



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2CYZ / pdb_00002cyz
Title : photo-activation state of Fe-type NHase in anaerobic condition
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Deposited on : 2005-07-09
Resolution : 1.55 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

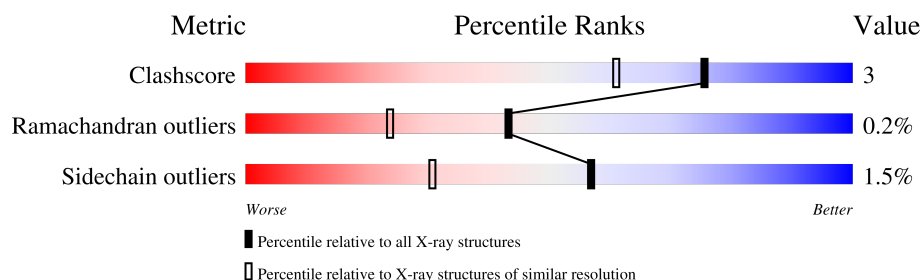
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	206	 86% 8% . .
2	B	212	 89% 9% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3924 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
1	A	197	Total	C	N	O	S	0	1	0
			1552	988	260	298	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	CSD	CYS	modified residue	UNP P13448
A	114	CSO	CYS	modified residue	UNP P13448

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	4	0
			1661	1054	282	315	10			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	337	Total	O	0	1
			338	338		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	370	Total	O	0	1
			371	371		

Note EDS was not executed.

- Chain A: 86% 8% ...



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.05Å 60.59Å 82.01Å 90.00° 124.96° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55	Depositor
% Data completeness (in resolution range)	86.4 (20.00-1.55)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.149 , 0.193	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3924	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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: CSO, FE, MG, CSD

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	0.59	0/1579	1.34	9/2156 (0.4%)
2	B	0.61	0/1729	1.31	6/2351 (0.3%)
All	All	0.60	0/3308	1.33	15/4507 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	CD-NE-CZ	12.81	142.34	124.40
1	A	70	ARG	NE-CZ-NH1	-6.71	114.79	121.50
1	A	54	ARG	NE-CZ-NH2	6.68	125.22	119.20
1	A	70	ARG	CD-NE-CZ	-6.51	115.29	124.40
2	B	195	ASP	CA-CB-CG	6.40	119.00	112.60
2	B	65	ARG	NE-CZ-NH1	-6.24	115.26	121.50
2	B	76	TYR	CA-CB-CG	-6.20	102.75	113.90
1	A	41	GLU	CA-C-N	6.15	126.77	119.94
1	A	41	GLU	C-N-CA	6.15	126.77	119.94
1	A	70	ARG	NE-CZ-NH2	5.91	124.52	119.20
2	B	103	PHE	CA-CB-CG	5.78	119.58	113.80
2	B	114	ARG	NE-CZ-NH1	-5.53	115.97	121.50
2	B	155	HIS	CA-CB-CG	5.37	119.17	113.80
1	A	141	ARG	CD-NE-CZ	5.13	131.58	124.40
1	A	66	ASP	CA-CB-CG	5.02	117.62	112.60

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	1552	0	1517	11	0
2	B	1661	0	1581	11	0
3	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	338	0	0	3	0
5	B	371	0	0	2	0
All	All	3924	0	3098	19	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 (19) 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:8:THR:HG23	1:A:11:ALA:HB2	1.46	0.95
1:A:98:GLU:HG3	5:A:554:HOH:O	1.90	0.70
1:A:34:LEU:HB3	2:B:47:LEU:HD21	1.78	0.66
1:A:125:THR:HG23	5:A:484:HOH:O	2.01	0.60
1:A:93:TYR:OH	2:B:155:HIS:HE1	1.93	0.52
2:B:128:ARG:HG2	2:B:152[A]:THR:HG22	1.91	0.51
2:B:34:HIS:H	2:B:34:HIS:CD2	2.31	0.48
1:A:70:ARG:HH11	1:A:70:ARG:HD2	1.43	0.47
2:B:118:VAL:HG13	5:B:1544:HOH:O	2.14	0.47
2:B:150[B]:VAL:HG22	2:B:188:GLU:OE2	2.16	0.45
1:A:8:THR:HG23	1:A:11:ALA:CB	2.34	0.45
1:A:137:VAL:HG23	5:A:371:HOH:O	2.18	0.44
1:A:8:THR:OG1	1:A:9:GLU:N	2.50	0.43
2:B:161:TRP:HB3	2:B:162:PRO:HD2	2.00	0.42
1:A:117:TRP:HB2	1:A:118:PRO:HD3	2.00	0.42
2:B:150[A]:VAL:HG23	5:B:1491:HOH:O	2.19	0.41
1:A:110:SER:HB2	2:B:8:ALA:HB2	2.03	0.40
2:B:35:LEU:N	2:B:36:PRO:HD2	2.36	0.40
2:B:166:ALA:HA	2:B:171:ARG:HD3	2.04	0.40

There are no symmetry-related clashes.

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	194/206 (94%)	190 (98%)	3 (2%)	1 (0%)	24	8
2	B	213/212 (100%)	209 (98%)	4 (2%)	0	100	100
All	All	407/418 (97%)	399 (98%)	7 (2%)	1 (0%)	43	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER

5.3.2 Protein sidechains

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	162/170 (95%)	160 (99%)	2 (1%)	63	40
2	B	177/173 (102%)	174 (98%)	3 (2%)	53	25
All	All	339/343 (99%)	334 (98%)	5 (2%)	57	31

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	153	SER
2	B	118	VAL
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	29	HIS
2	B	34	HIS
2	B	155	HIS
2	B	172	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	4,7,8	1.45	1 (25%)	1,8,10	1.36	0
1	CSO	A	114	1,3	3,6,7	0.84	0	1,6,8	0.68	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	112	1,3	-	1/2/6/8	-
1	CSO	A	114	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	112	CSD	OD1-SG	2.69	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	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.