



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:10 AM GMT

PDB ID : 3O8O
Title : Structure of phosphofructokinase from *Saccharomyces cerevisiae*
Authors : Banaszak, K.; Mechin, I.; Kopperschlager, G.; Rypniewski, W.
Deposited on : 2010-08-03
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
<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

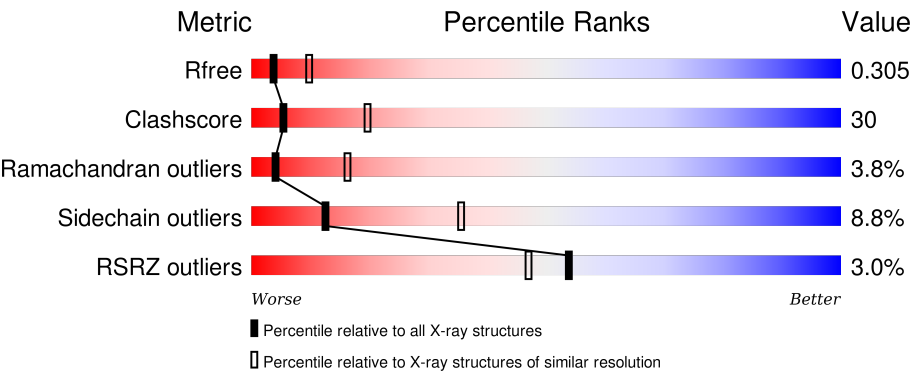
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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. 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	787	<div><div>3%</div><div>52%37%6% • 5%</div></div>
1	C	787	<div><div>4%</div><div>51%38%5% • 5%</div></div>
1	E	787	<div><div>3%</div><div>53%35%6% • •</div></div>
1	G	787	<div><div>4%</div><div>53%34%6% • 5%</div></div>
2	B	766	<div><div>3%</div><div>53%39%7% •</div></div>

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Mol	Chain	Length	Quality of chain
2	D	766	
2	F	766	
2	H	766	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FDP	C	3	-	-	-	X
4	FDP	H	8	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46645 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.

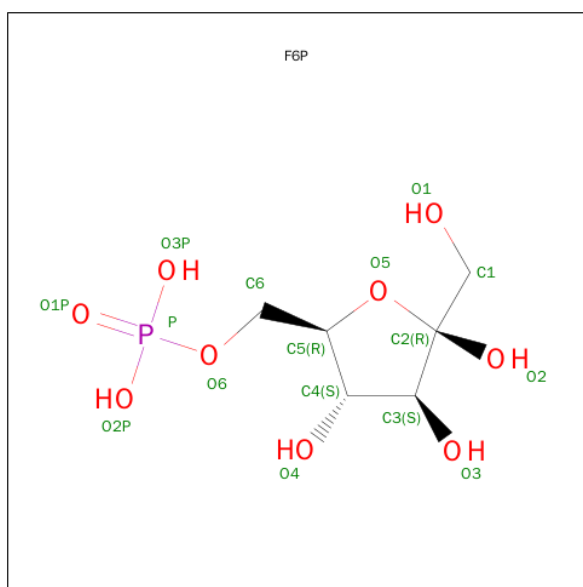
- Molecule 1 is a protein called 6-phosphofructokinase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	273	0	0
			5759	3620	1019	1098	22			
1	C	750	Total	C	N	O	S	196	0	0
			5759	3620	1019	1098	22			
1	E	752	Total	C	N	O	S	260	0	0
			5777	3631	1023	1101	22			
1	G	746	Total	C	N	O	S	289	0	0
			5733	3604	1015	1092	22			

- Molecule 2 is a protein called 6-phosphofructokinase subunit beta.

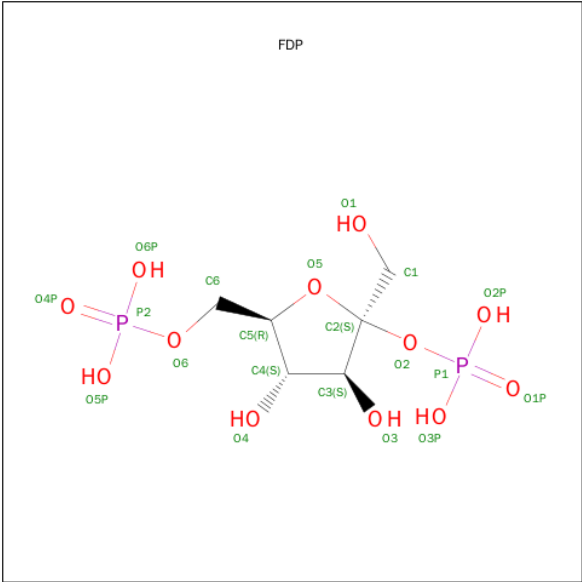
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	763	Total	C	N	O	S	364	0	0
			5834	3652	1034	1118	30			
2	D	763	Total	C	N	O	S	266	0	0
			5834	3652	1034	1118	30			
2	F	762	Total	C	N	O	S	279	0	0
			5827	3647	1033	1117	30			
2	H	763	Total	C	N	O	S	173	0	0
			5834	3652	1034	1118	30			

