



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 01:50 am BST

PDB ID : 6GG3
Title : Crystal structure of M2 PYK in complex with Alanine.
Authors : McNae, I.W.; Yuan, M.; Walkinshaw, M.D.
Deposited on : 2018-05-02
Resolution : 3.72 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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Mol	Chain	Length	Quality of chain
1	G	551	 % 87% 7% • 5%
1	H	551	 2% 87% 7% • 6%
1	I	551	 % 67% 8% • 24%
1	J	551	 2% 68% 7% • 24%
1	K	551	 % 85% 7% • 6%
1	L	551	 % 87% 8% • 5%

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
2	PO4	F	601	-	X	-	-
2	PO4	L	601	-	X	-	-
3	ALA	D	602	-	-	-	X
3	ALA	E	602	-	-	-	X
3	ALA	G	602	-	-	-	X
3	ALA	J	602	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46087 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 PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	Total 3973	C 2498	N 705	O 745	S 25	0	0	0
1	B	524	Total 4005	C 2519	N 710	O 751	S 25	0	0	0
1	C	521	Total 3988	C 2510	N 707	O 746	S 25	0	0	0
1	D	513	Total 3938	C 2478	N 699	O 736	S 25	0	0	0
1	E	481	Total 3685	C 2320	N 656	O 687	S 22	0	0	0
1	F	524	Total 4005	C 2519	N 710	O 751	S 25	0	0	0
1	G	524	Total 4005	C 2519	N 710	O 751	S 25	0	0	0
1	H	520	Total 3983	C 2507	N 706	O 745	S 25	0	0	0
1	I	418	Total 3215	C 2018	N 581	O 594	S 22	0	0	0
1	J	418	Total 3215	C 2018	N 581	O 594	S 22	0	0	0
1	K	516	Total 3944	C 2479	N 698	O 742	S 25	0	0	0
1	L	524	Total 4005	C 2519	N 710	O 751	S 25	0	0	0

