



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2017 – 06:56 PM EDT

PDB ID : 3QYG
Title : Crystal Structure of Co-type Nitrile Hydratase beta-E56Q from *Pseudomonas putida*.
Authors : Brodtkin, H.R.; Novak, W.R.P.; Ringe, D.; Petsko, G.A.
Deposited on : unknown
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

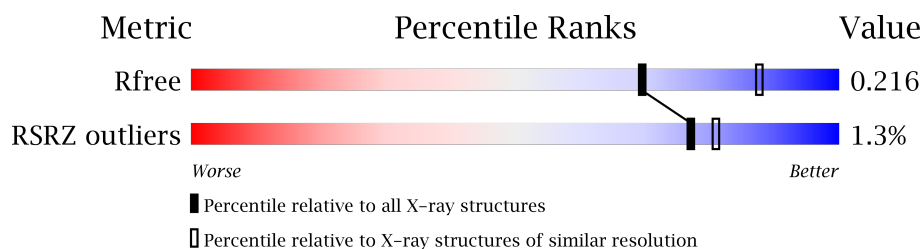
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14164 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 Co-type Nitrile Hydratase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1542	982	262	290	8			
1	C	201	Total	C	N	O	S	0	0	0
			1543	983	264	288	8			
1	E	200	Total	C	N	O	S	0	2	0
			1550	989	264	289	8			
1	G	200	Total	C	N	O	S	0	1	0
			1541	982	265	286	8			

- Molecule 2 is a protein called Co-type Nitrile Hydratase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	3	0
			1731	1093	312	322	4			
2	D	219	Total	C	N	O	S	0	3	0
			1727	1092	309	322	4			
2	F	219	Total	C	N	O	S	0	3	0
			1729	1093	311	321	4			
2	H	219	Total	C	N	O	S	0	3	0
			1721	1089	307	321	4			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is COBALT (III) ION (three-letter code: 3CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Co	0	0
			1	1		
4	A	1	Total	Co	0	0
			1	1		
4	C	1	Total	Co	0	0
			1	1		
4	E	1	Total	Co	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total	O	0	0
			147	147		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	146	Total 146	O 146	0	0
5	C	105	Total 105	O 105	0	0
5	D	146	Total 146	O 146	0	0
5	E	114	Total 114	O 114	0	0
5	F	138	Total 138	O 138	0	0
5	G	120	Total 120	O 120	0	0
5	H	136	Total 136	O 136	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.96Å 137.55Å 85.42Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	45.37 – 2.30 45.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (45.37-2.30) 96.1 (45.37-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.196 , 0.224 0.188 , 0.216	Depositor DCC
R_{free} test set	4037 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for l,k,-h 0.031 for h,-k,-l 0.107 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14164	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 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	115	1,4	4,7,8	1.25	0	2,8,10	2.09	1 (50%)
1	CSD	A	117	1,4	4,7,8	0.90	0	2,8,10	1.40	0
1	CSD	C	115	1,4	4,7,8	1.04	0	2,8,10	2.36	2 (100%)
1	CSD	C	117	1,4	4,7,8	0.87	0	2,8,10	1.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	E	115	1,4	4,7,8	1.34	0	2,8,10	1.72	1 (50%)
1	CSD	E	117	1,4	4,7,8	0.92	0	2,8,10	1.93	1 (50%)
1	CSD	G	115	1,4	4,7,8	1.06	0	2,8,10	2.68	2 (100%)
1	CSD	G	117	1,4	4,7,8	0.91	0	2,8,10	1.27	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	115	1,4	-	1/2/6/8	0/0/0/0
1	CSD	A	117	1,4	-	1/2/6/8	0/0/0/0
1	CSD	C	115	1,4	-	1/2/6/8	0/0/0/0
1	CSD	C	117	1,4	-	1/2/6/8	0/0/0/0
1	CSD	E	115	1,4	-	1/2/6/8	0/0/0/0
1	CSD	E	117	1,4	-	1/2/6/8	0/0/0/0
1	CSD	G	115	1,4	-	1/2/6/8	0/0/0/0
1	CSD	G	117	1,4	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	115	CSD	OD1-SG-CB	-2.94	100.09	105.61
1	A	115	CSD	O-C-CA	-2.66	117.67	125.02
1	E	115	CSD	O-C-CA	-2.42	118.33	125.02
1	C	115	CSD	OD1-SG-CB	-2.41	101.08	105.61
1	G	115	CSD	O-C-CA	-2.39	118.41	125.02

