



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 8, 2024 – 11:15 am GMT

PDB ID : 6GG6  
Title : Crystal structure of M2 PYK in complex with Serine.  
Authors : McNae, I.W.; Yuan, M.; Walkinshaw, M.D.  
Deposited on : 2018-05-02  
Resolution : 2.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

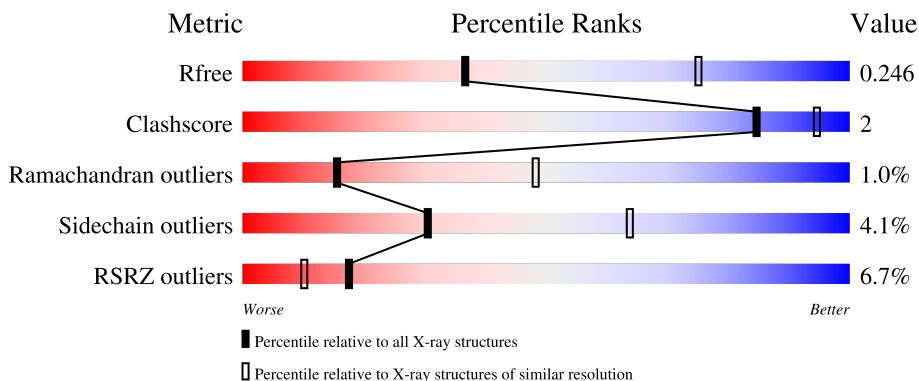
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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.



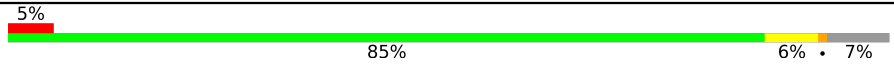

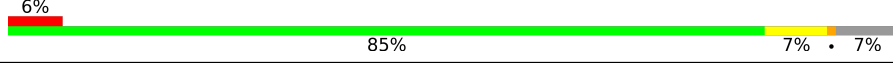
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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  $\geq 3$ , 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	
1	B	551	
1	C	551	
1	D	551	
1	E	551	

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Mol	Chain	Length	Quality of chain
1	F	551	 5% 85% 6% • 7%
1	G	551	 6% 85% 6% • 7%
1	H	551	 6% 85% 7% • 7%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31408 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	510	3912	2460	694	733	25	0	1	0
1	B	510	3912	2460	694	733	25	0	1	0
1	C	510	3912	2460	694	733	25	0	1	0
1	D	510	3912	2460	694	733	25	0	1	0
1	E	510	3912	2460	694	733	25	0	1	0
1	F	510	3912	2460	694	733	25	0	1	0
1	G	510	3912	2460	694	733	25	0	1	0
1	H	510	3912	2460	694	733	25	0	1	0

There are 160 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-	initiating methionine	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

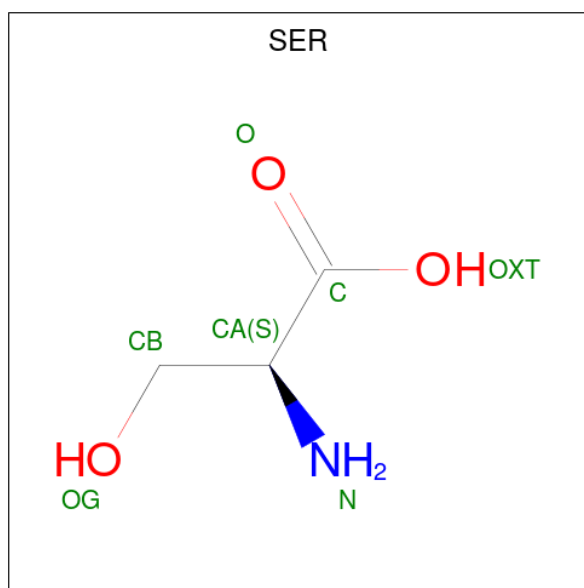
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0
2	G	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0

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



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

- Molecule 4 is SERINE (three-letter code: SER) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>3</sub>).



