



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:20 PM GMT

PDB ID : 1T5A
Title : Human Pyruvate Kinase M2
Authors : Dombrauckas, J.D.; Santarsiero, B.D.; Mesecar, A.D.
Deposited on : 2004-05-03
Resolution : 2.80 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

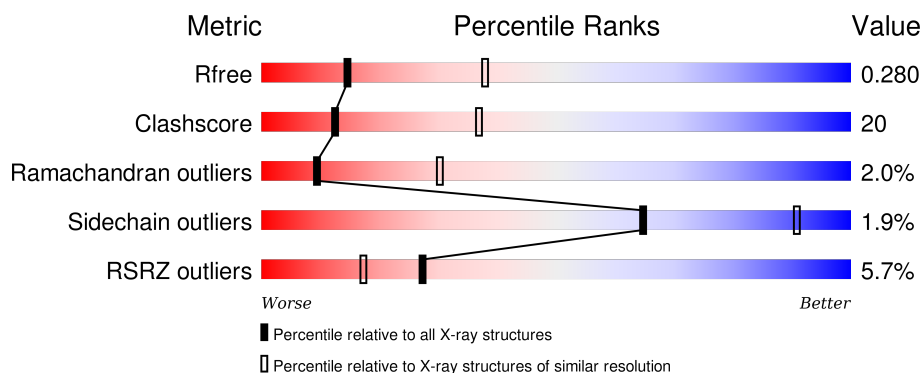
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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.

Mol	Chain	Length	Quality of chain
1	A	567	<div> <div>7%</div> <div>60%</div> <div>29%</div> <div>8%</div> </div>
1	B	567	<div> <div>6%</div> <div>62%</div> <div>27%</div> <div>8%</div> </div>
1	C	567	<div> <div>2%</div> <div>60%</div> <div>29%</div> <div>8%</div> </div>
1	D	567	<div> <div>6%</div> <div>61%</div> <div>28%</div> <div>8%</div> </div>

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
3	OXL	C	533	-	-	X	X
3	OXL	D	533	-	-	-	X
7	GOL	A	703	-	-	-	X
7	GOL	B	704	-	-	-	X
7	GOL	B	705	-	-	-	X
7	GOL	C	705	-	-	-	X
7	GOL	C	707	-	-	X	X
7	GOL	C	709	-	-	-	X
7	GOL	D	708	-	-	-	X
7	GOL	D	709	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16271 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 Pyruvate kinase, M2 isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3971	2496	704	746	25			
1	B	519	Total	C	N	O	S	0	0	0
			3971	2496	704	746	25			
1	C	519	Total	C	N	O	S	0	0	0
			3971	2496	704	746	25			
1	D	519	Total	C	N	O	S	0	0	0
			3971	2496	704	746	25			

