



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 11:23 AM UTC

PDB ID : 6GG3 / pdb_00006gg3
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

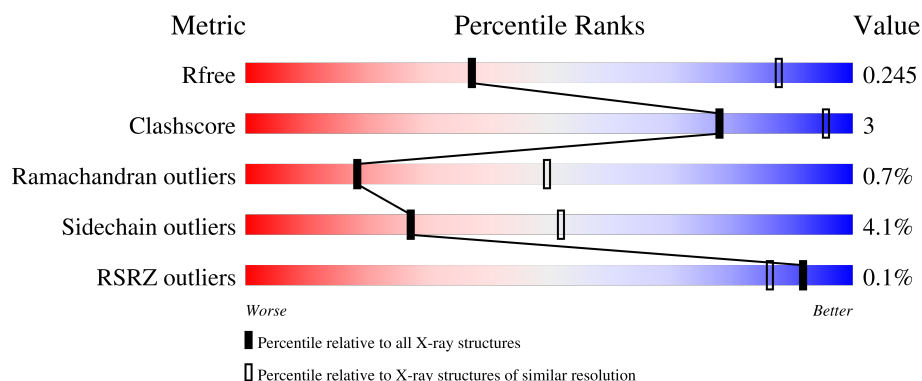
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.72 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}	180053	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	551	 84% 9% • 6%
1	B	551	 84% 9% • 5%
1	C	551	 85% 8% • 5%
1	D	551	 84% 8% • 7%
1	E	551	 77% 9% • 13%

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Mol	Chain	Length	Quality of chain
1	F	551	 86%8% • 5%
1	G	551	 86%8% • 5%
1	H	551	 86%8% • 6%
1	I	551	 66%9% • 24%
1	J	551	 67%8% • 24%
1	K	551	 84%8% • 6%
1	L	551	 86%9% • 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	A	602	-	X	-	-
3	ALA	H	602	-	X	-	-
3	ALA	L	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
1	A	519	Total	C	N	O	S	0	0	0
			3973	2498	705	745	25			
1	B	524	Total	C	N	O	S	0	0	0
			4005	2519	710	751	25			
1	C	521	Total	C	N	O	S	0	0	0
			3988	2510	707	746	25			
1	D	513	Total	C	N	O	S	0	0	0
			3938	2478	699	736	25			
1	E	481	Total	C	N	O	S	0	0	0
			3685	2320	656	687	22			
1	F	524	Total	C	N	O	S	0	0	0
			4005	2519	710	751	25			
1	G	524	Total	C	N	O	S	0	0	0
			4005	2519	710	751	25			
1	H	520	Total	C	N	O	S	0	0	0
			3983	2507	706	745	25			
1	I	418	Total	C	N	O	S	0	0	0
			3215	2018	581	594	22			
1	J	418	Total	C	N	O	S	0	0	0
			3215	2018	581	594	22			
1	K	516	Total	C	N	O	S	0	0	0
			3944	2479	698	742	25			
1	L	524	Total	C	N	O	S	0	0	0
			4005	2519	710	751	25			