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-	initiating methionine	UNP P14618
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	-	initiating methionine	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-18	MET	-	initiating methionine	UNP P14618
D	-17	GLY	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	SER	-	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	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618
D	1	HIS	-	expression tag	UNP P14618
E	-19	MET	-	initiating methionine	UNP P14618
E	-18	GLY	-	expression tag	UNP P14618
E	-17	SER	-	expression tag	UNP P14618
E	-16	SER	-	expression tag	UNP P14618
E	-15	HIS	-	expression tag	UNP P14618
E	-14	HIS	-	expression tag	UNP P14618
E	-13	HIS	-	expression tag	UNP P14618
E	-12	HIS	-	expression tag	UNP P14618
E	-11	HIS	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP P14618
E	-9	SER	-	expression tag	UNP P14618
E	-8	SER	-	expression tag	UNP P14618
E	-7	GLY	-	expression tag	UNP P14618
E	-6	LEU	-	expression tag	UNP P14618
E	-5	VAL	-	expression tag	UNP P14618
E	-4	PRO	-	expression tag	UNP P14618
E	-3	ARG	-	expression tag	UNP P14618
E	-2	GLY	-	expression tag	UNP P14618
E	-1	SER	-	expression tag	UNP P14618
E	0	HIS	-	expression tag	UNP P14618
F	-19	MET	-	initiating methionine	UNP P14618
F	-18	GLY	-	expression tag	UNP P14618
F	-17	SER	-	expression tag	UNP P14618
F	-16	SER	-	expression tag	UNP P14618
F	-15	HIS	-	expression tag	UNP P14618
F	-14	HIS	-	expression tag	UNP P14618
F	-13	HIS	-	expression tag	UNP P14618
F	-12	HIS	-	expression tag	UNP P14618
F	-11	HIS	-	expression tag	UNP P14618
F	-10	HIS	-	expression tag	UNP P14618
F	-9	SER	-	expression tag	UNP P14618
F	-8	SER	-	expression tag	UNP P14618
F	-7	GLY	-	expression tag	UNP P14618
F	-6	LEU	-	expression tag	UNP P14618
F	-5	VAL	-	expression tag	UNP P14618
F	-4	PRO	-	expression tag	UNP P14618
F	-3	ARG	-	expression tag	UNP P14618
F	-2	GLY	-	expression tag	UNP P14618
F	-1	SER	-	expression tag	UNP P14618
F	0	HIS	-	expression tag	UNP P14618
G	-19	MET	-	initiating methionine	UNP P14618
G	-18	GLY	-	expression tag	UNP P14618
G	-17	SER	-	expression tag	UNP P14618
G	-16	SER	-	expression tag	UNP P14618
G	-15	HIS	-	expression tag	UNP P14618
G	-14	HIS	-	expression tag	UNP P14618
G	-13	HIS	-	expression tag	UNP P14618
G	-12	HIS	-	expression tag	UNP P14618
G	-11	HIS	-	expression tag	UNP P14618
G	-10	HIS	-	expression tag	UNP P14618
G	-9	SER	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	expression tag	UNP P14618
G	-7	GLY	-	expression tag	UNP P14618
G	-6	LEU	-	expression tag	UNP P14618
G	-5	VAL	-	expression tag	UNP P14618
G	-4	PRO	-	expression tag	UNP P14618
G	-3	ARG	-	expression tag	UNP P14618
G	-2	GLY	-	expression tag	UNP P14618
G	-1	SER	-	expression tag	UNP P14618
G	0	HIS	-	expression tag	UNP P14618
H	-19	MET	-	initiating methionine	UNP P14618
H	-18	GLY	-	expression tag	UNP P14618
H	-17	SER	-	expression tag	UNP P14618
H	-16	SER	-	expression tag	UNP P14618
H	-15	HIS	-	expression tag	UNP P14618
H	-14	HIS	-	expression tag	UNP P14618
H	-13	HIS	-	expression tag	UNP P14618
H	-12	HIS	-	expression tag	UNP P14618
H	-11	HIS	-	expression tag	UNP P14618
H	-10	HIS	-	expression tag	UNP P14618
H	-9	SER	-	expression tag	UNP P14618
H	-8	SER	-	expression tag	UNP P14618
H	-7	GLY	-	expression tag	UNP P14618
H	-6	LEU	-	expression tag	UNP P14618
H	-5	VAL	-	expression tag	UNP P14618
H	-4	PRO	-	expression tag	UNP P14618
H	-3	ARG	-	expression tag	UNP P14618
H	-2	GLY	-	expression tag	UNP P14618
H	-1	SER	-	expression tag	UNP P14618
H	0	HIS	-	expression tag	UNP P14618
I	-19	MET	-	initiating methionine	UNP P14618
I	-18	GLY	-	expression tag	UNP P14618
I	-17	SER	-	expression tag	UNP P14618
I	-16	SER	-	expression tag	UNP P14618
I	-15	HIS	-	expression tag	UNP P14618
I	-14	HIS	-	expression tag	UNP P14618
I	-13	HIS	-	expression tag	UNP P14618
I	-12	HIS	-	expression tag	UNP P14618
I	-11	HIS	-	expression tag	UNP P14618
I	-10	HIS	-	expression tag	UNP P14618
I	-9	SER	-	expression tag	UNP P14618
I	-8	SER	-	expression tag	UNP P14618
I	-7	GLY	-	expression tag	UNP P14618

