



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:12 PM GMT

PDB ID : 1JB1
Title : Lactobacillus casei HprK/P Bound to Phosphate
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Deposited on : 2001-06-01
Resolution : 2.80 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
<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 : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

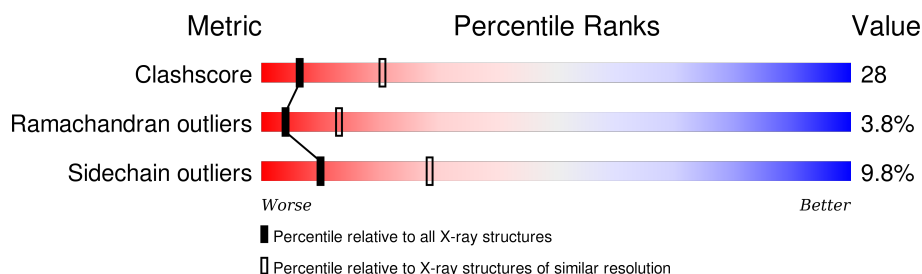
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	205	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1236 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 HPRK PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	Se	0	0	0
			1181	750	204	223	4			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	MSE	-	EXPRESSION TAG	UNP Q9RE09
A	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
A	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
A	118	SER	-	EXPRESSION TAG	UNP Q9RE09
A	119	HIS	-	EXPRESSION TAG	UNP Q9RE09
A	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
A	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
A	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
A	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
A	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
A	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
A	126	SER	-	EXPRESSION TAG	UNP Q9RE09
A	127	MSE	-	EXPRESSION TAG	UNP Q9RE09
A	139	MSE	MET	MODIFIED RESIDUE	UNP Q9RE09
A	214	MSE	MET	MODIFIED RESIDUE	UNP Q9RE09
A	282	MSE	MET	MODIFIED RESIDUE	UNP Q9RE09
A	289	MSE	MET	MODIFIED RESIDUE	UNP Q9RE09

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



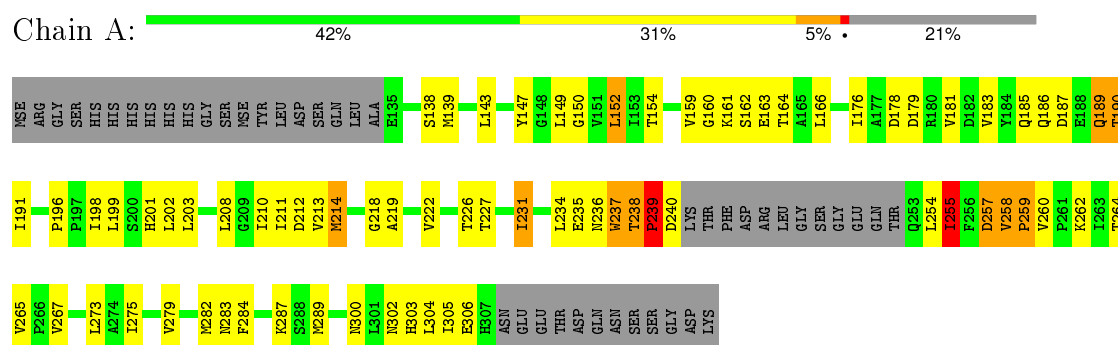
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		

Note EDS was not executed.

- Molecule 1: HPRK PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	107.74Å 107.74Å 66.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1236	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

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: 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	0.38	0/1191	0.67	1/1614 (0.1%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	239	PRO	N-CA-CB	5.52	109.92	103.30

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	1181	0	1177	65	0
2	A	5	0	0	0	0
3	A	50	0	0	1	0
All	All	1236	0	1177	65	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 28.