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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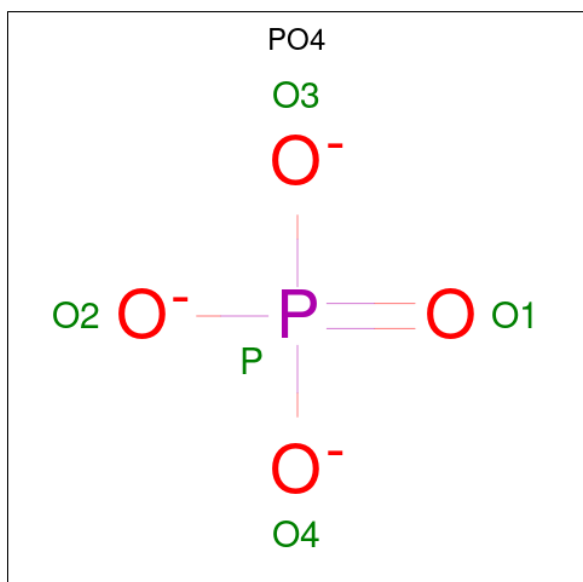
Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP P14618
I	-5	VAL	-	expression tag	UNP P14618
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I	-2	GLY	-	expression tag	UNP P14618
I	-1	SER	-	expression tag	UNP P14618
I	0	HIS	-	expression tag	UNP P14618
J	-19	MET	-	initiating 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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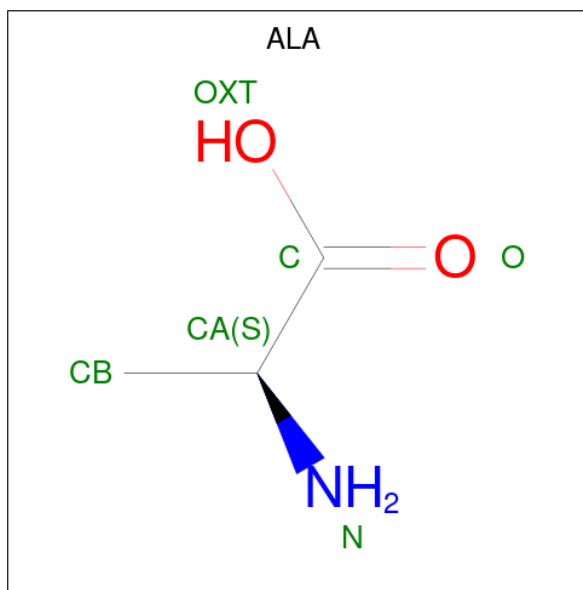
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP P14618
K	-3	ARG	-	expression tag	UNP P14618
K	-2	GLY	-	expression tag	UNP P14618
K	-1	SER	-	expression tag	UNP P14618
K	0	HIS	-	expression tag	UNP P14618
L	-19	MET	-	initiating methionine	UNP P14618
L	-18	GLY	-	expression tag	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 (CCD ID: 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 (CCD ID: ALA) (formula: $C_3H_7NO_2$).

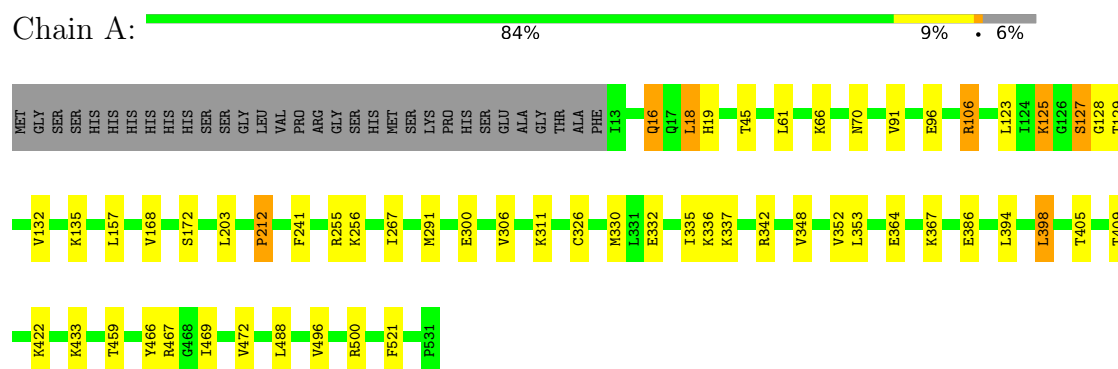


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	3	1	2		
3	C	1	Total	C	N	O	0	0
			6	3	1	2		
3	D	1	Total	C	N	O	0	0
			6	3	1	2		
3	E	1	Total	C	N	O	0	0
			6	3	1	2		
3	F	1	Total	C	N	O	0	0
			6	3	1	2		
3	G	1	Total	C	N	O	0	0
			6	3	1	2		
3	H	1	Total	C	N	O	0	0
			6	3	1	2		
3	I	1	Total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