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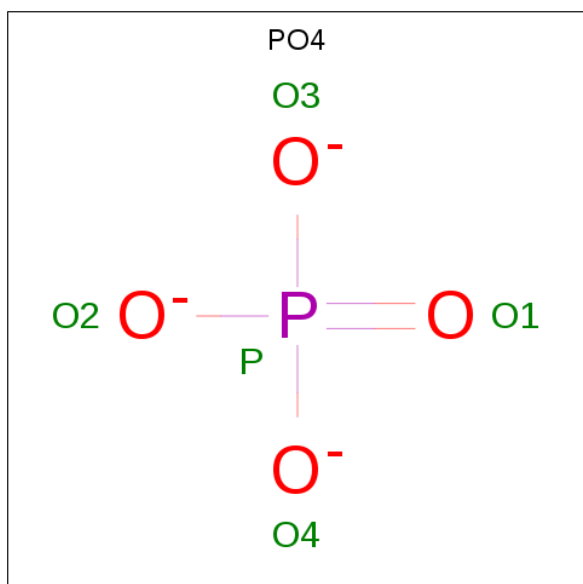
Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP P14618
I	-5	VAL	-	expression tag	UNP P14618
I	-4	PRO	-	expression tag	UNP P14618
I	-3	ARG	-	expression tag	UNP P14618
I	-2	GLY	-	expression tag	UNP P14618
I	-1	SER	-	expression tag	UNP P14618
I	0	HIS	-	expression tag	UNP P14618
J	-19	MET	-	initiating methionine	UNP P14618
J	-18	GLY	-	expression tag	UNP P14618
J	-17	SER	-	expression tag	UNP P14618
J	-16	SER	-	expression tag	UNP P14618
J	-15	HIS	-	expression tag	UNP P14618
J	-14	HIS	-	expression tag	UNP P14618
J	-13	HIS	-	expression tag	UNP P14618
J	-12	HIS	-	expression tag	UNP P14618
J	-11	HIS	-	expression tag	UNP P14618
J	-10	HIS	-	expression tag	UNP P14618
J	-9	SER	-	expression tag	UNP P14618
J	-8	SER	-	expression tag	UNP P14618
J	-7	GLY	-	expression tag	UNP P14618
J	-6	LEU	-	expression tag	UNP P14618
J	-5	VAL	-	expression tag	UNP P14618
J	-4	PRO	-	expression tag	UNP P14618
J	-3	ARG	-	expression tag	UNP P14618
J	-2	GLY	-	expression tag	UNP P14618
J	-1	SER	-	expression tag	UNP P14618
J	0	HIS	-	expression tag	UNP P14618
K	-19	MET	-	initiating methionine	UNP P14618
K	-18	GLY	-	expression tag	UNP P14618
K	-17	SER	-	expression tag	UNP P14618
K	-16	SER	-	expression tag	UNP P14618
K	-15	HIS	-	expression tag	UNP P14618
K	-14	HIS	-	expression tag	UNP P14618
K	-13	HIS	-	expression tag	UNP P14618
K	-12	HIS	-	expression tag	UNP P14618
K	-11	HIS	-	expression tag	UNP P14618
K	-10	HIS	-	expression tag	UNP P14618
K	-9	SER	-	expression tag	UNP P14618
K	-8	SER	-	expression tag	UNP P14618
K	-7	GLY	-	expression tag	UNP P14618
K	-6	LEU	-	expression tag	UNP P14618
K	-5	VAL	-	expression tag	UNP P14618

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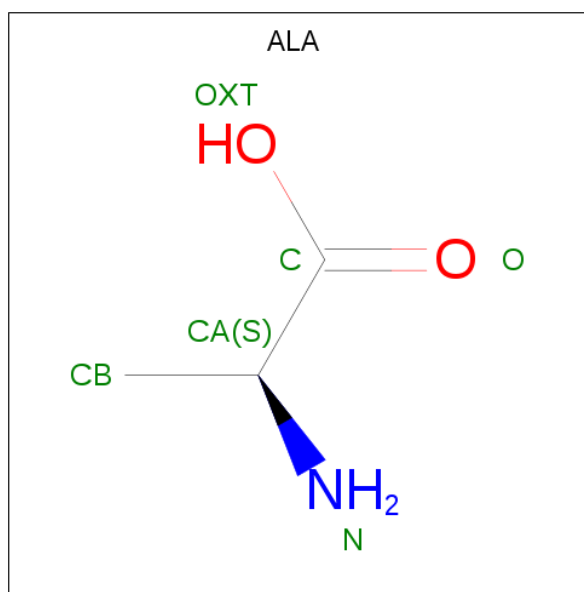
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP P14618
K	-3	ARG	-	expression tag	UNP P14618
K	-2	GLY	-	expression tag	UNP P14618
K	-1	SER	-	expression tag	UNP P14618
K	0	HIS	-	expression tag	UNP P14618
L	-19	MET	-	initiating methionine	UNP P14618
L	-18	GLY	-	expression tag	UNP P14618
L	-17	SER	-	expression tag	UNP P14618
L	-16	SER	-	expression tag	UNP P14618
L	-15	HIS	-	expression tag	UNP P14618
L	-14	HIS	-	expression tag	UNP P14618
L	-13	HIS	-	expression tag	UNP P14618
L	-12	HIS	-	expression tag	UNP P14618
L	-11	HIS	-	expression tag	UNP P14618
L	-10	HIS	-	expression tag	UNP P14618
L	-9	SER	-	expression tag	UNP P14618
L	-8	SER	-	expression tag	UNP P14618
L	-7	GLY	-	expression tag	UNP P14618
L	-6	LEU	-	expression tag	UNP P14618
L	-5	VAL	-	expression tag	UNP P14618
L	-4	PRO	-	expression tag	UNP P14618
L	-3	ARG	-	expression tag	UNP P14618
L	-2	GLY	-	expression tag	UNP P14618
L	-1	SER	-	expression tag	UNP P14618
L	0	HIS	-	expression tag	UNP P14618

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0

- Molecule 3 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).

