Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:03 PM GMT

PDB ID	:	3SRD
Title	:	Human M2 pyruvate kinase in complex with fructose 1-6 bisphosphate and Oxalate.
Authors	:	Morgan, H.P.; O'Reilly, F.; Palmer, R.; McNae, I.W.; Nowicki, M.W.; Wear, M.A.; Fothergill-Gilmore, L.A.; Walkinshaw, M.D.
Deposited on	:	2011-07-07
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

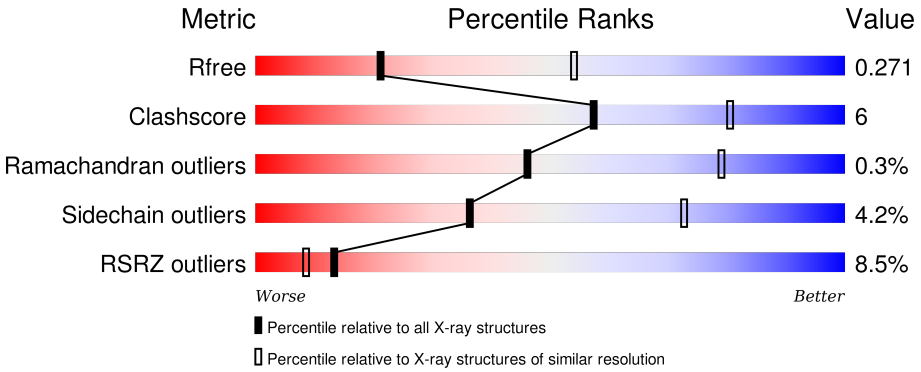
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	551	4% 77% 14% • 7%
1	B	551	17% 77% 15% • 7%
1	C	551	6% 78% 14% • 7%
1	D	551	5% 76% 16% • 7%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16047 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 isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			3951	2486	701	739	25			
1	B	512	Total	C	N	O	S	0	0	0
			3930	2473	698	734	25			
1	C	514	Total	C	N	O	S	0	0	0
			3947	2484	700	738	25			
1	D	515	Total	C	N	O	S	0	1	0
			3952	2484	702	741	25			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P14618
A	-18	GLY	-	EXPRESSION TAG	UNP P14618
A	-17	SER	-	EXPRESSION TAG	UNP P14618
A	-16	SER	-	EXPRESSION TAG	UNP P14618
A	-15	HIS	-	EXPRESSION TAG	UNP P14618
A	-14	HIS	-	EXPRESSION TAG	UNP P14618
A	-13	HIS	-	EXPRESSION TAG	UNP P14618
A	-12	HIS	-	EXPRESSION TAG	UNP P14618
A	-11	HIS	-	EXPRESSION TAG	UNP P14618
A	-10	HIS	-	EXPRESSION TAG	UNP P14618
A	-9	SER	-	EXPRESSION TAG	UNP P14618
A	-8	SER	-	EXPRESSION TAG	UNP P14618
A	-7	GLY	-	EXPRESSION TAG	UNP P14618
A	-6	LEU	-	EXPRESSION TAG	UNP P14618
A	-5	VAL	-	EXPRESSION TAG	UNP P14618
A	-4	PRO	-	EXPRESSION TAG	UNP P14618
A	-3	ARG	-	EXPRESSION TAG	UNP P14618
A	-2	GLY	-	EXPRESSION TAG	UNP P14618
A	-1	SER	-	EXPRESSION TAG	UNP P14618
A	0	HIS	-	EXPRESSION TAG	UNP P14618
B	-19	MET	-	EXPRESSION TAG	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP P14618
B	-17	SER	-	EXPRESSION TAG	UNP P14618
B	-16	SER	-	EXPRESSION TAG	UNP P14618
B	-15	HIS	-	EXPRESSION TAG	UNP P14618
B	-14	HIS	-	EXPRESSION TAG	UNP P14618
B	-13	HIS	-	EXPRESSION TAG	UNP P14618
B	-12	HIS	-	EXPRESSION TAG	UNP P14618
B	-11	HIS	-	EXPRESSION TAG	UNP P14618
B	-10	HIS	-	EXPRESSION TAG	UNP P14618
B	-9	SER	-	EXPRESSION TAG	UNP P14618
B	-8	SER	-	EXPRESSION TAG	UNP P14618
B	-7	GLY	-	EXPRESSION TAG	UNP P14618
B	-6	LEU	-	EXPRESSION TAG	UNP P14618
B	-5	VAL	-	EXPRESSION TAG	UNP P14618
B	-4	PRO	-	EXPRESSION TAG	UNP P14618
B	-3	ARG	-	EXPRESSION TAG	UNP P14618
B	-2	GLY	-	EXPRESSION TAG	UNP P14618
B	-1	SER	-	EXPRESSION TAG	UNP P14618
B	0	HIS	-	EXPRESSION TAG	UNP P14618
C	-19	MET	-	EXPRESSION TAG	UNP P14618
C	-18	GLY	-	EXPRESSION TAG	UNP P14618
C	-17	SER	-	EXPRESSION TAG	UNP P14618
C	-16	SER	-	EXPRESSION TAG	UNP P14618
C	-15	HIS	-	EXPRESSION TAG	UNP P14618
C	-14	HIS	-	EXPRESSION TAG	UNP P14618
C	-13	HIS	-	EXPRESSION TAG	UNP P14618
C	-12	HIS	-	EXPRESSION TAG	UNP P14618
C	-11	HIS	-	EXPRESSION TAG	UNP P14618
C	-10	HIS	-	EXPRESSION TAG	UNP P14618
C	-9	SER	-	EXPRESSION TAG	UNP P14618
C	-8	SER	-	EXPRESSION TAG	UNP P14618
C	-7	GLY	-	EXPRESSION TAG	UNP P14618
C	-6	LEU	-	EXPRESSION TAG	UNP P14618
C	-5	VAL	-	EXPRESSION TAG	UNP P14618
C	-4	PRO	-	EXPRESSION TAG	UNP P14618
C	-3	ARG	-	EXPRESSION TAG	UNP P14618
C	-2	GLY	-	EXPRESSION TAG	UNP P14618
C	-1	SER	-	EXPRESSION TAG	UNP P14618
C	0	HIS	-	EXPRESSION TAG	UNP P14618
D	-19	MET	-	EXPRESSION TAG	UNP P14618
D	-18	GLY	-	EXPRESSION TAG	UNP P14618
D	-17	SER	-	EXPRESSION TAG	UNP P14618

