



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:29 PM GMT

PDB ID : 4XYJ  
Title : Crystal structure of human phosphofructokinase-1 in complex with ATP and Mg, Northeast Structural Genomics Consortium Target HR9275  
Authors : Forouhar, F.; Webb, B.A.; Szu, F.-E.; Seetharaman, J.; Barber, D.L.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2015-02-02  
Resolution : 3.10 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](mailto: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.

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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

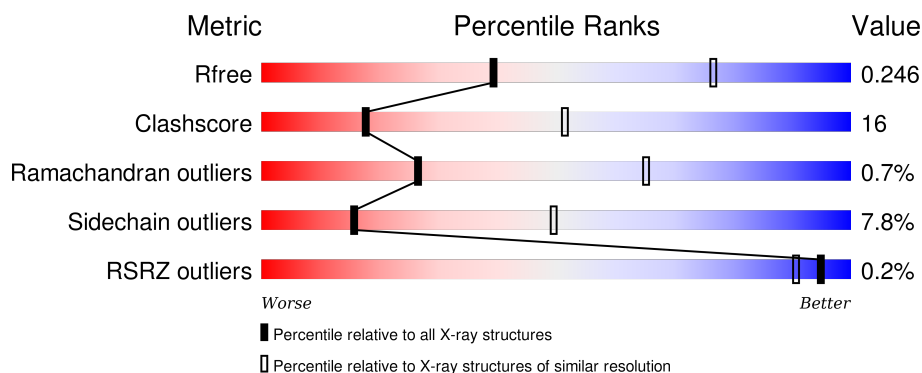
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 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	812	 63% 29% • 5%
1	B	812	 63% 28% • 5%
1	C	812	 62% 28% • 6%
1	D	812	 59% 31% • 6%
1	E	812	 60% 30% • 6%

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Mol	Chain	Length	Quality of chain
1	F	812	
1	G	812	
1	H	812	

