Full wwPDB X-ray Structure Validation Report ⓘ

Jan 9, 2023 – 12:27 pm GMT

PDB ID	:	7QOV
Title	:	The wild type nitrile hydratase from Geobacillus pallidus
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Deposited on	:	2021-12-29
Resolution	:	1.40 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:

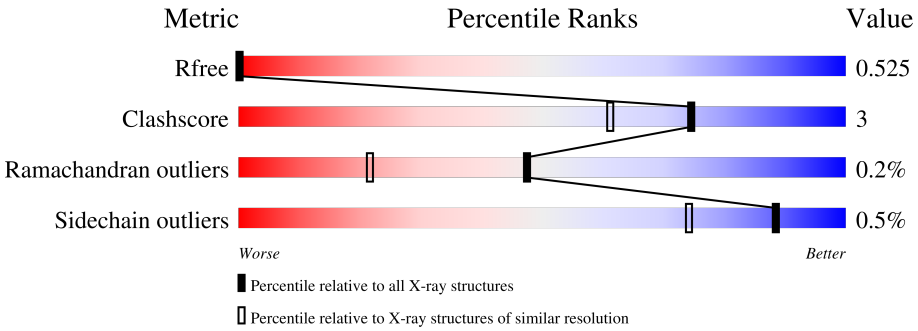
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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%

Mol	Chain	Length	Quality of chain
1	A	216	87% 7% 6%
2	B	229	87% 12% .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3988 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	202	Total	C	N	O	S	0	2	0
			1641	1046	284	303	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	4	0
			1876	1210	314	343	9			

- Molecule 3 is COBALT (III) ION (three-letter code: 3CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	2	Total	Cl	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	212	Total	O	0	0
			212	212		
5	B	255	Total	O	0	0
			255	255		

3 Residue-property plots (i)

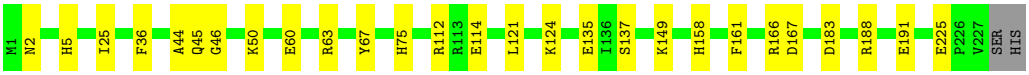
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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

Chain A:

- Molecule 2: Nitrile hydratase subunit beta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.48Å 105.48Å 83.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.59 – 1.40 27.59 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.59-1.40) 88.4 (27.59-1.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.10.1	Depositor
R, R_{free}	(Not available) , 0.180 0.542 , 0.525	Depositor DCC
R_{free} test set	5083 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	11.7	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 29.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.66	EDS
Total number of atoms	3988	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: 3CO, CL, 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	0.33	0/1676	0.55	0/2279
2	B	0.37	0/1940	0.62	0/2620
All	All	0.35	0/3616	0.59	0/4899

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	1641	0	1627	8	9
2	B	1876	0	1843	14	14
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	1	0
5	A	212	0	0	3	13
5	B	255	0	0	7	20
All	All	3988	0	3470	22	31

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:166:ARG:HH12	1.24	0.84
2:B:225:GLU:HG2	5:B:561:HOH:O	1.92	0.69
2:B:60:GLU:OE1	2:B:158:HIS:HD2	1.81	0.63
1:A:72[B]:THR:HG23	5:A:420:HOH:O	2.03	0.57
2:B:75:HIS:HD2	5:B:615:HOH:O	1.87	0.57
2:B:158:HIS:HE1	5:B:459:HOH:O	1.88	0.55
2:B:67:TYR:O	2:B:75:HIS:HE1	1.90	0.55
1:A:121:CSD:HB2	1:A:174:ARG:CZ	2.38	0.52
1:A:14:PHE:HB3	1:A:17:HIS:CD2	2.45	0.51
1:A:100:HIS:HD2	5:A:567:HOH:O	1.95	0.49
2:B:149:LYS:HE2	2:B:167:ASP:OD1	2.13	0.49
2:B:124:LYS:NZ	5:B:402:HOH:O	2.43	0.48
2:B:5:HIS:HD2	5:B:497:HOH:O	1.97	0.48
2:B:225:GLU:CG	5:B:561:HOH:O	2.55	0.47
1:A:17:HIS:HD2	5:A:586:HOH:O	1.98	0.45
2:B:121:LEU:HD23	2:B:121:LEU:C	2.37	0.44
1:A:68:ALA:O	1:A:72[B]:THR:HG22	2.17	0.44
2:B:63:ARG:HD2	4:B:302:CL:CL	2.54	0.43
2:B:225:GLU:CD	5:B:561:HOH:O	2.58	0.42
1:A:52:LYS:HB2	1:A:52:LYS:NZ	2.35	0.41
1:A:52:LYS:HB2	1:A:52:LYS:HZ2	1.84	0.41
2:B:161:PHE:CZ	2:B:166:ARG:HG2	2.56	0.40