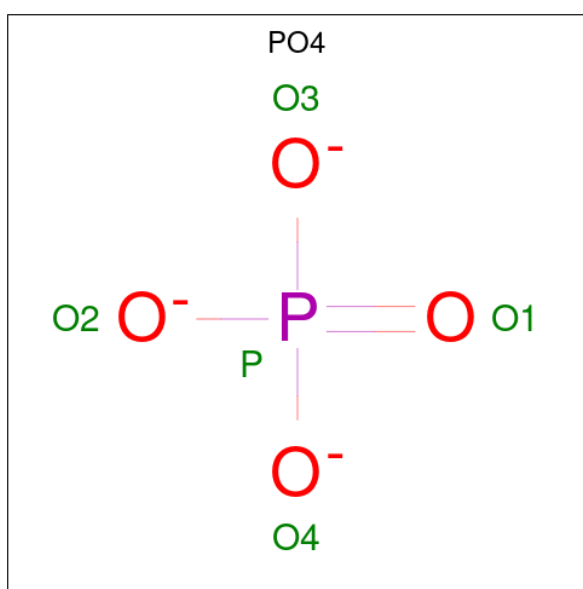
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 7 3 1 3	0	0
4	B	1	Total C N O 7 3 1 3	0	0
4	C	1	Total C N O 7 3 1 3	0	0
4	D	1	Total C N O 7 3 1 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			7	3	1	3		
4	F	1	Total	C	N	O	0	0
			7	3	1	3		
4	G	1	Total	C	N	O	0	0
			7	3	1	3		
4	H	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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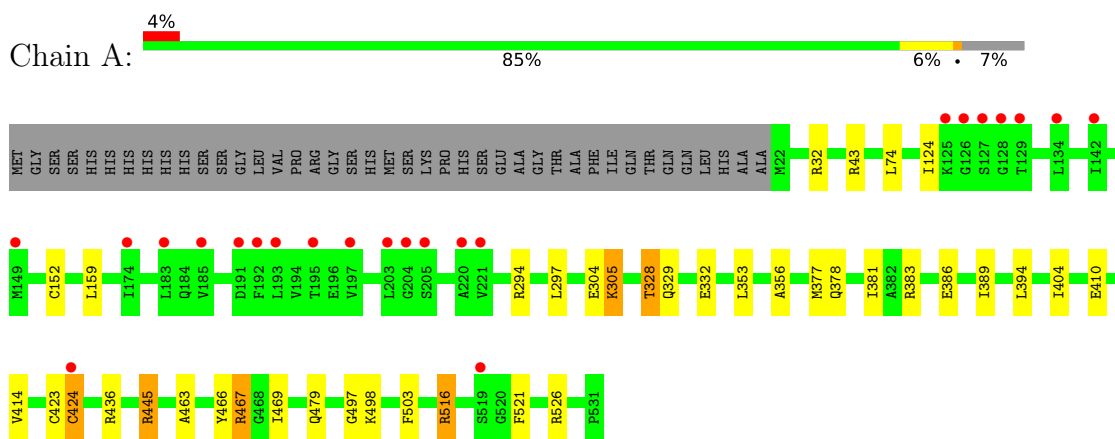
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
5	H	1	5	4	1	0	0

