Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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 ①) were used in the production of this report:

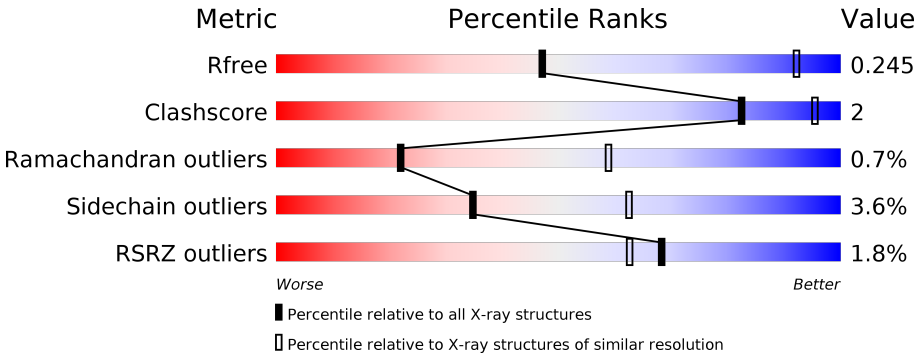
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	85% 8% • 6%
1	B	551	85% 8% • 5%
1	C	551	86% 8% • 5%
1	D	551	8% 84% 8% • 7%
1	E	551	79% 7% • 13%
1	F	551	86% 8% • 5%

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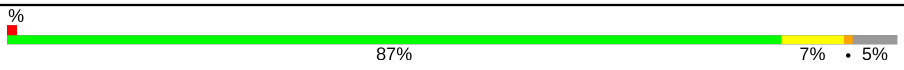
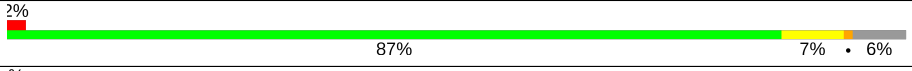
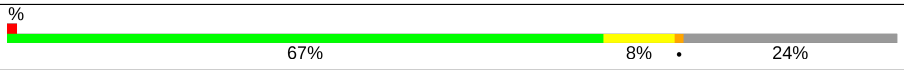
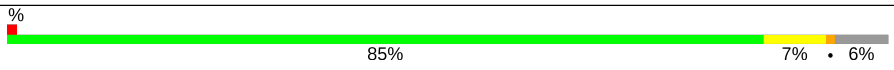
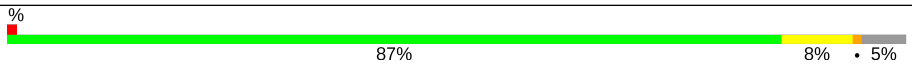
Mol	Chain	Length	Quality of chain
1	G	551	
1	H	551	
1	I	551	
1	J	551	
1	K	551	
1	L	551	

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
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
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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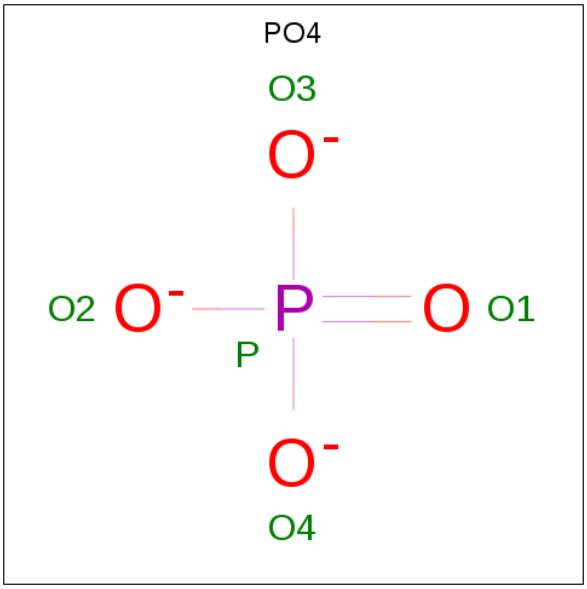
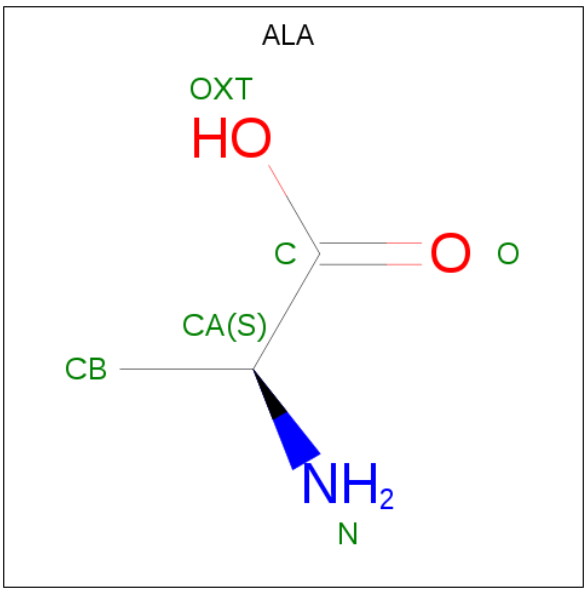
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP P14618
K	-3	ARG	-	expression tag	UNP P14618
K	-2	GLY	-	expression tag	UNP P14618
K	-1	SER	-	expression tag	UNP P14618
K	0	HIS	-	expression tag	UNP P14618
L	-19	MET	-	initiating methionine	UNP P14618
L	-18	GLY	-	expression tag	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: O_4P).



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: $C_3H_7NO_2$).

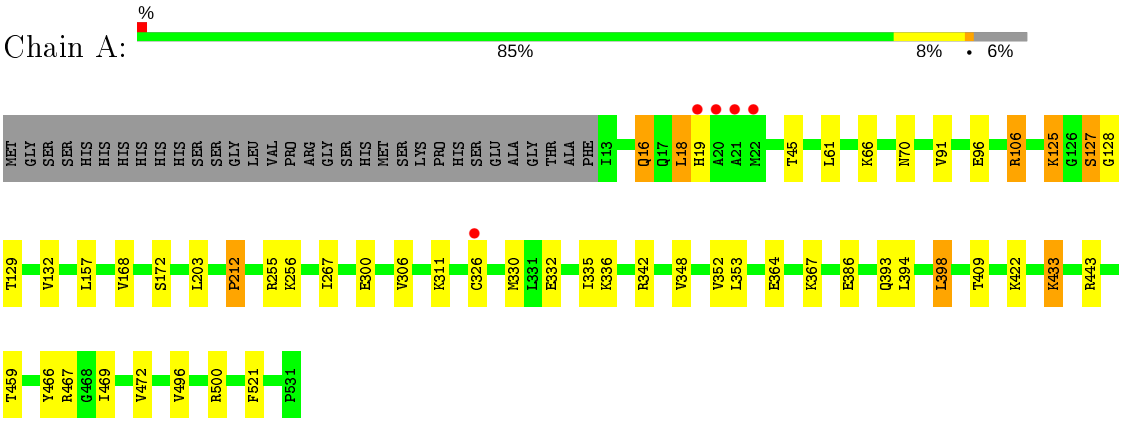


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	3	1	2		
3	C	1	Total	C	N	O	0	0
			6	3	1	2		
3	D	1	Total	C	N	O	0	0
			6	3	1	2		
3	E	1	Total	C	N	O	0	0
			6	3	1	2		
3	F	1	Total	C	N	O	0	0
			6	3	1	2		
3	G	1	Total	C	N	O	0	0
			6	3	1	2		
3	H	1	Total	C	N	O	0	0
			6	3	1	2		
3	I	1	Total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