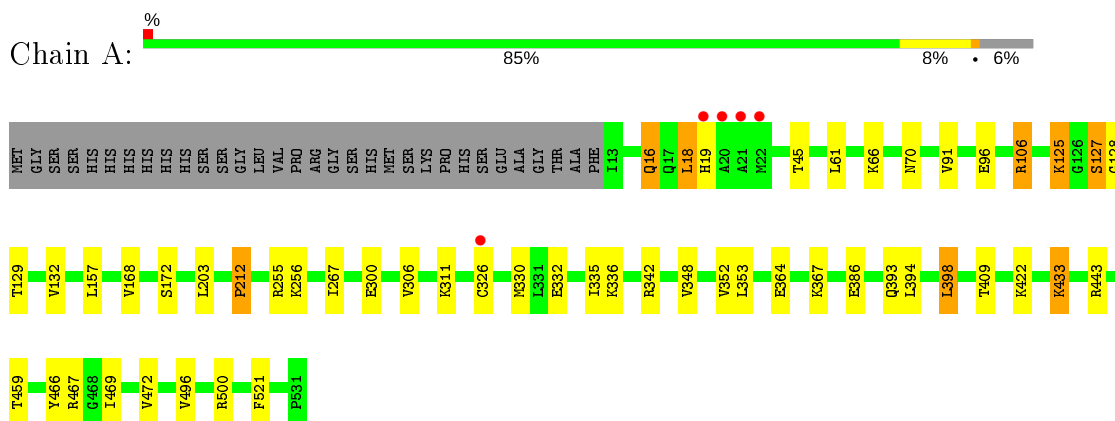


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 6	C 3	N 1	O 2	0	0
3	C	1	Total 6	C 3	N 1	O 2	0	0
3	D	1	Total 6	C 3	N 1	O 2	0	0
3	E	1	Total 6	C 3	N 1	O 2	0	0
3	F	1	Total 6	C 3	N 1	O 2	0	0
3	G	1	Total 6	C 3	N 1	O 2	0	0
3	H	1	Total 6	C 3	N 1	O 2	0	0
3	I	1	Total 6	C 3	N 1	O 2	0	0
3	J	1	Total 6	C 3	N 1	O 2	0	0
3	K	1	Total 6	C 3	N 1	O 2	0	0
3	L	1	Total 6	C 3	N 1	O 2	0	0

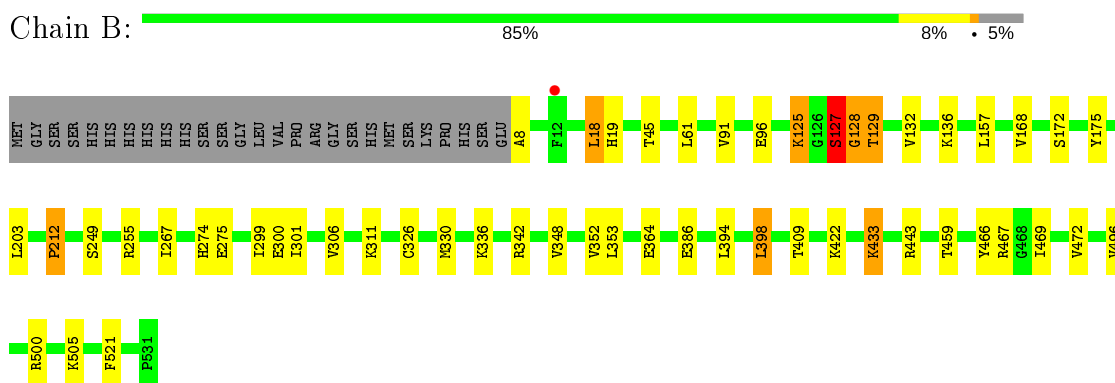
3 Residue-property plots [i](#)