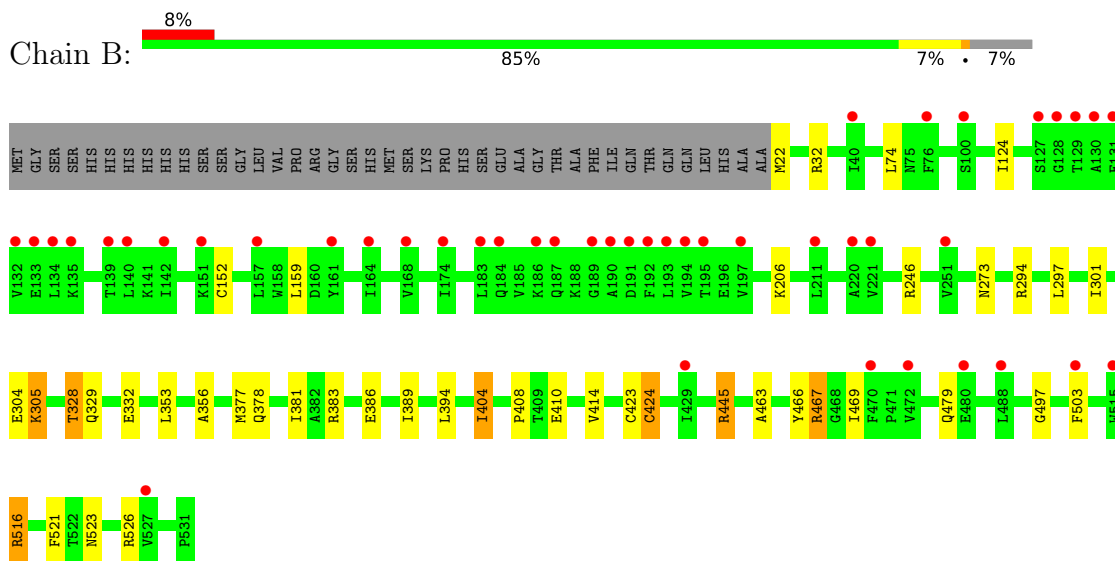
### 3 Residue-property plots [i](#)

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.