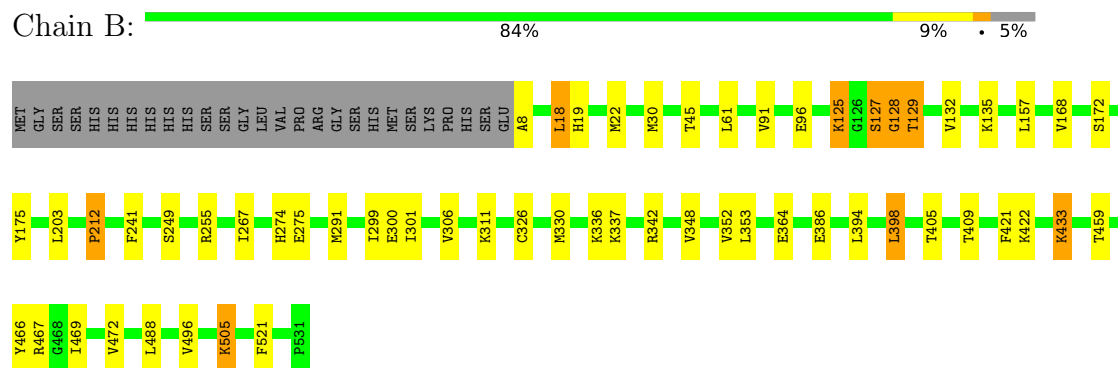
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

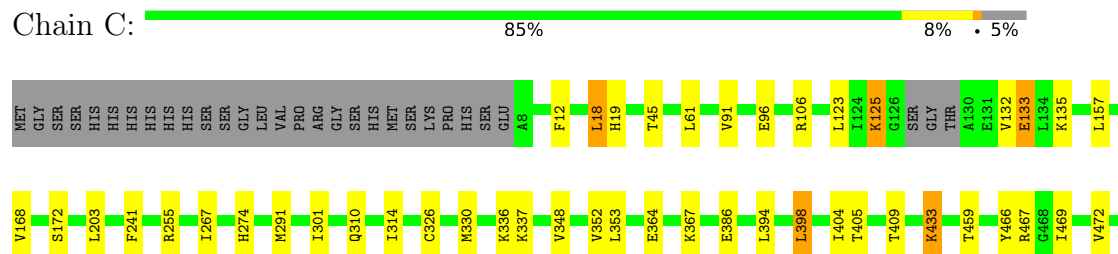
• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM



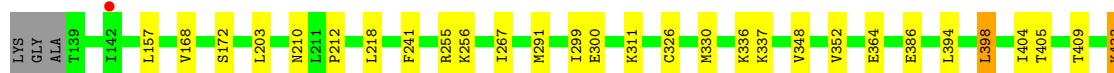
• Molecule 1: Pyruvate kinase PKM





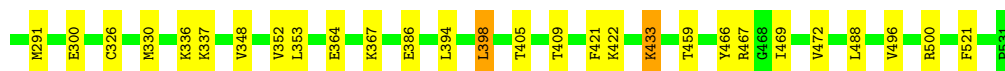
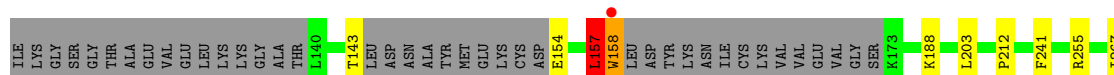
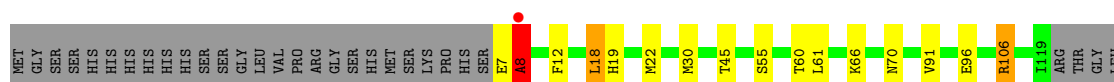
- Molecule 1: Pyruvate kinase PKM