- Molecule 3 is SUGAR (FRUCTOSE-6-PHOSPHATE) (three-letter code: F6P) (formula: C₆H₁₃O₉P).

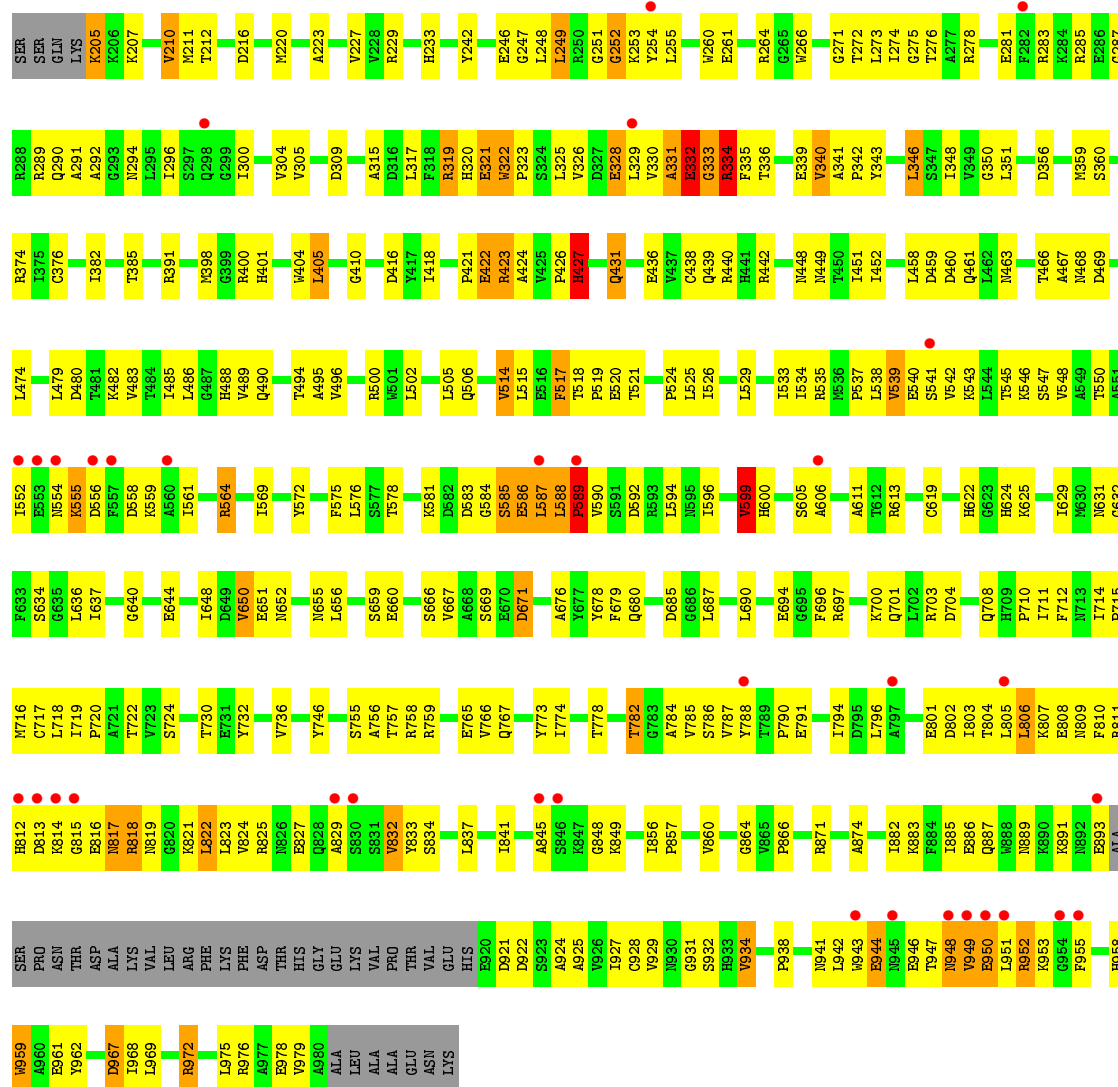


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		
3	E	1	Total	C	O	P	0	0
			16	6	9	1		
3	F	1	Total	C	O	P	0	0
			16	6	9	1		
3	G	1	Total	C	O	P	0	0
			16	6	9	1		
3	H	1	Total	C	O	P	0	0
			16	6	9	1		

