



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 07:44 PM EDT

PDB ID : 3A8H  
Title : Crystal structure of Nitrile Hydratase mutant S113A complexed with Trimethylacetamide  
Authors : Yamanaka, Y.; Hashimoto, K.; Ohtaki, A.; Noguchi, K.; Yohda, M.; Odaka, M.  
Deposited on : 2009-10-06  
Resolution : 1.66 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.36  
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) : 2.36

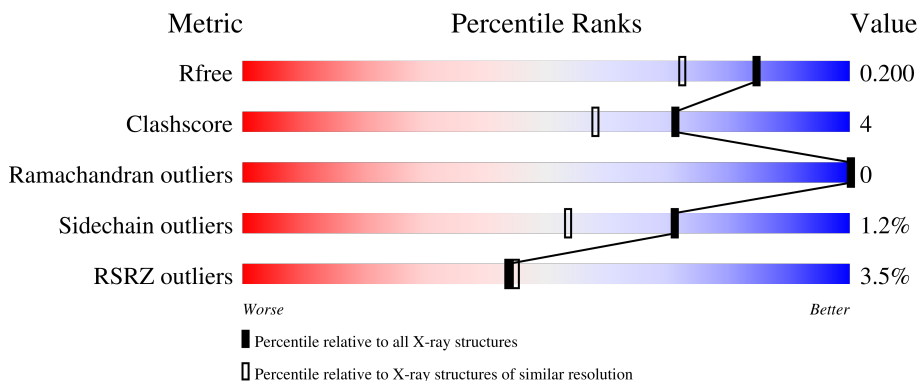
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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  $\leq 5\%$ . 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	207	
2	B	212	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3708 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	190	1484	950	245	283	6	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ALA	SER	engineered mutation	UNP P13448

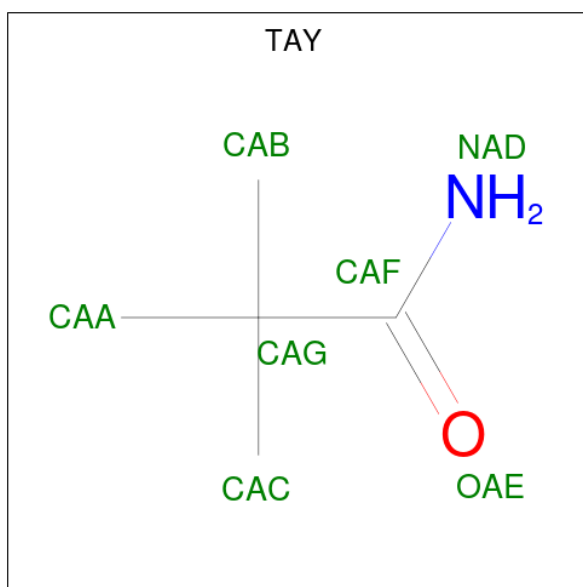
- Molecule 2 is a protein called Nitrile hydratase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	211	1686	1068	288	319	11	0	7	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is 2,2-dimethylpropanamide (three-letter code: TAY) (formula: C<sub>5</sub>H<sub>11</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	7	5	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	262	Total	O	0	0
			262	262		
5	B	268	Total	O	0	0
			268	268		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.61Å 60.01Å 81.50Å 90.00° 125.14° 90.00°	Depositor
Resolution (Å)	28.09 – 1.66 28.09 – 1.66	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.09-1.66) 99.8 (28.09-1.66)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 1.66Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.173 , 0.200 0.173 , 0.200	Depositor DCC
$R_{free}$ test set	2696 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.54	0/1504	0.61	0/2047
2	B	0.54	0/1754	0.61	0/2383
All	All	0.54	0/3258	0.61	0/4430

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1484	0	1446	16	0
2	B	1686	0	1605	8	0
3	A	1	0	0	0	0
4	B	7	0	11	0	0
5	A	262	0	0	11	0
5	B	268	0	0	1	0
All	All	3708	0	3062	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 4.