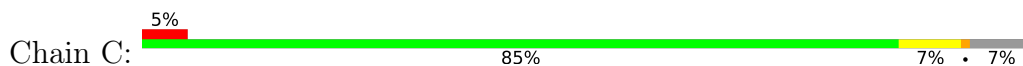
- Molecule 1: Pyruvate kinase PKM

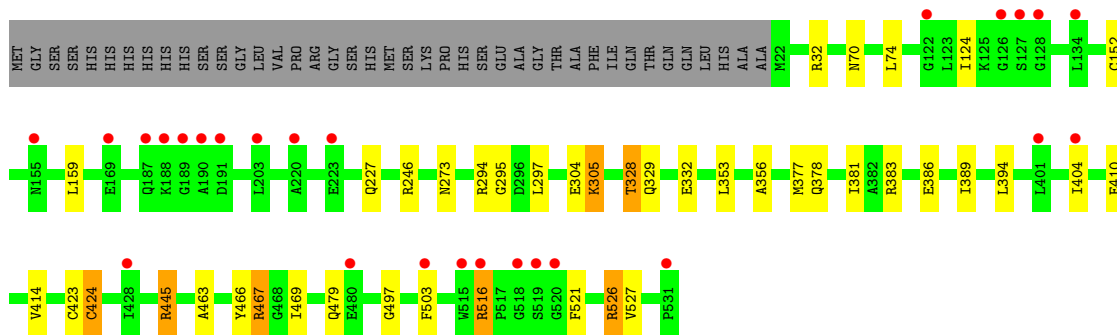


- Molecule 1: Pyruvate kinase PKM

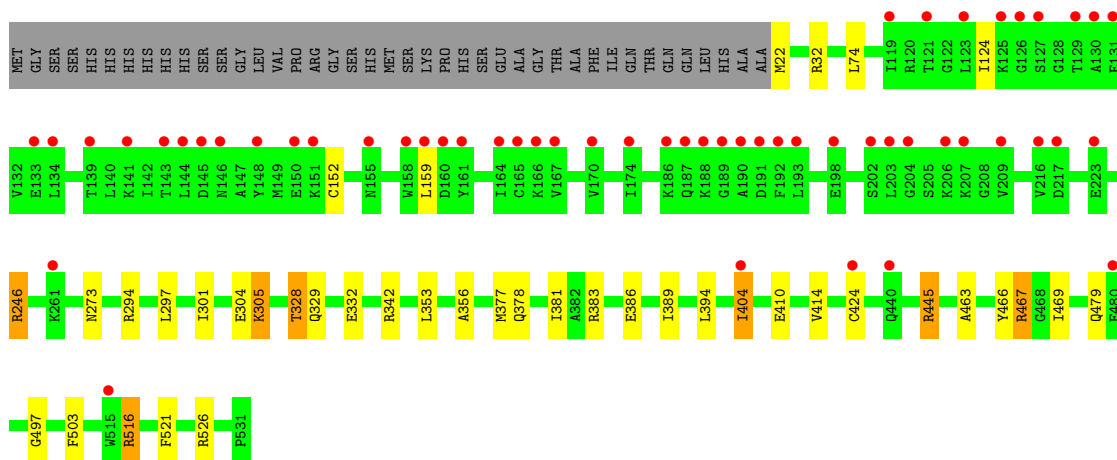
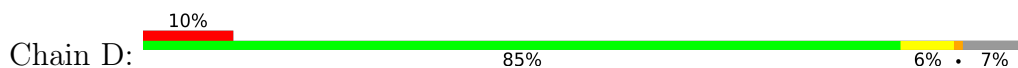


- Molecule 1: Pyruvate kinase PKM

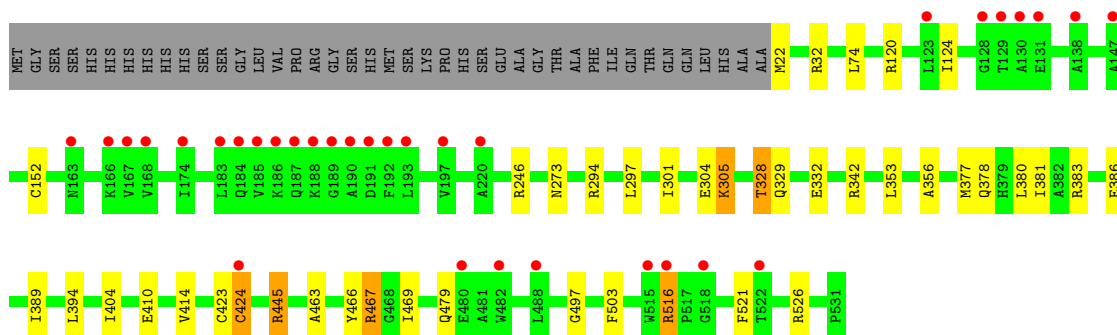
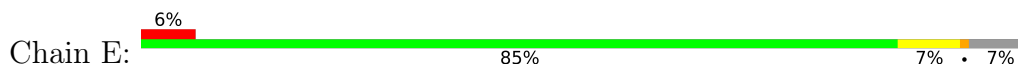




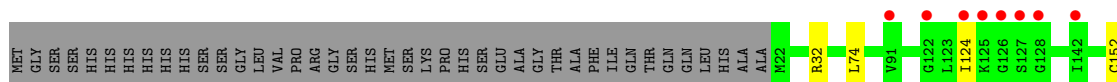
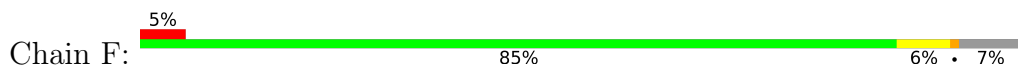
• Molecule 1: Pyruvate kinase PKM

