

Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2023 – 06:35 PM EST

PDB ID : 3FKJ

Title: Crystal structure of a putative phosphosugar isomerase (stm 0572) from

salmonella typhimurium lt2 at 2.12 A resolution

Authors : Joint Center for Structural Genomics (JCSG)

Deposited on : 2008-12-16

Resolution : 2.12 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 (i) 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 (1)) 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 : 2.31.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

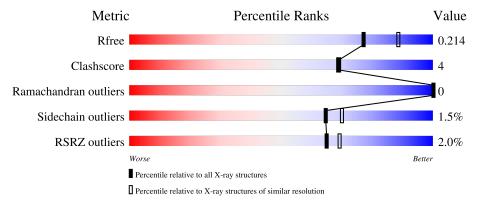
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.12 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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% 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	347	88%	8%	
1	В	347	84%	10%	7%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5520 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 Putative phosphosugar isomerases.

\mathbf{Mol}	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	335	Total 2647	C 1690		O 495			0	1	0
1	В	324	Total 2551	C 1632		O 475		Se 5	0	1	0

There are 38 discrepancies between the modelled and reference sequences:

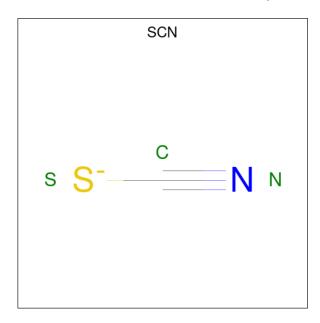
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	expression tag	UNP Q8ZR50
A	-17	GLY	-	expression tag	UNP Q8ZR50
A	-16	SER	-	expression tag	UNP Q8ZR50
A	-15	ASP	-	expression tag	UNP Q8ZR50
A	-14	LYS	-	expression tag	UNP Q8ZR50
A	-13	ILE	-	expression tag	UNP Q8ZR50
A	-12	HIS	-	expression tag	UNP Q8ZR50
A	-11	HIS	-	expression tag	UNP Q8ZR50
A	-10	HIS	-	expression tag	UNP Q8ZR50
A	-9	HIS	-	expression tag	UNP Q8ZR50
A	-8	HIS	-	expression tag	UNP Q8ZR50
A	-7	HIS	-	expression tag	UNP Q8ZR50
A	-6	GLU	-	expression tag	UNP Q8ZR50
A	-5	ASN	-	expression tag	UNP Q8ZR50
A	-4	LEU	-	expression tag	UNP Q8ZR50
A	-3	TYR	-	expression tag	UNP Q8ZR50
A	-2	PHE	-	expression tag	UNP Q8ZR50
A	-1	GLN	-	expression tag	UNP Q8ZR50
A	0	GLY	-	expression tag	UNP Q8ZR50
В	-18	MSE	-	expression tag	UNP Q8ZR50
В	-17	GLY	-	expression tag	UNP Q8ZR50
В	-16	SER	-	expression tag	UNP Q8ZR50
В	-15	ASP	-	expression tag	UNP Q8ZR50
В	-14	LYS	-	expression tag	UNP Q8ZR50
В	-13	ILE	-	expression tag	UNP Q8ZR50



 $Continued\ from\ previous\ page...$

Chain	Residue	Modelled	Actual	Comment	Reference
В	-12	HIS	-	expression tag	UNP Q8ZR50
В	-11	HIS	-	expression tag	UNP Q8ZR50
В	-10	HIS	-	expression tag	UNP Q8ZR50
В	-9	HIS	_	expression tag	UNP Q8ZR50
В	-8	HIS	-	expression tag	UNP Q8ZR50
В	-7	HIS	-	expression tag	UNP Q8ZR50
В	-6	GLU	-	expression tag	UNP Q8ZR50
В	-5	ASN	-	expression tag	UNP Q8ZR50
В	-4	LEU	-	expression tag	UNP Q8ZR50
В	-3	TYR	-	expression tag	UNP Q8ZR50
В	-2	PHE	-	expression tag	UNP Q8ZR50
В	-1	GLN	-	expression tag	UNP Q8ZR50
В	0	GLY	-	expression tag	UNP Q8ZR50

• Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mo	Chair	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total C N S 3 1 1 1	S 1	0	0
2	В	1	Total C N S 3 1 1	S 1	0	0

• Molecule 3 is water.