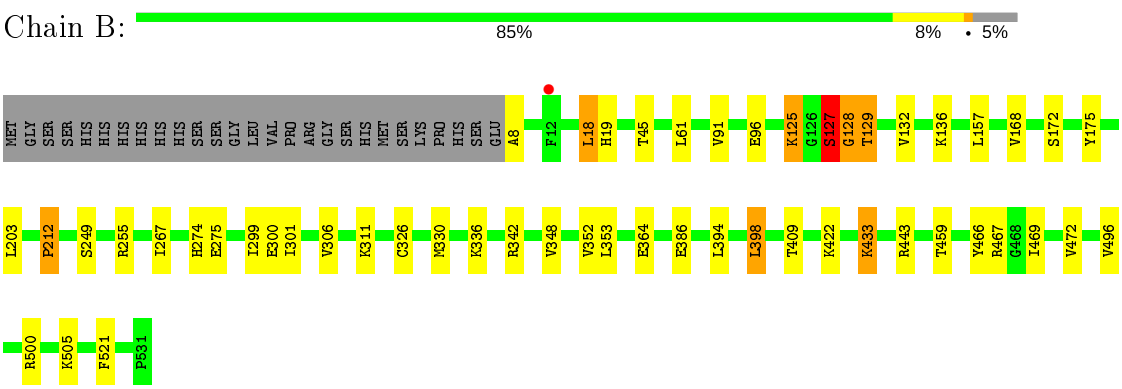
3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

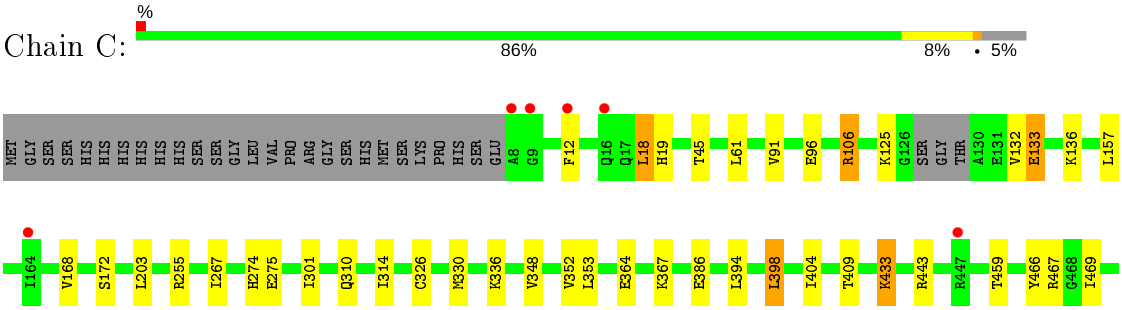
- Molecule 1: Pyruvate kinase PKM



- Molecule 1: Pyruvate kinase PKM

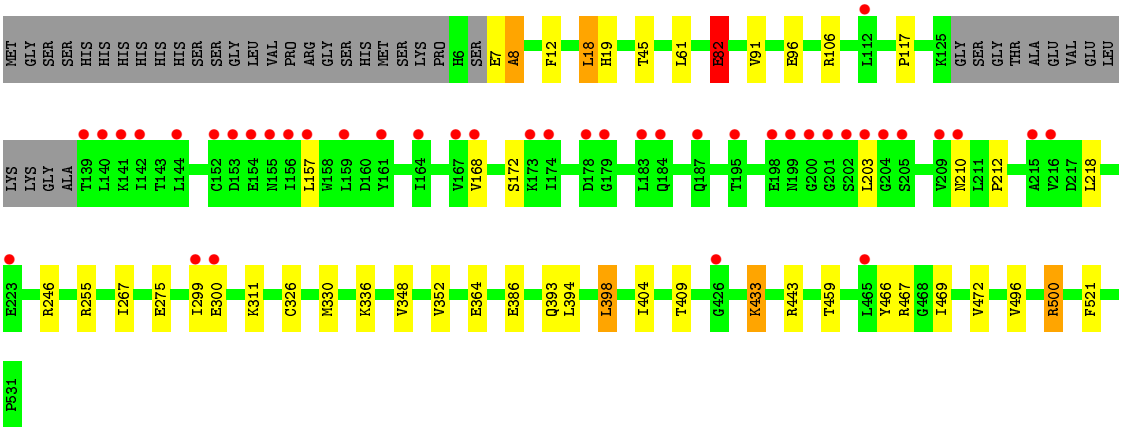


- Molecule 1: Pyruvate kinase PKM



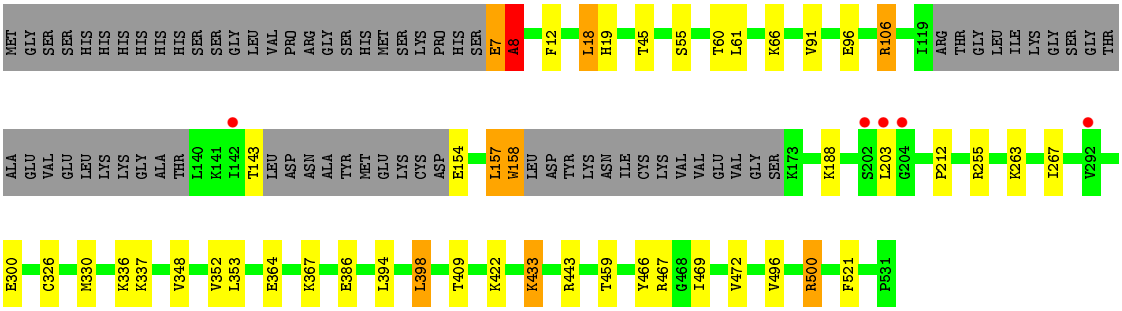
• Molecule 1: Pyruvate kinase PKM

Chain D:



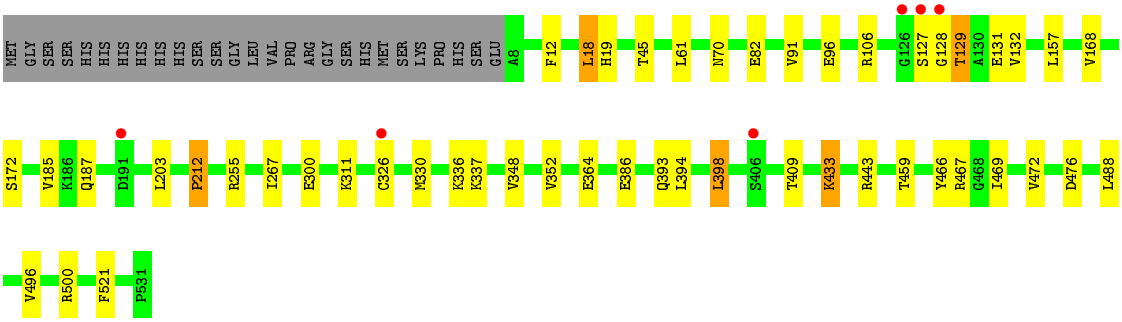
• Molecule 1: Pyruvate kinase PKM

Chain E:



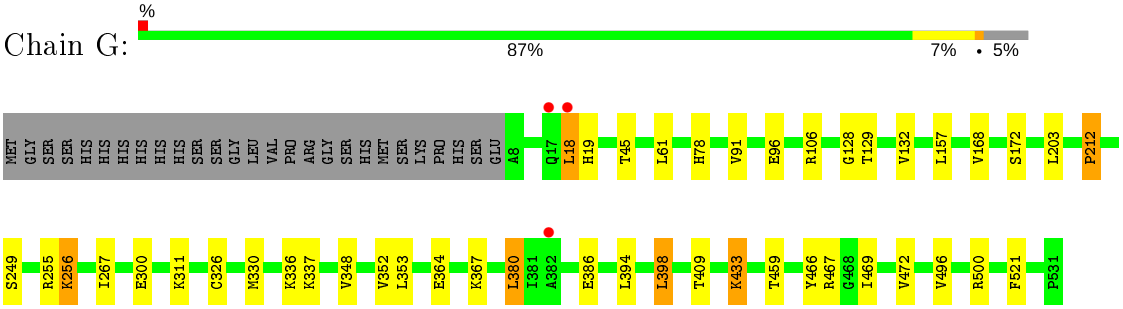
• Molecule 1: Pyruvate kinase PKM

Chain F:



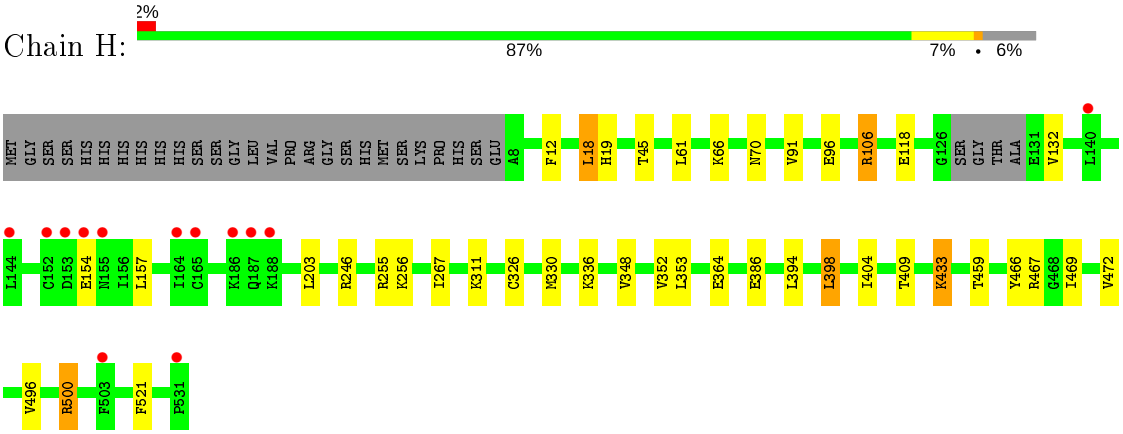
• Molecule 1: Pyruvate kinase PKM

Chain G:



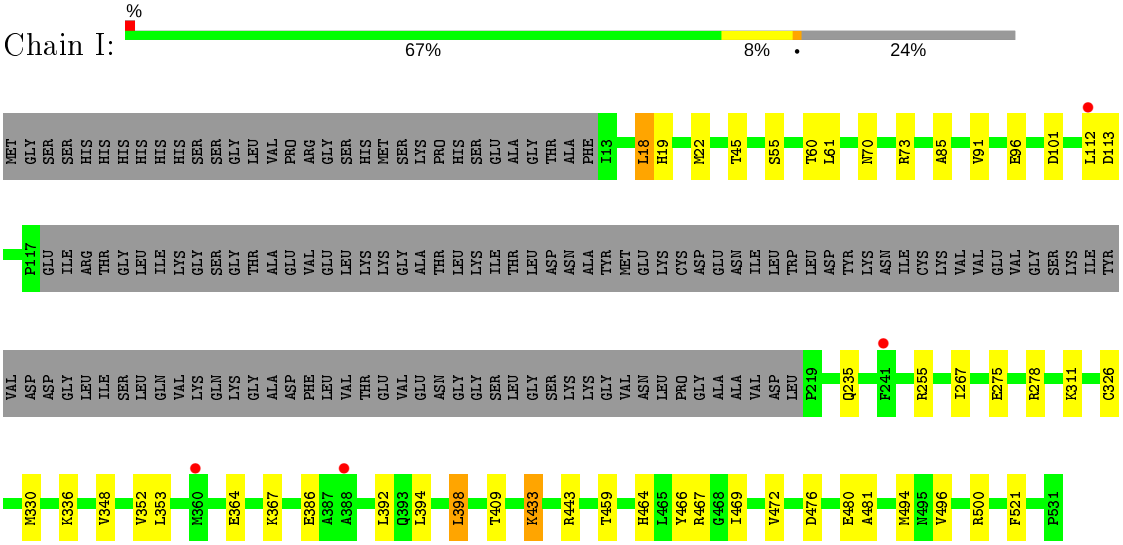
• Molecule 1: Pyruvate kinase PKM

Chain H:



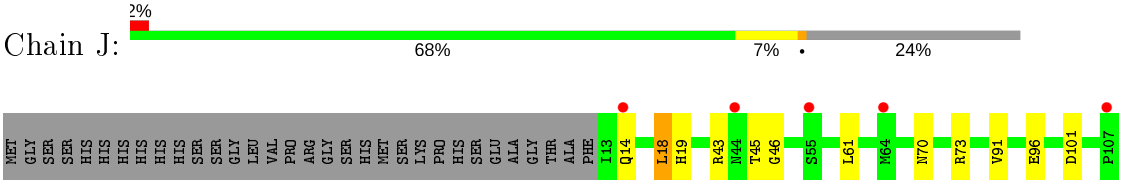
• Molecule 1: Pyruvate kinase PKM

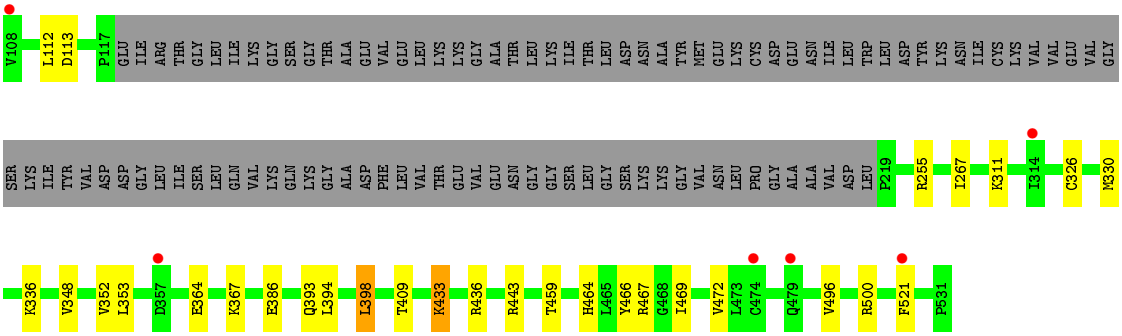
Chain I:



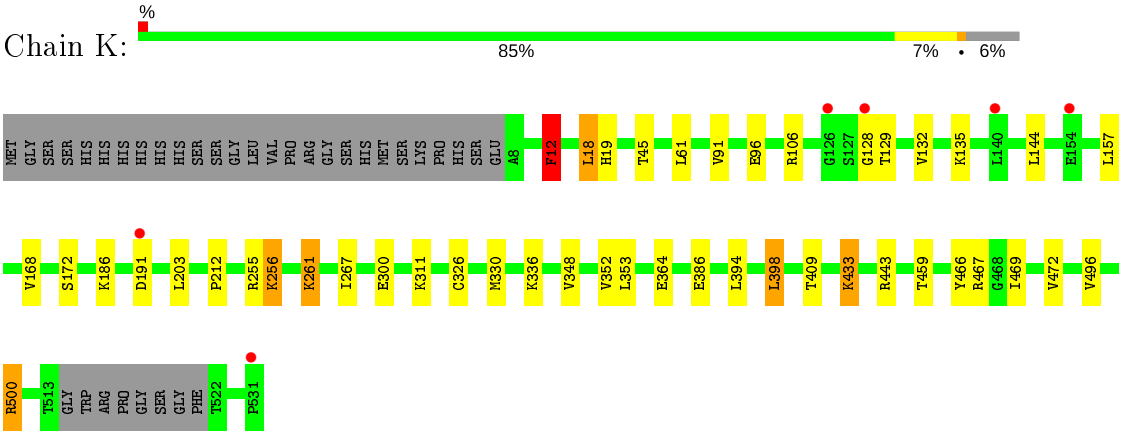
• Molecule 1: Pyruvate kinase PKM

Chain J:

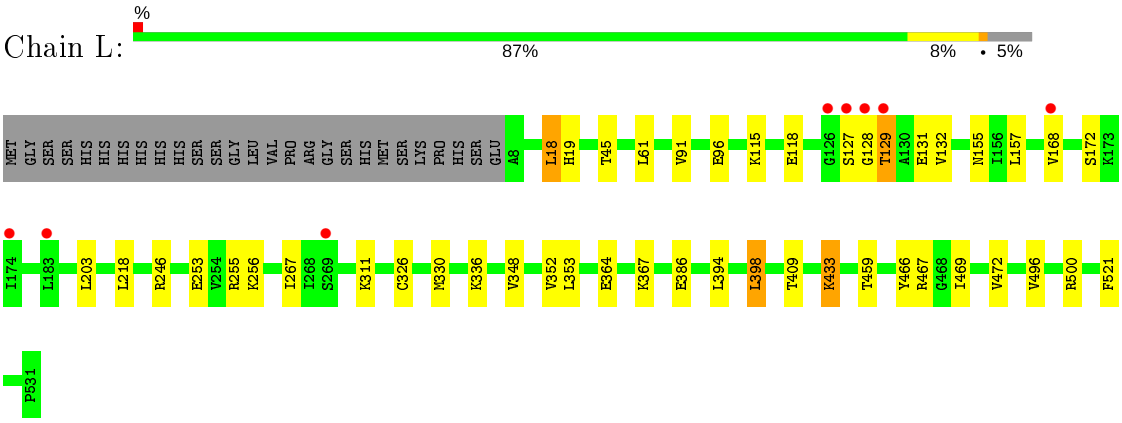




- Molecule 1: Pyruvate kinase PKM



- Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.03%)	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)	0.28 , 90.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	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

All (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
1	K	12	PHE	CA-CB	6.24	1.67	1.53
1	E	158	TRP	CA-C	-6.14	1.36	1.52
1	H	118	GLU	CD-OE1	-6.01	1.19	1.25
1	C	275	GLU	CD-OE1	-5.89	1.19	1.25
1	D	82	GLU	CD-OE2	-5.44	1.19	1.25
1	A	125	LYS	C-O	-5.11	1.13	1.23
1	C	133	GLU	CB-CG	5.10	1.61	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	L	500	ARG	CB-CG-CD	7.52	131.15	111.60
1	G	500	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	E	500	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	L	500	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	G	380	LEU	CB-CG-CD2	6.31	121.73	111.00
1	L	500	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	125	LYS	CA-C-N	5.86	127.92	116.20
1	A	16	GLN	CA-CB-CG	5.84	126.24	113.40
1	B	500	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	125	LYS	CA-C-O	-5.68	108.17	120.10
1	H	246	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	I	500	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	L	218	LEU	CB-CG-CD1	5.48	120.32	111.00
1	A	125	LYS	CA-C-N	5.21	126.61	116.20
1	K	12	PHE	N-CA-CB	5.12	119.82	110.60
1	A	127	SER	N-CA-CB	5.12	118.18	110.50
1	B	127	SER	N-CA-CB	5.08	118.12	110.50
1	B	128	GLY	N-CA-C	5.08	125.79	113.10
1	D	246	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	G	256	LYS	CD-CE-NZ	5.01	123.22	111.70

