Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:51 PM UTC

PDB ID	:	1IRE / pdb_00001ire
Title	:	Crystal Structure of Co-type nitrile hydratase from Pseudonocardia thermophila
Authors	:	Miyanaga, A.; Fushinobu, S.; Ito, K.; Wakagi, T.
Deposited on	:	2001-10-01
Resolution	:	1.80 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:

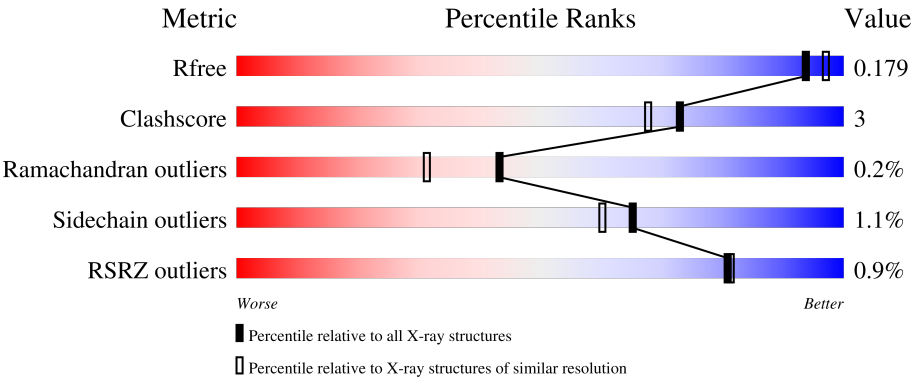
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

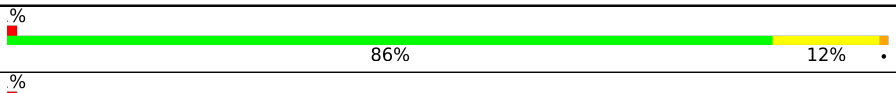
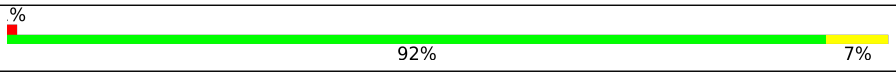
The reported resolution of this entry is 1.80 Å.

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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 <=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	204	
2	B	228	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3793 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 Nitrile Hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1616	1023	271	311	11			

- Molecule 2 is a protein called Nitrile Hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	228	Total	C	N	O	S	0	0	0
			1852	1182	320	344	6			

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		

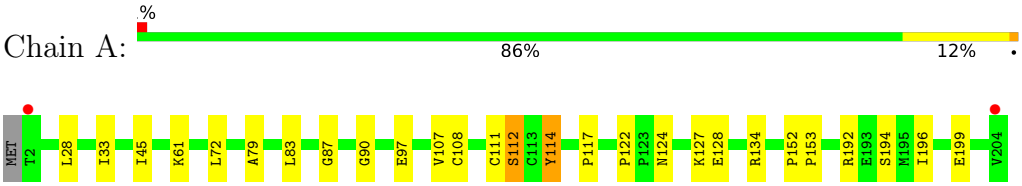
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		
4	B	192	Total	O	0	0
			192	192		

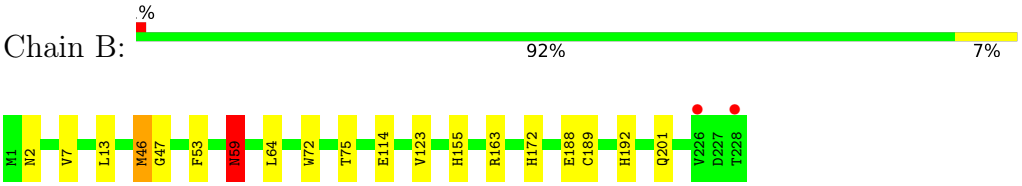
3 Residue-property plots (i)

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: Nitrile Hydratase



• Molecule 2: Nitrile Hydratase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	65.50Å 65.50Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.03 – 1.80 28.03 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.03-1.80) 99.9 (28.03-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 1.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.178 , 0.191 0.181 , 0.179	Depositor DCC
R_{free} test set	2192 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3793	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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

5.1 Standard geometry

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

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	0.37	0/1635	0.89	7/2215 (0.3%)
2	B	0.38	0/1914	0.86	3/2603 (0.1%)
All	All	0.37	0/3549	0.87	10/4818 (0.2%)