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

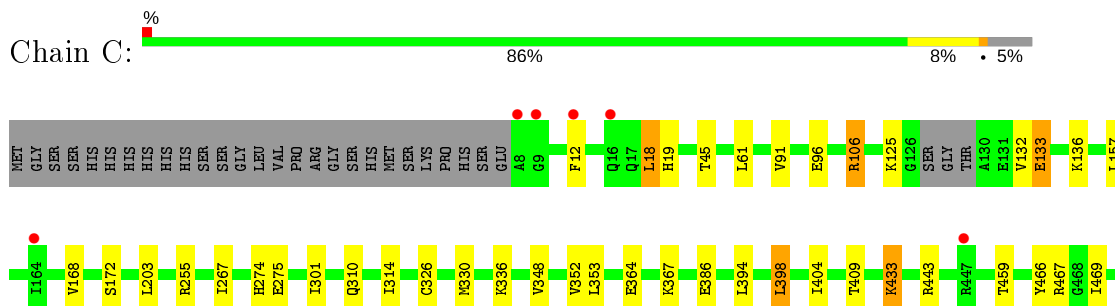
- Molecule 1: Pyruvate kinase PKM

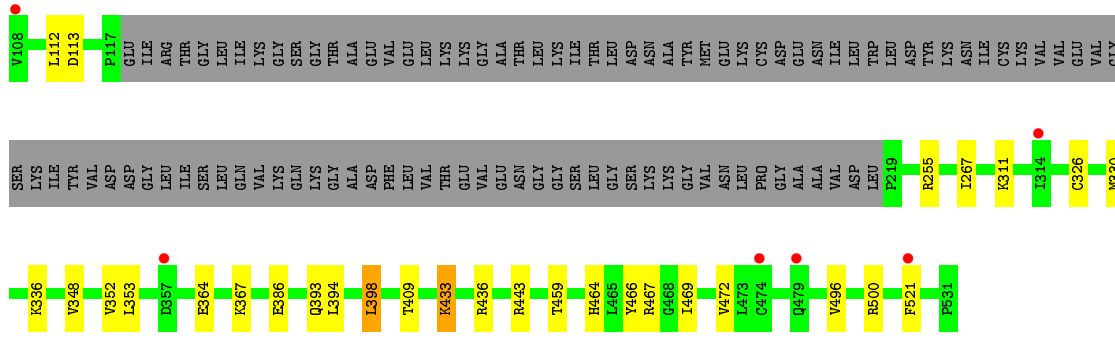


- Molecule 1: Pyruvate kinase PKM

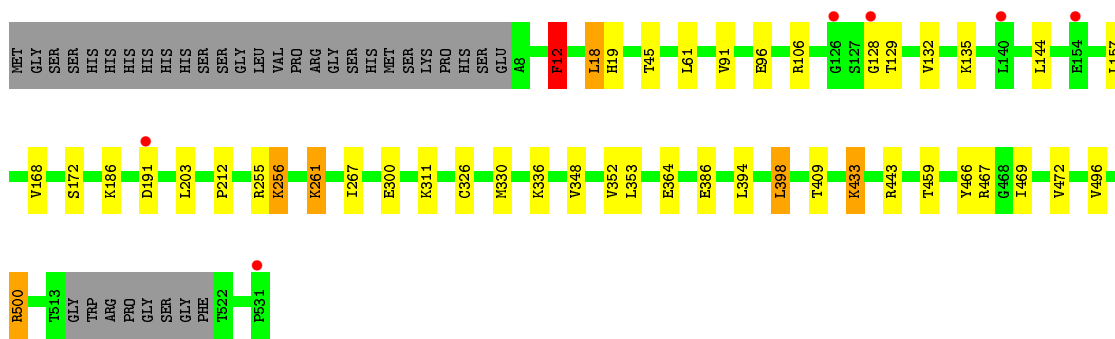
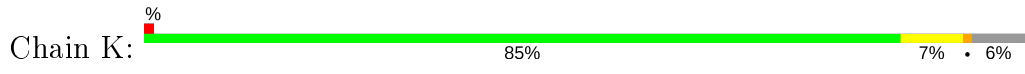