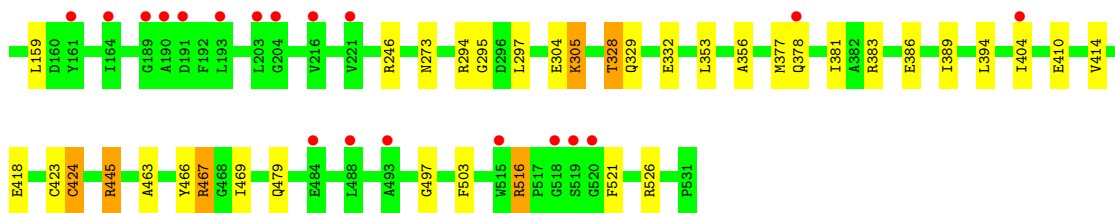


• Molecule 1: Pyruvate kinase PKM

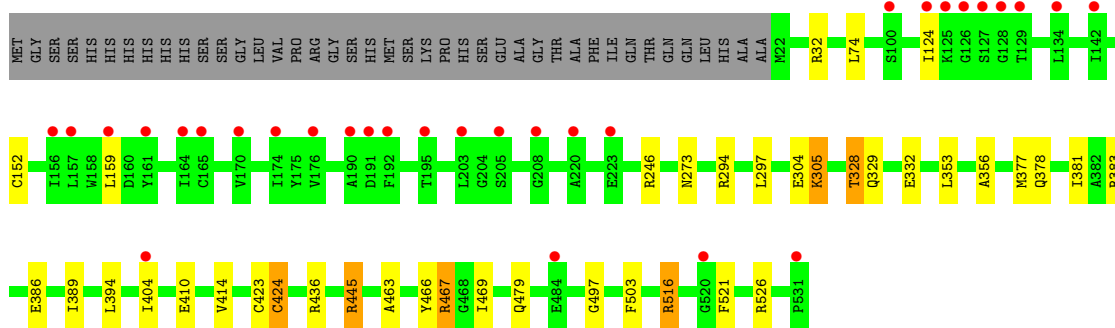
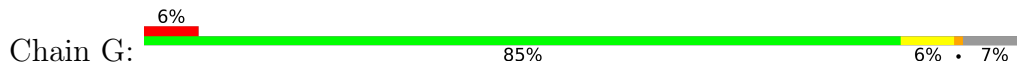


• Molecule 1: Pyruvate kinase PKM

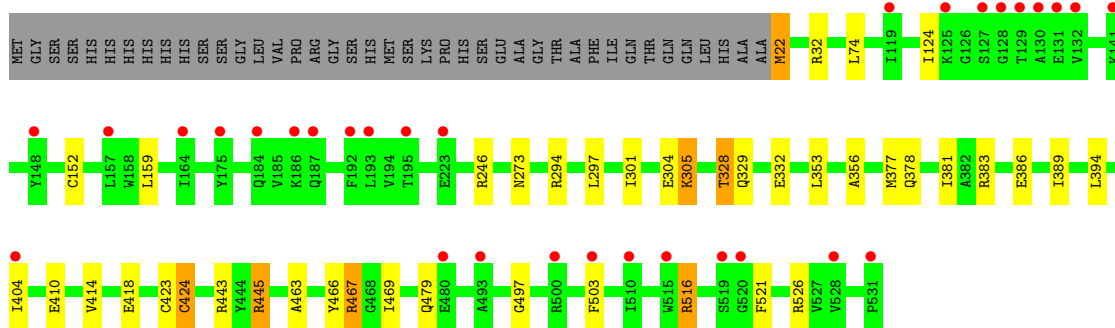
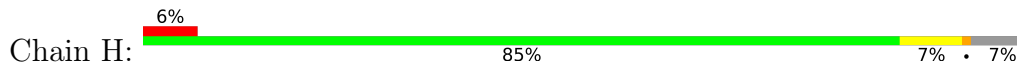




● Molecule 1: Pyruvate kinase PKM



● Molecule 1: Pyruvate kinase PKM



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.35Å 108.94Å 124.34Å 89.72° 71.13° 66.94°	Depositor
Resolution (Å)	116.50 – 2.96 116.50 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.6 (116.50-2.96) 98.6 (116.50-2.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.96Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.236 , 0.252 0.233 , 0.246	Depositor DCC
$R_{free}$ test set	4203 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.9	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	31408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9052e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: CSO, K, PO4, MG