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	CLONING ARTIFACT	UNP P14618
A	-34	ARG	-	CLONING ARTIFACT	UNP P14618
A	-33	GLY	-	CLONING ARTIFACT	UNP P14618
A	-32	SER	-	CLONING ARTIFACT	UNP P14618
A	-31	HIS	-	CLONING ARTIFACT	UNP P14618
A	-30	HIS	-	CLONING ARTIFACT	UNP P14618
A	-29	HIS	-	CLONING ARTIFACT	UNP P14618
A	-28	HIS	-	CLONING ARTIFACT	UNP P14618
A	-27	HIS	-	CLONING ARTIFACT	UNP P14618
A	-26	HIS	-	CLONING ARTIFACT	UNP P14618
A	-25	GLY	-	CLONING ARTIFACT	UNP P14618
A	-24	MET	-	CLONING ARTIFACT	UNP P14618
A	-23	ALA	-	CLONING ARTIFACT	UNP P14618
A	-22	SER	-	CLONING ARTIFACT	UNP P14618
A	-21	MET	-	CLONING ARTIFACT	UNP P14618
A	-20	THR	-	CLONING ARTIFACT	UNP P14618
A	-19	GLY	-	CLONING ARTIFACT	UNP P14618
A	-18	GLY	-	CLONING ARTIFACT	UNP P14618
A	-17	GLN	-	CLONING ARTIFACT	UNP P14618
A	-16	GLN	-	CLONING ARTIFACT	UNP P14618
A	-15	MET	-	CLONING ARTIFACT	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	GLY	-	CLONING ARTIFACT	UNP P14618
A	-13	ARG	-	CLONING ARTIFACT	UNP P14618
A	-12	ASP	-	CLONING ARTIFACT	UNP P14618
A	-11	LEU	-	CLONING ARTIFACT	UNP P14618
A	-10	TYR	-	CLONING ARTIFACT	UNP P14618
A	-9	ASP	-	CLONING ARTIFACT	UNP P14618
A	-8	ASP	-	CLONING ARTIFACT	UNP P14618
A	-7	ASP	-	CLONING ARTIFACT	UNP P14618
A	-6	ASP	-	CLONING ARTIFACT	UNP P14618
A	-5	LYS	-	CLONING ARTIFACT	UNP P14618
A	-4	ASP	-	CLONING ARTIFACT	UNP P14618
A	-3	HIS	-	CLONING ARTIFACT	UNP P14618
A	-2	PRO	-	CLONING ARTIFACT	UNP P14618
A	-1	PHE	-	CLONING ARTIFACT	UNP P14618
A	0	THR	-	CLONING ARTIFACT	UNP P14618
A	1	MET	-	INITIATING MET	UNP P14618
B	-35	MET	-	CLONING ARTIFACT	UNP P14618
B	-34	ARG	-	CLONING ARTIFACT	UNP P14618
B	-33	GLY	-	CLONING ARTIFACT	UNP P14618
B	-32	SER	-	CLONING ARTIFACT	UNP P14618
B	-31	HIS	-	CLONING ARTIFACT	UNP P14618
B	-30	HIS	-	CLONING ARTIFACT	UNP P14618
B	-29	HIS	-	CLONING ARTIFACT	UNP P14618
B	-28	HIS	-	CLONING ARTIFACT	UNP P14618
B	-27	HIS	-	CLONING ARTIFACT	UNP P14618
B	-26	HIS	-	CLONING ARTIFACT	UNP P14618
B	-25	GLY	-	CLONING ARTIFACT	UNP P14618
B	-24	MET	-	CLONING ARTIFACT	UNP P14618
B	-23	ALA	-	CLONING ARTIFACT	UNP P14618
B	-22	SER	-	CLONING ARTIFACT	UNP P14618
B	-21	MET	-	CLONING ARTIFACT	UNP P14618
B	-20	THR	-	CLONING ARTIFACT	UNP P14618
B	-19	GLY	-	CLONING ARTIFACT	UNP P14618
B	-18	GLY	-	CLONING ARTIFACT	UNP P14618
B	-17	GLN	-	CLONING ARTIFACT	UNP P14618
B	-16	GLN	-	CLONING ARTIFACT	UNP P14618
B	-15	MET	-	CLONING ARTIFACT	UNP P14618
B	-14	GLY	-	CLONING ARTIFACT	UNP P14618
B	-13	ARG	-	CLONING ARTIFACT	UNP P14618
B	-12	ASP	-	CLONING ARTIFACT	UNP P14618
B	-11	LEU	-	CLONING ARTIFACT	UNP P14618
B	-10	TYR	-	CLONING ARTIFACT	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	ASP	-	CLONING ARTIFACT	UNP P14618
B	-8	ASP	-	CLONING ARTIFACT	UNP P14618
B	-7	ASP	-	CLONING ARTIFACT	UNP P14618
B	-6	ASP	-	CLONING ARTIFACT	UNP P14618
B	-5	LYS	-	CLONING ARTIFACT	UNP P14618
B	-4	ASP	-	CLONING ARTIFACT	UNP P14618
B	-3	HIS	-	CLONING ARTIFACT	UNP P14618
B	-2	PRO	-	CLONING ARTIFACT	UNP P14618
B	-1	PHE	-	CLONING ARTIFACT	UNP P14618
B	0	THR	-	CLONING ARTIFACT	UNP P14618
B	1	MET	-	INITIATING MET	UNP P14618
C	-35	MET	-	CLONING ARTIFACT	UNP P14618
C	-34	ARG	-	CLONING ARTIFACT	UNP P14618
C	-33	GLY	-	CLONING ARTIFACT	UNP P14618
C	-32	SER	-	CLONING ARTIFACT	UNP P14618
C	-31	HIS	-	CLONING ARTIFACT	UNP P14618
C	-30	HIS	-	CLONING ARTIFACT	UNP P14618
C	-29	HIS	-	CLONING ARTIFACT	UNP P14618
C	-28	HIS	-	CLONING ARTIFACT	UNP P14618
C	-27	HIS	-	CLONING ARTIFACT	UNP P14618
C	-26	HIS	-	CLONING ARTIFACT	UNP P14618
C	-25	GLY	-	CLONING ARTIFACT	UNP P14618
C	-24	MET	-	CLONING ARTIFACT	UNP P14618
C	-23	ALA	-	CLONING ARTIFACT	UNP P14618
C	-22	SER	-	CLONING ARTIFACT	UNP P14618
C	-21	MET	-	CLONING ARTIFACT	UNP P14618
C	-20	THR	-	CLONING ARTIFACT	UNP P14618
C	-19	GLY	-	CLONING ARTIFACT	UNP P14618
C	-18	GLY	-	CLONING ARTIFACT	UNP P14618
C	-17	GLN	-	CLONING ARTIFACT	UNP P14618
C	-16	GLN	-	CLONING ARTIFACT	UNP P14618
C	-15	MET	-	CLONING ARTIFACT	UNP P14618
C	-14	GLY	-	CLONING ARTIFACT	UNP P14618
C	-13	ARG	-	CLONING ARTIFACT	UNP P14618
C	-12	ASP	-	CLONING ARTIFACT	UNP P14618
C	-11	LEU	-	CLONING ARTIFACT	UNP P14618
C	-10	TYR	-	CLONING ARTIFACT	UNP P14618
C	-9	ASP	-	CLONING ARTIFACT	UNP P14618
C	-8	ASP	-	CLONING ARTIFACT	UNP P14618
C	-7	ASP	-	CLONING ARTIFACT	UNP P14618
C	-6	ASP	-	CLONING ARTIFACT	UNP P14618
C	-5	LYS	-	CLONING ARTIFACT	UNP P14618

