



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2024 – 05:17 PM EDT

PDB ID : 2FFI
Title : Crystal Structure of Putative 2-Pyrone-4,6-Dicarboxylic Acid Hydrolase from *Pseudomonas putida*, Northeast Structural Genomics Target PpR23.
Authors : Forouhar, F.; Su, M.; Jayaraman, S.; Conover, K.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-12-19
Resolution : 2.61 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

<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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

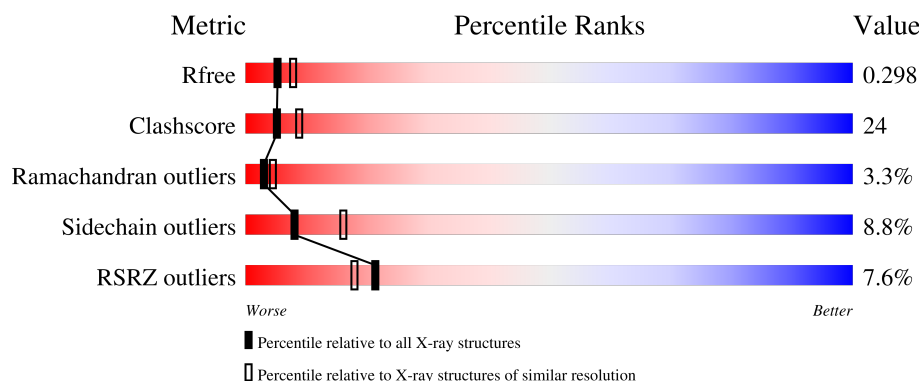
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (2.64-2.60)

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 $\leq 5\%$. 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	288	
1	B	288	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4331 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 2-pyrone-4,6-dicarboxylic acid hydrolase, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	Se	0	0	0
			2133	1347	394	385	2	5			
1	B	273	Total	C	N	O	S	Se	0	0	0
			2133	1347	394	385	2	5			

There are 30 discrepancies between the modelled and reference sequences:

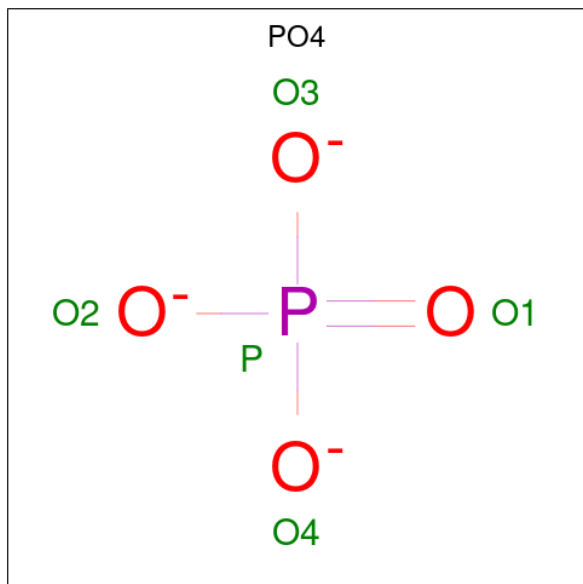
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q88M75
A	4	MSE	MET	modified residue	UNP Q88M75
A	88	MSE	MET	modified residue	UNP Q88M75
A	101	MSE	MET	modified residue	UNP Q88M75
A	114	MSE	MET	modified residue	UNP Q88M75
A	118	MSE	MET	modified residue	UNP Q88M75
A	232	MSE	MET	modified residue	UNP Q88M75
A	281	LEU	-	cloning artifact	UNP Q88M75
A	282	GLU	-	cloning artifact	UNP Q88M75
A	283	HIS	-	expression tag	UNP Q88M75
A	284	HIS	-	expression tag	UNP Q88M75
A	285	HIS	-	expression tag	UNP Q88M75
A	286	HIS	-	expression tag	UNP Q88M75
A	287	HIS	-	expression tag	UNP Q88M75
A	288	HIS	-	expression tag	UNP Q88M75
B	1	MSE	MET	modified residue	UNP Q88M75
B	4	MSE	MET	modified residue	UNP Q88M75
B	88	MSE	MET	modified residue	UNP Q88M75
B	101	MSE	MET	modified residue	UNP Q88M75
B	114	MSE	MET	modified residue	UNP Q88M75
B	118	MSE	MET	modified residue	UNP Q88M75
B	232	MSE	MET	modified residue	UNP Q88M75
B	281	LEU	-	cloning artifact	UNP Q88M75
B	282	GLU	-	cloning artifact	UNP Q88M75
B	283	HIS	-	expression tag	UNP Q88M75