Chain D: 84% 8% 7%



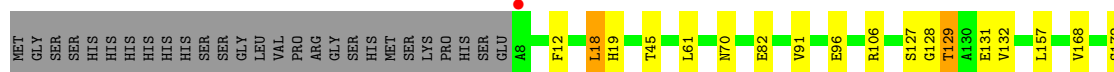
- Molecule 1: Pyruvate kinase PKM

Chain E: 77% 9% 13%



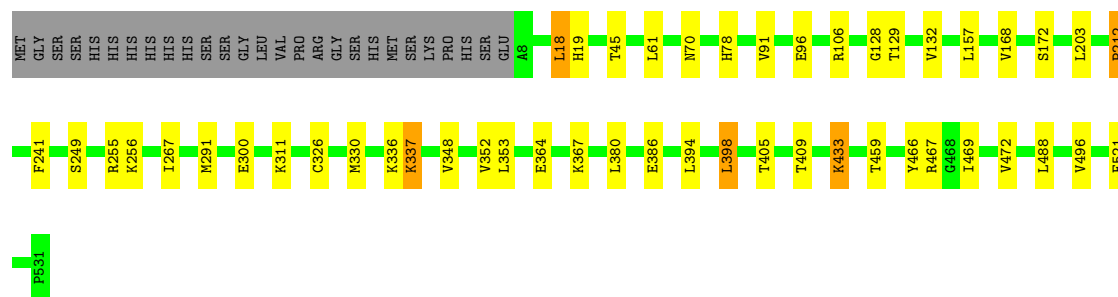
- Molecule 1: Pyruvate kinase PKM

Chain F: 86% 8% 5%

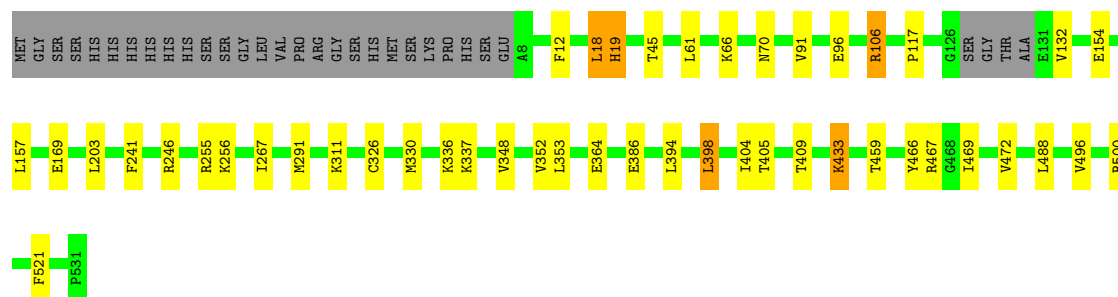
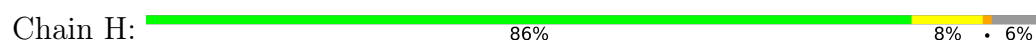


