



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 10:01 pm BST

PDB ID : 2GTA
Title : Crystal Structure of the putative pyrophosphatase YPJD from *Bacillus subtilis*. Northeast Structural Genomics Consortium Target SR428.
Authors : Vorobiev, S.M.; Zhou, W.; Seetharaman, J.; Wang, D.; Ma, L.C.; Acton, T.; Xio, R.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2006-04-27
Resolution : 2.90 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 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 : 2.11
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) : 2.11

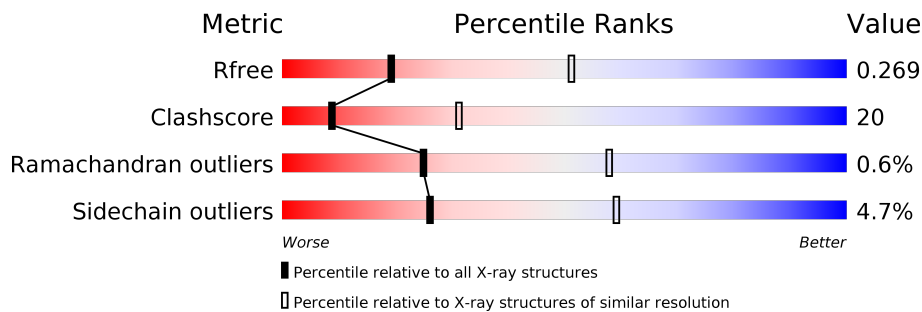
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	119	
1	B	119	
1	C	119	
1	D	119	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2968 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 Hypothetical protein ypjD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	98	767	478	129	153	1	6	0	0	0
1	B	96	748	468	129	144	1	6	0	0	0
1	C	86	666	420	114	126	1	5	0	0	0
1	D	97	757	474	128	149	1	5	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P42979
A	6	MSE	MET	MODIFIED RESIDUE	UNP P42979
A	30	MSE	MET	MODIFIED RESIDUE	UNP P42979
A	31	MSE	MET	MODIFIED RESIDUE	UNP P42979
A	63	MSE	MET	MODIFIED RESIDUE	UNP P42979
A	93	MSE	MET	MODIFIED RESIDUE	UNP P42979
A	112	LEU	-	EXPRESSION TAG	UNP P42979
A	113	GLU	-	EXPRESSION TAG	UNP P42979
A	114	HIS	-	EXPRESSION TAG	UNP P42979
A	115	HIS	-	EXPRESSION TAG	UNP P42979
A	116	HIS	-	EXPRESSION TAG	UNP P42979
A	117	HIS	-	EXPRESSION TAG	UNP P42979
A	118	HIS	-	EXPRESSION TAG	UNP P42979
A	119	HIS	-	EXPRESSION TAG	UNP P42979
B	1	MSE	MET	MODIFIED RESIDUE	UNP P42979
B	6	MSE	MET	MODIFIED RESIDUE	UNP P42979
B	30	MSE	MET	MODIFIED RESIDUE	UNP P42979
B	31	MSE	MET	MODIFIED RESIDUE	UNP P42979
B	63	MSE	MET	MODIFIED RESIDUE	UNP P42979
B	93	MSE	MET	MODIFIED RESIDUE	UNP P42979
B	112	LEU	-	EXPRESSION TAG	UNP P42979