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	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	134	ARG	N-CA-C	6.84	120.10	111.69
1	A	97	GLU	N-CA-C	5.85	118.26	108.96
1	A	124	ASN	N-CA-C	5.62	118.13	111.33
1	A	87	GLY	N-CA-C	5.42	117.03	111.56
2	B	7	VAL	N-CA-C	5.33	120.32	113.07
1	A	196	ILE	N-CA-C	-5.33	104.84	112.35
2	B	64	LEU	N-CA-C	5.18	117.66	111.71
1	A	128	GLU	CA-C-N	5.11	124.90	119.28
1	A	128	GLU	C-N-CA	5.11	124.90	119.28
2	B	59	ASN	N-CA-C	-5.08	100.69	109.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	TYR	Sidechain

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	1616	0	1602	12	0
2	B	1852	0	1738	11	0
3	A	1	0	0	0	0
4	A	132	0	0	1	0
4	B	192	0	0	1	0
All	All	3793	0	3340	22	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 3.

All (22) 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)
2:B:2:ASN:HD21	2:B:163:ARG:HH12	1.24	0.85
2:B:59:ASN:HD22	2:B:59:ASN:C	2.06	0.63
2:B:201:GLN:HG2	4:B:411:HOH:O	2.01	0.60
1:A:28:LEU:HD22	1:A:33:ILE:HD11	1.85	0.59
1:A:112:SER:HB2	1:A:127:LYS:HG2	1.93	0.50
2:B:72:TRP:O	2:B:75:THR:HG22	2.13	0.48
1:A:194:SER:HA	1:A:199:GLU:O	2.13	0.47
1:A:90:GLY:HA3	1:A:117:PRO:HG2	1.96	0.47
1:A:107:VAL:HG22	1:A:108:CYS:N	2.30	0.46
2:B:2:ASN:ND2	2:B:163:ARG:HH12	2.03	0.45
1:A:61:LYS:HD2	1:A:83:LEU:HD21	1.99	0.44
2:B:46:MET:HG2	2:B:47:GLY:O	2.17	0.44
2:B:53:PHE:CG	2:B:155:HIS:HB2	2.54	0.43
1:A:122:PRO:HG2	1:A:127:LYS:HD3	2.00	0.42
2:B:172:HIS:HE1	2:B:192:HIS:ND1	2.16	0.42
1:A:45:ILE:HG21	2:B:123:VAL:HG11	2.01	0.42
2:B:188:GLU:O	2:B:189:CYS:C	2.62	0.42
1:A:192:ARG:HD3	4:A:302:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HA	1:A:79:ALA:CB	2.51	0.40
1:A:114:TYR:CG	1:A:122:PRO:HB3	2.56	0.40
2:B:59:ASN:C	2:B:59:ASN:ND2	2.77	0.40
1:A:152:PRO:HA	1:A:153:PRO:HD3	1.87	0.40

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	199/204 (98%)	194 (98%)	4 (2%)	1 (0%)	24 14
2	B	226/228 (99%)	221 (98%)	5 (2%)	0	100 100
All	All	425/432 (98%)	415 (98%)	9 (2%)	1 (0%)	43 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER

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	177/178 (99%)	177 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	190/190 (100%)	186 (98%)	4 (2%)	47 36
All	All	367/368 (100%)	363 (99%)	4 (1%)	65 60

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

Mol	Chain	Res	Type
2	B	13	LEU
2	B	46	MET
2	B	59	ASN
2	B	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	2	ASN
2	B	59	ASN
2	B	172	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	111	1,3	4,7,8	1.60	1 (25%)	1,8,10	1.29	0
1	CSO	A	113	1,3	3,6,7	0.70	0	1,6,8	0.25	0

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	111	1,3	-	1/2/6/8	-
1	CSO	A	113	1,3	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	CSD	OD1-SG	3.04	1.50	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111	CSD	CA-CB-SG-OD1

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 monoatomic - 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

6.1 Protein, DNA and RNA chains

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			OWAB(Å^2)	Q<0.9
1	A	201/204 (98%)	-0.28	2 (0%)	79	80	11, 16, 27, 41	0
2	B	228/228 (100%)	-0.27	2 (0%)	81	81	10, 16, 27, 39	0
All	All	429/432 (99%)	-0.28	4 (0%)	81	81	10, 16, 27, 41	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	VAL	5.6
2	B	228	THR	3.5
1	A	2	THR	3.4
2	B	226	VAL	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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	B-factors(Å^2)	Q<0.9
1	CSO	A	113	7/8	0.98	0.06	11,12,14,15	0
1	CSD	A	111	8/9	0.99	0.05	9,11,14,14	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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	B-factors(Å^2)	Q<0.9
3	CO	A	301	1/1	1.00	0.01	13,13,13,13	0

6.5 Other polymers

There are no such residues in this entry.