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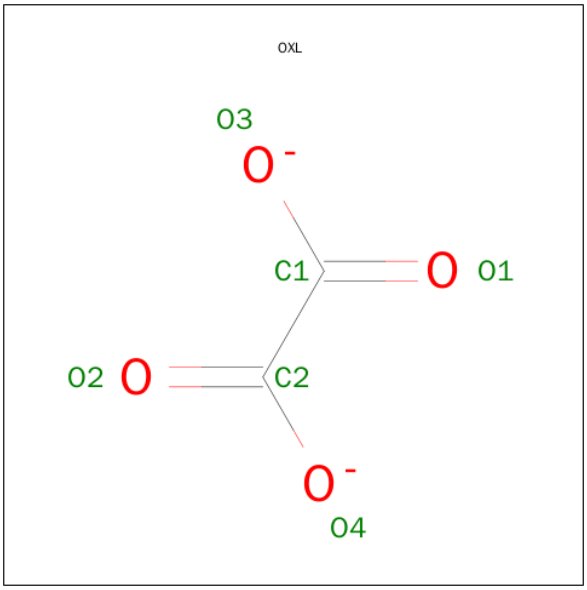
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP P14618
D	-15	HIS	-	EXPRESSION TAG	UNP P14618
D	-14	HIS	-	EXPRESSION TAG	UNP P14618
D	-13	HIS	-	EXPRESSION TAG	UNP P14618
D	-12	HIS	-	EXPRESSION TAG	UNP P14618
D	-11	HIS	-	EXPRESSION TAG	UNP P14618
D	-10	HIS	-	EXPRESSION TAG	UNP P14618
D	-9	SER	-	EXPRESSION TAG	UNP P14618
D	-8	SER	-	EXPRESSION TAG	UNP P14618
D	-7	GLY	-	EXPRESSION TAG	UNP P14618
D	-6	LEU	-	EXPRESSION TAG	UNP P14618
D	-5	VAL	-	EXPRESSION TAG	UNP P14618
D	-4	PRO	-	EXPRESSION TAG	UNP P14618
D	-3	ARG	-	EXPRESSION TAG	UNP P14618
D	-2	GLY	-	EXPRESSION TAG	UNP P14618
D	-1	SER	-	EXPRESSION TAG	UNP P14618
D	0	HIS	-	EXPRESSION TAG	UNP P14618

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



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

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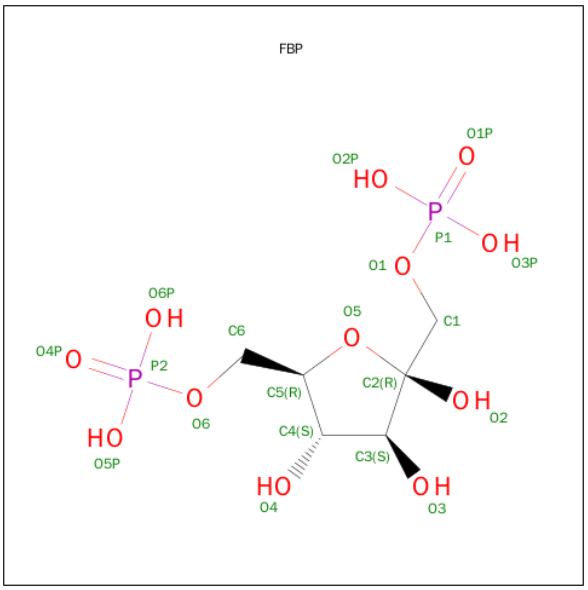
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 6 2 4	0	0

- Molecule 3 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



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

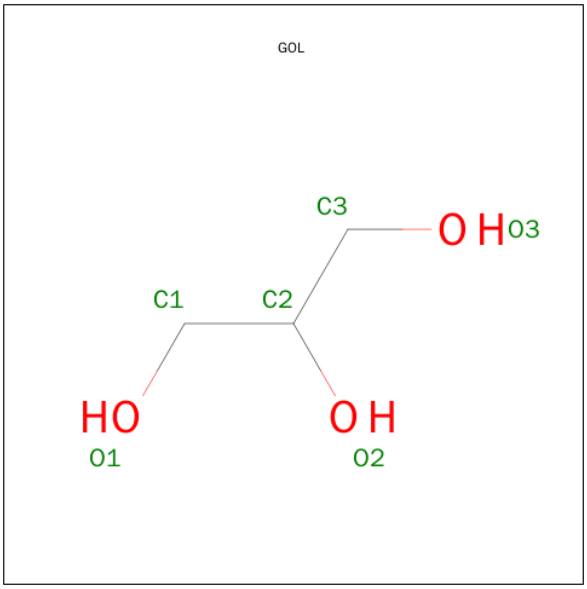
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0
4	C	1	Total K 1 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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

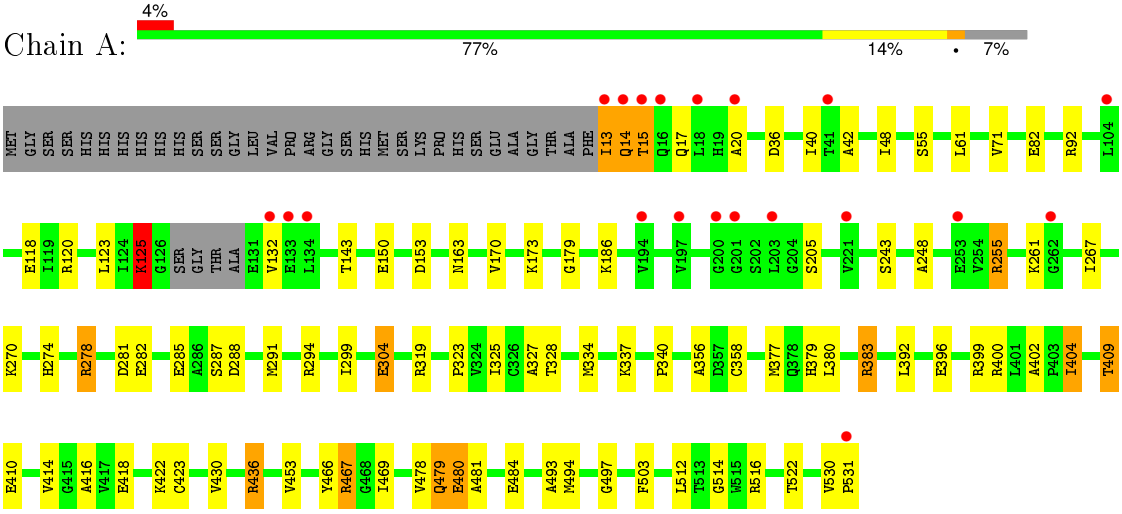
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	34	Total O 34 34	0	0
7	B	34	Total O 34 34	0	0
7	C	31	Total O 31 31	0	0
7	D	27	Total O 27 27	0	0

3 Residue-property plots (i)

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.