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	0.39	0/3970	0.61	0/5359
1	B	0.38	0/3970	0.61	0/5359
1	C	0.39	0/3970	0.62	0/5359
1	D	0.44	0/3970	0.63	1/5359 (0.0%)
1	E	0.41	0/3970	0.63	1/5359 (0.0%)
1	F	0.39	0/3970	0.62	0/5359
1	G	0.38	0/3970	0.61	0/5359
1	H	0.41	0/3970	0.65	4/5359 (0.1%)
All	All	0.40	0/31760	0.62	6/42872 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	22	MET	CG-SD-CE	7.05	111.48	100.20
1	H	22	MET	CA-CB-CG	6.35	124.10	113.30
1	E	120	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	H	22	MET	CB-CG-SD	5.56	129.07	112.40
1	D	246	ARG	NE-CZ-NH1	5.52	123.06	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3912	0	4001	18	1
1	B	3912	0	4001	20	0
1	C	3912	0	4001	22	1
1	D	3912	0	4001	18	0
1	E	3912	0	4002	19	0
1	F	3912	0	4001	19	0
1	G	3912	0	4001	17	0
1	H	3912	0	4001	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	7	0	4	1	0
4	B	7	0	4	0	0
4	C	7	0	4	1	0
4	D	7	0	4	0	0
4	E	7	0	4	0	0
4	F	7	0	4	0	0
4	G	7	0	4	0	0
4	H	7	0	4	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	0	0
5	H	5	0	0	0	0
All	All	31408	0	32041	143	1

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 143 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445[A]:ARG:HH11	1:C:445[A]:ARG:HG3	1.20	1.07
1:E:445[A]:ARG:HH11	1:E:445[A]:ARG:HG3	1.14	1.06
1:B:445[A]:ARG:HG3	1:B:445[A]:ARG:HH11	1.15	1.06
1:F:445[A]:ARG:HG3	1:F:445[A]:ARG:HH11	1.20	1.06
1:G:445[A]:ARG:HH11	1:G:445[A]:ARG:HG3	1.16	1.04

All (1) 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:A:498:LYS:O	1:C:227:GLN:NE2[1_455]	2.16	0.04

## 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	508/551 (92%)	483 (95%)	20 (4%)	5 (1%)	15	48
1	B	508/551 (92%)	483 (95%)	20 (4%)	5 (1%)	15	48
1	C	508/551 (92%)	484 (95%)	19 (4%)	5 (1%)	15	48
1	D	508/551 (92%)	482 (95%)	21 (4%)	5 (1%)	15	48
1	E	508/551 (92%)	484 (95%)	19 (4%)	5 (1%)	15	48
1	F	508/551 (92%)	482 (95%)	21 (4%)	5 (1%)	15	48
1	G	508/551 (92%)	483 (95%)	20 (4%)	5 (1%)	15	48
1	H	508/551 (92%)	484 (95%)	19 (4%)	5 (1%)	15	48
All	All	4064/4408 (92%)	3865 (95%)	159 (4%)	40 (1%)	15	48

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	CYS
1	B	424	CYS
1	C	424	CYS
1	D	424	CYS
1	E	424	CYS

### 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	420/452 (93%)	402 (96%)	18 (4%)	29 62
1	B	420/452 (93%)	400 (95%)	20 (5%)	25 59
1	C	420/452 (93%)	403 (96%)	17 (4%)	31 64
1	D	420/452 (93%)	401 (96%)	19 (4%)	27 61
1	E	420/452 (93%)	402 (96%)	18 (4%)	29 62
1	F	420/452 (93%)	403 (96%)	17 (4%)	31 64
1	G	420/452 (93%)	402 (96%)	18 (4%)	29 62
1	H	420/452 (93%)	401 (96%)	19 (4%)	27 61
All	All	3360/3616 (93%)	3214 (96%)	146 (4%)	30 62

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	378	GLN
1	H	516	ARG
1	G	436	ARG
1	H	159	LEU
1	C	445[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	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](#)