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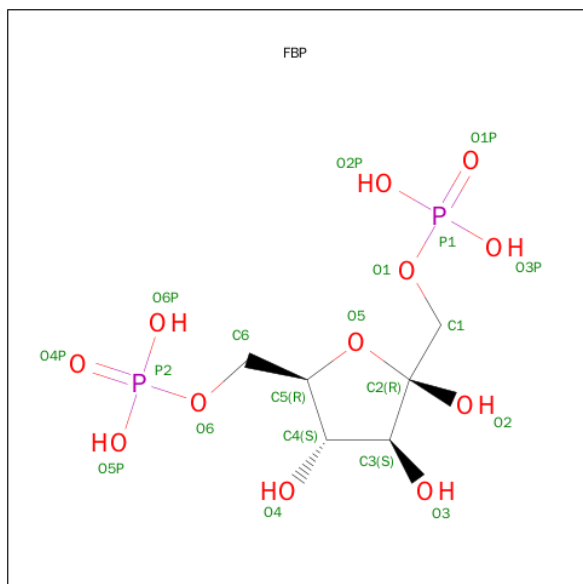
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	ASP	-	CLONING ARTIFACT	UNP P14618
C	-3	HIS	-	CLONING ARTIFACT	UNP P14618
C	-2	PRO	-	CLONING ARTIFACT	UNP P14618
C	-1	PHE	-	CLONING ARTIFACT	UNP P14618
C	0	THR	-	CLONING ARTIFACT	UNP P14618
C	1	MET	-	INITIATING MET	UNP P14618
D	-35	MET	-	CLONING ARTIFACT	UNP P14618
D	-34	ARG	-	CLONING ARTIFACT	UNP P14618
D	-33	GLY	-	CLONING ARTIFACT	UNP P14618
D	-32	SER	-	CLONING ARTIFACT	UNP P14618
D	-31	HIS	-	CLONING ARTIFACT	UNP P14618
D	-30	HIS	-	CLONING ARTIFACT	UNP P14618
D	-29	HIS	-	CLONING ARTIFACT	UNP P14618
D	-28	HIS	-	CLONING ARTIFACT	UNP P14618
D	-27	HIS	-	CLONING ARTIFACT	UNP P14618
D	-26	HIS	-	CLONING ARTIFACT	UNP P14618
D	-25	GLY	-	CLONING ARTIFACT	UNP P14618
D	-24	MET	-	CLONING ARTIFACT	UNP P14618
D	-23	ALA	-	CLONING ARTIFACT	UNP P14618
D	-22	SER	-	CLONING ARTIFACT	UNP P14618
D	-21	MET	-	CLONING ARTIFACT	UNP P14618
D	-20	THR	-	CLONING ARTIFACT	UNP P14618
D	-19	GLY	-	CLONING ARTIFACT	UNP P14618
D	-18	GLY	-	CLONING ARTIFACT	UNP P14618
D	-17	GLN	-	CLONING ARTIFACT	UNP P14618
D	-16	GLN	-	CLONING ARTIFACT	UNP P14618
D	-15	MET	-	CLONING ARTIFACT	UNP P14618
D	-14	GLY	-	CLONING ARTIFACT	UNP P14618
D	-13	ARG	-	CLONING ARTIFACT	UNP P14618
D	-12	ASP	-	CLONING ARTIFACT	UNP P14618
D	-11	LEU	-	CLONING ARTIFACT	UNP P14618
D	-10	TYR	-	CLONING ARTIFACT	UNP P14618
D	-9	ASP	-	CLONING ARTIFACT	UNP P14618
D	-8	ASP	-	CLONING ARTIFACT	UNP P14618
D	-7	ASP	-	CLONING ARTIFACT	UNP P14618
D	-6	ASP	-	CLONING ARTIFACT	UNP P14618
D	-5	LYS	-	CLONING ARTIFACT	UNP P14618
D	-4	ASP	-	CLONING ARTIFACT	UNP P14618
D	-3	HIS	-	CLONING ARTIFACT	UNP P14618
D	-2	PRO	-	CLONING ARTIFACT	UNP P14618
D	-1	PHE	-	CLONING ARTIFACT	UNP P14618
D	0	THR	-	CLONING ARTIFACT	UNP P14618