\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	173	Total O 173 173	0	0



 $Continued\ from\ previous\ page...$

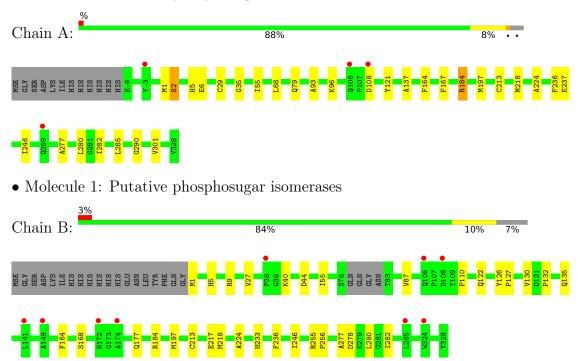
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	В	143	Total C 143 14	3	0	0



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: Putative phosphosugar isomerases





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	63.88Å 63.88Å 295.93Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.32 - 2.12	Depositor
Resolution (A)	29.32 - 2.12	EDS
% Data completeness	98.9 (29.32-2.12)	Depositor
(in resolution range)	98.9 (29.32-2.12)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.14 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
D.D.	0.165 , 0.212	Depositor
R, R_{free}	0.167 , 0.214	DCC
R_{free} test set	1899 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 46.4	EDS
L-test for twinning ²	$< L > = 0.46, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	0.093 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5520	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: SCN

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.69	0/2710	0.72	$2/3670 \ (0.1\%)$	
1	В	0.69	0/2612	0.70	1/3539 (0.0%)	
All	All	0.69	0/5322	0.71	3/7209 (0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Atoms Z		$\operatorname{Ideal}({}^{o})$
1	В	184	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	184	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	A	184	ARG	NE-CZ-NH1	-5.53	117.54	120.30

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	2647	0	2565	19	0
1	В	2551	0	2476	22	0
2	A	3	0	0	0	0
2	В	3	0	0	0	0
3	A	173	0	0	3	0
3	В	143	0	0	0	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5520	0	5041	38	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 4.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
1 D 100 CI M HD2	1 D 120 VAI II/01	distance (Å)	overlap (Å)
1:B:122:GLN:HB3	1:B:130:VAL:HG21	1.51	0.93
1:B:122:GLN:HB3	1:B:130:VAL:CG2	2.08	0.84
1:B:1:MSE:HE1	1:B:9[B]:ARG:NE	2.00	0.75
1:B:1:MSE:HE1	1:B:9[A]:ARG:HD3	1.78	0.66
1:A:282:ILE:HD13	1:A:285:LEU:HD12	1.78	0.65
1:A:277:ALA:HB1	1:A:282:ILE:HG13	1.91	0.53
1:B:1:MSE:HE2	1:B:5:HIS:CE1	2.43	0.53
1:A:1:MSE:HE1	3:A:608:HOH:O	2.07	0.53
1:B:177:GLN:NE2	1:B:280:LEU:HD23	2.23	0.53
1:A:213:CYS:O	1:A:218:MSE:HG3	2.08	0.52
1:A:55:ILE:HD12	3:A:476:HOH:O	2.10	0.52
1:A:79:GLN:HA	1:A:121:TYR:OH	2.12	0.49
1:B:122:GLN:HB3	1:B:130:VAL:HG22	1.93	0.49
1:A:167:PHE:HA	1:A:285:LEU:HD21	1.95	0.48
1:B:132:PRO:HG2	1:B:168:SER:HA	1.94	0.48
1:A:280:LEU:HD13	1:A:301:VAL:HG21	1.96	0.47
1:A:68:LEU:HD21	1:A:93:ALA:HA	1.96	0.47
1:B:40:LYS:NZ	1:B:44:ASP:OD2	2.44	0.47
1:A:29:CYS:HB3	1:B:233:HIS:CG	2.50	0.46
1:B:126:TYR:CG	1:B:127:PRO:HA	2.51	0.46
1:A:224:ALA:HB2	1:B:224:ALA:HB2	1.98	0.45
1:B:255:ARG:N	1:B:256:PRO:CD	2.80	0.45
1:A:1:MSE:HE3	1:A:6:GLU:CD	2.38	0.44
1:A:2:SER:HB3	1:A:5:HIS:H	1.83	0.44
1:B:27:VAL:HG22	1:B:55:ILE:CG2	2.48	0.43
1:B:126:TYR:CD1	1:B:127:PRO:HA	2.52	0.43
1:A:282:ILE:HD12	1:A:290:GLY:O	2.19	0.43
1:B:277:ALA:HB1	1:B:282:ILE:HG13	2.00	0.43
1:B:197:MSE:SE	1:B:246:ILE:HB	2.70	0.42
1:B:213:CYS:O	1:B:218:MSE:HG3	2.19	0.42
1:A:197:MSE:SE	1:A:246:ILE:HB	2.70	0.42
1:A:2:SER:HB2	1:A:5:HIS:HB2	2.01	0.41
1:A:237:GLU:HB2	1:B:217:GLU:HA	2.03	0.41
			ed on next page