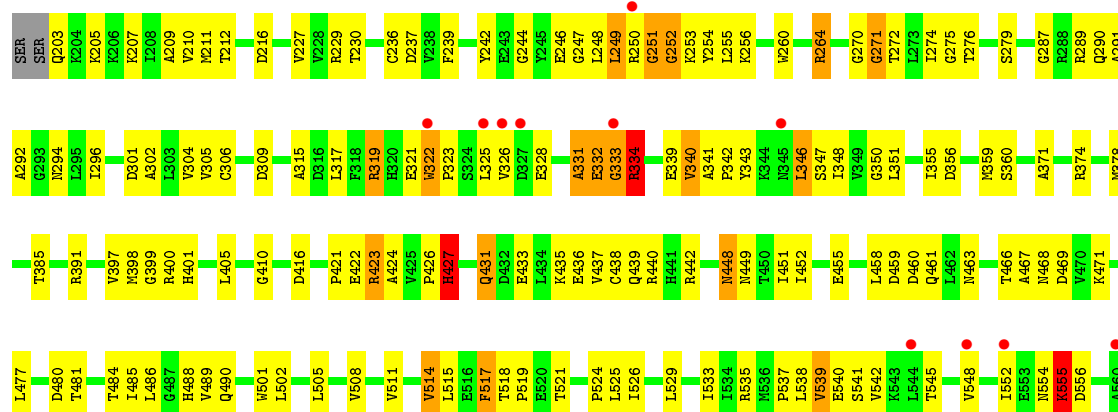
- Molecule 4 is SUGAR (FRUCTOSE-2,6-DIPHOSPHATE) (three-letter code: FDP) (formula: C₆H₁₄O₁₂P₂).

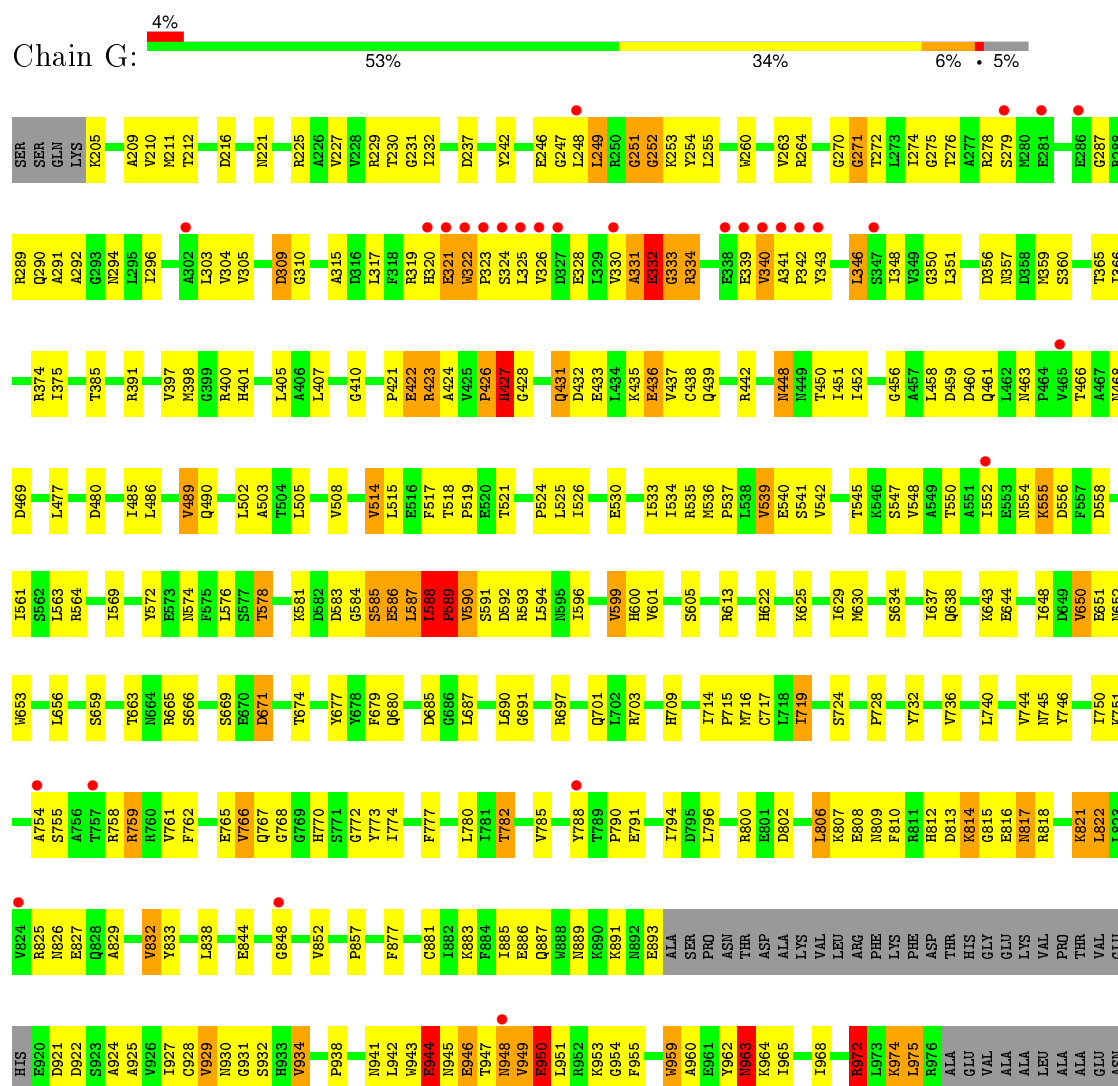
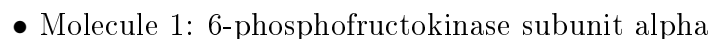