- Molecule 1: Pyruvate kinase PKM

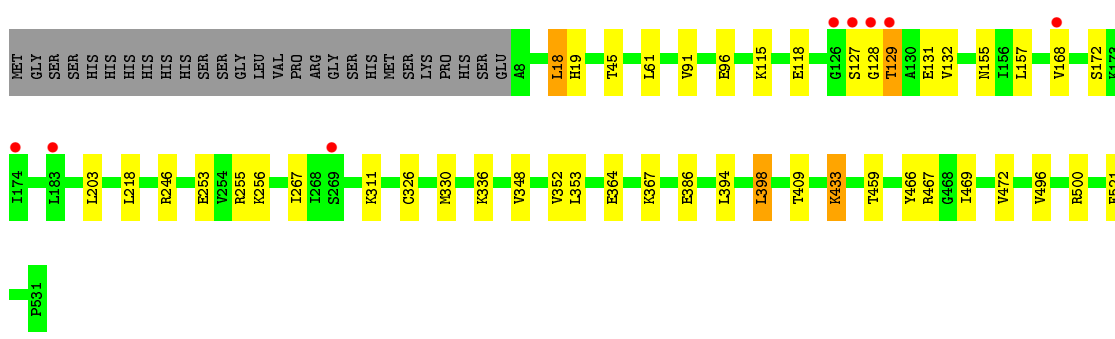
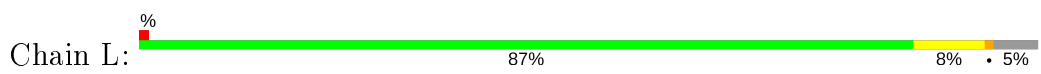




• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	160.72Å 199.36Å 243.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.19 – 3.72 154.19 – 3.72	Depositor EDS
% Data completeness (in resolution range)	94.7 (154.19-3.72) 94.7 (154.19-3.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.68Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.220 , 0.249 0.217 , 0.245	Depositor DCC
R_{free} test set	3932 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	110.8	Xtrriage
Anisotropy	0.365	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 90.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	46087	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.46	1/4037 (0.0%)	0.68	3/5452 (0.1%)
1	B	0.49	1/4070 (0.0%)	0.68	5/5497 (0.1%)
1	C	0.50	2/4052 (0.0%)	0.69	1/5471 (0.0%)
1	D	0.46	2/4003 (0.0%)	0.66	2/5407 (0.0%)
1	E	0.48	2/3745 (0.1%)	0.66	1/5057 (0.0%)
1	F	0.44	0/4070	0.66	0/5497
1	G	0.44	0/4070	0.67	3/5497 (0.1%)
1	H	0.48	2/4047 (0.0%)	0.67	2/5464 (0.0%)
1	I	0.44	0/3271	0.66	2/4418 (0.0%)
1	J	0.41	0/3271	0.65	0/4418
1	K	0.48	1/4004 (0.0%)	0.68	2/5406 (0.0%)
1	L	0.48	1/4070 (0.0%)	0.68	4/5497 (0.1%)
All	All	0.47	12/46710 (0.0%)	0.67	25/63081 (0.0%)

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	1
1	C	0	1
1	E	0	2
1	K	1	0
All	All	1	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	GLU	CD-OE1	8.70	1.35	1.25
1	H	246	ARG	CZ-NH1	8.36	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	7	GLU	CD-OE1	6.77	1.33	1.25
1	L	246	ARG	CZ-NH1	6.61	1.41	1.33
1	D	275	GLU	CD-OE1	6.24	1.32	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	12	PHE	CB-CA-C	9.43	129.25	110.40
1	C	133	GLU	CA-CB-CG	7.96	130.91	113.40
1	D	500	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	I	494	MET	CB-CG-SD	7.62	135.25	112.40
1	H	500	ARG	NE-CZ-NH1	7.53	124.06	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	K	12	PHE	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	8	ALA	Peptide
1	C	125	LYS	Peptide
1	E	157	LEU	Peptide
1	E	8	ALA	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3973	0	4060	21	0
1	B	4005	0	4089	23	1
1	C	3988	0	4073	18	1
1	D	3938	0	4012	21	1
1	E	3685	0	3753	19	0
1	F	4005	0	4089	25	0
1	G	4005	0	4089	20	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3983	0	4068	16	0
1	I	3215	0	3272	27	0
1	J	3215	0	3272	19	1
1	K	3944	0	4035	23	0
1	L	4005	0	4089	22	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	6	0	4	1	0
3	C	6	0	4	0	0
3	D	6	0	4	0	0
3	E	6	0	4	0	0
3	F	6	0	4	3	0
3	G	6	0	4	0	0
3	H	6	0	4	1	0
3	I	6	0	4	0	0
3	J	6	0	4	1	0
3	K	6	0	4	0	0
3	L	6	0	4	1	0
All	All	46087	0	46945	230	3

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 2.