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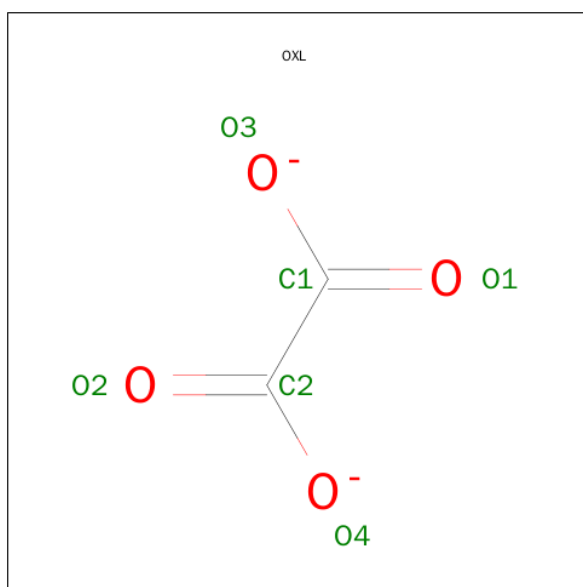
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	INITIATING MET	UNP P14618

- Molecule 2 is SUGAR (FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



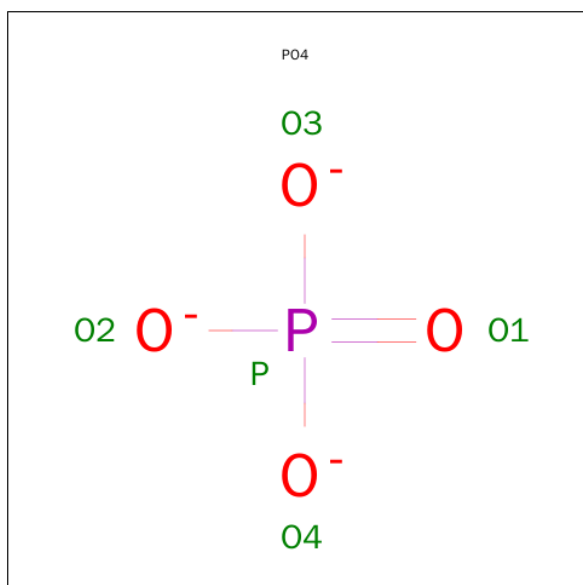
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

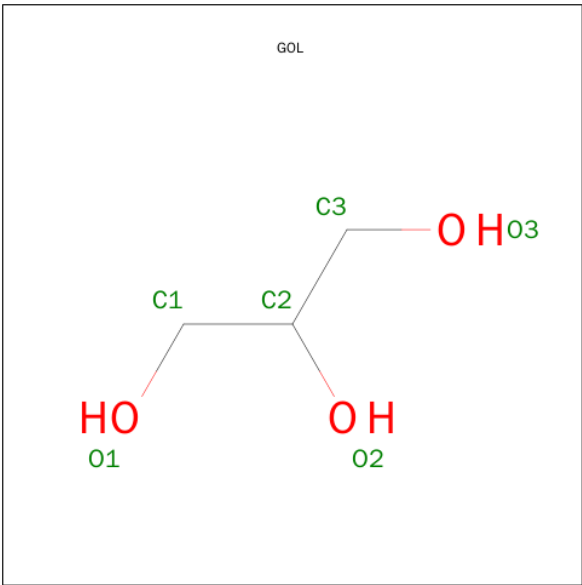
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0
6	A	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