All (31) 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)
5:A:568:HOH:O	5:B:431:HOH:O[8_777]	0.97	1.23
5:A:593:HOH:O	5:B:603:HOH:O[3_745]	1.25	0.95
5:B:606:HOH:O	5:B:612:HOH:O[4_574]	1.41	0.79
1:A:57:GLU:OE2	5:A:603:HOH:O[3_745]	1.59	0.61
2:B:188:ARG:O	5:B:536:HOH:O[4_574]	1.62	0.58
5:B:455:HOH:O	5:B:643:HOH:O[8_777]	1.68	0.52
5:B:534:HOH:O	5:B:583:HOH:O[4_574]	1.68	0.52
2:B:25[A]:ILE:CG2	5:B:513:HOH:O[3_745]	1.69	0.51
2:B:114:GLU:OE2	5:B:408:HOH:O[3_745]	1.69	0.51
2:B:25[B]:ILE:CG2	5:B:513:HOH:O[3_745]	1.74	0.46
2:B:135:GLU:OE2	5:B:629:HOH:O[4_574]	1.75	0.45
5:B:578:HOH:O	5:B:655:HOH:O[3_745]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:427:HOH:O	5:A:583:HOH:O[4_574]	1.80	0.40
5:A:468:HOH:O	5:B:496:HOH:O[3_745]	1.81	0.39
5:A:471:HOH:O	5:B:538:HOH:O[8_777]	1.82	0.38
1:A:56:HIS:CD2	2:B:45:GLN:O[3_745]	1.98	0.22
1:A:10:ILE:O	2:B:137:SER:N[5_747]	2.01	0.19
1:A:56:HIS:CD2	2:B:45:GLN:C[3_745]	2.01	0.19
5:B:517:HOH:O	5:B:596:HOH:O[4_574]	2.01	0.19
2:B:45:GLN:OE1	5:A:472:HOH:O[4_574]	2.03	0.17
2:B:191:GLU:N	5:B:557:HOH:O[4_574]	2.05	0.15
5:A:476:HOH:O	5:B:450:HOH:O[3_745]	2.07	0.13
5:A:537:HOH:O	5:B:456:HOH:O[5_747]	2.07	0.13
5:A:485:HOH:O	5:B:466:HOH:O[5_747]	2.10	0.10
1:A:13:ARG:CG	5:B:612:HOH:O[8_777]	2.13	0.07
1:A:40:GLY:O	5:A:606:HOH:O[4_574]	2.13	0.07
2:B:50:LYS:NZ	5:A:454:HOH:O[4_574]	2.14	0.06
2:B:112:ARG:NE	5:B:541:HOH:O[3_745]	2.15	0.05
1:A:41:HIS:CE1	5:A:402:HOH:O[4_574]	2.17	0.03
1:A:56:HIS:ND1	2:B:44:ALA:O[3_745]	2.18	0.02
1:A:56:HIS:NE2	2:B:46:GLY:N[3_745]	2.19	0.01

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	200/216 (93%)	194 (97%)	5 (2%)	1 (0%)	29 9
2	B	228/229 (100%)	223 (98%)	5 (2%)	0	100 100
All	All	428/445 (96%)	417 (97%)	10 (2%)	1 (0%)	47 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	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	179/190 (94%)	179 (100%)	0	100	100
2	B	198/196 (101%)	196 (99%)	2 (1%)	76	53
All	All	377/386 (98%)	375 (100%)	2 (0%)	88	74

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	36	PHE
2	B	183	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
2	B	2	ASN
2	B	5	HIS
2	B	75	HIS
2	B	152	ASN
2	B	158	HIS
2	B	211	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)