The worst 5 of 230 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:F:476:ASP:OD1	1:L:256:LYS:NZ	2.10	0.83
1:J:14:GLN:HE21	1:J:43:ARG:H	1.23	0.83
1:K:12:PHE:CD1	1:K:500:ARG:HD2	2.16	0.80
1:K:12:PHE:HD1	1:K:500:ARG:CD	1.97	0.78
1:G:256:LYS:NZ	1:I:476:ASP:OD1	2.17	0.77

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:PRO:O	1:L:155:ASN:ND2[4_495]	1.93	0.27
1:D:82:GLU:OE1	1:G:78:HIS:ND1[4_485]	2.04	0.16
1:B:249:SER:OG	1:J:101:ASP:OD2[1_455]	2.07	0.13

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	517/551 (94%)	487 (94%)	24 (5%)	6 (1%)	13	48
1	B	522/551 (95%)	495 (95%)	21 (4%)	6 (1%)	14	50
1	C	517/551 (94%)	489 (95%)	26 (5%)	2 (0%)	34	69
1	D	509/551 (92%)	485 (95%)	21 (4%)	3 (1%)	25	61
1	E	473/551 (86%)	450 (95%)	20 (4%)	3 (1%)	25	61
1	F	522/551 (95%)	496 (95%)	22 (4%)	4 (1%)	19	56
1	G	522/551 (95%)	495 (95%)	23 (4%)	4 (1%)	19	56
1	H	516/551 (94%)	491 (95%)	23 (4%)	2 (0%)	34	69
1	I	414/551 (75%)	398 (96%)	14 (3%)	2 (0%)	29	65
1	J	414/551 (75%)	397 (96%)	15 (4%)	2 (0%)	29	65
1	K	512/551 (93%)	487 (95%)	22 (4%)	3 (1%)	25	61
1	L	522/551 (95%)	495 (95%)	24 (5%)	3 (1%)	25	61
All	All	5960/6612 (90%)	5665 (95%)	255 (4%)	40 (1%)	22	59

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	LYS
1	A	127	SER

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Mol	Chain	Res	Type
1	A	128	GLY
1	A	364	GLU
1	B	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	427/453 (94%)	409 (96%)	18 (4%)	30	58
1	B	429/453 (95%)	416 (97%)	13 (3%)	41	65
1	C	427/453 (94%)	411 (96%)	16 (4%)	34	61
1	D	423/453 (93%)	410 (97%)	13 (3%)	40	65
1	E	394/453 (87%)	378 (96%)	16 (4%)	30	59
1	F	429/453 (95%)	413 (96%)	16 (4%)	34	61
1	G	429/453 (95%)	414 (96%)	15 (4%)	36	63
1	H	427/453 (94%)	414 (97%)	13 (3%)	41	65
1	I	344/453 (76%)	333 (97%)	11 (3%)	39	64
1	J	344/453 (76%)	330 (96%)	14 (4%)	30	59
1	K	424/453 (94%)	406 (96%)	18 (4%)	30	58
1	L	429/453 (95%)	417 (97%)	12 (3%)	43	67
All	All	4926/5436 (91%)	4751 (96%)	175 (4%)	35	62

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	96	GLU
1	G	132	VAL
1	K	443	ARG
1	F	129	THR
1	F	409	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such

sidechains are listed below:

Mol	Chain	Res	Type
1	E	318	ASN
1	F	70	ASN
1	J	14	GLN
1	D	318	ASN
1	H	318	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	H	601	-	4,4,4	0.92	0	6,6,6	1.29	1 (16%)
2	PO4	J	601	-	4,4,4	0.70	0	6,6,6	1.19	0
2	PO4	I	601	-	4,4,4	1.76	1 (25%)	6,6,6	0.89	0
2	PO4	L	601	-	4,4,4	2.71	3 (75%)	6,6,6	1.49	1 (16%)
2	PO4	K	601	-	4,4,4	1.77	1 (25%)	6,6,6	0.63	0
2	PO4	F	601	-	4,4,4	3.34	2 (50%)	6,6,6	2.95	4 (66%)
2	PO4	E	601	-	4,4,4	1.40	1 (25%)	6,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	G	601	-	4,4,4	2.15	2 (50%)	6,6,6	0.86	0
2	PO4	B	601	-	4,4,4	0.59	0	6,6,6	0.71	0
2	PO4	A	601	-	4,4,4	3.61	2 (50%)	6,6,6	1.35	0
2	PO4	D	601	-	4,4,4	4.71	2 (50%)	6,6,6	1.12	0
2	PO4	C	601	-	4,4,4	1.92	1 (25%)	6,6,6	0.95	0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	PO4	P-O1	8.02	1.69	1.50
2	A	601	PO4	P-O3	-6.56	1.34	1.54
2	F	601	PO4	P-O4	4.91	1.69	1.54
2	D	601	PO4	P-O4	-4.78	1.40	1.54
2	F	601	PO4	P-O3	-4.10	1.42	1.54