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 (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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:A:342:ARG:HG3	1:B:306:VAL:HG21	1.68	0.74
1:D:117:PRO:HB2	1:D:218:LEU:HD13	1.69	0.73
1:A:70:ASN:ND2	3:A:602:ALA:OXT	2.26	0.68
1:K:12:PHE:CE1	1:K:500:ARG:HD2	2.28	0.68
1:D:210:ASN:CG	1:D:299:ILE:HG21	2.14	0.68
1:K:12:PHE:CD1	1:K:500:ARG:CD	2.76	0.68
1:J:14:GLN:HE21	1:J:43:ARG:N	1.93	0.67
1:F:129:THR:OG1	1:F:131:GLU:O	2.13	0.67
1:F:12:PHE:CE1	1:F:500:ARG:HD3	2.31	0.65
1:L:129:THR:OG1	1:L:131:GLU:O	2.14	0.65
1:D:210:ASN:ND2	1:D:299:ILE:HG21	2.12	0.64
1:L:115:LYS:HG3	1:L:118:GLU:OE1	1.97	0.63
1:L:469:ILE:O	3:L:602:ALA:N	2.32	0.63
1:B:212:PRO:HA	1:B:300:GLU:HG3	1.82	0.60
1:K:144:LEU:HD12	1:K:191:ASP:OD1	2.02	0.59
1:A:306:VAL:HG21	1:B:342:ARG:HG3	1.86	0.58
1:C:157:LEU:HD13	1:C:203:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:VAL:HG21	1:D:496:VAL:HG21	1.88	0.56
1:K:311:LYS:HE3	1:L:353:LEU:HD13	1.87	0.56
1:C:472:VAL:HG21	1:C:496:VAL:HG21	1.88	0.56
1:B:472:VAL:HG21	1:B:496:VAL:HG21	1.88	0.55
1:I:472:VAL:HG21	1:I:496:VAL:HG21	1.89	0.55
1:H:472:VAL:HG21	1:H:496:VAL:HG21	1.89	0.55
1:L:127:SER:O	1:L:129:THR:N	2.38	0.55
1:D:157:LEU:HD13	1:D:203:LEU:HD21	1.89	0.55
1:F:472:VAL:HG21	1:F:496:VAL:HG21	1.88	0.55
1:L:472:VAL:HG21	1:L:496:VAL:HG21	1.89	0.54
1:A:342:ARG:HD2	1:B:306:VAL:HG11	1.90	0.54
1:G:472:VAL:HG21	1:G:496:VAL:HG21	1.88	0.54
1:J:472:VAL:HG21	1:J:496:VAL:HG21	1.89	0.54
1:E:472:VAL:HG21	1:E:496:VAL:HG21	1.88	0.54
1:L:115:LYS:CG	1:L:118:GLU:OE1	2.54	0.54
1:D:117:PRO:CB	1:D:218:LEU:HD13	2.37	0.54
1:F:70:ASN:HD21	3:F:602:ALA:C	2.10	0.54
1:K:157:LEU:HD13	1:K:203:LEU:HD21	1.90	0.54
1:E:143:THR:HG23	1:E:158:TRP:HA	1.90	0.54
1:G:353:LEU:HD13	1:H:311:LYS:HE3	1.90	0.54
1:A:472:VAL:HG21	1:A:496:VAL:HG21	1.88	0.53
1:B:157:LEU:HD13	1:B:203:LEU:HD21	1.90	0.53
1:B:422:LYS:O	1:C:404:ILE:HD11	2.08	0.53
1:A:157:LEU:HD13	1:A:203:LEU:HD21	1.89	0.53
1:G:311:LYS:HE3	1:H:353:LEU:HD13	1.90	0.53
1:K:472:VAL:HG21	1:K:496:VAL:HG21	1.89	0.53
1:K:353:LEU:HD13	1:L:311:LYS:HE3	1.91	0.53
1:F:157:LEU:HD13	1:F:203:LEU:HD21	1.90	0.53
1:B:127:SER:O	1:B:129:THR:N	2.40	0.53
1:G:45:THR:HG21	1:G:352:VAL:HG13	1.91	0.53
1:L:157:LEU:HD13	1:L:203:LEU:HD21	1.91	0.52
1:H:157:LEU:HD13	1:H:203:LEU:HD21	1.92	0.52
1:L:253:GLU:HG2	1:L:256:LYS:HZ1	1.74	0.52
1:F:127:SER:O	1:F:129:THR:N	2.38	0.52
1:K:45:THR:HG21	1:K:352:VAL:HG13	1.92	0.52
1:E:157:LEU:HD13	1:E:203:LEU:HD21	1.90	0.52
1:F:70:ASN:ND2	3:F:602:ALA:O	2.42	0.52
1:L:45:THR:HG21	1:L:352:VAL:HG13	1.91	0.52
1:B:175:TYR:CG	1:B:299:ILE:HG23	2.44	0.52
1:D:45:THR:HG21	1:D:352:VAL:HG13	1.92	0.52
1:A:332:GLU:O	1:A:335:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:THR:HG21	1:C:352:VAL:HG13	1.92	0.51
1:D:61:LEU:HD13	1:D:91:VAL:HA	1.93	0.51
1:B:61:LEU:HD13	1:B:91:VAL:HA	1.93	0.51
1:E:143:THR:CG2	1:E:158:TRP:HA	2.40	0.51
1:E:45:THR:HG21	1:E:352:VAL:HG13	1.92	0.51
1:F:61:LEU:HD13	1:F:91:VAL:HA	1.92	0.51
1:J:45:THR:HG21	1:J:352:VAL:HG13	1.92	0.51
1:B:45:THR:HG21	1:B:352:VAL:HG13	1.92	0.51
1:F:45:THR:HG21	1:F:352:VAL:HG13	1.92	0.51
1:I:22:MET:HE1	1:I:392:LEU:HD13	1.93	0.51
1:A:212:PRO:HA	1:A:300:GLU:HG3	1.93	0.51
1:J:61:LEU:HD13	1:J:91:VAL:HA	1.93	0.51
1:K:61:LEU:HD13	1:K:91:VAL:HA	1.92	0.51
1:G:212:PRO:HA	1:G:300:GLU:HG3	1.93	0.51
1:H:330:MET:CE	1:H:348:VAL:HG22	2.41	0.51
1:B:330:MET:CE	1:B:348:VAL:HG22	2.41	0.51
1:H:61:LEU:HD13	1:H:91:VAL:HA	1.92	0.51
1:A:61:LEU:HD13	1:A:91:VAL:HA	1.93	0.51
1:G:157:LEU:HD13	1:G:203:LEU:HD21	1.93	0.51
1:I:73:ARG:NH1	1:I:113:ASP:OD2	2.44	0.51
1:C:330:MET:CE	1:C:348:VAL:HG22	2.41	0.50
1:D:330:MET:CE	1:D:348:VAL:HG22	2.41	0.50
1:I:45:THR:HG21	1:I:352:VAL:HG13	1.92	0.50
1:J:14:GLN:NE2	1:J:43:ARG:HB3	2.26	0.50
1:A:330:MET:CE	1:A:348:VAL:HG22	2.41	0.50
1:E:330:MET:CE	1:E:348:VAL:HG22	2.41	0.50
1:L:330:MET:CE	1:L:348:VAL:HG22	2.41	0.50
1:L:61:LEU:HD13	1:L:91:VAL:HA	1.93	0.50
1:A:45:THR:HG21	1:A:352:VAL:HG13	1.92	0.50
1:G:330:MET:CE	1:G:348:VAL:HG22	2.41	0.50
1:G:61:LEU:HD13	1:G:91:VAL:HA	1.92	0.50
1:I:330:MET:CE	1:I:348:VAL:HG22	2.42	0.50
1:I:70:ASN:HB3	1:I:464:HIS:CD2	2.47	0.50
1:A:422:LYS:O	1:D:404:ILE:HD11	2.11	0.50
1:H:45:THR:HG21	1:H:352:VAL:HG13	1.91	0.50
1:J:330:MET:CE	1:J:348:VAL:HG22	2.41	0.50
1:I:275:GLU:HG3	1:I:278:ARG:HH12	1.76	0.50
1:K:330:MET:CE	1:K:348:VAL:HG22	2.42	0.50
1:F:330:MET:CE	1:F:348:VAL:HG22	2.41	0.50
1:J:73:ARG:NH1	1:J:113:ASP:OD2	2.45	0.50
1:C:61:LEU:HD13	1:C:91:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.94	0.50
1:J:70:ASN:HB3	1:J:464:HIS:CD2	2.46	0.50
1:E:386:GLU:OE2	1:E:467:ARG:NH2	2.45	0.49
1:F:212:PRO:HA	1:F:300:GLU:HG3	1.94	0.49
1:F:386:GLU:OE2	1:F:467:ARG:NH2	2.45	0.49
1:L:386:GLU:OE2	1:L:467:ARG:NH2	2.45	0.49
1:G:249:SER:HB3	1:I:101:ASP:OD1	2.13	0.49
1:J:466:TYR:HB2	1:J:469:ILE:HD12	1.94	0.49
1:B:386:GLU:OE2	1:B:467:ARG:NH2	2.46	0.49
1:E:61:LEU:HD13	1:E:91:VAL:HA	1.92	0.49
1:C:386:GLU:OE2	1:C:467:ARG:NH2	2.45	0.49
1:I:61:LEU:HD13	1:I:91:VAL:HA	1.93	0.49
1:J:386:GLU:OE2	1:J:467:ARG:NH2	2.45	0.49