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	119	1	3,7,8	0.63	0	1,8,10	0.20	0
1	CSD	A	121	1,3	3,7,8	0.72	0	1,8,10	0.13	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	119	1	-	0/2/6/8	-
1	CSD	A	121	1,3	-	0/2/6/8	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	121	CSD	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

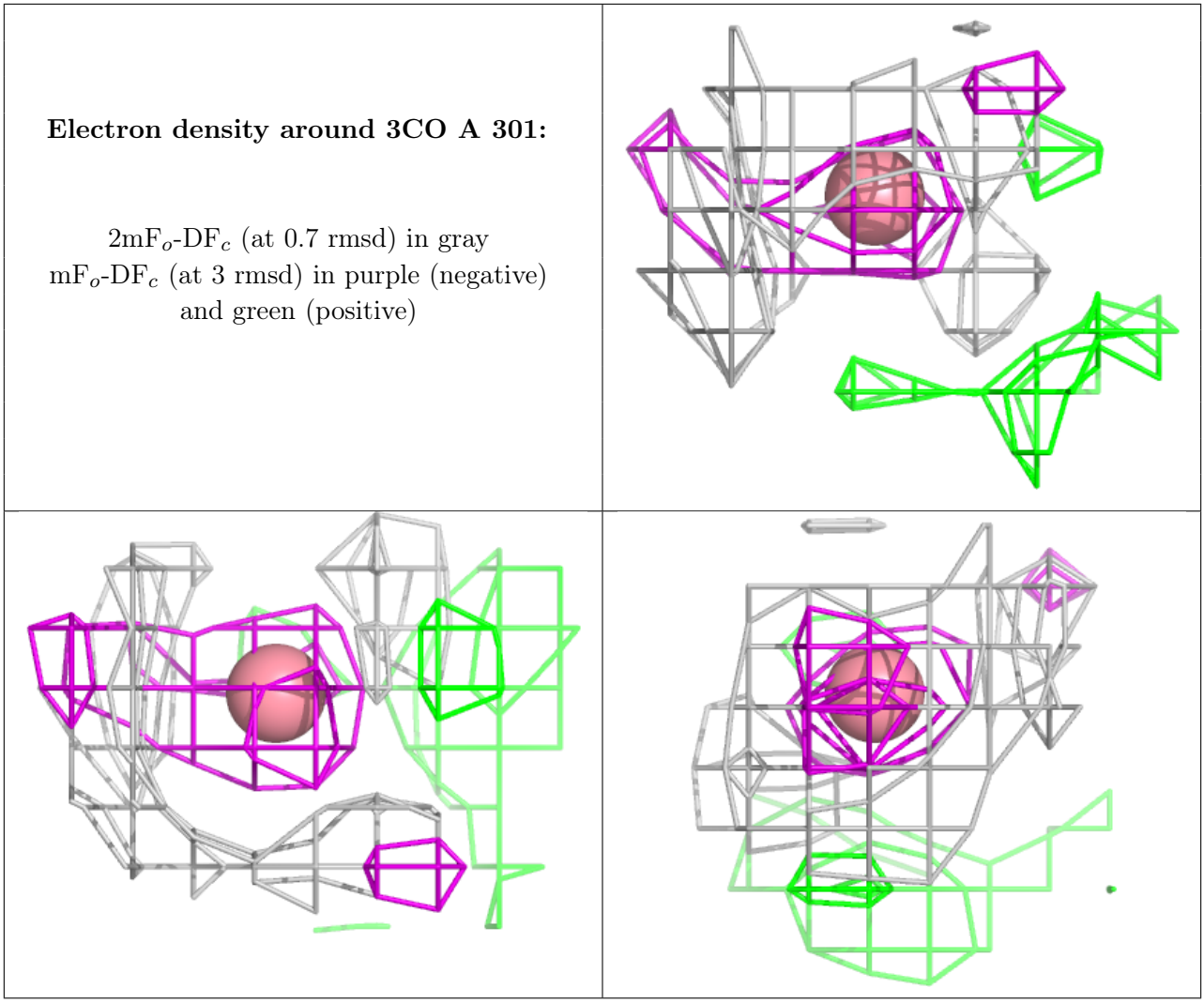
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 3CO A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.