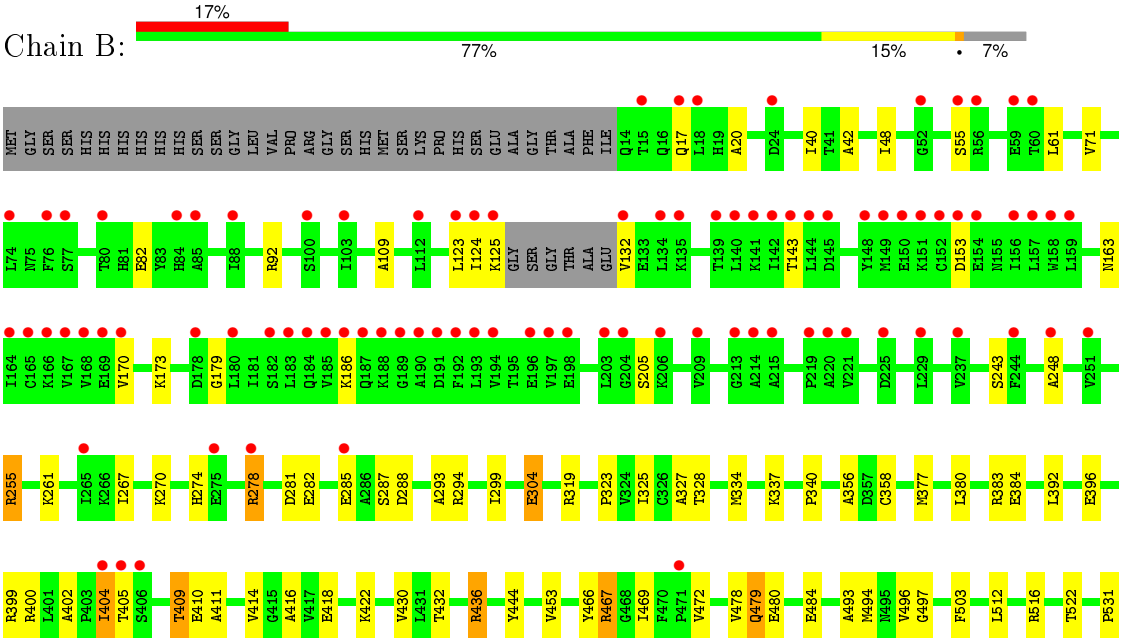
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain A:



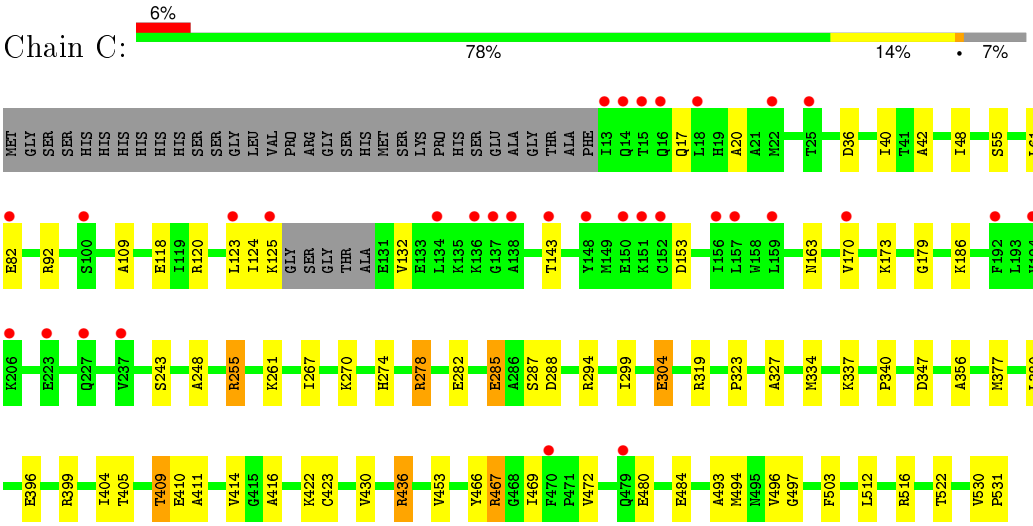
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain B:



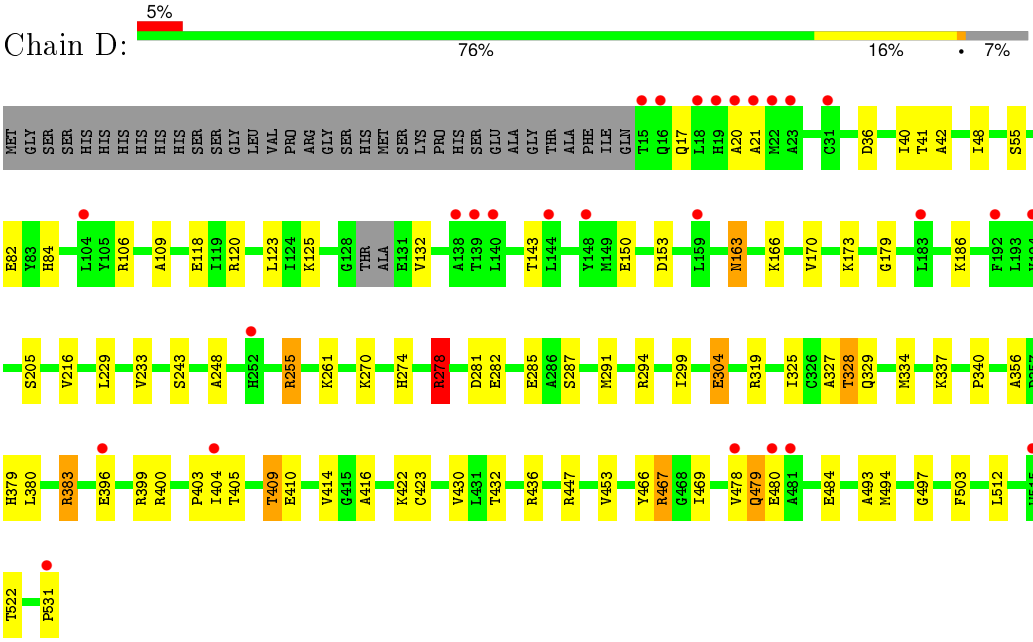
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain C:



- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.05Å 117.37Å 110.46Å 90.00° 113.56° 90.00°	Depositor
Resolution (Å)	54.18 – 2.90 54.18 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.18-2.90) 91.9 (54.18-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.253 , 0.279 0.249 , 0.271	Depositor DCC
R_{free} test set	2283 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.6	EDS
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 45322 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16047	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: OXL, GOL, MG, FBP, K

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	0.36	0/4014	0.75	16/5419 (0.3%)
1	B	0.36	0/3993	0.58	9/5391 (0.2%)
1	C	0.35	0/4010	0.60	9/5414 (0.2%)
1	D	0.39	2/4015 (0.0%)	0.58	7/5420 (0.1%)
All	All	0.37	2/16032 (0.0%)	0.63	41/21644 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	436	ARG	CG-CD	-6.60	1.35	1.51
1	D	278	ARG	CB-CG	-5.52	1.37	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ARG	NE-CZ-NH2	15.14	127.87	120.30
1	A	92	ARG	NE-CZ-NH1	-14.52	113.04	120.30
1	A	383	ARG	NE-CZ-NH2	13.47	127.04	120.30
1	A	383	ARG	NE-CZ-NH1	-13.43	113.58	120.30
1	A	436	ARG	NE-CZ-NH2	12.16	126.38	120.30
1	A	436	ARG	NE-CZ-NH1	-11.00	114.80	120.30
1	D	278	ARG	NE-CZ-NH2	10.50	125.55	120.30
1	C	436	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	C	436	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	B	436	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	14	GLN	N-CA-C	8.89	135.02	111.00
1	A	14	GLN	CB-CA-C	-8.86	92.69	110.40
1	B	436	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	A	278	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	C	278	ARG	NE-CZ-NH2	-7.79	116.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	436	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	C	285	GLU	CA-CB-CG	7.66	130.26	113.40
1	B	278	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	278	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	92	ARG	CD-NE-CZ	6.96	133.35	123.60
1	A	278	ARG	CG-CD-NE	-6.92	97.28	111.80
1	D	436	ARG	CG-CD-NE	6.87	126.22	111.80
1	B	278	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	125	LYS	CB-CA-C	-6.69	97.02	110.40
1	C	278	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	278	ARG	CG-CD-NE	-6.61	97.92	111.80
1	B	278	ARG	CG-CD-NE	-6.45	98.25	111.80
1	A	15	THR	N-CA-C	6.39	128.25	111.00
1	D	436	ARG	CB-CG-CD	-6.36	95.06	111.60
1	A	383	ARG	CD-NE-CZ	5.79	131.70	123.60
1	B	383	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	D	383	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	383	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	383	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	383	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	383	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	436	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	C	92	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	436	ARG	CD-NE-CZ	5.06	130.69	123.60
1	B	92	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	92	ARG	NE-CZ-NH2	-5.00	117.80	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	3951	0	4039	61	0
1	B	3930	0	4019	50	0
1	C	3947	0	4036	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3952	0	4033	62	0
2	A	6	0	0	0	0
2	B	6	0	0	1	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	20	0	10	1	0
3	B	20	0	10	1	0
3	C	20	0	10	0	0
3	D	20	0	10	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	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	6	0	8	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	12	0	16	1	0
7	A	34	0	0	0	0
7	B	34	0	0	1	0
7	C	31	0	0	0	0
7	D	27	0	0	4	0
All	All	16047	0	16207	194	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 6.