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	115	CSD	CA-CB-SG-OD1
1	G	115	CSD	CA-CB-SG-OD1
1	A	115	CSD	CA-CB-SG-OD1
1	C	115	CSD	CA-CB-SG-OD1
1	C	117	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	GOL	A	212	-	5,5,5	0.37	0	5,5,5	0.21	0
3	GOL	C	212	-	5,5,5	0.33	0	5,5,5	0.44	0
3	GOL	E	212	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	G	212	-	5,5,5	0.41	0	5,5,5	0.65	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
3	GOL	A	212	-	-	0/4/4/4	0/0/0/0
3	GOL	C	212	-	-	0/4/4/4	0/0/0/0
3	GOL	E	212	-	-	0/4/4/4	0/0/0/0
3	GOL	G	212	-	-	0/4/4/4	0/0/0/0

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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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, 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	199/226 (88%)	-0.13	0 100 100	18, 24, 32, 37	0
1	C	199/226 (88%)	-0.11	1 (0%) 90 93	18, 24, 33, 39	0
1	E	198/226 (87%)	-0.25	1 (0%) 90 93	18, 24, 32, 37	1 (0%)
1	G	198/226 (87%)	-0.19	2 (1%) 82 86	18, 24, 33, 38	0
2	B	219/219 (100%)	-0.08	1 (0%) 90 93	19, 23, 33, 47	1 (0%)
2	D	219/219 (100%)	-0.11	4 (1%) 69 74	19, 23, 31, 47	0
2	F	219/219 (100%)	-0.10	7 (3%) 48 55	19, 23, 35, 47	0
2	H	219/219 (100%)	-0.15	5 (2%) 61 67	19, 23, 34, 47	0
All	All	1670/1780 (93%)	-0.14	21 (1%) 77 81	18, 23, 33, 47	2 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	3.0
2	F	200	ALA	3.0
2	D	219	ALA	2.7
2	H	219	ALA	2.6
2	F	94	GLY	2.6

5.2 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
1	CSD	A	115	8/9	0.99	0.15	-	17,17,18,18	0
1	CSD	C	115	8/9	0.99	0.16	-	18,18,18,19	0
1	CSD	E	115	8/9	0.98	0.11	-	17,18,18,18	0
1	CSD	E	117	8/9	0.98	0.11	-	18,18,18,19	0
1	CSD	C	117	8/9	0.98	0.14	-	18,18,18,19	0
1	CSD	A	117	8/9	0.99	0.13	-	18,18,18,19	0
1	CSD	G	117	8/9	0.98	0.13	-	18,18,18,19	0
1	CSD	G	115	8/9	0.98	0.12	-	18,18,18,18	0

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	G	212	6/6	0.90	0.15	1.36	20,21,21,22	0
3	GOL	A	212	6/6	0.91	0.15	0.20	20,20,21,21	0
3	GOL	C	212	6/6	0.91	0.14	0.06	20,21,21,22	0
3	GOL	E	212	6/6	0.96	0.11	-0.61	20,20,21,21	0
4	3CO	G	213	1/1	0.99	0.14	-	18,18,18,18	0
4	3CO	E	213	1/1	0.99	0.12	-	18,18,18,18	0
4	3CO	C	213	1/1	1.00	0.13	-	18,18,18,18	0
4	3CO	A	213	1/1	1.00	0.14	-	18,18,18,18	0

5.5 Other polymers [i](#)

There are no such residues in this entry.