Continued from previous page...

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:35:GLY:O	1:A:137:ALA:HA	2.21	0.41
1:A:96:LYS:NZ	3:A:556:HOH:O	2.54	0.40
1:B:87:VAL:HG21	1:B:110:PRO:HB2	2.03	0.40
1:B:1:MSE:HE2	1:B:5:HIS:NE2	2.36	0.40
1:B:130:VAL:HG12	1:B:135:GLN:HE21	1.86	0.40

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	Perce	entiles
1	A	334/347~(96%)	325 (97%)	9 (3%)	0	100	100
1	В	321/347 (92%)	313 (98%)	8 (2%)	0	100	100
All	All	655/694~(94%)	638 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	273/280 (98%)	268 (98%)	5 (2%)	59 63
1	В	261/280 (93%)	258 (99%)	3 (1%)	73 79
All	All	534/560 (95%)	526 (98%)	8 (2%)	65 70



All	(8)	residues	with	a non-rotan	neric sic	dechain	are listed	below:
-----	-----	----------	------	-------------	-----------	---------	------------	--------

Mol	Chain	Res	Type
1	A	2	SER
1	A	108	ASP
1	A	164	PHE
1	A	184	ARG
1	A	236	PHE
1	В	164	PHE
1	В	236	PHE
1	В	278	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	135	GLN
1	В	156	GLN
1	В	177	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 monosaccharides 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	Trunc	Chain	Dag	Timle	В	ond leng	gths	В	ond ang	gles
MIOI	ol Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SCN	A	329	-	1,2,2	0.55	0	0,1,1	-	-
2	SCN	В	329	-	1,2,2	0.82	0	0,1,1	-	-

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 (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, 95^{th} 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	$OWAB(A^2)$	Q < 0.9
1	A	330/347 (95%)	-0.01	4 (1%) 79 82	28, 34, 50, 62	0
1	В	319/347 (91%)	0.16	9 (2%) 53 59	28, 34, 48, 62	0
All	All	649/694 (93%)	0.07	13 (2%) 65 69	28, 34, 49, 62	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	108	ASP	2.9
1	A	-3	TYR	2.7
1	В	172	HIS	2.6
1	A	269	GLN	2.6
1	В	141	LEU	2.6
1	В	174	ALA	2.5
1	A	108	ASP	2.4
1	В	285	LEU	2.3
1	В	149	ALA	2.2
1	В	38	PRO	2.1
1	A	106	GLN	2.1
1	В	324	TRP	2.1
1	В	106	GLN	2.0

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	SCN	В	329	3/3	0.97	0.06	41,41,43,46	0
2	SCN	A	329	3/3	0.98	0.09	29,29,31,35	0

6.5 Other polymers (i)

There are no such residues in this entry.