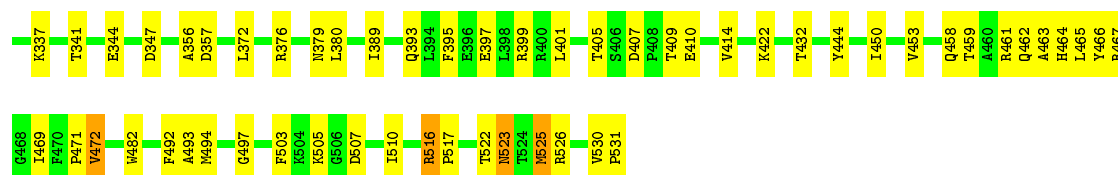
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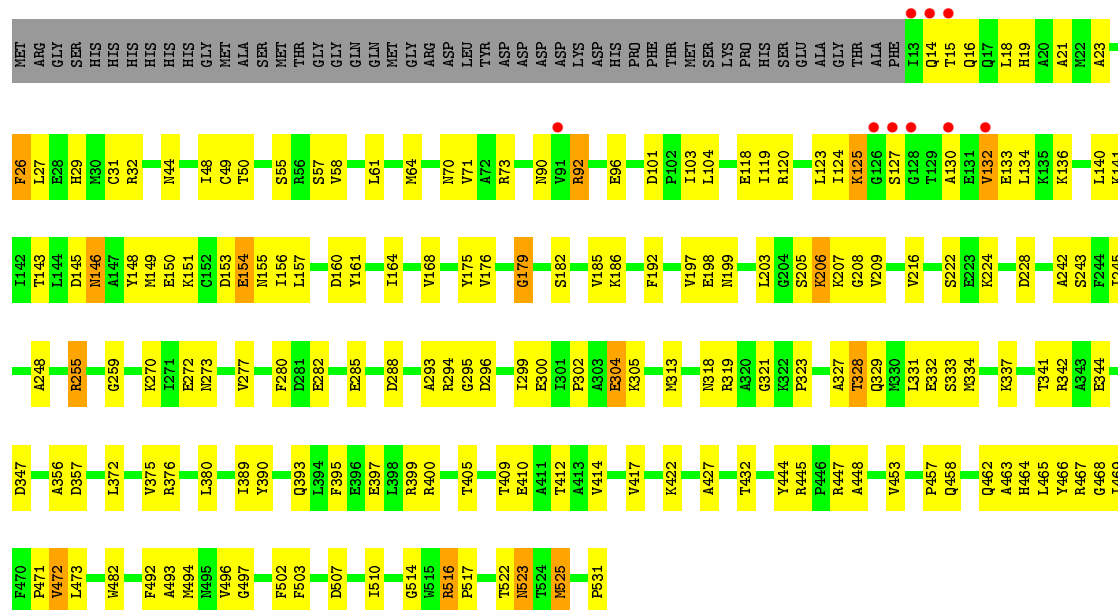
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0

- Molecule 8 is water.

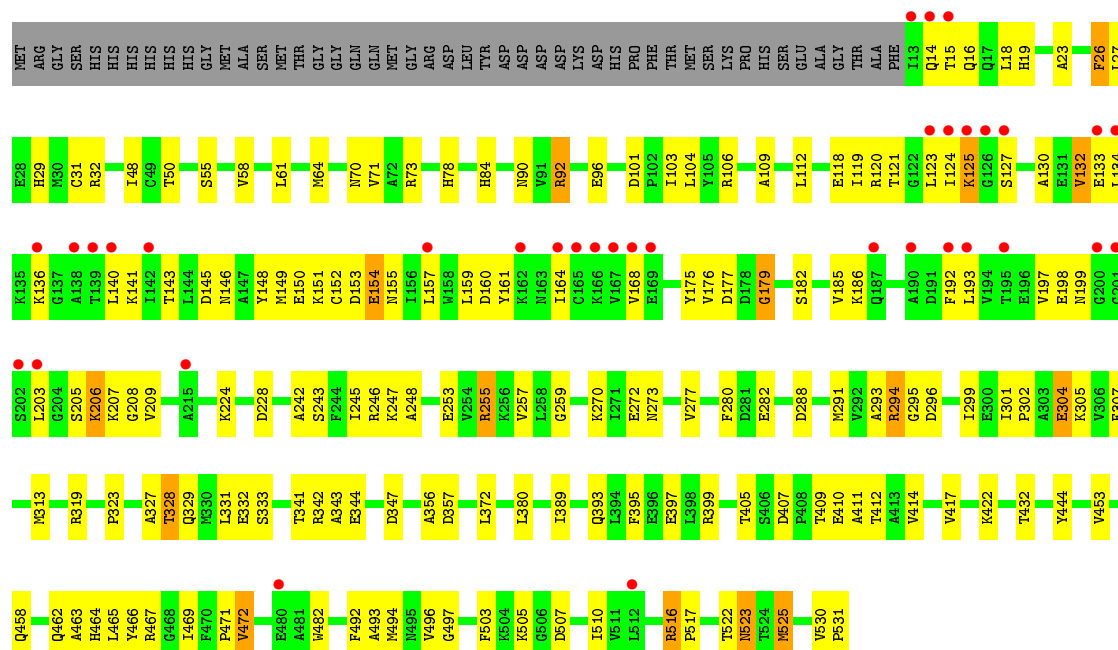
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	47	Total 47	O 47	0	0
8	B	28	Total 28	O 28	0	0
8	C	30	Total 30	O 30	0	0
8	D	30	Total 30	O 30	0	0