1:A:386:GLU:OE2	1:A:467:ARG:NH2	2.45	0.49
1:G:386:GLU:OE2	1:G:467:ARG:NH2	2.45	0.49
1:H:386:GLU:OE2	1:H:467:ARG:NH2	2.45	0.49
1:I:386:GLU:OE2	1:I:467:ARG:NH2	2.45	0.49
1:G:466:TYR:HB2	1:G:469:ILE:HD12	1.95	0.49
1:J:70:ASN:HB3	1:J:464:HIS:HD2	1.78	0.49
1:D:386:GLU:OE2	1:D:467:ARG:NH2	2.46	0.49
1:E:466:TYR:HB2	1:E:469:ILE:HD12	1.95	0.49
1:K:386:GLU:OE2	1:K:467:ARG:NH2	2.45	0.48
1:C:12:PHE:CZ	1:C:106:ARG:HG3	2.47	0.48
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.95	0.48
1:A:433:LYS:O	1:A:459:THR:HG21	2.14	0.48
1:J:433:LYS:O	1:J:459:THR:HG21	2.14	0.48
1:J:46:GLY:HA2	3:J:602:ALA:HA	1.96	0.48
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.95	0.48
1:B:433:LYS:O	1:B:459:THR:HG21	2.14	0.48
1:F:433:LYS:O	1:F:459:THR:HG21	2.14	0.48
1:I:480:GLU:CG	1:I:481:ALA:N	2.77	0.48
1:K:12:PHE:HD1	1:K:500:ARG:HD3	1.76	0.48
1:K:466:TYR:HB2	1:K:469:ILE:HD12	1.95	0.48
1:F:488:LEU:HD13	1:L:256:LYS:HD3	1.96	0.48
1:H:433:LYS:O	1:H:459:THR:HG21	2.14	0.48
1:I:433:LYS:O	1:I:459:THR:HG21	2.14	0.48
1:I:70:ASN:HB3	1:I:464:HIS:HD2	1.79	0.48
1:A:311:LYS:HE3	1:B:353:LEU:HD13	1.95	0.47
1:C:433:LYS:O	1:C:459:THR:HG21	2.14	0.47
1:D:433:LYS:O	1:D:459:THR:HG21	2.14	0.47
1:E:433:LYS:O	1:E:459:THR:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:433:LYS:O	1:L:459:THR:HG21	2.14	0.47
1:G:433:LYS:O	1:G:459:THR:HG21	2.14	0.47
1:L:466:TYR:HB2	1:L:469:ILE:HD12	1.96	0.47
1:H:466:TYR:HB2	1:H:469:ILE:HD12	1.96	0.47
1:I:112:LEU:C	1:I:112:LEU:HD23	2.35	0.47
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.95	0.46
1:G:249:SER:CB	1:I:101:ASP:OD1	2.63	0.46
1:J:112:LEU:HD23	1:J:112:LEU:C	2.35	0.46
1:K:433:LYS:O	1:K:459:THR:HG21	2.14	0.46
1:B:505:LYS:HG2	1:F:187:GLN:OE1	2.15	0.46
1:H:70:ASN:ND2	3:H:602:ALA:OXT	2.48	0.46
1:C:353:LEU:HD13	1:D:311:LYS:HE3	1.98	0.46
1:E:422:LYS:O	1:H:404:ILE:HD11	2.15	0.46
1:F:466:TYR:HB2	1:F:469:ILE:HD12	1.96	0.46
1:I:466:TYR:HB2	1:I:469:ILE:HD12	1.96	0.46
1:E:7:GLU:O	1:E:8:ALA:HB2	2.16	0.45
1:K:330:MET:HE3	1:K:348:VAL:HG22	1.98	0.45
1:A:168:VAL:HG13	1:A:172:SER:HB2	1.99	0.45
1:A:353:LEU:HD13	1:B:311:LYS:HE3	1.98	0.45
1:E:66:LYS:HA	1:E:106:ARG:NH1	2.32	0.45
1:D:168:VAL:HG13	1:D:172:SER:HB2	1.99	0.44
1:A:66:LYS:HA	1:A:106:ARG:NH1	2.32	0.44
1:F:168:VAL:HG13	1:F:172:SER:HB2	1.99	0.44
1:F:70:ASN:ND2	3:F:602:ALA:C	2.71	0.44
1:L:168:VAL:HG13	1:L:172:SER:HB2	1.99	0.44
1:H:255:ARG:CZ	1:H:267:ILE:HD12	2.48	0.44
1:K:168:VAL:HG13	1:K:172:SER:HB2	2.00	0.44
1:A:255:ARG:CZ	1:A:267:ILE:HD12	2.48	0.44
1:B:255:ARG:CZ	1:B:267:ILE:HD12	2.48	0.44
1:I:255:ARG:CZ	1:I:267:ILE:HD12	2.48	0.44
1:C:12:PHE:HA	1:C:106:ARG:NH2	2.32	0.44
1:C:255:ARG:CZ	1:C:267:ILE:HD12	2.48	0.44
1:L:255:ARG:CZ	1:L:267:ILE:HD12	2.48	0.44
1:H:66:LYS:HA	1:H:106:ARG:NH1	2.33	0.44
1:J:255:ARG:CZ	1:J:267:ILE:HD12	2.48	0.44
1:K:261:LYS:CD	1:K:261:LYS:H	2.31	0.44
1:C:168:VAL:HG13	1:C:172:SER:HB2	1.99	0.43
1:F:255:ARG:CZ	1:F:267:ILE:HD12	2.48	0.43
1:I:353:LEU:HD13	1:J:311:LYS:HE3	1.99	0.43
1:D:255:ARG:CZ	1:D:267:ILE:HD12	2.48	0.43
1:D:212:PRO:HA	1:D:300:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ARG:CZ	1:E:267:ILE:HD12	2.48	0.43
1:G:249:SER:OG	1:I:101:ASP:OD1	2.37	0.43
1:G:255:ARG:CZ	1:G:267:ILE:HD12	2.48	0.43
1:K:255:ARG:CZ	1:K:267:ILE:HD12	2.48	0.43
1:G:330:MET:HE3	1:G:348:VAL:HG22	2.01	0.42
1:G:256:LYS:CE	1:I:476:ASP:OD1	2.67	0.42
1:I:480:GLU:HG2	1:I:481:ALA:H	1.85	0.42
1:F:12:PHE:CZ	1:F:500:ARG:HD3	2.54	0.42
1:G:168:VAL:HG13	1:G:172:SER:HB2	2.00	0.42
1:B:168:VAL:HG13	1:B:172:SER:HB2	2.01	0.42
1:I:330:MET:HE3	1:I:348:VAL:HG22	2.00	0.42
1:F:330:MET:HE3	1:F:348:VAL:HG22	2.01	0.42
1:F:394:LEU:O	1:F:398:LEU:HD12	2.20	0.42
1:I:311:LYS:HE3	1:J:353:LEU:HD13	2.02	0.42
1:K:256:LYS:HE3	1:K:256:LYS:HB2	1.87	0.42
1:A:394:LEU:O	1:A:398:LEU:HD12	2.20	0.41
1:E:353:LEU:HD13	1:F:311:LYS:HE3	2.02	0.41
1:D:394:LEU:O	1:D:398:LEU:HD12	2.21	0.41
1:K:394:LEU:O	1:K:398:LEU:HD12	2.21	0.41
1:K:212:PRO:HA	1:K:300:GLU:HG3	2.02	0.41
1:L:394:LEU:O	1:L:398:LEU:HD12	2.21	0.41
1:D:12:PHE:CE1	1:D:500:ARG:HD3	2.55	0.41
1:D:7:GLU:O	1:D:8:ALA:HB2	2.20	0.41
1:E:212:PRO:HA	1:E:300:GLU:HG3	2.02	0.41
1:E:394:LEU:O	1:E:398:LEU:HD12	2.21	0.41
1:H:394:LEU:O	1:H:398:LEU:HD12	2.21	0.41
1:E:12:PHE:CE1	1:E:500:ARG:HD3	2.56	0.41
1:F:168:VAL:HG11	1:F:185:VAL:HG21	2.03	0.41
1:I:394:LEU:O	1:I:398:LEU:HD12	2.21	0.41
1:I:85:ALA:HA	1:I:235:GLN:HE21	1.86	0.41
1:H:12:PHE:CE1	1:H:500:ARG:HD3	2.56	0.41
1:C:394:LEU:O	1:C:398:LEU:HD12	2.20	0.40
1:E:55:SER:HA	1:E:60:THR:HG21	2.03	0.40
1:C:310:GLN:HG2	1:C:314:ILE:HD12	2.04	0.40
1:G:394:LEU:O	1:G:398:LEU:HD12	2.21	0.40
1:J:394:LEU:O	1:J:398:LEU:HD12	2.21	0.40
1:L:330:MET:HE3	1:L:348:VAL:HG22	2.02	0.40
1:B:274:HIS:ND1	1:B:301:ILE:HG22	2.36	0.40
1:B:330:MET:HE3	1:B:348:VAL:HG22	2.03	0.40
1:C:274:HIS:ND1	1:C:301:ILE:HG22	2.36	0.40
1:C:12:PHE:CZ	1:C:106:ARG:CG	3.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:MET:HE3	1:D:348:VAL:HG22	2.03	0.40
1:B:394:LEU:O	1:B:398:LEU:HD12	2.20	0.40
1:I:55:SER:HA	1:I:60:THR:HG21	2.04	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5960/6612 (90%)	5665 (95%)	255 (4%)	40 (1%)	22 59