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		
4	E	1	Total	C	O	P	0	0
			20	6	12	2		
4	F	1	Total	C	O	P	0	0
			20	6	12	2		
4	G	1	Total	C	O	P	0	0
			20	6	12	2		
4	H	1	Total	C	O	P	0	0
			20	6	12	2		



• Molecule 1: 6-phosphofructokinase subunit alpha

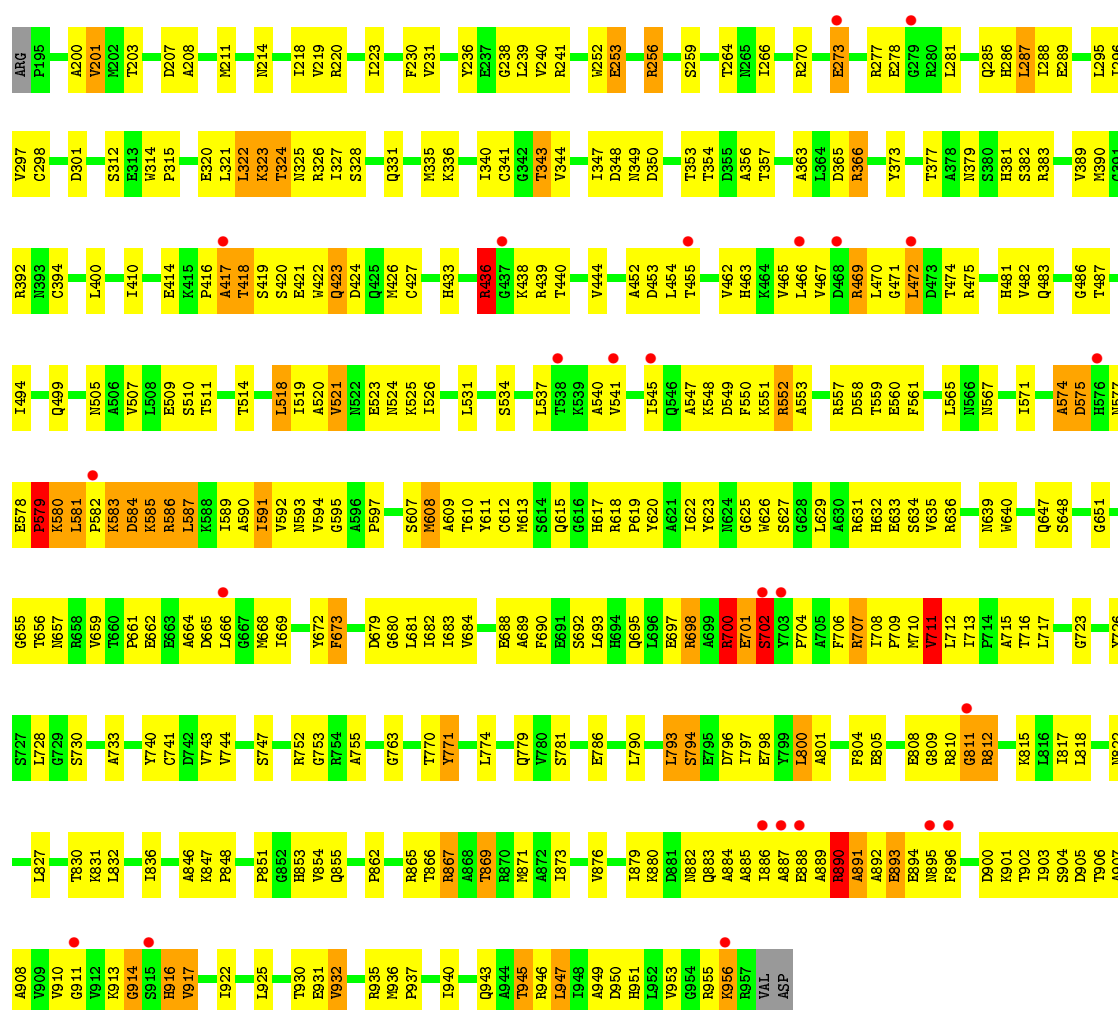




LVS

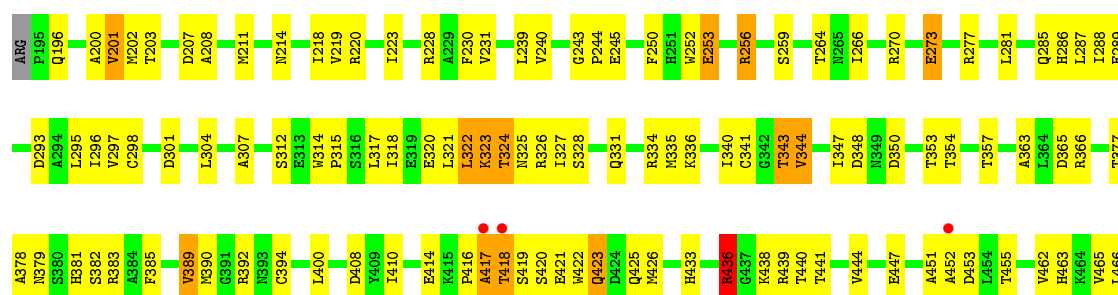
• Molecule 2: 6-phosphofructokinase subunit beta

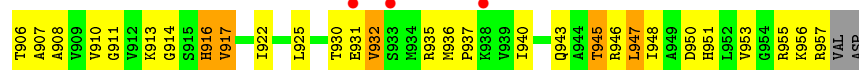
Chain B: 



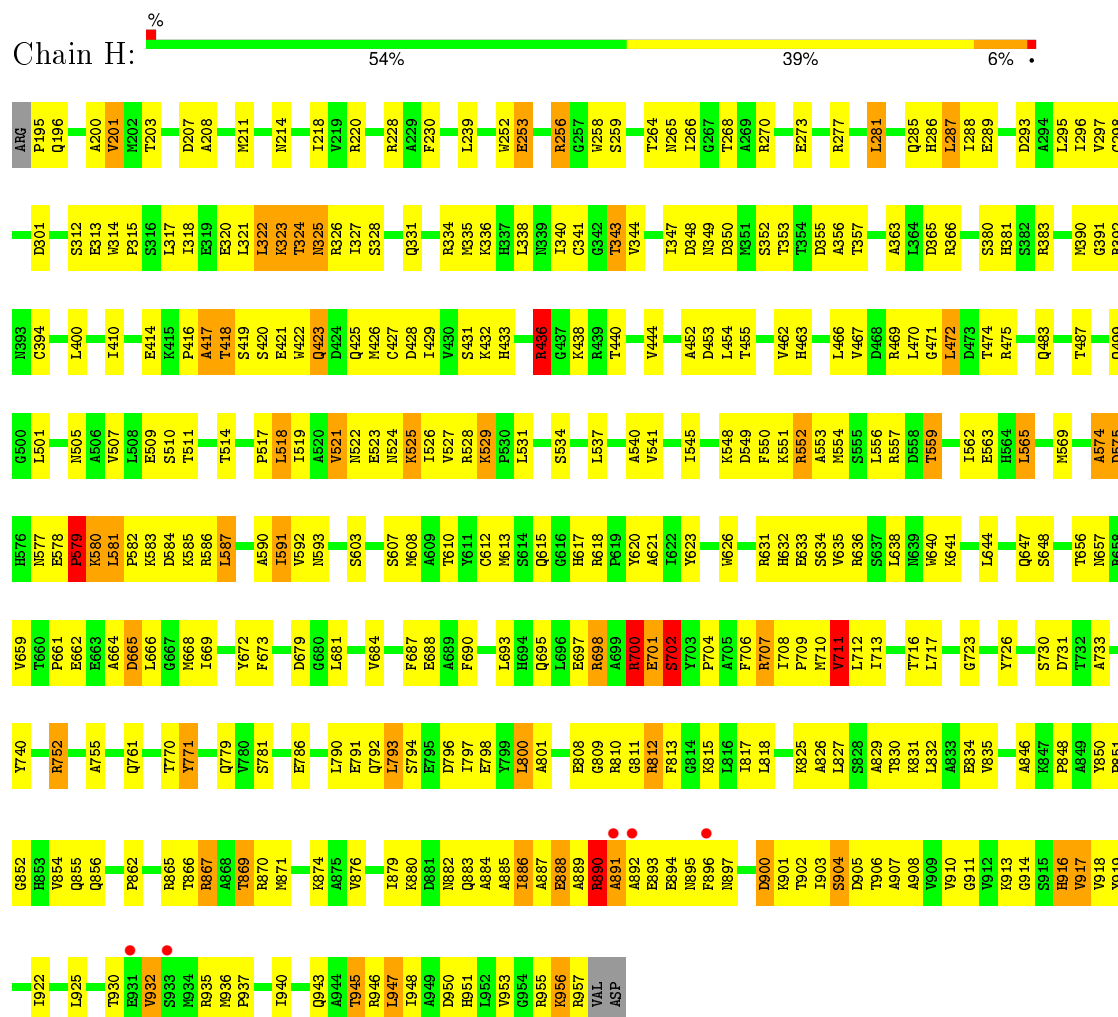
• Molecule 2: 6-phosphofructokinase subunit beta