• Molecule 1: Pyruvate kinase, M2 isozyme



• Molecule 1: Pyruvate kinase, M2 isozyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.21Å 145.01Å 159.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 48.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.80) 96.4 (48.30-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.231 , 0.278 0.235 , 0.280	Depositor DCC
R_{free} test set	3022 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60139 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16271	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, MG, FBP, K, OXL, 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	0.53	0/4034	0.74	3/5448 (0.1%)
1	B	0.51	1/4034 (0.0%)	0.69	2/5448 (0.0%)
1	C	0.52	0/4034	0.69	2/5448 (0.0%)
1	D	0.50	0/4034	0.68	2/5448 (0.0%)
All	All	0.51	1/16136 (0.0%)	0.70	9/21792 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	ASN	CB-CG	5.22	1.63	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	NE-CZ-NH1	-14.04	113.28	120.30
1	A	92	ARG	NE-CZ-NH2	13.29	126.95	120.30
1	D	92	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	92	ARG	CD-NE-CZ	7.46	134.04	123.60
1	B	92	ARG	NE-CZ-NH2	-6.94	116.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3971	0	4059	170	0
1	B	3971	0	4059	160	0
1	C	3971	0	4059	175	0
1	D	3971	0	4059	172	0
2	A	20	0	10	1	0
2	B	20	0	10	1	0
2	C	20	0	10	2	0
2	D	20	0	10	1	0
3	A	6	0	0	0	0
3	B	6	0	0	1	0
3	C	6	0	0	2	0
3	D	6	0	0	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	30	0	40	1	0
7	B	24	0	32	0	0
7	C	36	0	48	11	0
7	D	30	0	40	1	0
8	A	47	0	0	6	0
8	B	28	0	0	3	0
8	C	30	0	0	4	0
8	D	30	0	0	7	0
All	All	16271	0	16436	636	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 20.

The worst 5 of 636 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:132:VAL:HG12	1:C:133:GLU:H	1.13	1.08
1:A:132:VAL:HG12	1:A:133:GLU:H	1.14	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:HG12	1:B:133:GLU:H	1.16	1.04
1:B:132:VAL:HG21	1:B:153:ASP:HA	1.42	1.01
1:D:132:VAL:HG12	1:D:133:GLU:H	1.19	1.00

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	517/567 (91%)	479 (93%)	28 (5%)	10 (2%)	10	32
1	B	517/567 (91%)	477 (92%)	30 (6%)	10 (2%)	10	32
1	C	517/567 (91%)	482 (93%)	24 (5%)	11 (2%)	9	29
1	D	517/567 (91%)	479 (93%)	27 (5%)	11 (2%)	9	29
All	All	2068/2268 (91%)	1917 (93%)	109 (5%)	42 (2%)	9	30

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	GLU
1	B	154	GLU
1	C	154	GLU
1	D	154	GLU
1	A	125	LYS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/466 (92%)	418 (98%)	9 (2%)	61	90
1	B	427/466 (92%)	420 (98%)	7 (2%)	70	93
1	C	427/466 (92%)	419 (98%)	8 (2%)	65	91
1	D	427/466 (92%)	418 (98%)	9 (2%)	61	90
All	All	1708/1864 (92%)	1675 (98%)	33 (2%)	65	91

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	516	ARG
1	C	199	ASN
1	D	472	VAL
1	B	525	MET
1	C	26	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	393	GLN
1	C	14	GLN
1	C	439	HIS
1	B	90	ASN
1	D	84	HIS

