



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:26 AM GMT

PDB ID : 2QMH
Title : structure of V267F mutant HprK/P
Authors : Chaptal, V.; Vincent F.; Gueguen-Chaignon, V.; Poncet, S.; Deutscher, J.;
Nessler, S.; Morera, S.
Deposited on : 2007-07-16
Resolution : 2.60 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
<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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

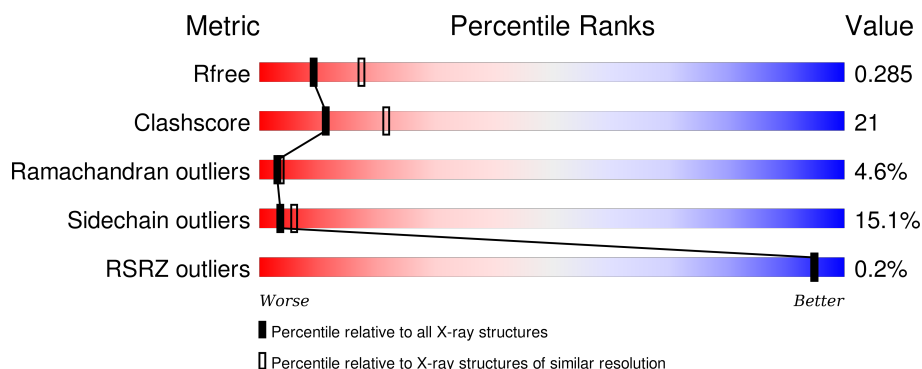
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 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.

Mol	Chain	Length	Quality of chain
1	A	205	 46% 24% 7% 21%
1	B	205	 55% 27% 5% 12%
1	C	205	 50% 24% 6% 20%
1	D	205	 54% 25% 8% 12%
1	E	205	 41% 33% 6% 20%

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Mol	Chain	Length	Quality of chain
1	F	205	<div><div></div><div>38%33%6%22%</div></div>
1	G	205	<div><div></div><div>42%26%9%22%</div></div>
1	H	205	<div><div></div><div>55%22%10%13%</div></div>
1	I	205	<div><div></div><div>43%27%6%22%</div></div>
1	J	205	<div><div></div><div>54%23%9%13%</div></div>
1	K	205	<div><div></div><div>40%30%8%21%</div></div>
1	L	205	<div><div></div><div>%47%22%8%21%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15591 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 HPr kinase/phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1242	787	218	233	4			
1	B	181	Total	C	N	O	S	0	0	0
			1405	887	245	269	4			
1	C	164	Total	C	N	O	S	0	0	0
			1269	806	223	236	4			
1	D	181	Total	C	N	O	S	0	0	0
			1405	887	245	269	4			
1	E	164	Total	C	N	O	S	0	0	0
			1265	799	222	240	4			
1	F	160	Total	C	N	O	S	0	0	0
			1235	783	215	233	4			
1	G	160	Total	C	N	O	S	0	0	0
			1238	785	217	232	4			
1	H	178	Total	C	N	O	S	0	0	0
			1380	872	241	263	4			
1	I	160	Total	C	N	O	S	0	0	0
			1238	785	217	232	4			
1	J	178	Total	C	N	O	S	0	0	0
			1383	873	241	265	4			
1	K	162	Total	C	N	O	S	0	0	0
			1250	791	220	235	4			
1	L	161	Total	C	N	O	S	0	0	0
			1246	789	219	234	4			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	MET	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	MET	-	EXPRESSION TAG	UNP Q9RE09
A	267	PHE	VAL	ENGINEERED	UNP Q9RE09
B	115	MET	-	EXPRESSION TAG	UNP Q9RE09
B	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
B	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
B	118	SER	-	EXPRESSION TAG	UNP Q9RE09
B	119	HIS	-	EXPRESSION TAG	UNP Q9RE09
B	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
B	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
B	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
B	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
B	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
B	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
B	126	SER	-	EXPRESSION TAG	UNP Q9RE09
B	127	MET	-	EXPRESSION TAG	UNP Q9RE09
B	267	PHE	VAL	ENGINEERED	UNP Q9RE09
C	115	MET	-	EXPRESSION TAG	UNP Q9RE09
C	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
C	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
C	118	SER	-	EXPRESSION TAG	UNP Q9RE09
C	119	HIS	-	EXPRESSION TAG	UNP Q9RE09
C	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
C	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
C	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
C	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
C	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
C	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
C	126	SER	-	EXPRESSION TAG	UNP Q9RE09
C	127	MET	-	EXPRESSION TAG	UNP Q9RE09
C	267	PHE	VAL	ENGINEERED	UNP Q9RE09
D	115	MET	-	EXPRESSION TAG	UNP Q9RE09
D	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
D	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
D	118	SER	-	EXPRESSION TAG	UNP Q9RE09
D	119	HIS	-	EXPRESSION TAG	UNP Q9RE09