- Molecule 1: Pyruvate kinase PKM

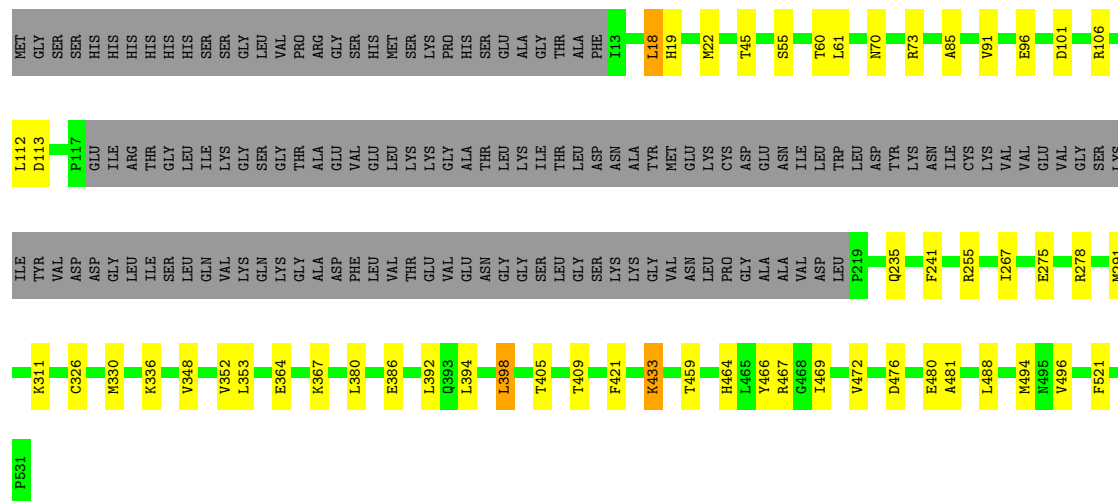
Chain G: 86% 8% 5%



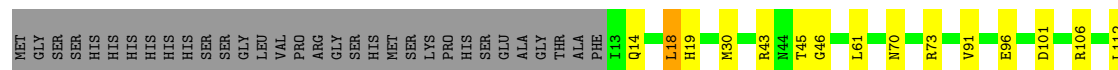
- Molecule 1: Pyruvate kinase PKM

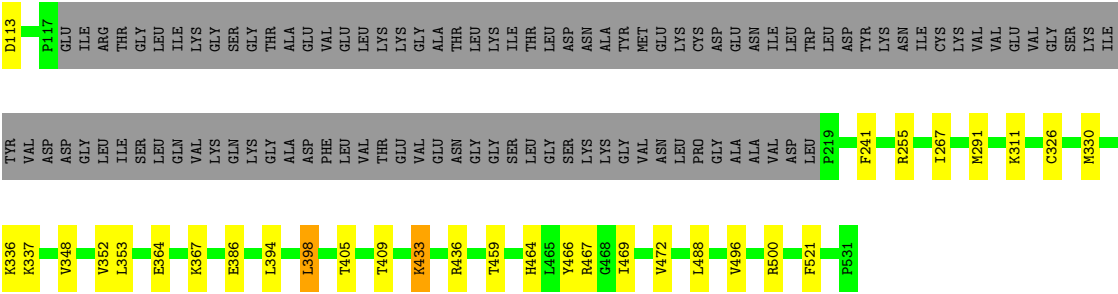


- Molecule 1: Pyruvate kinase PKM

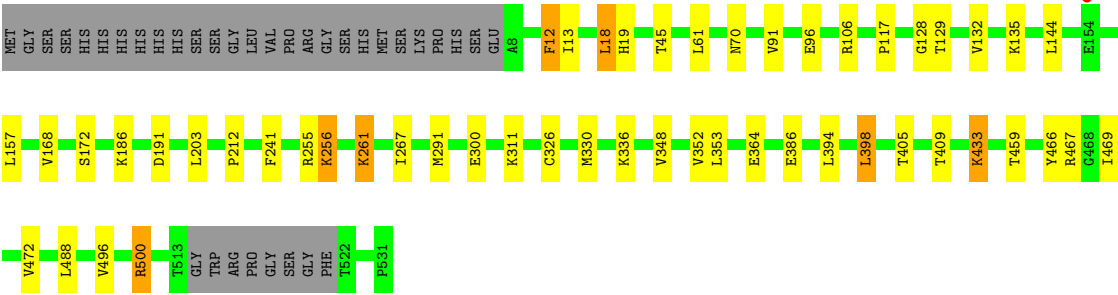
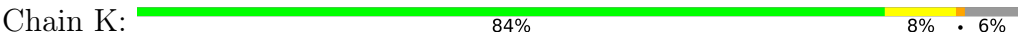


- Molecule 1: Pyruvate kinase PKM

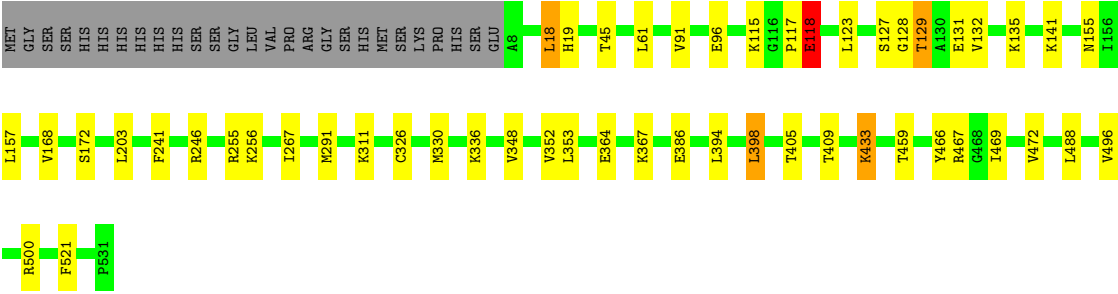
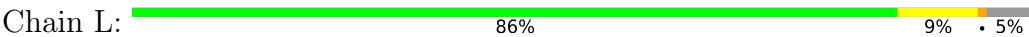




● Molecule 1: Pyruvate kinase PKM



● 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)	Xtriage
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 (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	46087	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