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	PO4	E	804	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 47023 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 ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	0	0	0
			5881	3689	1047	1106	39			
1	B	768	Total	C	N	O	S	0	0	0
			5880	3688	1047	1106	39			
1	C	760	Total	C	N	O	S	0	0	0
			5820	3652	1031	1098	39			
1	D	761	Total	C	N	O	S	0	0	0
			5825	3655	1032	1099	39			
1	E	765	Total	C	N	O	S	0	0	0
			5860	3675	1043	1103	39			
1	F	761	Total	C	N	O	S	0	0	0
			5823	3655	1030	1099	39			
1	G	760	Total	C	N	O	S	0	0	0
			5820	3652	1031	1098	39			
1	H	739	Total	C	N	O	S	0	0	0
			5644	3540	1003	1062	39			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q01813
A	-26	SER	-	expression tag	UNP Q01813
A	-25	TYR	-	expression tag	UNP Q01813
A	-24	TYR	-	expression tag	UNP Q01813
A	-23	HIS	-	expression tag	UNP Q01813
A	-22	HIS	-	expression tag	UNP Q01813
A	-21	HIS	-	expression tag	UNP Q01813
A	-20	HIS	-	expression tag	UNP Q01813
A	-19	HIS	-	expression tag	UNP Q01813
A	-18	HIS	-	expression tag	UNP Q01813
A	-17	ASP	-	expression tag	UNP Q01813
A	-16	TYR	-	expression tag	UNP Q01813
A	-15	ASP	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ILE	-	expression tag	UNP Q01813
A	-13	PRO	-	expression tag	UNP Q01813
A	-12	THR	-	expression tag	UNP Q01813
A	-11	THR	-	expression tag	UNP Q01813
A	-10	GLU	-	expression tag	UNP Q01813
A	-9	ASN	-	expression tag	UNP Q01813
A	-8	LEU	-	expression tag	UNP Q01813
A	-7	TYR	-	expression tag	UNP Q01813
A	-6	PHE	-	expression tag	UNP Q01813
A	-5	GLN	-	expression tag	UNP Q01813
A	-4	GLY	-	expression tag	UNP Q01813
A	-3	ALA	-	expression tag	UNP Q01813
A	-2	MET	-	expression tag	UNP Q01813
A	-1	ASP	-	expression tag	UNP Q01813
A	0	PRO	-	expression tag	UNP Q01813
B	-27	MET	-	initiating methionine	UNP Q01813
B	-26	SER	-	expression tag	UNP Q01813
B	-25	TYR	-	expression tag	UNP Q01813
B	-24	TYR	-	expression tag	UNP Q01813
B	-23	HIS	-	expression tag	UNP Q01813
B	-22	HIS	-	expression tag	UNP Q01813
B	-21	HIS	-	expression tag	UNP Q01813
B	-20	HIS	-	expression tag	UNP Q01813
B	-19	HIS	-	expression tag	UNP Q01813
B	-18	HIS	-	expression tag	UNP Q01813
B	-17	ASP	-	expression tag	UNP Q01813
B	-16	TYR	-	expression tag	UNP Q01813
B	-15	ASP	-	expression tag	UNP Q01813
B	-14	ILE	-	expression tag	UNP Q01813
B	-13	PRO	-	expression tag	UNP Q01813
B	-12	THR	-	expression tag	UNP Q01813
B	-11	THR	-	expression tag	UNP Q01813
B	-10	GLU	-	expression tag	UNP Q01813
B	-9	ASN	-	expression tag	UNP Q01813
B	-8	LEU	-	expression tag	UNP Q01813
B	-7	TYR	-	expression tag	UNP Q01813
B	-6	PHE	-	expression tag	UNP Q01813
B	-5	GLN	-	expression tag	UNP Q01813
B	-4	GLY	-	expression tag	UNP Q01813
B	-3	ALA	-	expression tag	UNP Q01813
B	-2	MET	-	expression tag	UNP Q01813
B	-1	ASP	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PRO	-	expression tag	UNP Q01813
C	-27	MET	-	initiating methionine	UNP Q01813
C	-26	SER	-	expression tag	UNP Q01813
C	-25	TYR	-	expression tag	UNP Q01813
C	-24	TYR	-	expression tag	UNP Q01813
C	-23	HIS	-	expression tag	UNP Q01813
C	-22	HIS	-	expression tag	UNP Q01813
C	-21	HIS	-	expression tag	UNP Q01813
C	-20	HIS	-	expression tag	UNP Q01813
C	-19	HIS	-	expression tag	UNP Q01813
C	-18	HIS	-	expression tag	UNP Q01813
C	-17	ASP	-	expression tag	UNP Q01813
C	-16	TYR	-	expression tag	UNP Q01813
C	-15	ASP	-	expression tag	UNP Q01813
C	-14	ILE	-	expression tag	UNP Q01813
C	-13	PRO	-	expression tag	UNP Q01813
C	-12	THR	-	expression tag	UNP Q01813
C	-11	THR	-	expression tag	UNP Q01813
C	-10	GLU	-	expression tag	UNP Q01813
C	-9	ASN	-	expression tag	UNP Q01813
C	-8	LEU	-	expression tag	UNP Q01813
C	-7	TYR	-	expression tag	UNP Q01813
C	-6	PHE	-	expression tag	UNP Q01813
C	-5	GLN	-	expression tag	UNP Q01813
C	-4	GLY	-	expression tag	UNP Q01813
C	-3	ALA	-	expression tag	UNP Q01813
C	-2	MET	-	expression tag	UNP Q01813
C	-1	ASP	-	expression tag	UNP Q01813
C	0	PRO	-	expression tag	UNP Q01813
D	-27	MET	-	initiating methionine	UNP Q01813
D	-26	SER	-	expression tag	UNP Q01813
D	-25	TYR	-	expression tag	UNP Q01813
D	-24	TYR	-	expression tag	UNP Q01813
D	-23	HIS	-	expression tag	UNP Q01813
D	-22	HIS	-	expression tag	UNP Q01813
D	-21	HIS	-	expression tag	UNP Q01813
D	-20	HIS	-	expression tag	UNP Q01813
D	-19	HIS	-	expression tag	UNP Q01813
D	-18	HIS	-	expression tag	UNP Q01813
D	-17	ASP	-	expression tag	UNP Q01813
D	-16	TYR	-	expression tag	UNP Q01813
D	-15	ASP	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	ILE	-	expression tag	UNP Q01813
D	-13	PRO	-	expression tag	UNP Q01813
D	-12	THR	-	expression tag	UNP Q01813
D	-11	THR	-	expression tag	UNP Q01813
D	-10	GLU	-	expression tag	UNP Q01813
D	-9	ASN	-	expression tag	UNP Q01813
D	-8	LEU	-	expression tag	UNP Q01813
D	-7	TYR	-	expression tag	UNP Q01813
D	-6	PHE	-	expression tag	UNP Q01813
D	-5	GLN	-	expression tag	UNP Q01813
D	-4	GLY	-	expression tag	UNP Q01813
D	-3	ALA	-	expression tag	UNP Q01813
D	-2	MET	-	expression tag	UNP Q01813
D	-1	ASP	-	expression tag	UNP Q01813
D	0	PRO	-	expression tag	UNP Q01813
E	-27	MET	-	initiating methionine	UNP Q01813
E	-26	SER	-	expression tag	UNP Q01813
E	-25	TYR	-	expression tag	UNP Q01813
E	-24	TYR	-	expression tag	UNP Q01813
E	-23	HIS	-	expression tag	UNP Q01813
E	-22	HIS	-	expression tag	UNP Q01813
E	-21	HIS	-	expression tag	UNP Q01813
E	-20	HIS	-	expression tag	UNP Q01813
E	-19	HIS	-	expression tag	UNP Q01813
E	-18	HIS	-	expression tag	UNP Q01813
E	-17	ASP	-	expression tag	UNP Q01813
E	-16	TYR	-	expression tag	UNP Q01813
E	-15	ASP	-	expression tag	UNP Q01813
E	-14	ILE	-	expression tag	UNP Q01813
E	-13	PRO	-	expression tag	UNP Q01813
E	-12	THR	-	expression tag	UNP Q01813
E	-11	THR	-	expression tag	UNP Q01813
E	-10	GLU	-	expression tag	UNP Q01813
E	-9	ASN	-	expression tag	UNP Q01813
E	-8	LEU	-	expression tag	UNP Q01813
E	-7	TYR	-	expression tag	UNP Q01813
E	-6	PHE	-	expression tag	UNP Q01813
E	-5	GLN	-	expression tag	UNP Q01813
E	-4	GLY	-	expression tag	UNP Q01813
E	-3	ALA	-	expression tag	UNP Q01813
E	-2	MET	-	expression tag	UNP Q01813
E	-1	ASP	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	PRO	-	expression tag	UNP Q01813
F	-27	MET	-	initiating methionine	UNP Q01813
F	-26	SER	-	expression tag	UNP Q01813
F	-25	TYR	-	expression tag	UNP Q01813
F	-24	TYR	-	expression tag	UNP Q01813
F	-23	HIS	-	expression tag	UNP Q01813
F	-22	HIS	-	expression tag	UNP Q01813
F	-21	HIS	-	expression tag	UNP Q01813
F	-20	HIS	-	expression tag	UNP Q01813
F	-19	HIS	-	expression tag	UNP Q01813
F	-18	HIS	-	expression tag	UNP Q01813
F	-17	ASP	-	expression tag	UNP Q01813
F	-16	TYR	-	expression tag	UNP Q01813
F	-15	ASP	-	expression tag	UNP Q01813
F	-14	ILE	-	expression tag	UNP Q01813
F	-13	PRO	-	expression tag	UNP Q01813
F	-12	THR	-	expression tag	UNP Q01813
F	-11	THR	-	expression tag	UNP Q01813
F	-10	GLU	-	expression tag	UNP Q01813
F	-9	ASN	-	expression tag	UNP Q01813
F	-8	LEU	-	expression tag	UNP Q01813
F	-7	TYR	-	expression tag	UNP Q01813
F	-6	PHE	-	expression tag	UNP Q01813
F	-5	GLN	-	expression tag	UNP Q01813
F	-4	GLY	-	expression tag	UNP Q01813
F	-3	ALA	-	expression tag	UNP Q01813
F	-2	MET	-	expression tag	UNP Q01813
F	-1	ASP	-	expression tag	UNP Q01813
F	0	PRO	-	expression tag	UNP Q01813
G	-27	MET	-	initiating methionine	UNP Q01813
G	-26	SER	-	expression tag	UNP Q01813
G	-25	TYR	-	expression tag	UNP Q01813
G	-24	TYR	-	expression tag	UNP Q01813
G	-23	HIS	-	expression tag	UNP Q01813
G	-22	HIS	-	expression tag	UNP Q01813
G	-21	HIS	-	expression tag	UNP Q01813
G	-20	HIS	-	expression tag	UNP Q01813
G	-19	HIS	-	expression tag	UNP Q01813
G	-18	HIS	-	expression tag	UNP Q01813
G	-17	ASP	-	expression tag	UNP Q01813
G	-16	TYR	-	expression tag	UNP Q01813
G	-15	ASP	-	expression tag	UNP Q01813