All (65) 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:237:TRP:HE3	1:A:238:THR:H	1.31	0.79
1:A:191:ILE:HD11	1:A:258:VAL:HG21	1.64	0.76
1:A:235:GLU:HG2	1:A:236:ASN:H	1.48	0.76
1:A:139:MSE:HE3	1:A:183:VAL:HG11	1.70	0.73
1:A:187:ASP:HB3	1:A:189:GLN:HE22	1.55	0.71
1:A:255:ILE:HG22	1:A:260:VAL:N	2.07	0.69
1:A:305:ILE:HG22	1:A:306:GLU:OE2	1.93	0.69
1:A:202:LEU:HD13	1:A:210:ILE:HD11	1.76	0.68
1:A:304:LEU:HD12	1:A:304:LEU:H	1.58	0.67
1:A:187:ASP:HB2	1:A:190:THR:HG23	1.76	0.66
1:A:196:PRO:HD2	1:A:199:LEU:HD12	1.77	0.65
1:A:258:VAL:O	1:A:258:VAL:HG12	1.97	0.64
1:A:258:VAL:HG22	3:A:406:HOH:O	1.98	0.64
1:A:191:ILE:HD11	1:A:258:VAL:CG2	2.28	0.62
1:A:139:MSE:HE3	1:A:183:VAL:CG1	2.28	0.61
1:A:208:LEU:HD12	1:A:211:ILE:HD11	1.85	0.58
1:A:201:HIS:ND1	1:A:214:MSE:HG3	2.18	0.58
1:A:152:LEU:HD13	1:A:154:THR:HG23	1.85	0.58
1:A:139:MSE:CE	1:A:183:VAL:HG11	2.33	0.56
1:A:257:ASP:O	1:A:258:VAL:HG23	2.05	0.56
1:A:235:GLU:CG	1:A:236:ASN:H	2.19	0.55
1:A:150:GLY:HA3	1:A:227:THR:O	2.06	0.55
1:A:234:LEU:HD23	1:A:265:VAL:CG2	2.37	0.54
1:A:185:GLN:HG2	1:A:187:ASP:O	2.08	0.54
1:A:254:LEU:C	1:A:255:ILE:HG12	2.27	0.54
1:A:231:ILE:HG12	1:A:262:LYS:HG3	1.91	0.53
1:A:201:HIS:CE1	1:A:214:MSE:HG3	2.43	0.53
1:A:214:MSE:HE3	1:A:219:ALA:N	2.24	0.53
1:A:238:THR:HG22	1:A:239:PRO:N	2.24	0.52
1:A:187:ASP:HB3	1:A:189:GLN:NE2	2.22	0.52
1:A:235:GLU:O	1:A:267:VAL:HG23	2.09	0.52
1:A:152:LEU:HD13	1:A:154:THR:CG2	2.40	0.52
1:A:149:LEU:HD11	1:A:284:PHE:CE2	2.46	0.51
1:A:160:GLY:HA2	1:A:163:GLU:OE2	2.11	0.50
1:A:176:ILE:HG12	1:A:226:THR:HG22	1.93	0.50
1:A:160:GLY:O	1:A:164:THR:HG22	2.11	0.50
1:A:159:VAL:HG22	1:A:267:VAL:HG21	1.95	0.49
1:A:186:GLN:HB3	1:A:190:THR:OG1	2.14	0.48
1:A:214:MSE:HE3	1:A:218:GLY:C	2.34	0.48
1:A:304:LEU:N	1:A:304:LEU:HD12	2.26	0.48
1:A:162:SER:HB3	1:A:203:LEU:HD21	1.96	0.47
1:A:202:LEU:CD1	1:A:210:ILE:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LYS:O	1:A:164:THR:HG22	2.15	0.46
1:A:212:ASP:OD1	1:A:212:ASP:C	2.54	0.46
1:A:300:ASN:O	1:A:303:HIS:HB3	2.16	0.45
1:A:161:LYS:O	1:A:164:THR:CG2	2.64	0.45
1:A:187:ASP:CB	1:A:189:GLN:HE22	2.27	0.45
1:A:275:ILE:O	1:A:279:VAL:HG23	2.18	0.44
1:A:147:TYR:HE1	1:A:282:MSE:HG3	1.83	0.43
1:A:147:TYR:CE1	1:A:282:MSE:HG3	2.53	0.43
1:A:264:THR:O	1:A:264:THR:HG23	2.19	0.43
1:A:212:ASP:OD1	1:A:214:MSE:N	2.52	0.43
1:A:139:MSE:CE	1:A:183:VAL:HG21	2.48	0.43
1:A:138:SER:HA	1:A:181:VAL:O	2.19	0.43
1:A:302:ASN:O	1:A:303:HIS:C	2.58	0.42
1:A:159:VAL:CG2	1:A:267:VAL:HG21	2.49	0.42
1:A:255:ILE:HG22	1:A:260:VAL:C	2.40	0.42
1:A:189:GLN:NE2	1:A:189:GLN:N	2.67	0.41
1:A:178:ASP:O	1:A:179:ASP:HB2	2.19	0.41
1:A:304:LEU:CD1	1:A:304:LEU:H	2.31	0.41
1:A:273:LEU:N	1:A:273:LEU:HD12	2.35	0.41
1:A:239:PRO:O	1:A:240:ASP:CB	2.69	0.41
1:A:287:LYS:O	1:A:289:MSE:N	2.53	0.41
1:A:213:VAL:HG23	1:A:222:VAL:CG1	2.51	0.40
1:A:187:ASP:CB	1:A:189:GLN:NE2	2.84	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	Percentiles
1	A	157/205 (77%)	130 (83%)	21 (13%)	6 (4%)	4 13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	THR
1	A	239	PRO
1	A	257	ASP
1	A	258	VAL
1	A	259	PRO
1	A	255	ILE

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	122/168 (73%)	110 (90%)	12 (10%)	10	28

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	152	LEU
1	A	166	LEU
1	A	189	GLN
1	A	190	THR
1	A	198	ILE
1	A	214	MSE
1	A	231	ILE
1	A	237	TRP
1	A	255	ILE
1	A	259	PRO
1	A	283	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	186	GLN
1	A	189	GLN
1	A	215	ASN

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Mol	Chain	Res	Type
1	A	283	ASN
1	A	300	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	400	-	4,4,4	1.02	0	6,6,6	0.27	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
2	PO4	A	400	-	-	0/0/0/0	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.

5.7 Other polymers

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.