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	0.62	2/4037 (0.0%)	0.86	2/5452 (0.0%)
1	B	0.65	2/4070 (0.0%)	0.86	2/5497 (0.0%)
1	C	0.64	0/4052	0.86	1/5471 (0.0%)
1	D	0.61	0/4003	0.85	2/5407 (0.0%)
1	E	0.63	2/3745 (0.1%)	0.84	0/5057
1	F	0.61	0/4070	0.84	0/5497
1	G	0.61	0/4070	0.85	1/5497 (0.0%)
1	H	0.63	2/4047 (0.0%)	0.85	1/5464 (0.0%)
1	I	0.60	0/3271	0.86	1/4418 (0.0%)
1	J	0.58	0/3271	0.85	0/4418
1	K	0.65	2/4004 (0.0%)	0.87	3/5406 (0.1%)
1	L	0.65	3/4070 (0.1%)	0.87	4/5497 (0.1%)
All	All	0.62	13/46710 (0.0%)	0.85	17/63081 (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 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	117	PRO	C-O	-9.16	1.14	1.23
1	K	12	PHE	CA-CB	8.77	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	LYS	C-O	-8.20	1.13	1.24
1	H	246	ARG	CZ-NH1	7.98	1.44	1.32
1	E	158	TRP	CA-C	-7.61	1.36	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	12	PHE	CB-CA-C	9.25	129.25	110.38
1	B	125	LYS	CA-C-O	-8.63	108.17	120.51
1	L	500	ARG	CB-CG-CD	8.63	131.15	111.30
1	C	133	GLU	CA-CB-CG	8.40	130.91	114.10
1	I	494	MET	CB-CG-SD	7.52	135.25	112.70

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 ⓘ

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	24	0
1	B	4005	0	4089	26	1
1	C	3988	0	4073	20	1
1	D	3938	0	4012	22	1
1	E	3685	0	3753	24	0
1	F	4005	0	4089	26	0
1	G	4005	0	4089	22	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3983	0	4068	18	0
1	I	3215	0	3272	30	0
1	J	3215	0	3272	22	1
1	K	3944	0	4035	25	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	2	0
3	C	6	0	4	0	0
3	D	6	0	4	0	0
3	E	6	0	4	1	0
3	F	6	0	4	3	0
3	G	6	0	4	1	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	1	0
3	L	6	0	4	1	0
All	All	46087	0	46945	257	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 3.

The worst 5 of 257 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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/551 (94%)	487 (94%)	24 (5%)	6 (1%)	10	39
1	B	522/551 (95%)	495 (95%)	21 (4%)	6 (1%)	11	41
1	C	517/551 (94%)	489 (95%)	26 (5%)	2 (0%)	30	60
1	D	509/551 (92%)	485 (95%)	21 (4%)	3 (1%)	21	52
1	E	473/551 (86%)	450 (95%)	20 (4%)	3 (1%)	21	52
1	F	522/551 (95%)	496 (95%)	22 (4%)	4 (1%)	16	47
1	G	522/551 (95%)	495 (95%)	23 (4%)	4 (1%)	16	47
1	H	516/551 (94%)	491 (95%)	23 (4%)	2 (0%)	30	60
1	I	414/551 (75%)	398 (96%)	14 (3%)	2 (0%)	24	56
1	J	414/551 (75%)	397 (96%)	15 (4%)	2 (0%)	24	56
1	K	512/551 (93%)	487 (95%)	22 (4%)	3 (1%)	21	52
1	L	522/551 (95%)	495 (95%)	24 (5%)	3 (1%)	21	52
All	All	5960/6612 (90%)	5665 (95%)	255 (4%)	40 (1%)	18	49

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 ⓘ

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%)	407 (95%)	20 (5%)	23	48
1	B	429/453 (95%)	413 (96%)	16 (4%)	30	53
1	C	427/453 (94%)	408 (96%)	19 (4%)	25	50
1	D	423/453 (93%)	408 (96%)	15 (4%)	32	54
1	E	394/453 (87%)	378 (96%)	16 (4%)	27	52
1	F	429/453 (95%)	413 (96%)	16 (4%)	30	53
1	G	429/453 (95%)	412 (96%)	17 (4%)	28	52
1	H	427/453 (94%)	410 (96%)	17 (4%)	28	52
1	I	344/453 (76%)	330 (96%)	14 (4%)	27	52
1	J	344/453 (76%)	328 (95%)	16 (5%)	23	48
1	K	424/453 (94%)	406 (96%)	18 (4%)	26	51
1	L	429/453 (95%)	411 (96%)	18 (4%)	26	51
All	All	4926/5436 (91%)	4724 (96%)	202 (4%)	27	52