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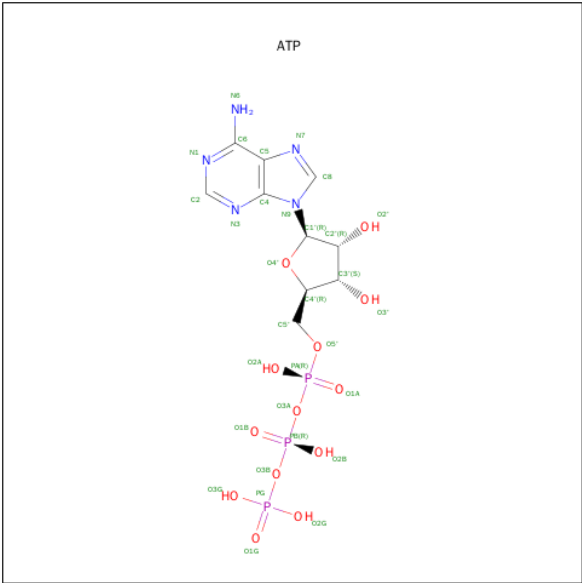
Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	ILE	-	expression tag	UNP Q01813
G	-13	PRO	-	expression tag	UNP Q01813
G	-12	THR	-	expression tag	UNP Q01813
G	-11	THR	-	expression tag	UNP Q01813
G	-10	GLU	-	expression tag	UNP Q01813
G	-9	ASN	-	expression tag	UNP Q01813
G	-8	LEU	-	expression tag	UNP Q01813
G	-7	TYR	-	expression tag	UNP Q01813
G	-6	PHE	-	expression tag	UNP Q01813
G	-5	GLN	-	expression tag	UNP Q01813
G	-4	GLY	-	expression tag	UNP Q01813
G	-3	ALA	-	expression tag	UNP Q01813
G	-2	MET	-	expression tag	UNP Q01813
G	-1	ASP	-	expression tag	UNP Q01813
G	0	PRO	-	expression tag	UNP Q01813
H	-27	MET	-	initiating methionine	UNP Q01813
H	-26	SER	-	expression tag	UNP Q01813
H	-25	TYR	-	expression tag	UNP Q01813
H	-24	TYR	-	expression tag	UNP Q01813
H	-23	HIS	-	expression tag	UNP Q01813
H	-22	HIS	-	expression tag	UNP Q01813
H	-21	HIS	-	expression tag	UNP Q01813
H	-20	HIS	-	expression tag	UNP Q01813
H	-19	HIS	-	expression tag	UNP Q01813
H	-18	HIS	-	expression tag	UNP Q01813
H	-17	ASP	-	expression tag	UNP Q01813
H	-16	TYR	-	expression tag	UNP Q01813
H	-15	ASP	-	expression tag	UNP Q01813
H	-14	ILE	-	expression tag	UNP Q01813
H	-13	PRO	-	expression tag	UNP Q01813
H	-12	THR	-	expression tag	UNP Q01813
H	-11	THR	-	expression tag	UNP Q01813
H	-10	GLU	-	expression tag	UNP Q01813
H	-9	ASN	-	expression tag	UNP Q01813
H	-8	LEU	-	expression tag	UNP Q01813
H	-7	TYR	-	expression tag	UNP Q01813
H	-6	PHE	-	expression tag	UNP Q01813
H	-5	GLN	-	expression tag	UNP Q01813
H	-4	GLY	-	expression tag	UNP Q01813
H	-3	ALA	-	expression tag	UNP Q01813
H	-2	MET	-	expression tag	UNP Q01813
H	-1	ASP	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	PRO	-	expression tag	UNP Q01813

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

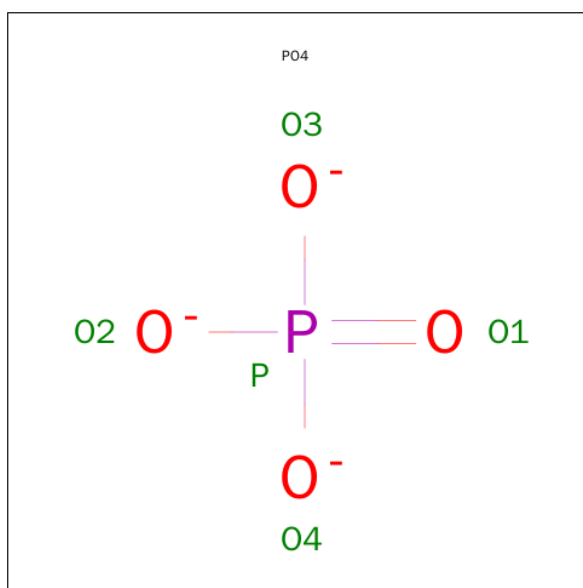


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0
3	E	2	Total Mg 2 2	0	0
3	H	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	F	2	Total Mg 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Co	0	0
			1	1		
5	F	1	Total	Co	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	B	28	Total	O	0	0
			28	28		
6	C	11	Total	O	0	0
			11	11		
6	D	9	Total	O	0	0
			9	9		
6	E	18	Total	O	0	0
			18	18		
6	F	16	Total	O	0	0
			16	16		
6	G	21	Total	O	0	0
			21	21		