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)
1:A:46:THR:N	5:A:505:HOH:O	2.08	0.86
1:A:72:LEU:N	5:A:509:HOH:O	2.13	0.81
1:A:44:LYS:C	5:A:216:HOH:O	2.29	0.70
1:A:70:ARG:C	5:A:225:HOH:O	2.29	0.69
1:A:154:ASP:HB2	5:A:519:HOH:O	1.91	0.69
1:A:185:GLN:N	5:A:500:HOH:O	2.26	0.67
1:A:69:PHE:N	5:A:506:HOH:O	2.30	0.65
1:A:8:THR:HG23	1:A:11:ALA:HB2	1.86	0.57
1:A:137:VAL:HG23	5:A:259:HOH:O	2.04	0.56
1:A:72:LEU:N	5:A:225:HOH:O	2.40	0.55
2:B:65[A]:ARG:O	2:B:69[A]:MET:HG3	2.08	0.52
1:A:183:GLN:C	5:A:500:HOH:O	2.50	0.51
2:B:40[A]:MET:HG3	2:B:55:VAL:HG21	1.94	0.49
2:B:172:ASN:HD22	2:B:172:ASN:C	2.16	0.48
1:A:108:VAL:HG22	1:A:109:CYS:N	2.30	0.46
2:B:29:HIS:HD2	5:B:377:HOH:O	2.00	0.45
2:B:172:ASN:HD22	2:B:173:ASP:N	2.14	0.45
1:A:10:ASN:OD1	2:B:65[B]:ARG:NE	2.44	0.45
1:A:46:THR:N	5:A:216:HOH:O	2.50	0.44
1:A:93:TYR:OH	2:B:155:HIS:HE1	2.01	0.43
1:A:124:PRO:HD3	1:A:192:LYS:HE3	2.03	0.41
2:B:120:THR:HB	2:B:205:GLU:HG2	2.03	0.41

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	173/207 (84%)	168 (97%)	5 (3%)	0	100	100
2	B	216/212 (102%)	212 (98%)	4 (2%)	0	100	100
All	All	389/419 (93%)	380 (98%)	9 (2%)	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	154/170 (91%)	153 (99%)	1 (1%)	86	76
2	B	180/173 (104%)	177 (98%)	3 (2%)	60	39
All	All	334/343 (97%)	330 (99%)	4 (1%)	71	53

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

Mol	Chain	Res	Type
1	A	8	THR
2	B	103	PHE
2	B	165	ASP
2	B	172	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	105	ASN
2	B	21	ASN
2	B	34	HIS
2	B	155	HIS
2	B	172	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](#)

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	112	1,3	3,7,8	0.79	0	1,8,10	2.74	1 (100%)
1	CSO	A	114	1,3	3,6,7	0.71	0	0,6,8	-	-

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	112	1,3	-	1/2/6/8	-
1	CSO	A	114	1,3	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	CSD	OD1-SG-CB	-2.74	100.33	105.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	112	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
4	TAY	B	300	-	6,6,6	0.64	0	7,9,9	0.52	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
4	TAY	B	300	-	-	0/6/6/6	-

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	188/207 (90%)	0.05	11 (5%) 22 21	9, 16, 32, 45	0
2	B	211/212 (99%)	-0.27	3 (1%) 75 79	9, 16, 25, 31	0
All	All	399/419 (95%)	-0.12	14 (3%) 44 45	9, 16, 27, 45	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	THR	10.6
1	A	11	ALA	7.7
1	A	12	ALA	7.1
1	A	154	ASP	4.7
1	A	153	SER	3.8
1	A	10	ASN	3.6
1	A	13	PRO	3.3
1	A	9	GLU	3.1
2	B	118	VAL	3.0
1	A	14	ALA	2.9
1	A	203	VAL	2.8
1	A	204	PRO	2.3
2	B	112	GLU	2.3
2	B	128	ARG	2.2

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	CSO	A	114	7/8	0.98	0.12	9,10,14,16	0
1	CSD	A	112	8/9	0.99	0.08	9,10,10,10	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	TAY	B	300	7/7	0.78	0.21	40,41,41,41	0
3	FE	A	300	1/1	1.00	0.08	11,11,11,11	0

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

There are no such residues in this entry.