



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 10:21 pm BST

PDB ID : 7ZVY  
Title : Thermococcus kadokarensis phosphomannose isomerase  
Authors : Hoh, f.; Calio, A.  
Deposited on : 2022-05-17  
Resolution : 2.16 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](mailto: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>.

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

MolProbity : **FAILED**  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

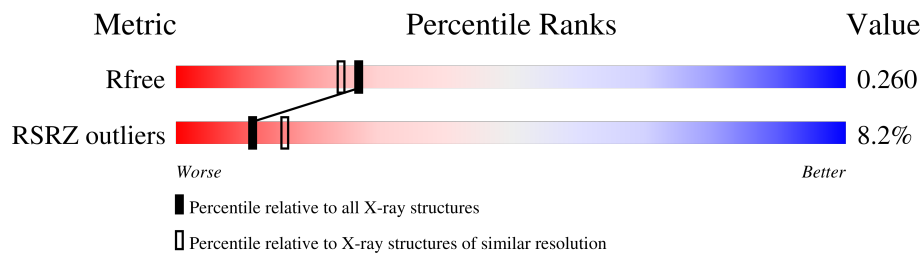
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7172 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 Cupin\_2 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	112	931	607	156	167	1	0	0	0
1	C	112	931	607	156	167	1	0	0	0
1	D	112	931	607	156	167	1	0	0	0
1	F	107	888	578	150	159	1	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	GLY	-	expression tag	UNP Q5JD98
A	115	SER	-	expression tag	UNP Q5JD98
A	116	PHE	-	expression tag	UNP Q5JD98
C	114	GLY	-	expression tag	UNP Q5JD98
C	115	SER	-	expression tag	UNP Q5JD98
C	116	PHE	-	expression tag	UNP Q5JD98
D	114	GLY	-	expression tag	UNP Q5JD98
D	115	SER	-	expression tag	UNP Q5JD98
D	116	PHE	-	expression tag	UNP Q5JD98
F	114	GLY	-	expression tag	UNP Q5JD98
F	115	SER	-	expression tag	UNP Q5JD98
F	116	PHE	-	expression tag	UNP Q5JD98

- Molecule 2 is a protein called Cupin\_2 domain-containing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	110	914	596	153	165	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	GLY	-	expression tag	UNP Q5JD98
B	115	SER	-	expression tag	UNP Q5JD98
B	116	PHE	-	expression tag	UNP Q5JD98

- Molecule 3 is a protein called Cupin\_2 domain-containing protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
3	E	106	Total	C	N	O	0	0	0
			883	576	148	159			
3	H	96	Total	C	N	O	0	0	0
			800	524	136	140			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	GLY	-	expression tag	UNP Q5JD98
E	115	SER	-	expression tag	UNP Q5JD98
E	116	PHE	-	expression tag	UNP Q5JD98
H	114	GLY	-	expression tag	UNP Q5JD98
H	115	SER	-	expression tag	UNP Q5JD98
H	116	PHE	-	expression tag	UNP Q5JD98

- Molecule 4 is a protein called Cupin\_2 domain-containing protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
4	G	101	Total	C	N	O	0	0	0
			840	550	139	151			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	114	GLY	-	expression tag	UNP Q5JD98
G	115	SER	-	expression tag	UNP Q5JD98
G	116	PHE	-	expression tag	UNP Q5JD98

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	F	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	B	6	Total	O	0	0
			6	6		
6	C	3	Total	O	0	0
			3	3		
6	D	5	Total	O	0	0
			5	5		
6	E	5	Total	O	0	0
			5	5		
6	F	13	Total	O	0	0
			13	13		
6	G	4	Total	O	0	0
			4	4		
6	H	3	Total	O	0	0
			3	3		

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### 3 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.16Å 91.16Å 113.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.79 – 2.16 64.79 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.1 (64.79-2.16) 98.3 (64.79-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.221 , 0.289 0.236 , 0.260	Depositor DCC
$R_{free}$ test set	2704 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.477 for -h,-k,l 0.469 for h,-h-k,-l 0.470 for -k,-h,-l	Xtrriage
Reported twinning fraction	0.288 for H, K, L 0.235 for K, H, -L 0.243 for -h,-k,l 0.233 for -K, -H, -L	Depositor
Outliers	0 of 55488 reflections	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 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.