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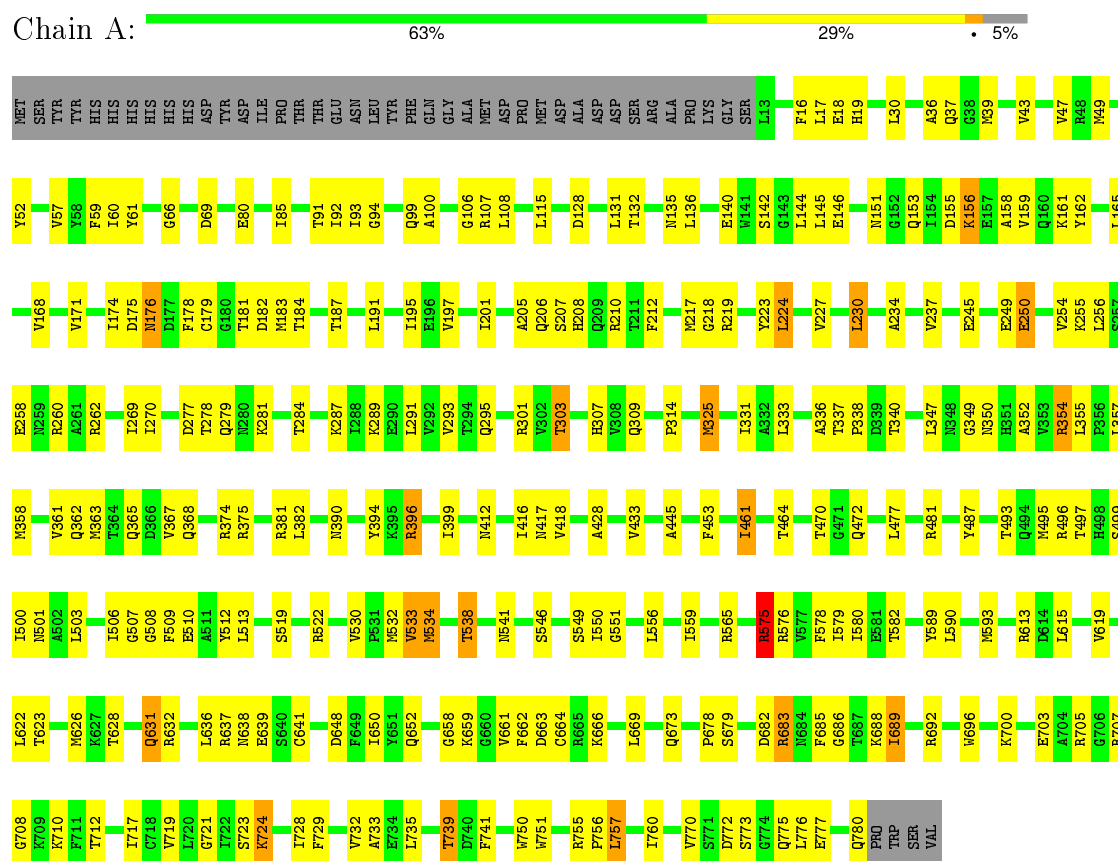
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	13	Total	O	0	0
			13	13		

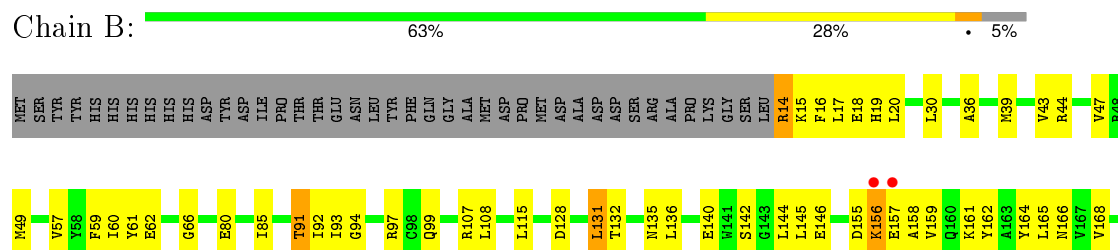
### 3 Residue-property plots

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.