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	PO4	O4-P-O2	4.50	122.41	107.97
2	F	601	PO4	O2-P-O1	-3.95	96.45	110.89
2	F	601	PO4	O3-P-O1	3.01	121.91	110.89
2	L	601	PO4	O3-P-O2	2.77	116.87	107.97
2	F	601	PO4	O3-P-O2	-2.60	99.63	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	519/551 (94%)	-0.10	5 (0%) 82 78	84, 120, 163, 204	0
1	B	524/551 (95%)	-0.10	1 (0%) 95 95	88, 144, 209, 251	0
1	C	521/551 (94%)	0.15	6 (1%) 79 74	82, 126, 157, 178	0
1	D	513/551 (93%)	0.43	42 (8%) 11 10	103, 147, 248, 283	0
1	E	481/551 (87%)	-0.00	5 (1%) 82 78	84, 119, 193, 231	0
1	F	524/551 (95%)	0.01	6 (1%) 80 76	77, 116, 187, 241	0
1	G	524/551 (95%)	-0.09	3 (0%) 89 87	86, 120, 159, 222	0
1	H	520/551 (94%)	-0.01	13 (2%) 57 49	94, 144, 228, 256	0
1	I	418/551 (75%)	0.11	4 (0%) 82 78	108, 148, 192, 206	0
1	J	418/551 (75%)	0.24	11 (2%) 56 47	118, 157, 190, 208	0
1	K	516/551 (93%)	-0.13	6 (1%) 79 74	84, 125, 188, 239	0
1	L	524/551 (95%)	0.02	8 (1%) 73 68	92, 132, 179, 265	0
All	All	6002/6612 (90%)	0.04	110 (1%) 68 62	77, 132, 197, 283	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	127	SER	10.1
1	L	128	GLY	10.0
1	D	157	LEU	7.5
1	D	167	VAL	5.7
1	L	129	THR	5.3

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. 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	B-factors(Å ²)	Q<0.9
3	ALA	J	602	6/6	0.71	1.42	161,165,169,171	0
3	ALA	H	602	6/6	0.75	0.38	119,121,121,123	0
3	ALA	G	602	6/6	0.75	0.40	110,113,115,118	0
3	ALA	D	602	6/6	0.76	0.75	123,124,125,126	0
2	PO4	D	601	5/5	0.76	0.19	124,129,135,135	0
3	ALA	E	602	6/6	0.79	0.42	106,108,110,114	0
3	ALA	F	602	6/6	0.82	0.51	97,102,105,107	0
3	ALA	A	602	6/6	0.83	0.35	146,149,149,150	0
3	ALA	K	602	6/6	0.83	0.39	128,130,132,132	0
3	ALA	L	602	6/6	0.84	0.69	124,128,130,133	0
2	PO4	K	601	5/5	0.84	0.19	115,121,123,125	0
3	ALA	I	602	6/6	0.85	0.52	146,149,149,152	0
2	PO4	J	601	5/5	0.88	0.12	128,133,136,139	0
2	PO4	F	601	5/5	0.88	0.17	91,92,94,98	0
3	ALA	C	602	6/6	0.91	0.35	114,115,118,121	0
2	PO4	H	601	5/5	0.91	0.20	131,133,139,148	0
2	PO4	I	601	5/5	0.92	0.15	130,131,135,144	0
2	PO4	G	601	5/5	0.92	0.20	86,89,96,97	0
2	PO4	A	601	5/5	0.93	0.19	115,119,122,123	0
2	PO4	C	601	5/5	0.94	0.20	100,102,105,109	0
2	PO4	B	601	5/5	0.94	0.22	137,138,139,142	0
2	PO4	L	601	5/5	0.95	0.15	108,108,116,117	0
2	PO4	E	601	5/5	0.96	0.13	97,100,103,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.