All (194) 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:14:GLN:CG	1:A:14:GLN:O	1.70	1.32
1:D:274:HIS:CD2	1:D:278:ARG:HH22	1.52	1.27
1:A:480:GLU:H	1:A:480:GLU:CD	1.54	1.08
1:D:278:ARG:HG3	1:D:278:ARG:NH2	1.56	1.06
1:D:278:ARG:HH21	1:D:278:ARG:CG	1.72	1.03
1:A:380:LEU:HB3	1:C:304:GLU:HG2	1.37	1.03
1:D:278:ARG:HH21	1:D:278:ARG:HG3	0.91	1.02
1:D:274:HIS:CD2	1:D:278:ARG:NH2	2.29	0.99
1:C:405:THR:O	1:D:423:CYS:HA	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:HB3	1:D:304:GLU:HG2	1.44	0.97
1:D:274:HIS:HD2	1:D:278:ARG:HH22	1.11	0.97
1:D:274:HIS:HD2	1:D:278:ARG:NH2	1.64	0.93
1:B:304:GLU:HG2	1:D:380:LEU:HB3	1.51	0.92
1:C:274:HIS:CD2	1:C:278:ARG:NH2	2.39	0.91
1:D:216:VAL:HG21	6:D:535:GOL:H32	1.54	0.89
1:A:274:HIS:CD2	1:A:278:ARG:NH2	2.42	0.88
1:B:274:HIS:CD2	1:B:278:ARG:NH2	2.42	0.87
1:D:278:ARG:NH2	1:D:278:ARG:CG	2.30	0.87
1:A:304:GLU:HG2	1:C:380:LEU:HB3	1.57	0.86
1:A:14:GLN:O	1:A:14:GLN:HG2	0.99	0.81
1:C:274:HIS:CD2	1:C:278:ARG:HH22	1.99	0.80
1:B:274:HIS:CD2	1:B:278:ARG:HH22	2.00	0.79
1:A:423:CYS:HA	1:B:405:THR:O	1.85	0.77
1:A:409:THR:HG22	1:A:522:THR:HB	1.68	0.76
1:B:494:MET:HG2	1:B:531:PRO:HD2	1.69	0.75
1:A:480:GLU:N	1:A:480:GLU:CD	2.31	0.75
1:A:274:HIS:CD2	1:A:278:ARG:HH22	2.02	0.75
1:C:494:MET:HG2	1:C:531:PRO:HD2	1.68	0.75
1:D:409:THR:HG22	1:D:522:THR:HB	1.69	0.74
1:A:494:MET:HG2	1:A:531:PRO:HD2	1.69	0.74
1:C:409:THR:HG22	1:C:522:THR:HB	1.70	0.74
1:D:494:MET:HG2	1:D:531:PRO:HD2	1.69	0.73
1:C:399:ARG:HH21	1:D:399:ARG:HH21	1.34	0.73
1:D:518:GLY:O	3:D:532:FBP:O4	2.07	0.73
1:C:422:LYS:NZ	1:D:403:PRO:O	2.22	0.71
1:B:409:THR:HG22	1:B:522:THR:HB	1.71	0.70
1:B:278:ARG:NH1	1:D:36:ASP:OD1	2.25	0.69
1:A:36:ASP:OD1	1:C:278:ARG:NH1	2.25	0.69
1:D:123:LEU:HD23	1:D:205:SER:HB3	1.80	0.62
1:B:123:LEU:HD23	1:B:205:SER:HB3	1.81	0.62
1:A:123:LEU:HD23	1:A:205:SER:HB3	1.81	0.61
1:C:123:LEU:HD23	1:C:205:SER:HB3	1.80	0.61
1:D:179:GLY:HA3	1:D:299:ILE:HD12	1.81	0.61
1:C:274:HIS:HD2	1:C:278:ARG:NH2	1.98	0.60
1:D:432:THR:HA	3:D:532:FBP:H61	1.83	0.60
1:A:294:ARG:HD3	1:A:327:ALA:O	2.01	0.60
1:A:179:GLY:HA3	1:A:299:ILE:HD12	1.82	0.60
1:B:179:GLY:HA3	1:B:299:ILE:HD12	1.84	0.59
1:C:399:ARG:NH2	1:D:399:ARG:HH21	2.00	0.59
1:C:179:GLY:HA3	1:C:299:ILE:HD12	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ARG:HE	1:B:392:LEU:HD11	1.67	0.59
1:A:13:ILE:O	1:A:13:ILE:CG2	2.50	0.58
1:D:356:ALA:O	1:D:467:ARG:NH1	2.37	0.57
1:C:294:ARG:HD3	1:C:327:ALA:O	2.05	0.57
1:D:84:HIS:HD2	7:D:555:HOH:O	1.88	0.57
1:B:274:HIS:HD2	1:B:278:ARG:NH2	2.01	0.57
1:C:356:ALA:O	1:C:467:ARG:NH1	2.37	0.57
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.41	0.56
1:B:356:ALA:O	1:B:467:ARG:NH1	2.38	0.55
1:D:294:ARG:HD3	1:D:327:ALA:O	2.07	0.55
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.42	0.55
1:C:392:LEU:HD11	1:D:400:ARG:HE	1.72	0.55
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.42	0.54
1:B:294:ARG:HD3	1:B:327:ALA:O	2.07	0.54
1:B:432:THR:HA	3:B:532:FBP:H61	1.89	0.54
1:A:423:CYS:HB3	1:B:411:ALA:HB2	1.89	0.53
1:A:356:ALA:O	1:A:467:ARG:NH1	2.41	0.53
1:D:453:VAL:HG21	1:D:493:ALA:HB2	1.91	0.53
1:B:17:GLN:HB3	1:B:20:ALA:HB3	1.91	0.53
1:A:453:VAL:HG21	1:A:493:ALA:HB2	1.91	0.52
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.91	0.52
1:C:422:LYS:HE3	1:D:405:THR:HG22	1.91	0.52
1:C:17:GLN:HB3	1:C:20:ALA:HB3	1.91	0.52
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.92	0.52
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.45	0.52
1:A:380:LEU:CB	1:C:304:GLU:HG2	2.26	0.51
1:D:17:GLN:HB3	1:D:20:ALA:HB3	1.91	0.51
1:D:243:SER:HA	1:D:270:LYS:HE2	1.93	0.51
1:A:17:GLN:HB3	1:A:20:ALA:HB3	1.92	0.51
1:C:40:ILE:HD12	1:C:42:ALA:HB3	1.92	0.50
1:C:453:VAL:HG21	1:C:493:ALA:HB2	1.94	0.50
1:A:278:ARG:NH1	1:C:36:ASP:OD1	2.45	0.50
1:B:430:VAL:HG22	1:B:512:LEU:HD12	1.94	0.50
1:C:248:ALA:HB2	1:C:282:GLU:HG2	1.94	0.50
1:D:40:ILE:HD12	1:D:42:ALA:HB3	1.93	0.50
1:A:430:VAL:HG22	1:A:512:LEU:HD12	1.94	0.49
1:D:340:PRO:HG3	1:D:377:MET:HG2	1.94	0.49
1:C:423:CYS:HA	1:D:405:THR:O	2.11	0.49
1:A:40:ILE:HD12	1:A:42:ALA:HB3	1.93	0.49
1:A:392:LEU:HD11	1:B:400:ARG:HE	1.77	0.49
1:A:410:GLU:O	1:A:414:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.94	0.49
1:B:410:GLU:O	1:B:414:VAL:HG23	2.13	0.49
1:D:410:GLU:O	1:D:414:VAL:HG23	2.13	0.49
1:C:410:GLU:O	1:C:414:VAL:HG23	2.13	0.48
1:A:118:GLU:OE2	1:A:120:ARG:NH1	2.46	0.48
1:A:243:SER:HA	1:A:270:LYS:HE2	1.95	0.48
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.95	0.48
1:D:430:VAL:HG22	1:D:512:LEU:HD12	1.94	0.48
1:A:248:ALA:HB2	1:A:282:GLU:HG2	1.95	0.48
1:C:170:VAL:HG13	1:C:186:LYS:O	2.13	0.48
1:B:40:ILE:HD12	1:B:42:ALA:HB3	1.95	0.48
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.95	0.48
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.94	0.48