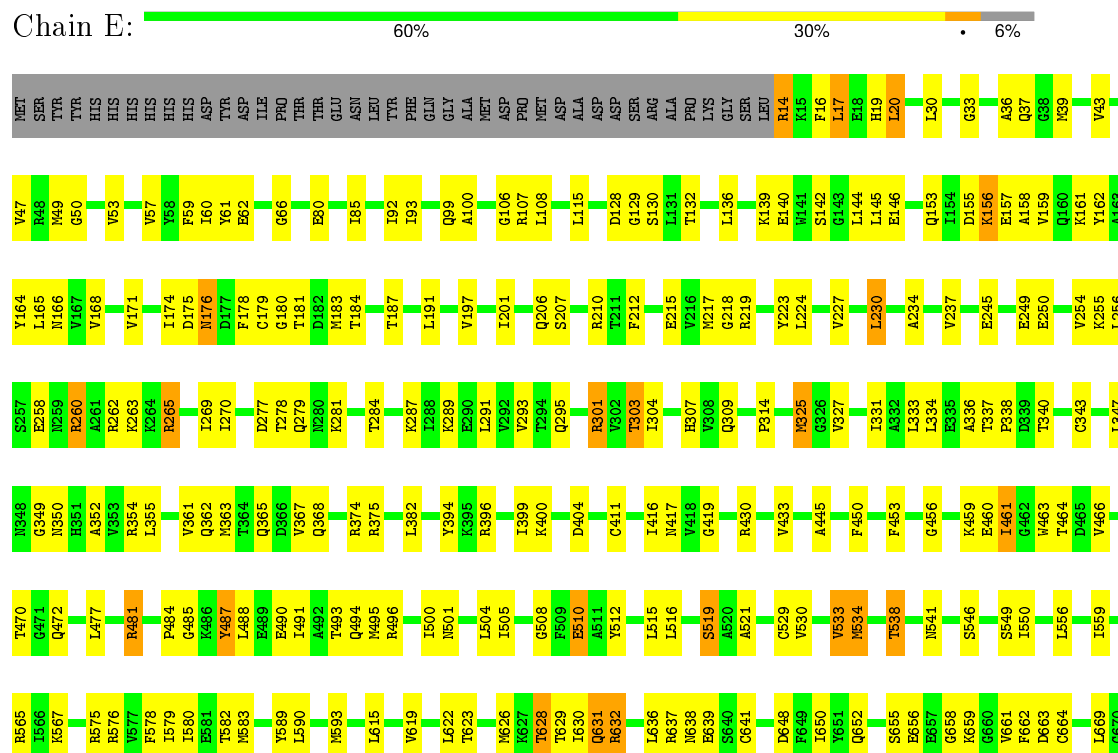
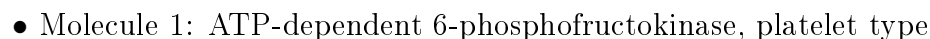
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



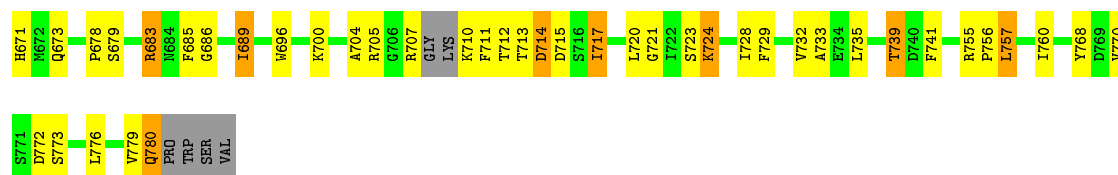
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type