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Chain	Residue	Modelled	Actual	Comment	Reference
D	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
D	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
D	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
D	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
D	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
D	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
D	126	SER	-	EXPRESSION TAG	UNP Q9RE09
D	127	MET	-	EXPRESSION TAG	UNP Q9RE09
D	267	PHE	VAL	ENGINEERED	UNP Q9RE09
E	115	MET	-	EXPRESSION TAG	UNP Q9RE09
E	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
E	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
E	118	SER	-	EXPRESSION TAG	UNP Q9RE09
E	119	HIS	-	EXPRESSION TAG	UNP Q9RE09
E	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
E	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
E	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
E	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
E	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
E	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
E	126	SER	-	EXPRESSION TAG	UNP Q9RE09
E	127	MET	-	EXPRESSION TAG	UNP Q9RE09
E	267	PHE	VAL	ENGINEERED	UNP Q9RE09
F	115	MET	-	EXPRESSION TAG	UNP Q9RE09
F	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
F	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
F	118	SER	-	EXPRESSION TAG	UNP Q9RE09
F	119	HIS	-	EXPRESSION TAG	UNP Q9RE09
F	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
F	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
F	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
F	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
F	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
F	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
F	126	SER	-	EXPRESSION TAG	UNP Q9RE09
F	127	MET	-	EXPRESSION TAG	UNP Q9RE09
F	267	PHE	VAL	ENGINEERED	UNP Q9RE09
G	115	MET	-	EXPRESSION TAG	UNP Q9RE09
G	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
G	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
G	118	SER	-	EXPRESSION TAG	UNP Q9RE09
G	119	HIS	-	EXPRESSION TAG	UNP Q9RE09

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Chain	Residue	Modelled	Actual	Comment	Reference
G	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
G	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
G	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
G	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
G	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
G	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
G	126	SER	-	EXPRESSION TAG	UNP Q9RE09
G	127	MET	-	EXPRESSION TAG	UNP Q9RE09
G	267	PHE	VAL	ENGINEERED	UNP Q9RE09
H	115	MET	-	EXPRESSION TAG	UNP Q9RE09
H	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
H	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
H	118	SER	-	EXPRESSION TAG	UNP Q9RE09
H	119	HIS	-	EXPRESSION TAG	UNP Q9RE09
H	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
H	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
H	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
H	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
H	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
H	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
H	126	SER	-	EXPRESSION TAG	UNP Q9RE09
H	127	MET	-	EXPRESSION TAG	UNP Q9RE09
H	267	PHE	VAL	ENGINEERED	UNP Q9RE09
I	115	MET	-	EXPRESSION TAG	UNP Q9RE09
I	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
I	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
I	118	SER	-	EXPRESSION TAG	UNP Q9RE09
I	119	HIS	-	EXPRESSION TAG	UNP Q9RE09
I	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
I	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
I	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
I	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
I	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
I	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
I	126	SER	-	EXPRESSION TAG	UNP Q9RE09
I	127	MET	-	EXPRESSION TAG	UNP Q9RE09
I	267	PHE	VAL	ENGINEERED	UNP Q9RE09
J	115	MET	-	EXPRESSION TAG	UNP Q9RE09
J	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
J	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
J	118	SER	-	EXPRESSION TAG	UNP Q9RE09
J	119	HIS	-	EXPRESSION TAG	UNP Q9RE09