1:B:248:ALA:HB2	1:B:282:GLU:HG2	1.96	0.48
1:C:411:ALA:HB2	1:D:423:CYS:HB3	1.96	0.48
1:C:430:VAL:HG22	1:C:512:LEU:HD12	1.96	0.48
1:B:170:VAL:HG13	1:B:186:LYS:O	2.13	0.48
1:C:410:GLU:HG3	1:D:422:LYS:HE2	1.96	0.48
1:A:480:GLU:OE1	1:A:481:ALA:N	2.47	0.47
1:B:293:ALA:HB1	2:B:533:OXL:C2	2.43	0.47
1:A:340:PRO:HG3	1:A:377:MET:HG2	1.96	0.47
1:C:340:PRO:HG3	1:C:377:MET:HG2	1.95	0.47
1:A:170:VAL:HG13	1:A:186:LYS:O	2.14	0.47
1:B:404:ILE:H	1:B:404:ILE:HG13	1.44	0.47
1:A:13:ILE:O	1:A:13:ILE:HG22	2.13	0.47
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.97	0.47
1:D:270:LYS:HD2	1:D:291:MET:SD	2.54	0.47
1:D:118:GLU:OE2	1:D:120:ARG:NH1	2.47	0.47
1:D:41:THR:HG21	7:D:553:HOH:O	2.14	0.47
1:D:106:ARG:HG2	7:D:562:HOH:O	2.14	0.47
1:B:243:SER:HA	1:B:270:LYS:HE2	1.97	0.47
1:A:40:ILE:O	1:A:383:ARG:HD3	2.15	0.46
1:B:384:GLU:HG2	7:B:561:HOH:O	2.15	0.46
1:D:248:ALA:HB2	1:D:282:GLU:HG2	1.97	0.46
1:D:170:VAL:HG13	1:D:186:LYS:O	2.16	0.46
1:A:274:HIS:HD2	1:A:278:ARG:NH2	2.03	0.46
1:D:255:ARG:NH1	7:D:559:HOH:O	2.45	0.46
1:A:132:VAL:HG21	1:A:153:ASP:HA	1.97	0.46
1:C:243:SER:HA	1:C:270:LYS:HE2	1.98	0.46
1:A:379:HIS:HE2	1:A:383:ARG:HH11	1.62	0.46
1:D:379:HIS:HE2	1:D:383:ARG:NH1	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:VAL:HG21	1:D:153:ASP:HA	1.99	0.45
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.98	0.45
1:D:325:ILE:HG12	1:D:358:CYS:HB2	1.98	0.44
1:A:270:LYS:HD2	1:A:291:MET:SD	2.57	0.44
1:A:48:ILE:HG12	1:A:71:VAL:HB	1.98	0.44
1:A:55:SER:O	1:A:61:LEU:HD13	2.17	0.44
1:A:288:ASP:O	1:A:323:PRO:HD2	2.18	0.44
1:D:55:SER:O	1:D:61:LEU:HD13	2.17	0.44
1:A:255:ARG:HG2	1:A:267:ILE:HD12	2.00	0.44
1:C:334:MET:HA	1:C:337:LYS:O	2.17	0.44
1:D:281:ASP:O	1:D:285:GLU:HB2	2.17	0.44
1:B:281:ASP:O	1:B:285:GLU:HB2	2.18	0.44
1:B:132:VAL:HG21	1:B:153:ASP:HA	1.99	0.44
1:A:416:ALA:HB2	1:A:512:LEU:HD21	2.00	0.43
1:B:416:ALA:HB2	1:B:512:LEU:HD21	2.00	0.43
1:B:48:ILE:HG12	1:B:71:VAL:HB	2.00	0.43
1:D:334:MET:HA	1:D:337:LYS:O	2.19	0.43
1:D:478:VAL:HG12	1:D:479:GLN:O	2.19	0.43
1:B:55:SER:O	1:B:61:LEU:HD13	2.18	0.43
1:C:132:VAL:HG21	1:C:153:ASP:HA	2.00	0.43
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.00	0.43
1:D:416:ALA:HB2	1:D:512:LEU:HD21	2.01	0.43
1:B:288:ASP:O	1:B:323:PRO:HD2	2.19	0.43
1:B:255:ARG:HG2	1:B:267:ILE:HD12	2.01	0.43
1:C:124:ILE:O	1:C:125:LYS:C	2.56	0.42
1:D:123:LEU:HD12	1:D:150:GLU:HG2	2.02	0.42
1:B:478:VAL:HG12	1:B:479:GLN:O	2.19	0.42
1:B:124:ILE:O	1:B:125:LYS:C	2.58	0.42
1:C:255:ARG:HG2	1:C:267:ILE:HD12	2.01	0.42
1:A:404:ILE:H	1:A:404:ILE:HG13	1.43	0.42
1:C:118:GLU:OE2	1:C:120:ARG:NH1	2.52	0.42
1:B:325:ILE:HG12	1:B:358:CYS:HB2	2.02	0.42
1:A:281:ASP:O	1:A:285:GLU:HB2	2.19	0.42
1:A:325:ILE:HG12	1:A:358:CYS:HB2	2.01	0.42
1:C:405:THR:HG22	1:D:422:LYS:HE3	2.00	0.42
1:A:402:ALA:HB1	1:B:422:LYS:NZ	2.34	0.42
1:C:48:ILE:HG12	1:C:71:VAL:HB	2.02	0.41
1:A:125:LYS:HE2	1:A:125:LYS:HB3	1.16	0.41
1:A:514:GLY:HA3	3:A:532:FBP:O3	2.20	0.41
1:A:399:ARG:HH21	1:B:399:ARG:HH21	1.67	0.41
1:B:334:MET:HA	1:B:337:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:VAL:HG21	1:B:496:VAL:HG11	2.02	0.41
1:A:418:GLU:HB2	1:B:418:GLU:HG2	2.03	0.41
1:A:418:GLU:HG2	1:B:418:GLU:HB2	2.02	0.41
1:C:288:ASP:O	1:C:323:PRO:HD2	2.21	0.41
1:B:414:VAL:HG22	1:B:444:TYR:CZ	2.56	0.41
1:D:71:VAL:HG22	1:D:109:ALA:HB3	2.03	0.41
1:A:494:MET:HG3	1:A:530:VAL:HG13	2.02	0.41
1:A:123:LEU:HD12	1:A:150:GLU:HG2	2.02	0.41
1:A:334:MET:HA	1:A:337:LYS:O	2.20	0.41
1:A:480:GLU:N	1:A:480:GLU:OE1	2.46	0.40
1:D:163:ASN:OD1	1:D:166:LYS:HD2	2.20	0.40
1:B:71:VAL:HG22	1:B:109:ALA:HB3	2.02	0.40
1:D:21:ALA:CB	1:D:447:ARG:HH22	2.34	0.40
1:C:494:MET:HG3	1:C:530:VAL:HG13	2.02	0.40
1:C:294:ARG:NH2	1:C:347:ASP:OD1	2.54	0.40
1:C:55:SER:O	1:C:61:LEU:HD13	2.21	0.40
1:D:229:LEU:O	1:D:233:VAL:HG23	2.21	0.40
1:D:328:THR:HG22	1:D:329:GLN:HG3	2.03	0.40
1:A:478:VAL:HG12	1:A:479:GLN:O	2.21	0.40
1:A:422:LYS:NZ	1:B:402:ALA:HB1	2.36	0.40
1:C:472:VAL:HG21	1:C:496:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	511/551 (93%)	485 (95%)	24 (5%)	2 (0%)	39 74
1	B	508/551 (92%)	480 (94%)	26 (5%)	2 (0%)	39 74
1	C	510/551 (93%)	480 (94%)	30 (6%)	0	100 100
1	D	512/551 (93%)	483 (94%)	26 (5%)	3 (1%)	30 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2041/2204 (93%)	1928 (94%)	106 (5%)	7 (0%)	46 79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	125	LYS
1	B	479	GLN
1	D	479	GLN
1	A	479	GLN
1	A	328	THR
1	B	328	THR
1	D	328	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	425/453 (94%)	405 (95%)	20 (5%)	32 68
1	B	423/453 (93%)	406 (96%)	17 (4%)	38 74
1	C	425/453 (94%)	407 (96%)	18 (4%)	36 73
1	D	425/453 (94%)	408 (96%)	17 (4%)	38 74
All	All	1698/1812 (94%)	1626 (96%)	72 (4%)	36 73