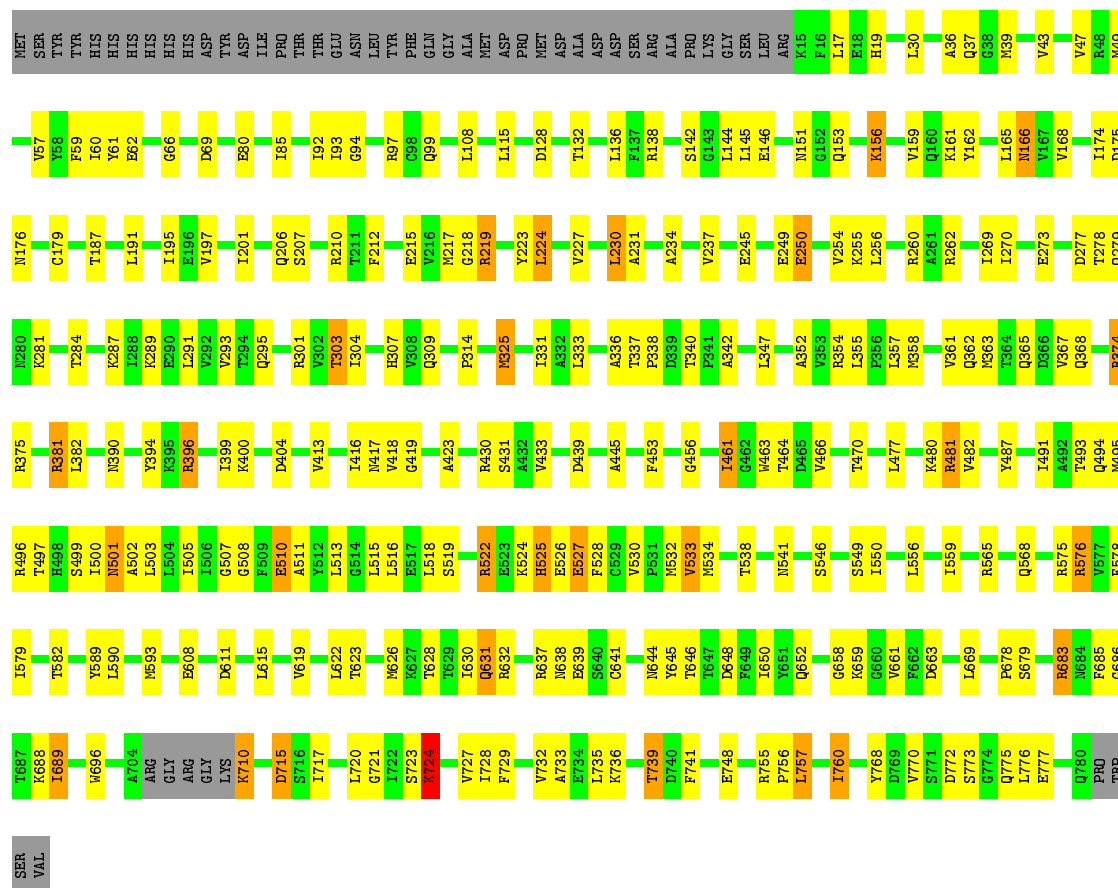




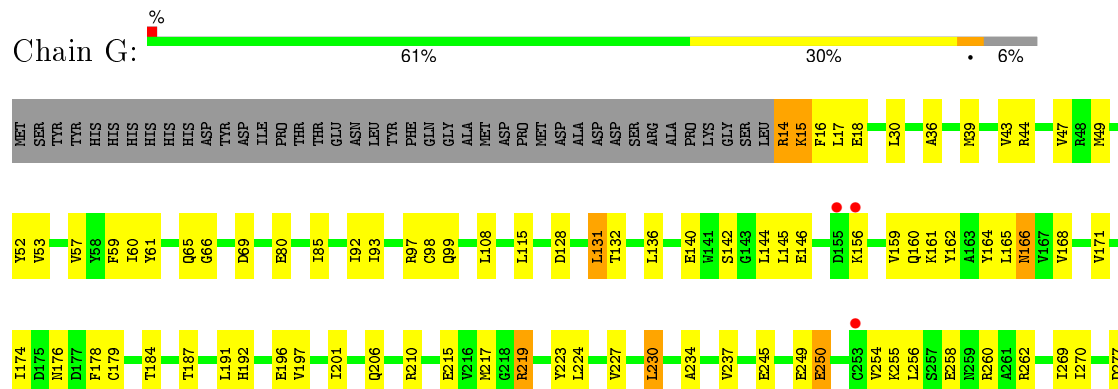


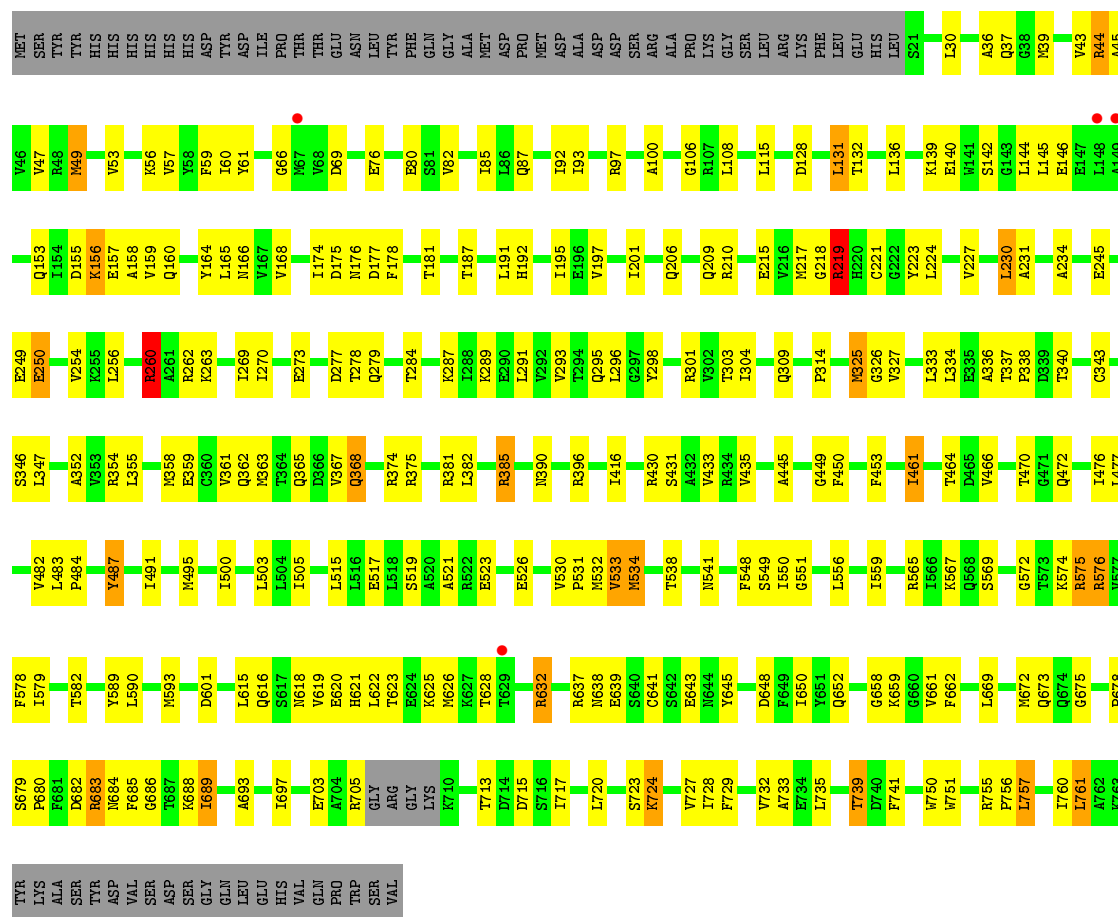
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain F:



- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.20Å 159.33Å 170.53Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	49.69 – 3.10 49.69 – 3.08	Depositor EDS
% Data completeness (in resolution range)	85.0 (49.69-3.10) 84.2 (49.69-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.07Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.221 , 0.246 0.221 , 0.246	Depositor DCC
$R_{free}$ test set	10980 reflections (10.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 121769 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	47023	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CO, PO4, ATP

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	0.46	1/5977 (0.0%)	1.25	29/8067 (0.4%)
1	B	0.45	0/5977	0.75	8/8068 (0.1%)
1	C	0.42	0/5915	0.77	12/7986 (0.2%)
1	D	0.42	0/5920	0.75	8/7993 (0.1%)
1	E	0.42	0/5955	0.85	12/8037 (0.1%)
1	F	0.42	0/5918	0.86	12/7990 (0.2%)
1	G	0.41	0/5915	0.70	8/7986 (0.1%)
1	H	0.43	0/5734	0.83	12/7741 (0.2%)
All	All	0.43	1/47311 (0.0%)	0.86	101/63868 (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	B	0	4
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	3
1	G	0	1
1	H	0	6
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	CYS	CB-SG	-5.67	1.72	1.81

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ARG	NE-CZ-NH2	-27.87	106.36	120.30
1	A	575	ARG	NE-CZ-NH2	-26.89	106.85	120.30
1	H	219	ARG	NE-CZ-NH1	-26.18	107.21	120.30
1	A	613	ARG	NE-CZ-NH1	-26.11	107.24	120.30
1	F	138	ARG	NE-CZ-NH2	-26.08	107.26	120.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	219	ARG	Sidechain
1	B	260	ARG	Sidechain
1	B	665	ARG	Sidechain
1	B	97	ARG	Sidechain
1	C	396	ARG	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	5881	0	5912	195	0
1	B	5880	0	5908	186	0
1	C	5820	0	5837	183	0
1	D	5825	0	5842	197	0
1	E	5860	0	5884	211	0
1	F	5823	0	5842	191	0
1	G	5820	0	5837	198	0
1	H	5644	0	5678	180	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	1	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
6	A	29	0	0	0	0
6	B	28	0	0	1	0
6	C	11	0	0	0	0
6	D	9	0	0	0	0
6	E	18	0	0	0	0
6	F	16	0	0	0	0
6	G	21	0	0	1	0
6	H	13	0	0	2	0
All	All	47023	0	46836	1489	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 16.