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Chain	Residue	Modelled	Actual	Comment	Reference
J	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
J	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
J	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
J	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
J	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
J	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
J	126	SER	-	EXPRESSION TAG	UNP Q9RE09
J	127	MET	-	EXPRESSION TAG	UNP Q9RE09
J	267	PHE	VAL	ENGINEERED	UNP Q9RE09
K	115	MET	-	EXPRESSION TAG	UNP Q9RE09
K	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
K	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
K	118	SER	-	EXPRESSION TAG	UNP Q9RE09
K	119	HIS	-	EXPRESSION TAG	UNP Q9RE09
K	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
K	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
K	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
K	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
K	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
K	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
K	126	SER	-	EXPRESSION TAG	UNP Q9RE09
K	127	MET	-	EXPRESSION TAG	UNP Q9RE09
K	267	PHE	VAL	ENGINEERED	UNP Q9RE09
L	115	MET	-	EXPRESSION TAG	UNP Q9RE09
L	116	ARG	-	EXPRESSION TAG	UNP Q9RE09
L	117	GLY	-	EXPRESSION TAG	UNP Q9RE09
L	118	SER	-	EXPRESSION TAG	UNP Q9RE09
L	119	HIS	-	EXPRESSION TAG	UNP Q9RE09
L	120	HIS	-	EXPRESSION TAG	UNP Q9RE09
L	121	HIS	-	EXPRESSION TAG	UNP Q9RE09
L	122	HIS	-	EXPRESSION TAG	UNP Q9RE09
L	123	HIS	-	EXPRESSION TAG	UNP Q9RE09
L	124	HIS	-	EXPRESSION TAG	UNP Q9RE09
L	125	GLY	-	EXPRESSION TAG	UNP Q9RE09
L	126	SER	-	EXPRESSION TAG	UNP Q9RE09
L	127	MET	-	EXPRESSION TAG	UNP Q9RE09
L	267	PHE	VAL	ENGINEERED	UNP Q9RE09

- Molecule 2 is water.

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

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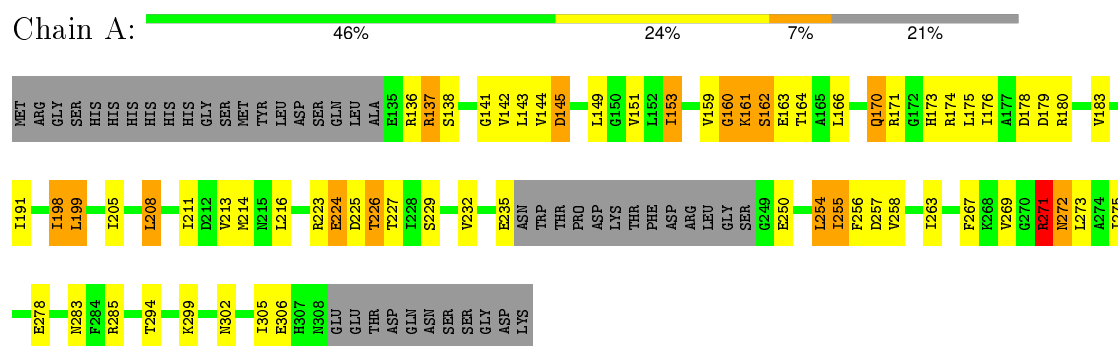
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	O 2	0	0
2	C	3	Total 3	O 3	0	0
2	D	2	Total 2	O 2	0	0
2	F	3	Total 3	O 3	0	0
2	G	10	Total 10	O 10	0	0
2	H	6	Total 6	O 6	0	0
2	I	4	Total 4	O 4	0	0
2	K	1	Total 1	O 1	0	0
2	L	3	Total 3	O 3	0	0

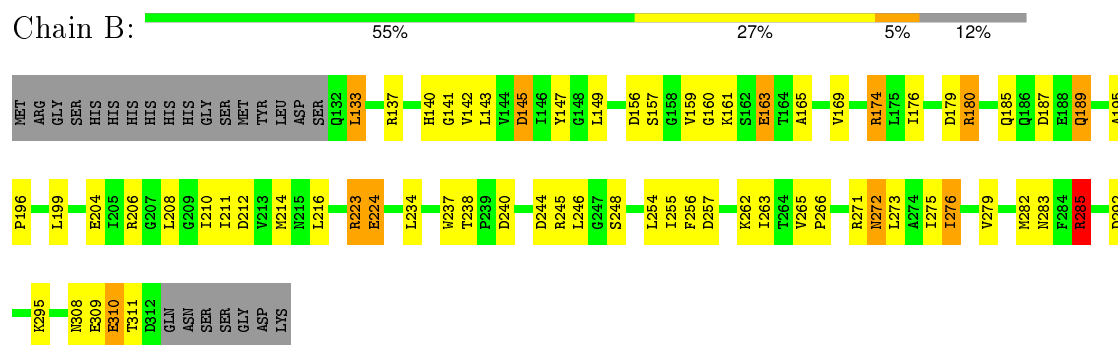
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