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	284	HIS	-	expression tag	UNP Q88M75
B	285	HIS	-	expression tag	UNP Q88M75
B	286	HIS	-	expression tag	UNP Q88M75
B	287	HIS	-	expression tag	UNP Q88M75
B	288	HIS	-	expression tag	UNP Q88M75

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

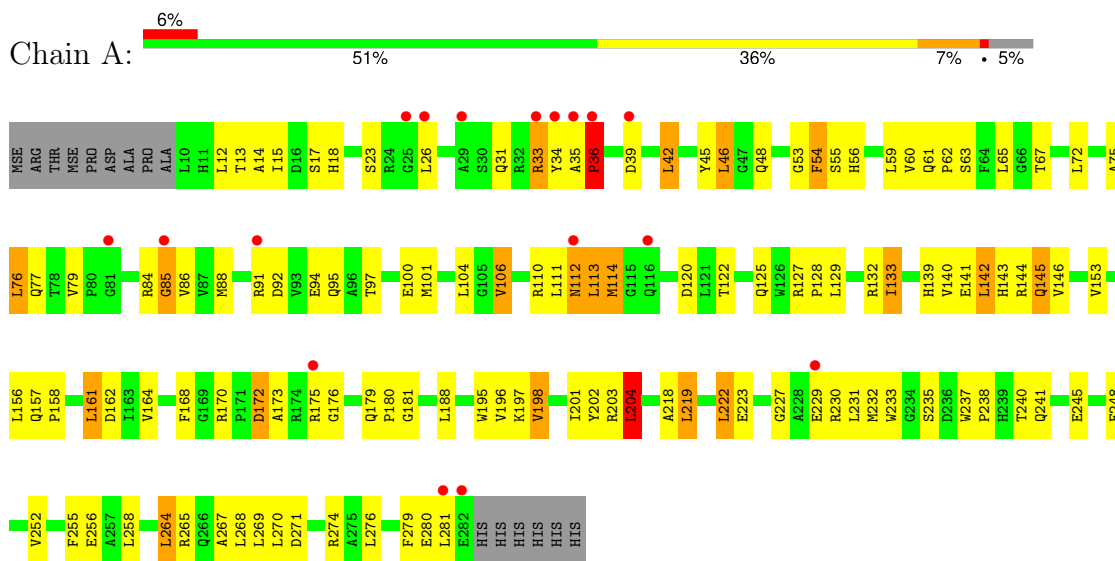
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	29	Total	O	0	0
			29	29		

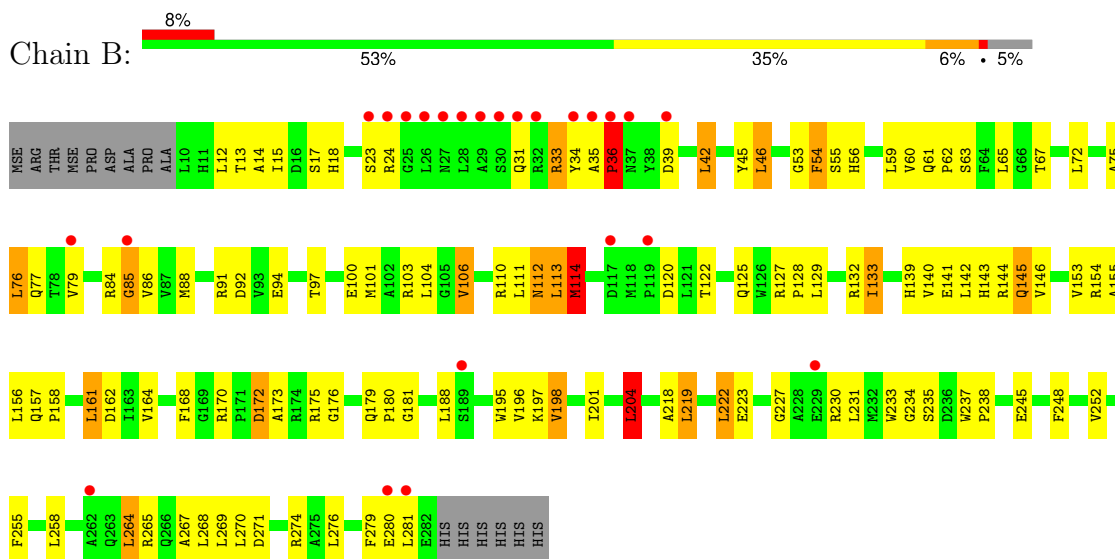
3 Residue-property plots [i](#)