8 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSO	C	474	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	H	474	1	3,6,7	0.57	0	0,6,8	-	-
1	CSO	F	474	1	3,6,7	0.65	0	0,6,8	-	-
1	CSO	E	474	1	3,6,7	0.72	0	0,6,8	-	-
1	CSO	D	474	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	B	474	1	3,6,7	0.66	0	0,6,8	-	-
1	CSO	G	474	1	3,6,7	0.65	0	0,6,8	-	-
1	CSO	A	474	1	3,6,7	0.61	0	0,6,8	-	-

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
1	CSO	C	474	1	-	0/1/5/7	-
1	CSO	H	474	1	-	0/1/5/7	-
1	CSO	F	474	1	-	0/1/5/7	-
1	CSO	E	474	1	-	0/1/5/7	-
1	CSO	D	474	1	-	0/1/5/7	-
1	CSO	B	474	1	-	0/1/5/7	-
1	CSO	G	474	1	-	0/1/5/7	-
1	CSO	A	474	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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
5	PO4	G	604	-	4,4,4	0.91	0	6,6,6	0.63	0
4	SER	F	603	-	5,6,6	0.97	1 (20%)	5,7,7	1.56	2 (40%)
5	PO4	A	604	-	4,4,4	0.96	0	6,6,6	0.49	0
5	PO4	F	604	-	4,4,4	0.96	0	6,6,6	0.59	0
5	PO4	E	604	-	4,4,4	0.89	0	6,6,6	0.49	0
5	PO4	D	604	-	4,4,4	0.95	0	6,6,6	0.43	0
4	SER	A	603	-	5,6,6	1.06	1 (20%)	5,7,7	1.60	2 (40%)
4	SER	H	603	-	5,6,6	1.00	1 (20%)	5,7,7	1.63	2 (40%)
5	PO4	H	604	-	4,4,4	0.88	0	6,6,6	0.53	0
4	SER	E	603	-	5,6,6	1.08	1 (20%)	5,7,7	1.69	2 (40%)
4	SER	D	603	-	5,6,6	1.07	1 (20%)	5,7,7	1.73	2 (40%)
4	SER	C	603	-	5,6,6	1.03	1 (20%)	5,7,7	1.98	2 (40%)
4	SER	B	603	-	5,6,6	1.10	1 (20%)	5,7,7	1.48	1 (20%)
5	PO4	C	604	-	4,4,4	0.88	0	6,6,6	0.52	0
5	PO4	B	604	-	4,4,4	0.83	0	6,6,6	0.57	0
4	SER	G	603	-	5,6,6	1.02	1 (20%)	5,7,7	1.50	2 (40%)

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
4	SER	F	603	-	-	0/6/6/6	-
4	SER	A	603	-	-	2/6/6/6	-
4	SER	H	603	-	-	0/6/6/6	-
4	SER	E	603	-	-	2/6/6/6	-
4	SER	D	603	-	-	2/6/6/6	-
4	SER	C	603	-	-	2/6/6/6	-
4	SER	B	603	-	-	1/6/6/6	-
4	SER	G	603	-	-	2/6/6/6	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	SER	OXT-C	-2.40	1.22	1.30
4	E	603	SER	OXT-C	-2.36	1.22	1.30
4	D	603	SER	OXT-C	-2.34	1.22	1.30
4	A	603	SER	OXT-C	-2.30	1.23	1.30
4	C	603	SER	OXT-C	-2.25	1.23	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	SER	OXT-C-O	-3.62	115.87	124.09
4	D	603	SER	OXT-C-O	-2.88	117.55	124.09
4	E	603	SER	OXT-C-O	-2.82	117.69	124.09
4	A	603	SER	OXT-C-O	-2.81	117.71	124.09
4	H	603	SER	OXT-C-O	-2.54	118.33	124.09