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	LYS
1	A	127	SER
1	A	128	GLY
1	A	364	GLU
1	B	125	LYS
1	B	127	SER
1	B	128	GLY
1	B	364	GLU
1	C	364	GLU
1	D	8	ALA
1	D	364	GLU
1	E	8	ALA
1	E	364	GLU
1	F	128	GLY
1	F	364	GLU
1	G	128	GLY
1	G	364	GLU
1	H	364	GLU
1	I	364	GLU
1	J	364	GLU
1	K	128	GLY
1	K	364	GLU
1	L	128	GLY
1	L	364	GLU
1	G	18	LEU
1	H	18	LEU
1	L	18	LEU
1	B	18	LEU
1	C	18	LEU
1	D	18	LEU
1	E	18	LEU
1	F	18	LEU
1	I	18	LEU
1	J	18	LEU
1	K	18	LEU
1	A	18	LEU
1	B	212	PRO

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Mol	Chain	Res	Type
1	A	212	PRO
1	F	212	PRO
1	G	212	PRO

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

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	18	LEU
1	A	19	HIS
1	A	96	GLU
1	A	106	ARG
1	A	129	THR
1	A	132	VAL

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Mol	Chain	Res	Type
1	A	256	LYS
1	A	326	CYS
1	A	336	LYS
1	A	367	LYS
1	A	393	GLN
1	A	398	LEU
1	A	409	THR
1	A	433	LYS
1	A	443	ARG
1	A	500	ARG
1	A	521	PHE
1	B	18	LEU
1	B	19	HIS
1	B	96	GLU
1	B	129	THR
1	B	132	VAL
1	B	136	LYS
1	B	326	CYS
1	B	336	LYS
1	B	398	LEU
1	B	409	THR
1	B	433	LYS
1	B	443	ARG
1	B	521	PHE
1	C	18	LEU
1	C	19	HIS
1	C	96	GLU
1	C	106	ARG
1	C	132	VAL
1	C	133	GLU
1	C	136	LYS
1	C	326	CYS
1	C	336	LYS
1	C	367	LYS
1	C	398	LEU
1	C	409	THR
1	C	433	LYS
1	C	443	ARG
1	C	500	ARG
1	C	521	PHE
1	D	18	LEU
1	D	19	HIS

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Mol	Chain	Res	Type
1	D	82	GLU
1	D	96	GLU
1	D	106	ARG
1	D	326	CYS
1	D	336	LYS
1	D	393	GLN
1	D	398	LEU
1	D	409	THR
1	D	433	LYS
1	D	443	ARG
1	D	521	PHE
1	E	18	LEU
1	E	19	HIS
1	E	96	GLU
1	E	106	ARG
1	E	154	GLU
1	E	188	LYS
1	E	263	LYS
1	E	326	CYS
1	E	336	LYS
1	E	337	LYS
1	E	367	LYS
1	E	398	LEU
1	E	409	THR
1	E	433	LYS
1	E	443	ARG
1	E	521	PHE
1	F	18	LEU
1	F	19	HIS
1	F	82	GLU
1	F	96	GLU
1	F	106	ARG
1	F	129	THR
1	F	132	VAL
1	F	326	CYS
1	F	336	LYS
1	F	337	LYS
1	F	393	GLN
1	F	398	LEU
1	F	409	THR
1	F	433	LYS
1	F	443	ARG