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	15	THR
1	A	82	GLU
1	A	125	LYS
1	A	143	THR
1	A	163	ASN
1	A	173	LYS
1	A	255	ARG

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Mol	Chain	Res	Type
1	A	261	LYS
1	A	287	SER
1	A	304	GLU
1	A	319	ARG
1	A	396	GLU
1	A	404	ILE
1	A	409	THR
1	A	436	ARG
1	A	467	ARG
1	A	480	GLU
1	A	484	GLU
1	A	516	ARG
1	B	82	GLU
1	B	143	THR
1	B	163	ASN
1	B	173	LYS
1	B	255	ARG
1	B	261	LYS
1	B	287	SER
1	B	304	GLU
1	B	319	ARG
1	B	396	GLU
1	B	404	ILE
1	B	409	THR
1	B	436	ARG
1	B	467	ARG
1	B	480	GLU
1	B	484	GLU
1	B	516	ARG
1	C	82	GLU
1	C	143	THR
1	C	163	ASN
1	C	173	LYS
1	C	255	ARG
1	C	261	LYS
1	C	285	GLU
1	C	287	SER
1	C	304	GLU
1	C	319	ARG
1	C	396	GLU
1	C	404	ILE
1	C	409	THR

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Mol	Chain	Res	Type
1	C	436	ARG
1	C	467	ARG
1	C	480	GLU
1	C	484	GLU
1	C	516	ARG
1	D	82	GLU
1	D	143	THR
1	D	163	ASN
1	D	173	LYS
1	D	255	ARG
1	D	261	LYS
1	D	278	ARG
1	D	287	SER
1	D	304	GLU
1	D	319	ARG
1	D	396	GLU
1	D	404	ILE
1	D	409	THR
1	D	467	ARG
1	D	480	GLU
1	D	484	GLU
1	D	516	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	274	HIS
1	A	393	GLN
1	B	146	ASN
1	B	274	HIS
1	C	146	ASN
1	C	274	HIS
1	C	318	ASN
1	D	84	HIS
1	D	146	ASN
1	D	184	GLN
1	D	252	HIS
1	D	274	HIS
1	D	393	GLN

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 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
3	FBP	A	532	-	18,20,20	0.91	1 (5%)	21,32,32	0.65	0
2	OXL	A	533	5	0,5,5	0.00	-	0,6,6	0.00	-
6	GOL	A	536	-	5,5,5	0.33	0	5,5,5	0.31	0
3	FBP	B	532	-	18,20,20	0.90	1 (5%)	21,32,32	0.61	0
2	OXL	B	533	5	0,5,5	0.00	-	0,6,6	0.00	-
6	GOL	B	534	-	5,5,5	0.33	0	5,5,5	0.22	0
3	FBP	C	532	-	18,20,20	0.87	1 (5%)	21,32,32	0.73	1 (4%)
2	OXL	C	533	5	0,5,5	0.00	-	0,6,6	0.00	-
6	GOL	C	534	-	5,5,5	0.38	0	5,5,5	0.16	0
3	FBP	D	532	-	18,20,20	0.92	1 (5%)	21,32,32	0.88	1 (4%)
2	OXL	D	533	5	0,5,5	0.00	-	0,6,6	0.00	-
6	GOL	D	534	-	5,5,5	0.32	0	5,5,5	0.23	0
6	GOL	D	535	-	5,5,5	0.35	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
3	FBP	A	532	-	-	0/13/32/32	0/1/1/1
2	OXL	A	533	5	-	0/0/4/4	0/0/0/0
6	GOL	A	536	-	-	0/4/4/4	0/0/0/0
3	FBP	B	532	-	-	0/13/32/32	0/1/1/1
2	OXL	B	533	5	-	0/0/4/4	0/0/0/0
6	GOL	B	534	-	-	0/4/4/4	0/0/0/0
3	FBP	C	532	-	-	0/13/32/32	0/1/1/1
2	OXL	C	533	5	-	0/0/4/4	0/0/0/0
6	GOL	C	534	-	-	0/4/4/4	0/0/0/0
3	FBP	D	532	-	-	0/13/32/32	0/1/1/1
2	OXL	D	533	5	-	0/0/4/4	0/0/0/0
6	GOL	D	534	-	-	0/4/4/4	0/0/0/0
6	GOL	D	535	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	532	FBP	O2-C2	2.68	1.45	1.41
3	A	532	FBP	O2-C2	2.71	1.45	1.41
3	D	532	FBP	O2-C2	2.73	1.45	1.41
3	B	532	FBP	O2-C2	2.87	1.45	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	532	FBP	O6P-P2-O6	2.07	112.53	106.56
3	D	532	FBP	O5-C5-C6	2.53	115.26	109.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	532	FBP	1	0
3	B	532	FBP	1	0
2	B	533	OXL	1	0
3	D	532	FBP	2	0
6	D	535	GOL	1	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