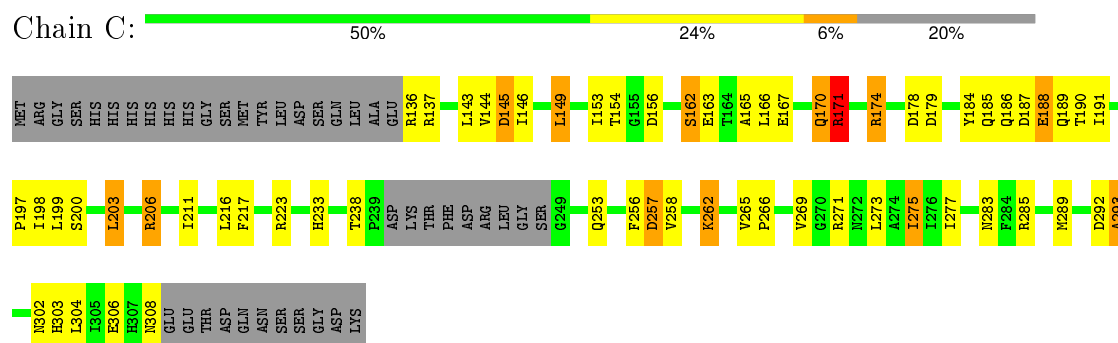
- Molecule 1: HPr kinase/phosphorylase



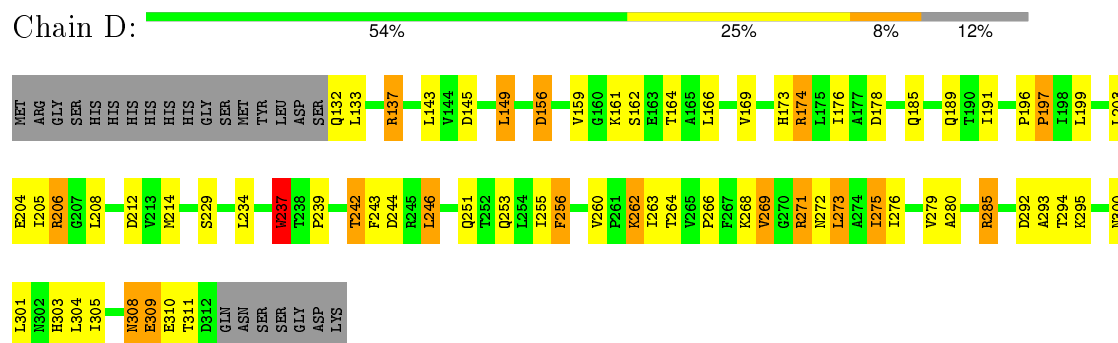
- Molecule 1: HPr kinase/phosphorylase



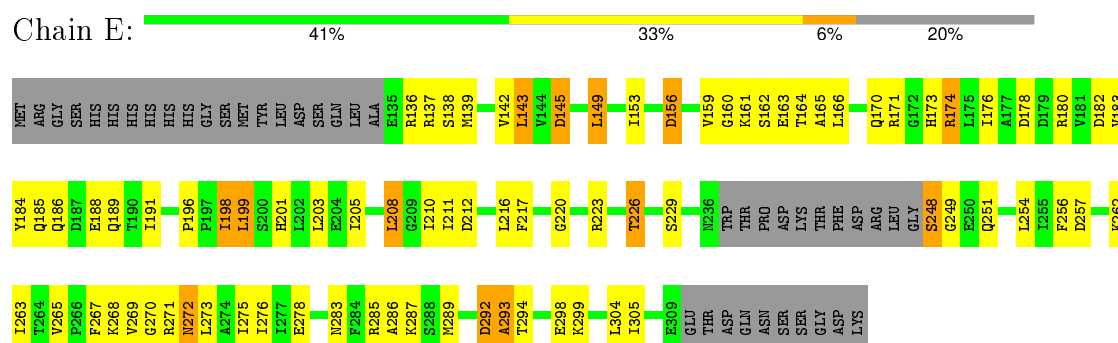
- Molecule 1: HPr kinase/phosphorylase



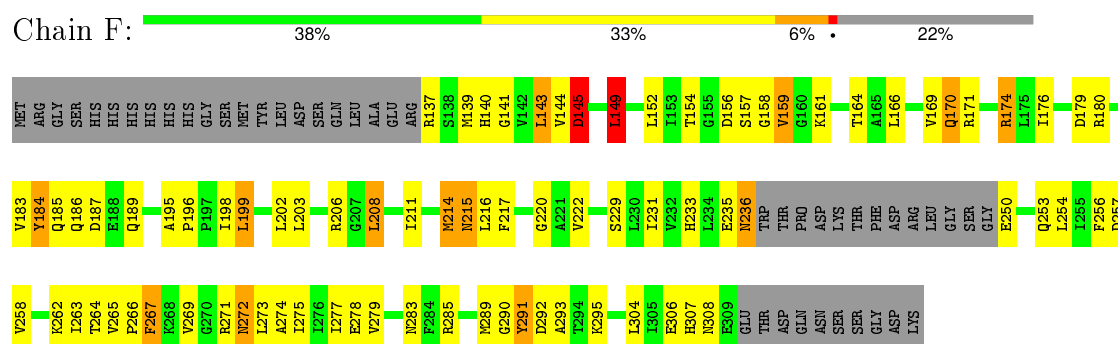
- Molecule 1: HPr kinase/phosphorylase



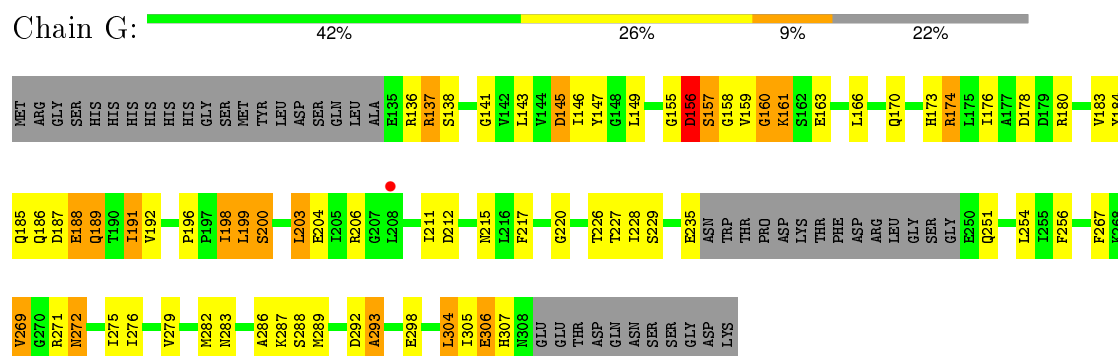
- Molecule 1: HPr kinase/phosphorylase



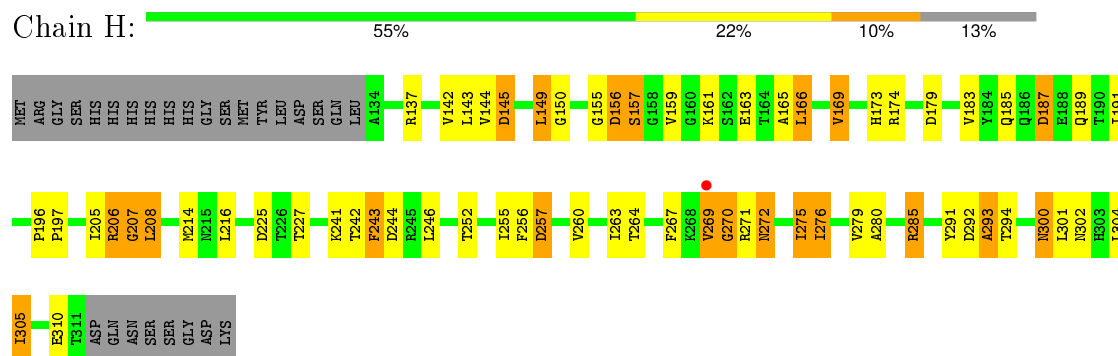
- Molecule 1: HPr kinase/phosphorylase



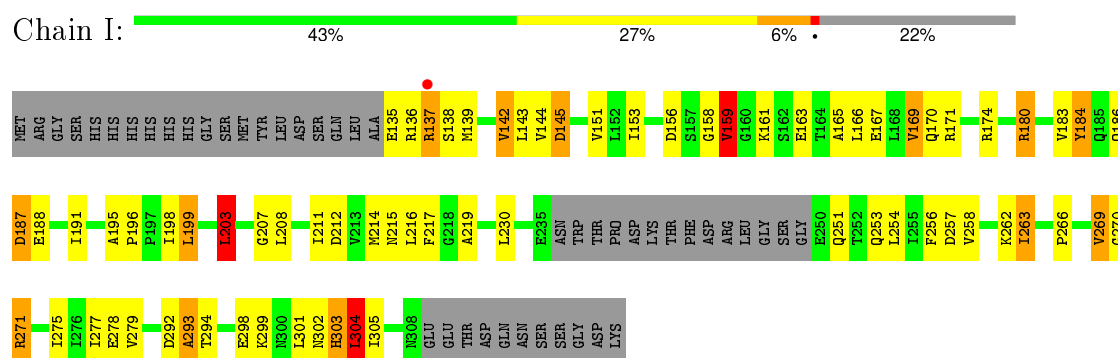
- Molecule 1: HPr kinase/phosphorylase

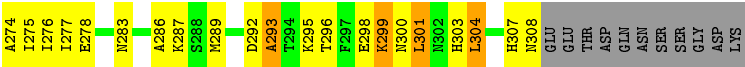


- Molecule 1: HPr kinase/phosphorylase

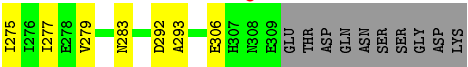


- Molecule 1: HPr kinase/phosphorylase





● Molecule 1: HPr kinase/phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.06 Å 106.37 Å 106.49 Å 119.50° 90.02° 89.96°	Depositor
Resolution (Å)	19.43 – 2.60 19.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.43-2.60) 82.2 (19.43-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.59 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.298 0.212 , 0.285	Depositor DCC