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	409	THR
1	I	380	LEU
1	L	433	LYS
1	H	18	LEU
1	H	398	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31

such sidechains are listed below:

Mol	Chain	Res	Type
1	F	458	GLN
1	K	70	ASN
1	H	155	ASN
1	L	252	HIS
1	J	19	HIS

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 oligosaccharides 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	L	601	-	4,4,4	2.80	3 (75%)	6,6,6	1.54	1 (16%)
3	ALA	D	602	-	5,5,5	1.25	1 (20%)	6,6,6	1.40	1 (16%)
2	PO4	D	601	-	4,4,4	4.86	2 (50%)	6,6,6	1.14	0
2	PO4	K	601	-	4,4,4	1.84	1 (25%)	6,6,6	0.66	0
2	PO4	G	601	-	4,4,4	2.21	2 (50%)	6,6,6	0.90	0
3	ALA	A	602	-	5,5,5	3.19	2 (40%)	6,6,6	2.03	2 (33%)
3	ALA	C	602	-	5,5,5	1.05	0	6,6,6	1.83	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ALA	J	602	-	5,5,5	0.51	0	6,6,6	1.42	2 (33%)
3	ALA	L	602	-	5,5,5	4.30	2 (40%)	6,6,6	2.55	3 (50%)
2	PO4	H	601	-	4,4,4	0.97	0	6,6,6	1.34	1 (16%)
3	ALA	G	602	-	5,5,5	3.24	1 (20%)	6,6,6	1.14	1 (16%)
2	PO4	F	601	-	4,4,4	3.46	2 (50%)	6,6,6	3.05	4 (66%)
3	ALA	F	602	-	5,5,5	2.43	2 (40%)	6,6,6	2.10	3 (50%)
3	ALA	E	602	-	5,5,5	1.89	1 (20%)	6,6,6	1.09	0
3	ALA	H	602	-	5,5,5	2.76	2 (40%)	6,6,6	2.29	3 (50%)
3	ALA	K	602	-	5,5,5	1.59	1 (20%)	6,6,6	1.63	2 (33%)
2	PO4	B	601	-	4,4,4	0.62	0	6,6,6	0.74	0
2	PO4	C	601	-	4,4,4	1.99	1 (25%)	6,6,6	0.99	0
2	PO4	E	601	-	4,4,4	1.47	1 (25%)	6,6,6	0.54	0
2	PO4	A	601	-	4,4,4	3.72	2 (50%)	6,6,6	1.40	0
3	ALA	I	602	-	5,5,5	1.73	2 (40%)	6,6,6	1.66	1 (16%)
2	PO4	I	601	-	4,4,4	1.82	1 (25%)	6,6,6	0.93	0
2	PO4	J	601	-	4,4,4	0.69	0	6,6,6	1.24	1 (16%)

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	ALA	G	602	-	-	0/4/4/4	-
3	ALA	K	602	-	-	2/4/4/4	-
3	ALA	D	602	-	-	2/4/4/4	-
3	ALA	F	602	-	-	0/4/4/4	-
3	ALA	A	602	-	-	2/4/4/4	-
3	ALA	C	602	-	-	2/4/4/4	-
3	ALA	I	602	-	-	0/4/4/4	-
3	ALA	E	602	-	-	2/4/4/4	-
3	ALA	J	602	-	-	3/4/4/4	-
3	ALA	H	602	-	-	3/4/4/4	-
3	ALA	L	602	-	-	3/4/4/4	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	602	ALA	CA-C	-8.90	1.44	1.54
2	D	601	PO4	P-O1	8.26	1.69	1.50
3	G	602	ALA	O-C	7.22	1.43	1.22
2	A	601	PO4	P-O3	-6.79	1.34	1.54
3	A	602	ALA	CA-C	6.61	1.61	1.54