Chain D: 





● Molecule 2: 6-phosphofructokinase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	180.05Å 186.21Å 236.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.90 34.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.90) 98.4 (34.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.309 0.257 , 0.305	Depositor DCC
R_{free} test set	3446 reflections (1.99%)	DCC
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.3	EDS
Estimated twinning fraction	0.000 for k,h,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 172763 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	46645	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FDP, F6P

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	0.53	0/5860	0.80	13/7925 (0.2%)
1	C	0.58	1/5860 (0.0%)	0.83	11/7925 (0.1%)
1	E	0.57	0/5878	0.82	17/7948 (0.2%)
1	G	0.59	1/5834 (0.0%)	0.80	9/7889 (0.1%)
2	B	0.52	1/5940 (0.0%)	0.79	14/8038 (0.2%)
2	D	0.55	1/5940 (0.0%)	0.83	20/8038 (0.2%)
2	F	0.51	0/5932	0.80	17/8027 (0.2%)
2	H	0.59	0/5940	0.84	19/8038 (0.2%)
All	All	0.56	4/47184 (0.0%)	0.81	120/63828 (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
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	376	CYS	CB-SG	-7.40	1.69	1.82
2	B	741	CYS	CB-SG	-5.75	1.72	1.81
2	D	760	CYS	CB-SG	-5.12	1.73	1.81
1	G	881	CYS	CB-SG	-5.10	1.73	1.81

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	759	ARG	NE-CZ-NH1	-9.97	115.32	120.30
1	C	283	ARG	NE-CZ-NH2	9.78	125.19	120.30
2	H	436	ARG	NE-CZ-NH1	-9.71	115.44	120.30
1	A	289	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	C	283	ARG	NE-CZ-NH1	-9.64	115.48	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	771	TYR	Sidechain
2	D	771	TYR	Sidechain
2	F	771	TYR	Sidechain
2	H	771	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	5759	0	5758	334	0
1	C	5759	0	5758	326	0
1	E	5777	0	5779	323	0
1	G	5733	0	5733	306	0
2	B	5834	0	5799	366	0
2	D	5834	0	5799	349	0
2	F	5827	0	5791	327	1
2	H	5834	0	5799	373	1
3	A	16	0	11	4	0
3	B	16	0	11	4	0
3	C	16	0	11	1	0
3	D	16	0	11	3	0
3	E	16	0	11	2	0
3	F	16	0	11	4	0
3	G	16	0	11	2	0
3	H	16	0	11	5	0
4	A	20	0	10	6	0
4	B	20	0	10	3	0
4	C	20	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	20	0	10	2	0
4	E	20	0	10	0	0
4	F	20	0	10	3	0
4	G	20	0	10	0	0
4	H	20	0	10	2	0
All	All	46645	0	46384	2612	1

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 30.