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: 2-pyrone-4,6-dicarboxylic acid hydrolase, putative



- Molecule 1: 2-pyrone-4,6-dicarboxylic acid hydrolase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.39Å 46.29Å 64.08Å 80.86° 76.86° 80.61°	Depositor
Resolution (Å)	28.91 – 2.61 28.91 – 2.61	Depositor EDS
% Data completeness (in resolution range)	78.4 (28.91-2.61) 91.8 (28.91-2.61)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, R_{free}	0.228 , 0.287 0.249 , 0.298	Depositor DCC
R_{free} test set	1318 reflections (9.29%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4331	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.42	0/2177	0.60	0/2944
1	B	0.43	1/2177 (0.0%)	0.60	0/2944
All	All	0.43	1/4354 (0.0%)	0.60	0/5888

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	MSE	CG-SE	-5.20	1.77	1.95

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	2133	0	2095	103	0
1	B	2133	0	2095	101	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	26	0	0	2	0
3	B	29	0	0	2	0
All	All	4331	0	4190	204	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 24.

The worst 5 of 204 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:229:GLU:HG3	3:A:322:HOH:O	1.72	0.87
1:B:12:LEU:HD21	1:B:274:ARG:HD3	1.65	0.78
1:A:12:LEU:HD21	1:A:274:ARG:HD3	1.67	0.76
1:A:173:ALA:HB2	1:A:204:LEU:HB3	1.67	0.76
1:B:110:ARG:HD3	1:B:112:ASN:HB2	1.69	0.75

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	271/288 (94%)	229 (84%)	33 (12%)	9 (3%)	3	4
1	B	271/288 (94%)	231 (85%)	31 (11%)	9 (3%)	3	4
All	All	542/576 (94%)	460 (85%)	64 (12%)	18 (3%)	3	4

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	TYR
1	A	280	GLU
1	B	34	TYR
1	B	114	MSE
1	B	280	GLU

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	217/224 (97%)	198 (91%)	19 (9%)	8	16
1	B	217/224 (97%)	198 (91%)	19 (9%)	8	16
All	All	434/448 (97%)	396 (91%)	38 (9%)	8	16

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	142	LEU
1	B	222	LEU
1	B	145	GLN
1	B	198	VAL
1	B	264	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	ASN
1	B	143	HIS
1	B	254	GLN
1	B	217	GLN
1	B	136	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
2	PO4	A	301	-	4,4,4	1.78	2 (50%)	6,6,6	0.47	0
2	PO4	B	302	-	4,4,4	1.88	2 (50%)	6,6,6	0.46	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	PO4	P-O3	-2.25	1.48	1.54
2	B	302	PO4	P-O2	-2.14	1.48	1.54
2	A	301	PO4	P-O3	-2.07	1.48	1.54
2	A	301	PO4	P-O4	-2.01	1.48	1.54

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 ⓘ

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, 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	268/288 (93%)	0.59	17 (6%) 27 23	5, 23, 47, 51	0
1	B	268/288 (93%)	0.69	24 (8%) 17 14	4, 24, 48, 54	0
All	All	536/576 (93%)	0.64	41 (7%) 21 18	4, 24, 48, 54	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	GLY	9.0
1	B	39	ASP	5.4
1	B	30	SER	4.9
1	A	26	LEU	4.4
1	B	28	LEU	4.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	B-factors(\AA^2)	Q<0.9
2	PO4	B	302	5/5	0.96	0.07	15,18,18,21	0
2	PO4	A	301	5/5	0.97	0.07	15,16,17,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.