The worst 5 of 1489 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:307:HIS:HE1	1:B:303:THR:HG22	1.04	1.16
1:B:481:ARG:HB2	1:B:481:ARG:HH11	1.01	1.13
1:H:166:ASN:ND2	1:H:336:ALA:HB3	1.63	1.12
1:H:166:ASN:HD21	1:H:336:ALA:CB	1.64	1.10
1:E:710:LYS:HE2	1:E:710:LYS:HA	1.38	1.02

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	766/812 (94%)	706 (92%)	57 (7%)	3 (0%)	39	75
1	B	766/812 (94%)	699 (91%)	60 (8%)	7 (1%)	21	61
1	C	756/812 (93%)	686 (91%)	62 (8%)	8 (1%)	17	55
1	D	757/812 (93%)	694 (92%)	57 (8%)	6 (1%)	24	63
1	E	761/812 (94%)	697 (92%)	58 (8%)	6 (1%)	24	63
1	F	757/812 (93%)	691 (91%)	60 (8%)	6 (1%)	24	63
1	G	756/812 (93%)	693 (92%)	58 (8%)	5 (1%)	26	65
1	H	735/812 (90%)	672 (91%)	59 (8%)	4 (0%)	34	72
All	All	6054/6496 (93%)	5538 (92%)	471 (8%)	45 (1%)	26	65

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	486	LYS
1	H	713	THR
1	A	278	THR
1	A	724	LYS
1	B	278	THR

### 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	619/658 (94%)	573 (93%)	46 (7%)	17	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	619/658 (94%)	567 (92%)	52 (8%)	14	46
1	C	614/658 (93%)	568 (92%)	46 (8%)	17	51
1	D	614/658 (93%)	564 (92%)	50 (8%)	15	47
1	E	617/658 (94%)	570 (92%)	47 (8%)	16	51
1	F	614/658 (93%)	563 (92%)	51 (8%)	14	46
1	G	614/658 (93%)	568 (92%)	46 (8%)	17	51
1	H	594/658 (90%)	549 (92%)	45 (8%)	16	51
All	All	4905/5264 (93%)	4522 (92%)	383 (8%)	16	49

5 of 383 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	470	THR
1	E	362	GLN
1	H	250	GLU
1	D	533	VAL
1	E	14	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	618	ASN
1	E	417	ASN
1	H	176	ASN
1	D	673	GLN
1	E	151	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 ⓘ

Of 37 ligands modelled in this entry, 17 are monoatomic - leaving 20 for Mogul analysis.

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	ATP	A	801	3	24,33,33	1.52	3 (12%)	31,52,52	2.55	4 (12%)
4	PO4	A	804	-	4,4,4	1.08	0	6,6,6	0.27	0
4	PO4	A	805	-	4,4,4	1.11	0	6,6,6	0.27	0
2	ATP	B	801	3	24,33,33	1.48	4 (16%)	31,52,52	2.50	4 (12%)
4	PO4	B	804	-	4,4,4	1.08	0	6,6,6	0.27	0
4	PO4	B	805	-	4,4,4	1.09	0	6,6,6	0.27	0
2	ATP	C	801	3	24,33,33	1.21	2 (8%)	31,52,52	2.30	4 (12%)
4	PO4	C	804	-	4,4,4	1.09	0	6,6,6	0.27	0
2	ATP	D	801	3	24,33,33	1.54	4 (16%)	31,52,52	2.37	4 (12%)
4	PO4	D	803	-	4,4,4	1.14	0	6,6,6	0.27	0
2	ATP	E	801	3	24,33,33	1.43	3 (12%)	31,52,52	2.36	4 (12%)
4	PO4	E	804	-	4,4,4	1.12	0	6,6,6	0.27	0
2	ATP	F	801	3	24,33,33	1.29	2 (8%)	31,52,52	2.44	4 (12%)
4	PO4	F	804	-	4,4,4	1.06	0	6,6,6	0.27	0
4	PO4	F	805	-	4,4,4	1.10	0	6,6,6	0.27	0
2	ATP	G	801	3	24,33,33	1.45	3 (12%)	31,52,52	2.50	4 (12%)
4	PO4	G	804	-	4,4,4	1.04	0	6,6,6	0.27	0
4	PO4	G	805	-	4,4,4	1.09	0	6,6,6	0.27	0
2	ATP	H	801	3	24,33,33	1.49	2 (8%)	31,52,52	2.39	4 (12%)
4	PO4	H	804	-	4,4,4	1.11	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	ATP	A	801	3	-	0/18/38/38	0/3/3/3
4	PO4	A	804	-	-	0/0/0/0	0/0/0/0
4	PO4	A	805	-	-	0/0/0/0	0/0/0/0
2	ATP	B	801	3	-	0/18/38/38	0/3/3/3
4	PO4	B	804	-	-	0/0/0/0	0/0/0/0
4	PO4	B	805	-	-	0/0/0/0	0/0/0/0
2	ATP	C	801	3	-	0/18/38/38	0/3/3/3
4	PO4	C	804	-	-	0/0/0/0	0/0/0/0
2	ATP	D	801	3	-	0/18/38/38	0/3/3/3
4	PO4	D	803	-	-	0/0/0/0	0/0/0/0
2	ATP	E	801	3	-	0/18/38/38	0/3/3/3
4	PO4	E	804	-	-	0/0/0/0	0/0/0/0
2	ATP	F	801	3	-	0/18/38/38	0/3/3/3
4	PO4	F	804	-	-	0/0/0/0	0/0/0/0
4	PO4	F	805	-	-	0/0/0/0	0/0/0/0
2	ATP	G	801	3	-	0/18/38/38	0/3/3/3
4	PO4	G	804	-	-	0/0/0/0	0/0/0/0
4	PO4	G	805	-	-	0/0/0/0	0/0/0/0
2	ATP	H	801	3	-	0/18/38/38	0/3/3/3
4	PO4	H	804	-	-	0/0/0/0	0/0/0/0