The worst 5 of 2612 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:C:427:HIS:HB3	1:C:460:ASP:HB2	1.33	1.10
1:A:665:ARG:HH21	4:A:1:FDP:H62	1.12	1.07
1:A:427:HIS:HB3	1:A:460:ASP:HB2	1.35	1.06
2:H:874:LYS:HD3	2:H:917:VAL:HG11	1.34	1.06
1:G:427:HIS:HB3	1:G:460:ASP:HB2	1.40	1.03

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:333:GLU:OE2	2:H:578:GLU:OE1[4_446]	2.14	0.06

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	746/787 (95%)	630 (84%)	87 (12%)	29 (4%)	4 15
1	C	746/787 (95%)	634 (85%)	85 (11%)	27 (4%)	4 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	748/787 (95%)	643 (86%)	74 (10%)	31 (4%)	3	14
1	G	742/787 (94%)	632 (85%)	79 (11%)	31 (4%)	3	13
2	B	761/766 (99%)	675 (89%)	61 (8%)	25 (3%)	5	20
2	D	761/766 (99%)	672 (88%)	59 (8%)	30 (4%)	4	15
2	F	760/766 (99%)	674 (89%)	58 (8%)	28 (4%)	4	17
2	H	761/766 (99%)	680 (89%)	53 (7%)	28 (4%)	4	17
All	All	6025/6212 (97%)	5240 (87%)	556 (9%)	229 (4%)	4	16

5 of 229 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLY
1	A	321	GLU
1	A	331	ALA
1	A	585	SER
1	A	587	LEU

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	614/645 (95%)	567 (92%)	47 (8%)	16	42
1	C	614/645 (95%)	567 (92%)	47 (8%)	16	42
1	E	616/645 (96%)	565 (92%)	51 (8%)	14	38
1	G	612/645 (95%)	561 (92%)	51 (8%)	14	38
2	B	612/615 (100%)	552 (90%)	60 (10%)	10	30
2	D	612/615 (100%)	552 (90%)	60 (10%)	10	30
2	F	611/615 (99%)	554 (91%)	57 (9%)	11	32
2	H	612/615 (100%)	553 (90%)	59 (10%)	10	31
All	All	4903/5040 (97%)	4471 (91%)	432 (9%)	12	35

5 of 432 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	701	GLU
1	E	578	THR
2	H	552	ARG
2	D	794	SER
1	E	306	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	792	GLN
1	E	767	GLN
2	H	463	HIS
2	D	897	ASN
1	E	463	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](#)

16 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FDP	A	1	-	20,20,20	0.98	0	27,32,32	0.85	1 (3%)
3	F6P	A	988	-	15,16,16	0.94	0	16,25,25	3.85	5 (31%)
4	FDP	B	2	-	20,20,20	0.98	0	27,32,32	0.90	1 (3%)
3	F6P	B	980	-	15,16,16	1.05	1 (6%)	16,25,25	1.01	1 (6%)
4	FDP	C	3	-	20,20,20	1.00	0	27,32,32	0.88	1 (3%)
3	F6P	C	988	-	15,16,16	0.92	0	16,25,25	0.86	0
4	FDP	D	4	-	20,20,20	0.97	0	27,32,32	0.91	2 (7%)
3	F6P	D	982	-	15,16,16	0.90	0	16,25,25	0.75	0
4	FDP	E	5	-	20,20,20	0.98	0	27,32,32	0.99	2 (7%)
3	F6P	E	988	-	15,16,16	0.84	0	16,25,25	0.76	0
4	FDP	F	6	-	20,20,20	0.99	0	27,32,32	1.02	3 (11%)
3	F6P	F	984	-	15,16,16	0.90	0	16,25,25	0.88	0
4	FDP	G	7	-	20,20,20	0.98	0	27,32,32	0.93	2 (7%)
3	F6P	G	988	-	15,16,16	1.10	2 (13%)	16,25,25	3.76	6 (37%)
4	FDP	H	8	-	20,20,20	1.00	0	27,32,32	1.03	1 (3%)
3	F6P	H	986	-	15,16,16	0.85	0	16,25,25	0.75	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
4	FDP	A	1	-	-	0/12/34/34	0/1/1/1
3	F6P	A	988	-	-	0/9/28/28	0/1/1/1
4	FDP	B	2	-	-	0/12/34/34	0/1/1/1
3	F6P	B	980	-	-	0/9/28/28	0/1/1/1
4	FDP	C	3	-	-	0/12/34/34	0/1/1/1
3	F6P	C	988	-	-	0/9/28/28	0/1/1/1
4	FDP	D	4	-	-	0/12/34/34	0/1/1/1
3	F6P	D	982	-	-	0/9/28/28	0/1/1/1
4	FDP	E	5	-	-	0/12/34/34	0/1/1/1
3	F6P	E	988	-	-	0/9/28/28	0/1/1/1
4	FDP	F	6	-	-	0/12/34/34	0/1/1/1
3	F6P	F	984	-	-	0/9/28/28	0/1/1/1
4	FDP	G	7	-	-	0/12/34/34	0/1/1/1
3	F6P	G	988	-	-	0/9/28/28	0/1/1/1
4	FDP	H	8	-	-	0/12/34/34	0/1/1/1
3	F6P	H	986	-	-	0/9/28/28	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	988	F6P	O5-C2	-2.20	1.39	1.43
3	G	988	F6P	P-O2P	2.05	1.62	1.54
3	B	980	F6P	P-O3P	2.35	1.63	1.54