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^{th} 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	515/551 (93%)	0.58	20 (3%) 43 36	39, 71, 101, 149	0
1	B	512/551 (92%)	1.02	92 (17%) 2 1	48, 82, 127, 160	0
1	C	514/551 (93%)	0.67	34 (6%) 22 16	46, 77, 108, 161	0
1	D	515/551 (93%)	0.57	29 (5%) 28 21	43, 69, 107, 148	0
All	All	2056/2204 (93%)	0.71	175 (8%) 13 8	39, 75, 114, 161	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	HIS	6.7
1	A	15	THR	6.6
1	B	143	THR	6.3
1	C	13	ILE	6.0
1	B	187	GLN	5.9
1	B	168	VAL	5.5
1	B	186	LYS	5.4
1	B	188	LYS	5.4
1	B	165	CYS	5.1
1	D	15	THR	4.9
1	B	215	ALA	4.9
1	A	14	GLN	4.8
1	A	20	ALA	4.7
1	B	167	VAL	4.7
1	B	76	PHE	4.7
1	A	18	LEU	4.6
1	B	194	VAL	4.6
1	B	80	THR	4.6
1	B	157	LEU	4.6
1	C	143	THR	4.5
1	B	159	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	158	TRP	4.5
1	B	192	PHE	4.4
1	B	214	ALA	4.4
1	D	16	GLN	4.4
1	B	189	GLY	4.3
1	B	156	ILE	4.3
1	C	14	GLN	4.2
1	B	153	ASP	4.2
1	B	183	LEU	4.1
1	C	134	LEU	4.1
1	B	170	VAL	4.1
1	B	151	LYS	3.9
1	B	148	TYR	3.9
1	C	137	GLY	3.9
1	B	150	GLU	3.8
1	C	123	LEU	3.7
1	A	13	ILE	3.7
1	C	157	LEU	3.7
1	D	531	PRO	3.7
1	B	251	VAL	3.7
1	B	144	LEU	3.7
1	B	198	GLU	3.6
1	A	203	LEU	3.6
1	B	124	ILE	3.6
1	B	166	LYS	3.5
1	B	237	VAL	3.5
1	B	134	LEU	3.5
1	D	18	LEU	3.5
1	B	125	LYS	3.5
1	B	123	LEU	3.4
1	D	31	CYS	3.4
1	C	479	GLN	3.3
1	B	152	CYS	3.3
1	B	190	ALA	3.3
1	D	23	ALA	3.3
1	A	200	GLY	3.3
1	B	193	LEU	3.3
1	B	182	SER	3.3
1	B	197	VAL	3.2
1	B	132	VAL	3.2
1	B	84	HIS	3.2
1	B	219	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	531	PRO	3.1
1	B	221	VAL	3.1
1	B	139	THR	3.1
1	B	149	MET	3.1
1	A	104	LEU	3.1
1	C	125	LYS	3.1
1	A	132	VAL	3.0
1	A	201	GLY	3.0
1	A	16	GLN	3.0
1	B	404	ILE	3.0
1	A	262	GLY	3.0
1	C	156	ILE	3.0
1	A	133	GLU	2.9
1	B	169	GLU	2.9
1	B	229	LEU	2.9
1	B	100	SER	2.9
1	B	142	ILE	2.9
1	B	185	VAL	2.8
1	D	198	GLU	2.8
1	B	55	SER	2.8
1	D	183	LEU	2.7
1	B	145	ASP	2.7
1	B	103	ILE	2.7
1	D	515	TRP	2.7
1	D	201	GLY	2.7
1	B	206	LYS	2.7
1	B	77	SER	2.7
1	B	15	THR	2.7
1	C	150	GLU	2.7
1	C	15	THR	2.6
1	B	285	GLU	2.6
1	D	22	MET	2.6
1	B	196	GLU	2.6
1	A	197	VAL	2.6
1	C	198	GLU	2.6
1	D	144	LEU	2.6
1	B	164	ILE	2.5
1	D	138	ALA	2.5
1	D	21	ALA	2.5
1	D	148	TYR	2.5
1	C	170	VAL	2.5
1	B	213	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	480	GLU	2.5
1	B	24	ASP	2.5
1	B	191	ASP	2.5
1	B	204	GLY	2.5
1	C	206	LYS	2.4
1	D	20	ALA	2.4
1	B	203	LEU	2.4
1	D	404	ILE	2.4
1	B	60	THR	2.4
1	B	405	THR	2.4
1	B	74	LEU	2.3
1	C	152	CYS	2.3
1	B	141	LYS	2.3
1	B	184	GLN	2.3
1	D	192	PHE	2.3
1	A	134	LEU	2.3
1	B	154	GLU	2.3
1	B	178	ASP	2.3
1	B	59	GLU	2.3
1	D	194	VAL	2.3
1	B	140	LEU	2.3
1	C	192	PHE	2.3
1	B	248	ALA	2.3
1	B	18	LEU	2.3
1	B	225	ASP	2.2
1	D	140	LEU	2.3
1	A	221	VAL	2.2
1	C	223	GLU	2.2
1	C	100	SER	2.2
1	C	237	VAL	2.2
1	A	41	THR	2.2
1	B	112	LEU	2.2
1	B	56	ARG	2.2
1	D	478	VAL	2.2
1	B	275	GLU	2.2
1	D	481	ALA	2.2
1	B	244	PHE	2.2
1	B	135	LYS	2.2
1	B	265	ILE	2.2
1	A	194	VAL	2.2
1	B	209	VAL	2.2
1	C	194	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	180	LEU	2.2
1	C	18	LEU	2.2
1	C	227	GLN	2.2
1	B	220	ALA	2.2
1	C	151	LYS	2.2
1	C	16	GLN	2.1
1	C	25	THR	2.1
1	D	159	LEU	2.1
1	C	148	TYR	2.1
1	C	82	GLU	2.1
1	C	138	ALA	2.1
1	B	17	GLN	2.1
1	C	81	HIS	2.1
1	C	470	PHE	2.1
1	B	88	ILE	2.1
1	C	159	LEU	2.1
1	D	252	HIS	2.1
1	A	253	GLU	2.1
1	B	52	GLY	2.0
1	B	406	SER	2.0
1	B	85	ALA	2.0
1	D	104	LEU	2.0
1	B	471	PRO	2.0
1	C	136	LYS	2.0
1	B	278	ARG	2.0
1	D	139	THR	2.0
1	C	22	MET	2.0
1	D	396	GLU	2.0

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, 95^{th} 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
6	GOL	C	534	6/6	0.90	0.33	1.62	72,72,73,73	0
6	GOL	A	536	6/6	0.92	0.27	1.35	67,68,68,69	0
6	GOL	D	534	6/6	0.91	0.27	1.31	65,66,67,67	0
6	GOL	D	535	6/6	0.94	0.28	0.88	60,61,61,61	0
6	GOL	B	534	6/6	0.91	0.24	0.30	55,58,59,60	0
2	OXL	C	533	6/6	0.95	0.17	-0.35	66,66,66,66	0
3	FBP	B	532	20/20	0.91	0.17	-1.08	70,74,78,79	0
3	FBP	C	532	20/20	0.91	0.18	-1.10	71,77,81,81	0
3	FBP	D	532	20/20	0.96	0.16	-1.26	62,63,66,66	0
2	OXL	B	533	6/6	0.85	0.16	-1.41	82,83,84,84	0
3	FBP	A	532	20/20	0.94	0.17	-1.49	71,72,76,76	0
2	OXL	A	533	6/6	0.94	0.13	-2.22	52,52,53,53	0
4	K	D	704	1/1	0.86	0.16	-2.32	64,64,64,64	0
2	OXL	D	533	6/6	0.95	0.14	-3.41	42,43,43,43	0
4	K	C	703	1/1	0.84	0.15	-3.47	78,78,78,78	0
4	K	A	534	1/1	0.97	0.08	-5.28	56,56,56,56	0
5	MG	C	603	1/1	0.97	0.12	-	50,50,50,50	0
5	MG	A	535	1/1	0.94	0.13	-	31,31,31,31	0
5	MG	B	602	1/1	0.73	0.28	-	133,133,133,133	0
5	MG	D	604	1/1	0.91	0.26	-	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.