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 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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	FBP	A	532	-	18,20,20	1.53	4 (22%)	21,32,32	0.86	0
3	OXL	A	533	5	0,5,5	0.00	-	0,6,6	0.00	-
4	PO4	A	534	-	4,4,4	1.49	1 (25%)	6,6,6	0.31	0
7	GOL	A	702	-	5,5,5	0.56	0	5,5,5	0.21	0
7	GOL	A	703	-	5,5,5	0.73	0	5,5,5	0.15	0
7	GOL	A	704	-	5,5,5	0.78	0	5,5,5	0.40	0
7	GOL	A	705	-	5,5,5	0.77	0	5,5,5	0.14	0
7	GOL	A	706	-	5,5,5	0.90	0	5,5,5	0.46	0
2	FBP	B	532	-	18,20,20	1.60	4 (22%)	21,32,32	0.93	1 (4%)
3	OXL	B	533	5	0,5,5	0.00	-	0,6,6	0.00	-
4	PO4	B	534	-	4,4,4	1.67	2 (50%)	6,6,6	0.30	0
7	GOL	B	703	-	5,5,5	0.59	0	5,5,5	0.28	0
7	GOL	B	704	-	5,5,5	0.90	0	5,5,5	0.20	0
7	GOL	B	705	-	5,5,5	0.77	0	5,5,5	0.28	0
7	GOL	B	706	-	5,5,5	0.96	0	5,5,5	0.15	0
2	FBP	C	532	-	18,20,20	1.56	4 (22%)	21,32,32	0.83	0
3	OXL	C	533	5	0,5,5	0.00	-	0,6,6	0.00	-
4	PO4	C	534	-	4,4,4	1.11	0	6,6,6	0.32	0
7	GOL	C	704	-	5,5,5	0.73	0	5,5,5	0.24	0
7	GOL	C	705	-	5,5,5	0.93	0	5,5,5	0.26	0
7	GOL	C	706	-	5,5,5	0.37	0	5,5,5	0.51	0
7	GOL	C	707	-	5,5,5	0.61	0	5,5,5	0.35	0
7	GOL	C	708	-	5,5,5	0.77	0	5,5,5	0.18	0
7	GOL	C	709	-	5,5,5	0.65	0	5,5,5	0.29	0
2	FBP	D	532	-	18,20,20	1.51	3 (16%)	21,32,32	0.81	0
3	OXL	D	533	5	0,5,5	0.00	-	0,6,6	0.00	-
4	PO4	D	534	-	4,4,4	1.56	0	6,6,6	0.29	0
7	GOL	D	705	-	5,5,5	0.73	0	5,5,5	0.24	0
7	GOL	D	706	-	5,5,5	1.12	0	5,5,5	0.39	0
7	GOL	D	707	-	5,5,5	0.57	0	5,5,5	0.23	0
7	GOL	D	708	-	5,5,5	1.00	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	D	709	-	5,5,5	1.14	0	5,5,5	0.36	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	FBP	A	532	-	-	0/13/32/32	0/1/1/1
3	OXL	A	533	5	-	0/0/4/4	0/0/0/0
4	PO4	A	534	-	-	0/0/0/0	0/0/0/0
7	GOL	A	702	-	-	0/4/4/4	0/0/0/0
7	GOL	A	703	-	-	0/4/4/4	0/0/0/0
7	GOL	A	704	-	-	0/4/4/4	0/0/0/0
7	GOL	A	705	-	-	0/4/4/4	0/0/0/0
7	GOL	A	706	-	-	0/4/4/4	0/0/0/0
2	FBP	B	532	-	-	0/13/32/32	0/1/1/1
3	OXL	B	533	5	-	0/0/4/4	0/0/0/0
4	PO4	B	534	-	-	0/0/0/0	0/0/0/0
7	GOL	B	703	-	-	0/4/4/4	0/0/0/0
7	GOL	B	704	-	-	0/4/4/4	0/0/0/0
7	GOL	B	705	-	-	0/4/4/4	0/0/0/0
7	GOL	B	706	-	-	0/4/4/4	0/0/0/0
2	FBP	C	532	-	-	0/13/32/32	0/1/1/1
3	OXL	C	533	5	-	0/0/4/4	0/0/0/0
4	PO4	C	534	-	-	0/0/0/0	0/0/0/0
7	GOL	C	704	-	-	0/4/4/4	0/0/0/0
7	GOL	C	705	-	-	0/4/4/4	0/0/0/0
7	GOL	C	706	-	-	0/4/4/4	0/0/0/0
7	GOL	C	707	-	-	0/4/4/4	0/0/0/0
7	GOL	C	708	-	-	0/4/4/4	0/0/0/0
7	GOL	C	709	-	-	0/4/4/4	0/0/0/0
2	FBP	D	532	-	-	0/13/32/32	0/1/1/1
3	OXL	D	533	5	-	0/0/4/4	0/0/0/0
4	PO4	D	534	-	-	0/0/0/0	0/0/0/0
7	GOL	D	705	-	-	0/4/4/4	0/0/0/0
7	GOL	D	706	-	-	0/4/4/4	0/0/0/0
7	GOL	D	707	-	-	0/4/4/4	0/0/0/0
7	GOL	D	708	-	-	0/4/4/4	0/0/0/0
7	GOL	D	709	-	-	0/4/4/4	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	532	FBP	P1-O3P	-3.81	1.41	1.54
2	A	532	FBP	P1-O3P	-3.55	1.42	1.54
2	C	532	FBP	P1-O3P	-3.42	1.42	1.54
2	D	532	FBP	P1-O3P	-3.34	1.42	1.54
2	B	532	FBP	P1-O2P	-2.60	1.45	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	532	FBP	O2-C2-O5	2.16	113.82	109.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	532	FBP	1	0
7	A	704	GOL	1	0
2	B	532	FBP	1	0
3	B	533	OXL	1	0
2	C	532	FBP	2	0
3	C	533	OXL	2	0
7	C	704	GOL	1	0
7	C	706	GOL	1	0
7	C	707	GOL	7	0
7	C	709	GOL	2	0
2	D	532	FBP	1	0
3	D	533	OXL	1	0
4	D	534	PO4	1	0
7	D	705	GOL	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 [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	519/567 (91%)	0.14	38 (7%) 18 10	23, 60, 99, 99	0
1	B	519/567 (91%)	0.18	36 (6%) 20 11	29, 65, 99, 99	0
1	C	519/567 (91%)	-0.03	9 (1%) 73 63	26, 65, 97, 99	0
1	D	519/567 (91%)	0.19	35 (6%) 21 12	34, 69, 99, 99	0
All	All	2076/2268 (91%)	0.12	118 (5%) 27 17	23, 65, 99, 99	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ILE	6.4
1	C	13	ILE	5.9
1	D	140	LEU	5.9
1	A	13	ILE	5.8
1	A	134	LEU	5.7

