Å 81.80Å 33.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70 10.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.70) 96.6 (10.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.70Å)	Xtrriage
Refinement program	FAST-FOURIER LEAST-SQUARES REFINEMENT	Depositor
R, R_{free}	0.171 , (Not available) 0.165 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.027 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1931	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	5/1713 (0.3%)	2.02	44/2338 (1.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	GLN	CD-OE1	5.28	1.33	1.23
1	A	60	GLN	CD-OE1	5.14	1.33	1.23
1	A	88	ASN	CG-OD1	5.09	1.33	1.23
1	A	125	GLN	CD-OE1	5.05	1.33	1.23
1	A	199	ASN	CG-OD1	5.04	1.33	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASP	CA-CB-CG	-19.04	93.56	112.60
1	A	66	ASP	CA-CB-CG	-13.93	98.67	112.60
1	A	76	PHE	CA-CB-CG	-11.64	102.16	113.80
1	A	172	GLU	CB-CG-CD	11.37	131.93	112.60
1	A	28	PHE	CA-CB-CG	-11.23	102.57	113.80
1	A	142	ASP	CA-CB-CG	-10.47	102.13	112.60
1	A	61	ASN	CA-CB-CG	-8.91	103.69	112.60
1	A	172	GLU	N-CA-CB	-8.35	96.78	110.81
1	A	49	SER	N-CA-C	7.54	120.35	108.67
1	A	107	TYR	CA-CB-CG	-7.52	100.36	113.90
1	A	171	THR	CA-C-N	-7.09	110.42	122.33
1	A	171	THR	C-N-CA	-7.09	110.42	122.33
1	A	145	LYS	CA-CB-CG	-7.04	100.02	114.10
1	A	95	ASP	CA-C-N	-6.95	115.99	122.17
1	A	95	ASP	C-N-CA	-6.95	115.99	122.17
1	A	2	PRO	CB-CA-C	-6.79	102.05	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	VAL	N-CA-C	6.54	117.30	110.62
1	A	94	GLN	CA-CB-CG	6.46	127.02	114.10
1	A	100	VAL	N-CA-CB	-6.16	102.16	110.54
1	A	38	ASN	CA-CB-CG	-6.13	106.47	112.60
1	A	94	GLN	CB-CG-CD	-5.84	102.68	112.60
1	A	114	GLU	CB-CG-CD	-5.83	102.68	112.60
1	A	96	GLY	O-C-N	5.81	128.43	123.95
1	A	94	GLN	CB-CA-C	-5.77	97.37	110.07
1	A	217	LYS	CA-C-N	-5.55	111.71	121.70
1	A	217	LYS	C-N-CA	-5.55	111.71	121.70
1	A	105	GLN	N-CA-CB	-5.50	101.47	110.21
1	A	63	ARG	CD-NE-CZ	5.46	132.04	124.40
1	A	162	HIS	CA-CB-CG	-5.44	108.36	113.80
1	A	195	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	A	90	PRO	N-CA-CB	5.32	108.97	103.38
1	A	55	ASP	CA-CB-CG	5.30	117.91	112.60
1	A	145	LYS	O-C-N	5.30	127.74	122.12
1	A	146	GLN	CB-CG-CD	-5.22	103.72	112.60
1	A	188	TRP	CE2-CD2-CE3	5.21	124.01	118.80
1	A	98	CYS	CA-C-N	-5.20	115.50	122.42
1	A	98	CYS	C-N-CA	-5.20	115.50	122.42
1	A	105	GLN	CB-CA-C	5.19	119.37	110.81
1	A	50	GLU	N-CA-C	-5.14	105.37	111.69
1	A	63	ARG	N-CA-CB	-5.14	103.37	111.23
1	A	130	TYR	CB-CA-C	-5.11	99.99	109.29
1	A	146	GLN	OE1-CD-NE2	5.10	127.70	122.60
1	A	72	ASP	N-CA-C	-5.06	106.61	112.89
1	A	217	LYS	CB-CA-C	5.05	118.24	110.62

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:NH1	1:A:58[A]:ARG:CG	2.71	0.51
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:97:ASP:OD2	1:A:97:ASP:N	2.48	0.42
1:A:157:GLY:O	1:A:206:CYS:HA	2.20	0.42
1:A:63:ARG:HB2	3:A:446:HOH:O	2.20	0.41
1:A:137:LEU:HD21	1:A:164:ILE:HD12	2.02	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	Interatomic distance (Å)	Clash overlap (Å)
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	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	Rotameric	Outliers	Percentiles	
1	A	175/173 (101%)	172 (98%)	3 (2%)	53	38

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	137	LEU
1	A	164	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	103	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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	A	25	1	4,7,8	19.20	1 (25%)	1,8,10	7.50	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	Res	Link	Chirals	Torsions	Rings
1	CSD	A	25	1	-	0/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	CSD	OD1-SG	38.39	1.82	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	CSD	OD1-SG-CB	-7.50	91.79	105.60

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 oligosaccharides 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, 95th 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	OWAB(Å ²)	Q<0.9
1	A	217/220 (98%)	-0.49	0 100 100	5, 9, 23, 33	5 (2%)

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, 95th 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	B-factors(Å ²)	Q<0.9
1	CSD	A	25	8/9	0.94	0.07	5,7,15,22	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	B-factors(Å ²)	Q<0.9
2	NH4	A	221	1/1	0.99	0.06	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.