#### 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 [i](#)

### 5.1 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	112/116 (96%)	0.81	13 (11%) 4 6	41, 62, 101, 135	0
1	C	112/116 (96%)	0.63	8 (7%) 16 22	42, 70, 104, 130	0
1	D	112/116 (96%)	0.95	13 (11%) 4 6	38, 60, 100, 124	0
1	F	107/116 (92%)	0.73	10 (9%) 8 13	41, 60, 94, 128	0
2	B	110/114 (96%)	0.73	7 (6%) 19 26	42, 63, 100, 119	0
3	E	106/110 (96%)	0.59	8 (7%) 14 19	42, 70, 102, 123	0
3	H	96/110 (87%)	0.67	6 (6%) 20 27	40, 64, 90, 105	0
4	G	101/105 (96%)	0.57	5 (4%) 28 37	44, 66, 99, 119	0
All	All	856/903 (94%)	0.71	70 (8%) 11 16	38, 64, 100, 135	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	LEU	10.6
2	B	112	LEU	5.8
1	A	110	VAL	5.7
1	D	110	VAL	5.7
2	B	110	VAL	5.5
1	F	107	ASP	5.2
1	F	45	TYR	5.1
1	D	109	SER	4.9
1	D	82	LYS	4.9
3	H	87	VAL	4.7
2	B	106	GLY	4.7
1	D	45	TYR	4.7
1	A	112	LEU	4.6
1	C	91	LYS	4.6
2	B	70	GLN	4.5
2	B	111	TRP	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	12	GLY	4.0
1	D	111	TRP	3.9
1	F	82	LYS	3.8
1	A	65	GLY	3.8
1	F	106	GLY	3.8
1	A	111	TRP	3.7
1	D	107	ASP	3.4
3	E	24	LEU	3.4
1	D	50	TYR	3.4
3	E	25	PRO	3.4
1	A	102	LEU	3.4
1	D	5	ILE	3.3
3	H	27	GLY	3.3
2	B	50	TYR	3.3
1	D	106	GLY	3.2
3	H	90	GLU	3.2
1	C	60	ALA	3.2
4	G	90	GLU	3.1
1	F	64	ILE	3.1
1	D	108	ASP	3.0
1	A	107	ASP	2.9
3	H	88	VAL	2.9
4	G	104	TYR	2.8
4	G	25	PRO	2.7
1	C	26	GLU	2.7
1	C	1	MET	2.6
1	F	105	HIS	2.5
1	F	50	TYR	2.5
3	H	45	TYR	2.5
1	F	65	GLY	2.5
1	D	47	GLU	2.4
2	B	45	TYR	2.4
1	A	82	LYS	2.3
3	E	91	LYS	2.3
1	D	65	GLY	2.3
3	E	45	TYR	2.2
1	C	89	ASN	2.2
1	F	53	PHE	2.2
1	A	6	LYS	2.2
1	C	25	PRO	2.2
1	A	45	TYR	2.1
3	E	103	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	19	LEU	2.1
1	A	101	LYS	2.1
1	A	59	GLU	2.1
3	E	104	TYR	2.1
1	C	5	ILE	2.1
1	A	79	VAL	2.0
1	A	53	PHE	2.0
1	F	93	GLU	2.0
3	E	95	PHE	2.0
4	G	89	ASN	2.0
4	G	93	GLU	2.0
3	H	38	LYS	2.0

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

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

## 5.3 Carbohydrates [i](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
5	ZN	G	201	1/1	0.95	0.04	50,50,50,50	0
5	ZN	A	201	1/1	0.98	0.04	50,50,50,50	0
5	ZN	A	202	1/1	0.99	0.07	50,50,50,50	0
5	ZN	F	201	1/1	1.00	0.04	50,50,50,50	0

## 5.5 Other polymers [i](#)

There are no such residues in this entry.