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	602	ALA	OXT-C-O	-4.95	112.85	124.08
2	F	601	PO4	O4-P-O2	4.66	122.41	107.91
3	H	602	ALA	OXT-C-O	-4.52	113.83	124.08
3	A	602	ALA	OXT-C-O	-4.22	114.51	124.08
2	F	601	PO4	O2-P-O1	-4.10	96.45	110.95

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	602	ALA	OXT-C-CA-CB
3	E	602	ALA	O-C-CA-CB
3	E	602	ALA	OXT-C-CA-CB
3	H	602	ALA	O-C-CA-CB
3	H	602	ALA	OXT-C-CA-CB

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	ALA	2	0
3	J	602	ALA	1	0
3	L	602	ALA	1	0
3	G	602	ALA	1	0
3	F	602	ALA	3	0
3	E	602	ALA	1	0
3	H	602	ALA	1	0
3	K	602	ALA	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 [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%)	-0.58	0	100	100	84, 120, 163, 204	0
1	B	524/551 (95%)	-0.37	0	100	100	88, 144, 209, 251	0
1	C	521/551 (94%)	-0.56	0	100	100	82, 126, 157, 178	0
1	D	513/551 (93%)	-0.41	1 (0%)	91	80	103, 147, 248, 283	0
1	E	481/551 (87%)	-0.55	2 (0%)	88	72	84, 119, 193, 231	0
1	F	524/551 (95%)	-0.48	2 (0%)	88	72	77, 116, 187, 241	0
1	G	524/551 (95%)	-0.57	0	100	100	86, 120, 159, 222	0
1	H	520/551 (94%)	-0.55	0	100	100	94, 144, 228, 256	0
1	I	418/551 (75%)	-0.57	0	100	100	108, 148, 192, 206	0
1	J	418/551 (75%)	-0.50	0	100	100	118, 157, 190, 208	0
1	K	516/551 (93%)	-0.61	1 (0%)	91	80	84, 125, 188, 239	0
1	L	524/551 (95%)	-0.57	0	100	100	92, 132, 179, 265	0
All	All	6002/6612 (90%)	-0.53	6 (0%)	92	86	77, 132, 197, 283	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	8	ALA	4.0
1	K	154	GLU	3.0
1	D	142	ILE	2.3
1	E	158	TRP	2.2
1	F	317	CYS	2.1

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 oligosaccharides 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	H	602	6/6	0.76	0.14	119,121,121,123	0
3	ALA	J	602	6/6	0.77	0.15	161,165,169,171	0
3	ALA	E	602	6/6	0.81	0.15	106,108,110,114	0
3	ALA	K	602	6/6	0.82	0.15	128,130,132,132	0
3	ALA	I	602	6/6	0.84	0.10	146,149,149,152	0
3	ALA	L	602	6/6	0.85	0.17	124,128,130,133	0
2	PO4	F	601	5/5	0.86	0.11	91,92,94,98	0
2	PO4	H	601	5/5	0.86	0.09	131,133,139,148	0
3	ALA	G	602	6/6	0.88	0.11	110,113,115,118	0
2	PO4	E	601	5/5	0.88	0.10	97,100,103,105	0
3	ALA	F	602	6/6	0.88	0.17	97,102,105,107	0
3	ALA	D	602	6/6	0.89	0.15	123,124,125,126	0
2	PO4	K	601	5/5	0.89	0.07	115,121,123,125	0
3	ALA	A	602	6/6	0.89	0.14	146,149,149,150	0
2	PO4	I	601	5/5	0.90	0.06	130,131,135,144	0
2	PO4	G	601	5/5	0.90	0.09	86,89,96,97	0
2	PO4	A	601	5/5	0.91	0.07	115,119,122,123	0
2	PO4	C	601	5/5	0.92	0.07	100,102,105,109	0
2	PO4	L	601	5/5	0.92	0.07	108,108,116,117	0
2	PO4	D	601	5/5	0.93	0.06	124,129,135,135	0
2	PO4	B	601	5/5	0.93	0.05	137,138,139,142	0
2	PO4	J	601	5/5	0.93	0.07	128,133,136,139	0
3	ALA	C	602	6/6	0.94	0.11	114,115,118,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.