R_{free} test set	4029 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 12.7	EDS
Estimated twinning fraction	0.019 for h,-l,k+l 0.019 for h,k+l,-k 0.019 for h,-k-l,k 0.019 for h,l,-k-l 0.469 for h,-k,-l 0.020 for -h,k,-k-l 0.019 for -h,-k-l,l 0.469 for -h,-l,-k 0.467 for -h,l,k 0.019 for -h,-k,k+l 0.019 for -h,k+l,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 80370 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15591	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.85	0/1259	0.96	1/1703 (0.1%)
1	B	0.93	2/1427 (0.1%)	0.97	5/1934 (0.3%)
1	C	0.85	0/1289	0.95	4/1747 (0.2%)
1	D	0.94	0/1427	1.01	6/1934 (0.3%)
1	E	0.83	0/1282	0.97	3/1734 (0.2%)
1	F	0.85	0/1252	0.91	2/1695 (0.1%)
1	G	0.86	0/1255	0.94	2/1698 (0.1%)
1	H	0.94	0/1402	0.99	4/1900 (0.2%)
1	I	0.79	1/1255 (0.1%)	0.88	2/1698 (0.1%)
1	J	0.91	0/1405	1.03	6/1904 (0.3%)
1	K	0.84	0/1267	0.92	0/1714
1	L	0.84	1/1263 (0.1%)	0.95	1/1709 (0.1%)
All	All	0.87	4/15783 (0.0%)	0.96	36/21370 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	206	ARG	CB-CG	5.35	1.67	1.52
1	B	163	GLU	CG-CD	5.10	1.59	1.51
1	I	217	PHE	CE1-CZ	5.08	1.47	1.37
1	B	224	GLU	CB-CG	5.04	1.61	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	LEU	CA-CB-CG	10.25	138.87	115.30
1	C	171	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	D	285	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	J	285	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	E	285	ARG	NE-CZ-NH2	-7.59	116.51	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	300	ASN	Peptide

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	1242	0	1268	60	0
1	B	1405	0	1415	54	0
1	C	1269	0	1292	49	0
1	D	1405	0	1415	58	0
1	E	1265	0	1285	64	0
1	F	1235	0	1258	69	0
1	G	1238	0	1265	56	0
1	H	1380	0	1392	53	0
1	I	1238	0	1265	53	0
1	J	1383	0	1391	49	0
1	K	1250	0	1274	70	0
1	L	1246	0	1271	59	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
2	F	3	0	0	0	0
2	G	10	0	0	1	0
2	H	6	0	0	3	0
2	I	4	0	0	1	0
2	K	1	0	0	0	0
2	L	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15591	0	15791	646	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 21.