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	SER	N-CA-CB-OG
4	C	603	SER	OXT-C-CA-N
4	D	603	SER	OXT-C-CA-N
4	E	603	SER	OXT-C-CA-N
4	C	603	SER	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	SER	1	0
4	C	603	SER	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	509/551 (92%)	0.15	23 (4%) 33 21	45, 83, 132, 178	0
1	B	509/551 (92%)	0.38	45 (8%) 10 5	52, 99, 148, 187	0
1	C	509/551 (92%)	0.22	26 (5%) 28 17	48, 86, 147, 186	0
1	D	509/551 (92%)	0.57	55 (10%) 5 3	50, 88, 158, 188	0
1	E	509/551 (92%)	0.29	33 (6%) 18 11	52, 83, 130, 180	0
1	F	509/551 (92%)	0.23	27 (5%) 26 16	52, 94, 145, 183	0
1	G	509/551 (92%)	0.22	31 (6%) 21 12	46, 85, 146, 185	0
1	H	509/551 (92%)	0.18	31 (6%) 21 12	52, 88, 130, 176	0
All	All	4072/4408 (92%)	0.28	271 (6%) 17 10	45, 88, 145, 188	0

The worst 5 of 271 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	130	ALA	23.0
1	D	126	GLY	18.5
1	C	519	SER	16.4
1	H	128	GLY	13.4
1	D	121	THR	11.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSO	F	474	7/8	0.76	0.15	97,102,107,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSO	B	474	7/8	0.78	0.19	108,112,114,115	0
1	CSO	A	474	7/8	0.84	0.16	82,85,92,93	0
1	CSO	C	474	7/8	0.90	0.12	86,91,97,99	0
1	CSO	H	474	7/8	0.90	0.10	101,102,104,104	0
1	CSO	E	474	7/8	0.91	0.12	84,86,87,89	0
1	CSO	D	474	7/8	0.94	0.14	80,84,94,97	0
1	CSO	G	474	7/8	0.96	0.12	86,87,95,96	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	E	602	1/1	0.80	0.31	58,58,58,58	0
2	K	A	601	1/1	0.84	0.11	93,93,93,93	0
3	MG	B	602	1/1	0.86	0.21	49,49,49,49	0
2	K	C	601	1/1	0.88	0.13	70,70,70,70	0
3	MG	H	602	1/1	0.88	0.26	61,61,61,61	0
4	SER	H	603	7/7	0.88	0.17	74,77,77,79	0
2	K	G	601	1/1	0.90	0.08	86,86,86,86	0
4	SER	F	603	7/7	0.90	0.22	90,91,92,93	0
3	MG	F	602	1/1	0.90	0.37	66,66,66,66	0
4	SER	C	603	7/7	0.91	0.15	69,71,71,73	0
5	PO4	F	604	5/5	0.91	0.12	100,103,104,106	0
3	MG	C	602	1/1	0.92	0.34	58,58,58,58	0
5	PO4	B	604	5/5	0.93	0.09	119,121,122,123	0
3	MG	D	602	1/1	0.93	0.34	57,57,57,57	0
4	SER	E	603	7/7	0.94	0.18	79,82,86,88	0
3	MG	A	602	1/1	0.94	0.22	58,58,58,58	0
4	SER	B	603	7/7	0.94	0.19	85,86,86,87	0
3	MG	G	602	1/1	0.94	0.25	61,61,61,61	0
4	SER	D	603	7/7	0.94	0.18	69,72,75,76	0
4	SER	G	603	7/7	0.95	0.14	85,87,89,90	0
2	K	F	601	1/1	0.95	0.09	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PO4	H	604	5/5	0.95	0.13	93,95,96,97	0
2	K	B	601	1/1	0.96	0.12	94,94,94,94	0
5	PO4	G	604	5/5	0.96	0.10	86,86,88,88	0
4	SER	A	603	7/7	0.96	0.15	81,83,86,88	0
5	PO4	A	604	5/5	0.97	0.10	87,88,89,90	0
2	K	E	601	1/1	0.97	0.11	72,72,72,72	0
5	PO4	E	604	5/5	0.97	0.10	83,83,84,86	0
2	K	H	601	1/1	0.98	0.09	80,80,80,80	0
5	PO4	D	604	5/5	0.98	0.10	86,87,88,90	0
2	K	D	601	1/1	0.98	0.04	77,77,77,77	0
5	PO4	C	604	5/5	0.99	0.07	72,72,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.