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Mol	Chain	Res	Type
1	F	521	PHE
1	G	18	LEU
1	G	19	HIS
1	G	96	GLU
1	G	106	ARG
1	G	129	THR
1	G	132	VAL
1	G	326	CYS
1	G	336	LYS
1	G	337	LYS
1	G	367	LYS
1	G	380	LEU
1	G	398	LEU
1	G	409	THR
1	G	433	LYS
1	G	521	PHE
1	H	18	LEU
1	H	19	HIS
1	H	96	GLU
1	H	106	ARG
1	H	132	VAL
1	H	154	GLU
1	H	256	LYS
1	H	326	CYS
1	H	336	LYS
1	H	398	LEU
1	H	409	THR
1	H	433	LYS
1	H	521	PHE
1	I	18	LEU
1	I	19	HIS
1	I	96	GLU
1	I	326	CYS
1	I	336	LYS
1	I	367	LYS
1	I	398	LEU
1	I	409	THR
1	I	433	LYS
1	I	443	ARG
1	I	521	PHE
1	J	18	LEU
1	J	19	HIS

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Mol	Chain	Res	Type
1	J	96	GLU
1	J	326	CYS
1	J	336	LYS
1	J	367	LYS
1	J	393	GLN
1	J	398	LEU
1	J	409	THR
1	J	433	LYS
1	J	436	ARG
1	J	443	ARG
1	J	500	ARG
1	J	521	PHE
1	K	12	PHE
1	K	18	LEU
1	K	19	HIS
1	K	96	GLU
1	K	106	ARG
1	K	129	THR
1	K	132	VAL
1	K	135	LYS
1	K	186	LYS
1	K	256	LYS
1	K	261	LYS
1	K	326	CYS
1	K	336	LYS
1	K	398	LEU
1	K	409	THR
1	K	433	LYS
1	K	443	ARG
1	K	500	ARG
1	L	18	LEU
1	L	19	HIS
1	L	96	GLU
1	L	129	THR
1	L	132	VAL
1	L	326	CYS
1	L	336	LYS
1	L	367	LYS
1	L	398	LEU
1	L	409	THR
1	L	433	LYS
1	L	521	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	ASN
1	B	210	ASN
1	B	318	ASN
1	C	318	ASN
1	D	210	ASN
1	D	318	ASN
1	E	318	ASN
1	F	70	ASN
1	F	318	ASN
1	G	318	ASN
1	H	19	HIS
1	H	318	ASN
1	J	14	GLN
1	K	318	ASN
1	L	318	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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
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

All (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
2	C	601	PO4	P-O2	-3.69	1.43	1.54
2	G	601	PO4	P-O4	3.63	1.65	1.54
2	L	601	PO4	P-O4	3.63	1.65	1.54
2	L	601	PO4	P-O3	-3.20	1.45	1.54
2	K	601	PO4	P-O3	-3.15	1.45	1.54
2	L	601	PO4	P-O2	-2.43	1.47	1.54
2	I	601	PO4	P-O3	-2.30	1.47	1.54
2	E	601	PO4	P-O2	-2.17	1.48	1.54
2	A	601	PO4	P-O4	2.14	1.61	1.54
2	G	601	PO4	P-O3	-2.01	1.48	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	PO4	O4-P-O1	-2.48	101.83	110.89

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	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

All (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
1	D	202	SER	5.2
1	D	142	ILE	5.0
1	D	152	CYS	4.9
1	D	140	LEU	4.9
1	D	203	LEU	4.6
1	H	187	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	159	LEU	4.5
1	D	184	GLN	4.5
1	D	161	TYR	4.4
1	D	164	ILE	4.4
1	D	156	ILE	4.3
1	D	153	ASP	4.3
1	G	18	LEU	4.3
1	D	179	GLY	4.3
1	D	201	GLY	4.2
1	D	216	VAL	4.1
1	E	204	GLY	4.1
1	D	154	GLU	3.9
1	D	183	LEU	3.7
1	K	128	GLY	3.6
1	A	20	ALA	3.6
1	C	9	GLY	3.3
1	C	16	GLN	3.1
1	H	164	ILE	3.1
1	C	8	ALA	3.1
1	D	200	GLY	3.1
1	H	503	PHE	3.0
1	F	128	GLY	2.9
1	D	187	GLN	2.9
1	H	165	CYS	2.9
1	D	168	VAL	2.9
1	F	191	ASP	2.9
1	J	107	PRO	2.9
1	D	210	ASN	2.9
1	C	164	ILE	2.8
1	G	17	GLN	2.8
1	E	203	LEU	2.8
1	J	55	SER	2.8
1	D	139	THR	2.8
1	D	174	ILE	2.8
1	D	173	LYS	2.8
1	J	474	CYS	2.8
1	K	531	PRO	2.7
1	A	21	ALA	2.7
1	H	531	PRO	2.7
1	A	22	MET	2.7
1	C	12	PHE	2.7
1	F	126	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	12	PHE	2.7
1	H	154	GLU	2.7
1	L	183	LEU	2.7
1	L	168	VAL	2.7
1	D	300	GLU	2.6
1	H	155	ASN	2.6
1	H	186	LYS	2.6
1	D	155	ASN	2.6
1	F	127	SER	2.6
1	A	326	CYS	2.5
1	D	178	ASP	2.5
1	J	44	ASN	2.5
1	D	223	GLU	2.5
1	J	108	VAL	2.5
1	E	202	SER	2.4
1	K	191	ASP	2.4
1	D	141	LYS	2.4
1	K	126	GLY	2.4
1	D	299	ILE	2.3
1	D	112	LEU	2.3
1	D	195	THR	2.3
1	L	126	GLY	2.3
1	I	112	LEU	2.3
1	H	144	LEU	2.3
1	L	174	ILE	2.3
1	J	314	ILE	2.2
1	D	199	ASN	2.2
1	D	204	GLY	2.2
1	H	152	CYS	2.2
1	D	426	GLY	2.2
1	I	241	PHE	2.2
1	D	205	SER	2.2
1	H	140	LEU	2.2
1	E	292	VAL	2.2
1	H	153	ASP	2.2
1	D	198	GLU	2.1
1	G	382	ALA	2.1
1	J	521	PHE	2.1
1	K	154	GLU	2.1
1	D	215	ALA	2.1
1	J	14	GLN	2.1
1	A	19	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	388	ALA	2.1
1	L	269	SER	2.1
1	J	357	ASP	2.1
1	E	142	ILE	2.1
1	J	64	MET	2.1
1	C	447	ARG	2.1
1	F	406	SER	2.0
1	D	209	VAL	2.0
1	I	360	MET	2.0
1	J	479	GLN	2.0
1	K	140	LEU	2.0
1	F	326	CYS	2.0
1	D	144	LEU	2.0
1	D	465	LEU	2.0
1	H	188	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.