The worst 5 of 646 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:E:137:ARG:HG2	1:E:138:SER:H	1.10	1.13
1:L:206:ARG:HD2	1:L:206:ARG:H	0.97	1.11
1:D:253:GLN:HB2	1:D:262:LYS:NZ	1.69	1.06
1:H:302:ASN:HA	1:H:305:ILE:HG22	1.41	1.02
1:G:198:ILE:HG13	1:G:199:LEU:H	1.25	0.99

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%)	127 (81%)	23 (15%)	7 (4%)	3	4
1	B	179/205 (87%)	161 (90%)	16 (9%)	2 (1%)	17	36
1	C	160/205 (78%)	140 (88%)	12 (8%)	8 (5%)	3	3
1	D	179/205 (87%)	155 (87%)	17 (10%)	7 (4%)	4	5
1	E	160/205 (78%)	132 (82%)	23 (14%)	5 (3%)	5	8
1	F	156/205 (76%)	142 (91%)	10 (6%)	4 (3%)	7	11
1	G	156/205 (76%)	130 (83%)	14 (9%)	12 (8%)	1	1
1	H	176/205 (86%)	149 (85%)	17 (10%)	10 (6%)	2	2
1	I	156/205 (76%)	134 (86%)	11 (7%)	11 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	176/205 (86%)	151 (86%)	18 (10%)	7 (4%)	4	4
1	K	158/205 (77%)	129 (82%)	20 (13%)	9 (6%)	2	2
1	L	157/205 (77%)	130 (83%)	19 (12%)	8 (5%)	2	3
All	All	1970/2460 (80%)	1680 (85%)	200 (10%)	90 (5%)	3	3

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	226	THR
1	B	133	LEU
1	D	269	VAL
1	D	293	ALA

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	135/174 (78%)	113 (84%)	22 (16%)	3	5
1	B	153/174 (88%)	132 (86%)	21 (14%)	4	8
1	C	138/174 (79%)	118 (86%)	20 (14%)	4	6
1	D	153/174 (88%)	130 (85%)	23 (15%)	3	6
1	E	138/174 (79%)	117 (85%)	21 (15%)	3	6
1	F	135/174 (78%)	115 (85%)	20 (15%)	4	6
1	G	135/174 (78%)	116 (86%)	19 (14%)	4	7
1	H	150/174 (86%)	128 (85%)	22 (15%)	4	6
1	I	135/174 (78%)	115 (85%)	20 (15%)	4	6
1	J	151/174 (87%)	127 (84%)	24 (16%)	3	5
1	K	136/174 (78%)	112 (82%)	24 (18%)	2	3
1	L	136/174 (78%)	116 (85%)	20 (15%)	4	6
All	All	1695/2088 (81%)	1439 (85%)	256 (15%)	3	6

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	189	GLN
1	G	305	ILE
1	L	143	LEU
1	F	208	LEU
1	G	149	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	272	ASN
1	H	189	GLN
1	L	186	GLN
1	G	140	HIS
1	H	272	ASN

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](#)

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9	
1	A	161/205 (78%)	-0.27	0	100	100	23, 53, 79, 88	0
1	B	181/205 (88%)	-0.30	0	100	100	22, 44, 85, 98	0
1	C	164/205 (80%)	-0.20	0	100	100	30, 54, 89, 102	0
1	D	181/205 (88%)	-0.26	0	100	100	23, 43, 85, 101	0
1	E	164/205 (80%)	-0.33	0	100	100	27, 51, 78, 91	0
1	F	160/205 (78%)	-0.23	0	100	100	32, 52, 89, 98	0
1	G	160/205 (78%)	-0.24	1 (0%)	90	88	23, 51, 78, 84	0
1	H	178/205 (86%)	-0.32	1 (0%)	90	88	21, 43, 81, 101	0
1	I	160/205 (78%)	-0.24	1 (0%)	90	88	33, 54, 86, 97	0
1	J	178/205 (86%)	-0.26	0	100	100	23, 43, 82, 100	0
1	K	162/205 (79%)	-0.31	0	100	100	21, 52, 78, 82	0
1	L	161/205 (78%)	-0.18	2 (1%)	81	77	30, 54, 87, 106	0
All	All	2010/2460 (81%)	-0.26	5 (0%)	95	95	21, 50, 85, 106	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	250	GLU	3.2
1	L	308	ASN	2.8
1	G	208	LEU	2.7
1	H	269	VAL	2.6
1	I	137	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.