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Chain	Residue	Modelled	Actual	Comment	Reference
B	113	GLU	-	EXPRESSION TAG	UNP P42979
B	114	HIS	-	EXPRESSION TAG	UNP P42979
B	115	HIS	-	EXPRESSION TAG	UNP P42979
B	116	HIS	-	EXPRESSION TAG	UNP P42979
B	117	HIS	-	EXPRESSION TAG	UNP P42979
B	118	HIS	-	EXPRESSION TAG	UNP P42979
B	119	HIS	-	EXPRESSION TAG	UNP P42979
C	1	MSE	MET	MODIFIED RESIDUE	UNP P42979
C	6	MSE	MET	MODIFIED RESIDUE	UNP P42979
C	30	MSE	MET	MODIFIED RESIDUE	UNP P42979
C	31	MSE	MET	MODIFIED RESIDUE	UNP P42979
C	63	MSE	MET	MODIFIED RESIDUE	UNP P42979
C	93	MSE	MET	MODIFIED RESIDUE	UNP P42979
C	112	LEU	-	EXPRESSION TAG	UNP P42979
C	113	GLU	-	EXPRESSION TAG	UNP P42979
C	114	HIS	-	EXPRESSION TAG	UNP P42979
C	115	HIS	-	EXPRESSION TAG	UNP P42979
C	116	HIS	-	EXPRESSION TAG	UNP P42979
C	117	HIS	-	EXPRESSION TAG	UNP P42979
C	118	HIS	-	EXPRESSION TAG	UNP P42979
C	119	HIS	-	EXPRESSION TAG	UNP P42979
D	1	MSE	MET	MODIFIED RESIDUE	UNP P42979
D	6	MSE	MET	MODIFIED RESIDUE	UNP P42979
D	30	MSE	MET	MODIFIED RESIDUE	UNP P42979
D	31	MSE	MET	MODIFIED RESIDUE	UNP P42979
D	63	MSE	MET	MODIFIED RESIDUE	UNP P42979
D	93	MSE	MET	MODIFIED RESIDUE	UNP P42979
D	112	LEU	-	EXPRESSION TAG	UNP P42979
D	113	GLU	-	EXPRESSION TAG	UNP P42979
D	114	HIS	-	EXPRESSION TAG	UNP P42979
D	115	HIS	-	EXPRESSION TAG	UNP P42979
D	116	HIS	-	EXPRESSION TAG	UNP P42979
D	117	HIS	-	EXPRESSION TAG	UNP P42979
D	118	HIS	-	EXPRESSION TAG	UNP P42979
D	119	HIS	-	EXPRESSION TAG	UNP P42979

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	2	Total O 2 2	0	0
3	C	10	Total O 10 10	0	0
3	D	5	Total O 5 5	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.75Å 79.69Å 119.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 2.90 49.01 – 2.38	Depositor EDS
% Data completeness (in resolution range)	80.1 (29.89-2.90) 86.8 (49.01-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.53 (at 2.37Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.263 0.233 , 0.269	Depositor DCC
R_{free} test set	1139 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtrriage
Anisotropy	1.245	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2968	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.39	0/773	0.58	0/1030
1	B	0.40	0/753	0.58	0/1002
1	C	0.39	0/670	0.57	0/893
1	D	0.44	0/760	0.69	2/1008 (0.2%)
All	All	0.40	0/2956	0.61	2/3933 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	LEU	CA-CB-CG	5.37	127.64	115.30
1	D	113	GLU	N-CA-C	5.26	125.19	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	767	0	725	36	0
1	B	748	0	703	39	0
1	C	666	0	619	28	0
1	D	757	0	712	50	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	9	0	0	1	0
3	B	2	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
All	All	2968	0	2759	116	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 20.

The worst 5 of 116 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:B:53:PRO:HD2	1:D:110:GLY:HA3	1.46	0.97
1:C:48:ARG:HB2	1:C:48:ARG:HH11	1.29	0.95
1:A:35:THR:HG21	1:B:35:THR:HG21	1.59	0.85
1:B:38:LEU:HD22	1:C:38:LEU:HD22	1.61	0.83
1:A:45:VAL:HG11	1:D:31:MSE:HE3	1.61	0.82

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	96/119 (81%)	90 (94%)	5 (5%)	1 (1%)	15	45
1	B	92/119 (77%)	88 (96%)	4 (4%)	0	100	100
1	C	82/119 (69%)	79 (96%)	3 (4%)	0	100	100
1	D	91/119 (76%)	86 (94%)	4 (4%)	1 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	361/476 (76%)	343 (95%)	16 (4%)	2 (1%)	25 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	110	GLY
1	A	96	PHE

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	80/100 (80%)	75 (94%)	5 (6%)	18 46
1	B	75/100 (75%)	72 (96%)	3 (4%)	31 65
1	C	66/100 (66%)	64 (97%)	2 (3%)	41 75
1	D	77/100 (77%)	73 (95%)	4 (5%)	23 55
All	All	298/400 (74%)	284 (95%)	14 (5%)	26 59

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	B	100	ASP
1	D	38	LEU
1	B	34	LEU
1	D	33	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	GLN
1	B	46	ASN
1	C	46	ASN

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Mol	Chain	Res	Type
1	B	10	GLN
1	C	19	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.

6.5 Other polymers

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