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
7	GOL	C	707	6/6	0.77	0.45	8.28	66,66,66,66	0
7	GOL	D	709	6/6	0.93	0.35	7.44	42,42,42,42	0
7	GOL	B	704	6/6	0.79	0.30	6.09	66,66,66,66	0
7	GOL	C	705	6/6	0.77	0.48	5.48	66,66,66,66	0
7	GOL	A	703	6/6	0.90	0.25	3.71	66,66,66,66	0
7	GOL	B	705	6/6	0.76	0.28	3.17	66,66,66,66	0
7	GOL	D	708	6/6	0.78	0.32	2.73	66,66,66,66	0
7	GOL	C	709	6/6	0.90	0.22	2.45	42,42,42,42	0
3	OXL	C	533	6/6	0.92	0.26	2.43	66,66,66,66	0
3	OXL	D	533	6/6	0.95	0.21	2.31	66,66,66,66	0
7	GOL	A	704	6/6	0.85	0.34	1.69	66,66,66,66	0
7	GOL	A	705	6/6	0.84	0.26	1.51	66,66,66,66	0
7	GOL	D	706	6/6	0.80	0.26	1.49	66,66,66,66	0
7	GOL	C	708	6/6	0.72	0.31	0.84	66,66,66,66	0
6	K	B	702	1/1	0.93	0.21	0.72	66,66,66,66	0
2	FBP	A	532	20/20	0.97	0.17	0.59	66,66,66,66	0
7	GOL	D	707	6/6	0.92	0.25	0.46	66,66,66,66	0
7	GOL	A	706	6/6	0.85	0.35	0.38	42,42,42,42	0
6	K	A	701	1/1	0.90	0.19	0.31	66,66,66,66	0
2	FBP	B	532	20/20	0.95	0.16	0.25	66,66,66,66	0
7	GOL	C	706	6/6	0.92	0.20	0.13	66,66,66,66	0
3	OXL	B	533	6/6	0.98	0.17	-0.35	66,66,66,66	0
7	GOL	B	706	6/6	0.92	0.16	-0.66	42,42,42,42	0
6	K	C	703	1/1	0.82	0.13	-0.98	66,66,66,66	0
2	FBP	D	532	20/20	0.92	0.14	-1.14	66,66,66,66	0
2	FBP	C	532	20/20	0.94	0.12	-1.51	66,66,66,66	0
3	OXL	A	533	6/6	0.89	0.14	-1.54	66,66,66,66	0
6	K	D	704	1/1	0.98	0.09	-4.87	66,66,66,66	0
4	PO4	B	534	5/5	0.95	0.17	-	66,66,66,66	0
4	PO4	D	534	5/5	0.94	0.17	-	66,66,66,66	0
5	MG	C	603	1/1	0.97	0.33	-	66,66,66,66	0
4	PO4	C	534	5/5	0.93	0.14	-	66,66,66,66	0
5	MG	D	604	1/1	0.95	0.16	-	66,66,66,66	0
5	MG	A	601	1/1	0.94	0.22	-	66,66,66,66	0
7	GOL	C	704	6/6	0.90	0.13	-	66,66,66,66	0
5	MG	B	602	1/1	0.94	0.24	-	66,66,66,66	0
7	GOL	A	702	6/6	0.94	0.15	-	66,66,66,66	0
4	PO4	A	534	5/5	0.94	0.20	-	66,66,66,66	0
7	GOL	B	703	6/6	0.87	0.19	-	66,66,66,66	0
7	GOL	D	705	6/6	0.86	0.25	-	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.