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ATP	PG-O3G	2.24	1.62	1.54
2	D	801	ATP	PG-O2G	2.25	1.62	1.54
2	C	801	ATP	PG-O3G	2.28	1.62	1.54
2	A	801	ATP	PG-O3G	2.57	1.63	1.54
2	D	801	ATP	PB-O1B	2.59	1.60	1.51

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	801	ATP	N3-C2-N1	-11.11	120.38	128.89
2	F	801	ATP	N3-C2-N1	-10.81	120.61	128.89
2	H	801	ATP	N3-C2-N1	-10.67	120.72	128.89
2	C	801	ATP	N3-C2-N1	-10.51	120.85	128.89
2	A	801	ATP	N3-C2-N1	-10.48	120.87	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	801	ATP	1	0

## 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 ⓘ

### 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, 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	768/812 (94%)	-0.22	0 100 100	25, 56, 83, 113	0
1	B	768/812 (94%)	-0.20	2 (0%) 94 88	26, 55, 83, 114	0
1	C	760/812 (93%)	-0.13	3 (0%) 93 85	36, 62, 93, 114	0
1	D	761/812 (93%)	-0.25	0 100 100	36, 59, 86, 113	0
1	E	765/812 (94%)	-0.18	0 100 100	37, 59, 86, 114	0
1	F	761/812 (93%)	-0.24	0 100 100	36, 60, 86, 114	0
1	G	760/812 (93%)	-0.15	5 (0%) 89 78	36, 62, 89, 113	0
1	H	739/812 (91%)	-0.11	4 (0%) 91 83	38, 61, 87, 114	0
All	All	6082/6496 (93%)	-0.18	14 (0%) 95 91	25, 60, 87, 114	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	155	ASP	3.2
1	H	629	THR	3.1
1	H	67	MET	2.7
1	H	148	LEU	2.6
1	B	157	GLU	2.4

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	E	804	5/5	0.98	0.27	2.60	77,78,78,78	0
3	MG	B	802	1/1	0.97	0.26	1.60	13,13,13,13	0
4	PO4	B	805	5/5	0.82	0.28	1.44	120,120,121,121	0
4	PO4	F	804	5/5	0.89	0.26	1.24	104,105,105,105	0
4	PO4	C	804	5/5	0.86	0.21	0.72	113,113,114,114	0
3	MG	F	802	1/1	0.79	0.20	0.67	54,54,54,54	0
3	MG	D	802	1/1	0.89	0.20	0.55	37,37,37,37	0
4	PO4	G	804	5/5	0.91	0.20	0.52	90,91,91,92	0
3	MG	E	802	1/1	0.95	0.18	0.17	39,39,39,39	0
2	ATP	F	801	31/31	0.94	0.20	0.16	45,54,62,62	0
4	PO4	D	803	5/5	0.94	0.18	0.08	83,83,84,84	0
2	ATP	D	801	31/31	0.95	0.17	0.01	55,69,82,83	0
4	PO4	A	804	5/5	0.94	0.19	-0.26	65,66,67,67	0
2	ATP	E	801	31/31	0.92	0.20	-0.37	79,88,95,95	0
4	PO4	A	805	5/5	0.91	0.18	-0.45	103,103,103,104	0
4	PO4	H	804	5/5	0.93	0.17	-0.45	75,75,76,76	0
3	MG	H	803	1/1	0.75	0.18	-0.53	67,67,67,67	0
3	MG	G	803	1/1	0.85	0.14	-0.58	40,40,40,40	0
2	ATP	G	801	31/31	0.95	0.16	-0.58	72,75,78,78	0
2	ATP	C	801	31/31	0.94	0.17	-0.63	78,86,92,93	0
3	MG	A	802	1/1	0.79	0.16	-0.79	43,43,43,43	0
2	ATP	H	801	31/31	0.93	0.17	-0.82	74,83,85,86	0
4	PO4	B	804	5/5	0.97	0.17	-0.85	66,67,67,69	0
3	MG	G	802	1/1	0.85	0.12	-1.08	36,36,36,36	0
2	ATP	A	801	31/31	0.96	0.14	-1.33	46,50,53,54	0
3	MG	C	802	1/1	0.92	0.12	-1.41	60,60,60,60	0
4	PO4	F	805	5/5	0.93	0.13	-1.60	90,91,91,91	0
2	ATP	B	801	31/31	0.97	0.15	-1.69	36,45,53,53	0
4	PO4	G	805	5/5	0.94	0.14	-1.83	113,113,114,114	0
3	MG	E	803	1/1	0.93	0.12	-1.92	40,40,40,40	0
5	CO	B	806	1/1	0.98	0.12	-1.95	48,48,48,48	0
3	MG	H	802	1/1	0.80	0.15	-2.07	47,47,47,47	0
3	MG	C	803	1/1	0.92	0.09	-2.19	34,34,34,34	0
3	MG	A	803	1/1	0.98	0.13	-2.31	18,18,18,18	0
3	MG	F	803	1/1	0.94	0.09	-2.73	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	803	1/1	0.98	0.07	-6.78	13,13,13,13	0
5	CO	F	806	1/1	0.98	0.03	-	71,71,71,71	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.