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	988	F6P	O3P-P-O1P	-8.22	84.12	110.58
3	A	988	F6P	O3P-P-O6	-8.07	83.32	106.56
3	G	988	F6P	O3P-P-O6	-8.00	83.52	106.56
3	G	988	F6P	O3P-P-O1P	-7.72	85.74	110.58
3	A	988	F6P	O3P-P-O2P	-6.35	83.21	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	FDP	6	0
3	A	988	F6P	4	0
4	B	2	FDP	3	0
3	B	980	F6P	4	0
4	C	3	FDP	1	0
3	C	988	F6P	1	0
4	D	4	FDP	2	0
3	D	982	F6P	3	0
3	E	988	F6P	2	0
4	F	6	FDP	3	0
3	F	984	F6P	4	0
3	G	988	F6P	2	0
4	H	8	FDP	2	0
3	H	986	F6P	5	0

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 [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, 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(Å ²)	Q<0.9
1	A	750/787 (95%)	0.02	26 (3%)	48	40	22, 61, 81, 81	67 (8%)
1	C	750/787 (95%)	0.06	34 (4%)	37	31	16, 56, 81, 81	49 (6%)
1	E	752/787 (95%)	-0.06	22 (2%)	55	49	22, 53, 81, 81	58 (7%)
1	G	744/787 (94%)	-0.10	29 (3%)	43	36	19, 52, 81, 81	60 (8%)
2	B	763/766 (99%)	0.06	25 (3%)	50	42	27, 70, 81, 81	88 (11%)
2	D	761/766 (99%)	-0.14	16 (2%)	67	62	20, 60, 81, 81	54 (7%)
2	F	762/766 (99%)	-0.07	22 (2%)	55	49	25, 61, 81, 81	61 (8%)
2	H	763/766 (99%)	-0.30	5 (0%)	89	88	21, 47, 79, 81	37 (4%)
All	All	6045/6212 (97%)	-0.07	179 (2%)	54	47	16, 57, 81, 81	474 (7%)

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	812	HIS	7.1
1	C	815	GLY	7.0
1	G	327	ASP	6.6
1	G	326	VAL	6.2
1	C	949	VAL	6.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
4	FDP	C	3	20/20	0.85	0.34	3.73	79,82,82,82	0
4	FDP	H	8	20/20	0.85	0.33	2.73	81,82,82,82	0
4	FDP	F	6	20/20	0.89	0.27	1.96	81,82,82,82	0
3	F6P	D	982	16/16	0.94	0.22	1.63	65,67,70,71	0
3	F6P	G	988	16/16	0.96	0.20	1.48	61,62,64,68	0
4	FDP	A	1	20/20	0.91	0.21	1.09	77,82,82,82	0
4	FDP	B	2	20/20	0.95	0.17	0.89	65,68,70,71	0
3	F6P	E	988	16/16	0.94	0.19	0.56	62,66,66,68	0
3	F6P	C	988	16/16	0.92	0.19	0.50	75,78,80,80	0
3	F6P	H	986	16/16	0.97	0.16	0.45	41,47,47,49	0
3	F6P	F	984	16/16	0.95	0.18	0.35	56,57,63,64	0
3	F6P	A	988	16/16	0.91	0.17	0.14	79,82,82,82	0
4	FDP	G	7	20/20	0.91	0.18	0.14	80,82,82,82	0
4	FDP	D	4	20/20	0.96	0.14	-0.44	52,54,56,57	0
3	F6P	B	980	16/16	0.93	0.16	-0.80	77,80,82,82	0
4	FDP	E	5	20/20	0.95	0.15	-0.85	66,70,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.