



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2025 – 05:27 pm BST

PDB ID : 9R3I / pdb\_00009r3i  
Title : Structure of liver pyruvate kinase in complex with fluorescent probe 4c  
Authors : Bogucka, A.; Nilsson, O.; Grotli, M.; Hyvonen, M.  
Deposited on : 2025-05-05  
Resolution : 2.58 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](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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

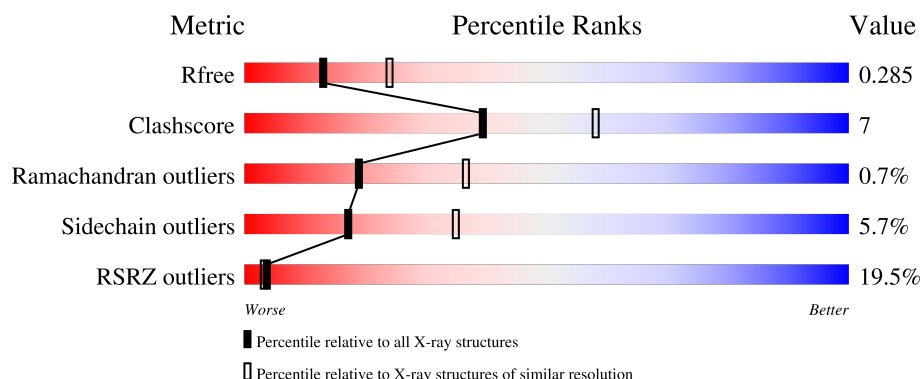
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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))
$R_{free}$	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	447	
1	B	447	
1	C	447	
1	D	447	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13329 atoms, of which 48 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 Isoform L-type of Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	1	0
			3185	1995	580	592	18			
1	B	420	Total	C	N	O	S	0	1	0
			3190	1998	583	591	18			
1	C	430	Total	C	N	O	S	0	2	0
			3269	2051	591	608	19			
1	D	426	Total	C	N	O	S	0	2	0
			3242	2035	589	600	18			

There are 416 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30613
A	0	SER	-	expression tag	UNP P30613
A	12	ASP	SER	conflict	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	SER	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	SER	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	ASP	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	ALA	deletion	UNP P30613
A	?	-	PHE	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	ALA	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	TRP	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	ASP	deletion	UNP P30613
A	?	-	TYR	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	TYR	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	ASP	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	SER	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	?	-	LYS	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	SER	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	LYS	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	ALA	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	130	GLY	VAL	linker	UNP P30613
A	131	SER	ASP	linker	UNP P30613
A	132	GLY	LEU	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P30613
B	12	ASP	SER	conflict	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	THR	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	SER	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	LYS	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	SER	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	THR	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	ASP	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	ALA	deletion	UNP P30613
B	?	-	PHE	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	THR	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613
B	?	-	ALA	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613
B	?	-	THR	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TRP	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	ASP	deletion	UNP P30613
B	?	-	TYR	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	TYR	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	ASP	deletion	UNP P30613
B	?	-	ASP	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	SER	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	?	-	LYS	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	THR	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	SER	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	LYS	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	ALA	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	130	GLY	VAL	linker	UNP P30613
B	131	SER	ASP	linker	UNP P30613
B	132	GLY	LEU	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	SER	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	LYS	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	ALA	deletion	UNP P30613
C	?	-	PHE	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	ALA	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	TRP	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	TYR	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	TYR	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	SER	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	?	-	LYS	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	SER	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	LYS	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	ALA	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	130	GLY	VAL	linker	UNP P30613
C	131	SER	ASP	linker	UNP P30613
C	132	GLY	LEU	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	12	ASP	SER	conflict	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	SER	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	LYS	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	SER	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	ASP	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	ALA	deletion	UNP P30613
D	?	-	PHE	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	ALA	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	TRP	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613

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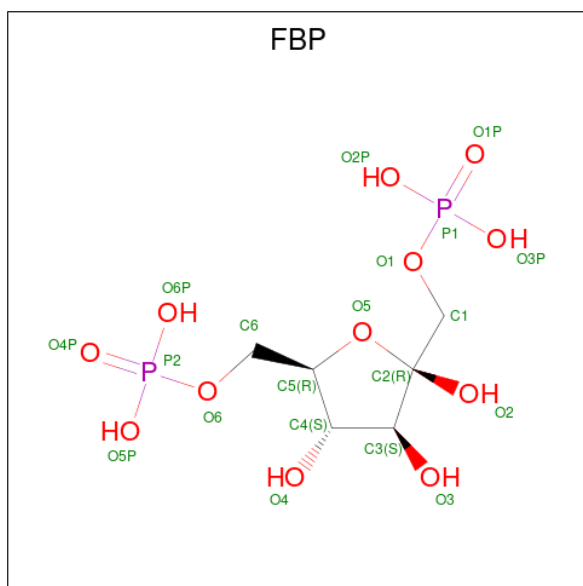
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	deletion	UNP P30613
D	?	-	TYR	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	TYR	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	ASP	deletion	UNP P30613
D	?	-	ASP	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	SER	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	?	-	LYS	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	VAL	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	SER	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	LYS	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	ALA	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	130	GLY	VAL	linker	UNP P30613
D	131	SER	ASP	linker	UNP P30613
D	132	GLY	LEU	linker	UNP P30613

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).



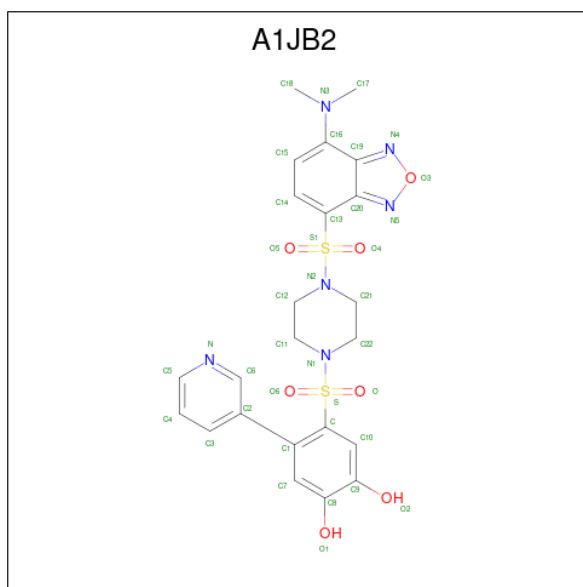
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		

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

- Molecule 3 is 4-[4-[[7-(dimethylamino)-2,1,3-benzoxadiazol-4-yl]sulfonyl]piperazin-1-yl]sulfonyl-5-pyridin-3-yl-benzene-1,2-diol (CCD ID: A1JB2) (formula: C<sub>23</sub>H<sub>24</sub>N<sub>6</sub>O<sub>7</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	S	24	0
			62	23	24	6	7	2		
3	D	1	Total	C	H	N	O	S	24	0
			62	23	24	6	7	2		

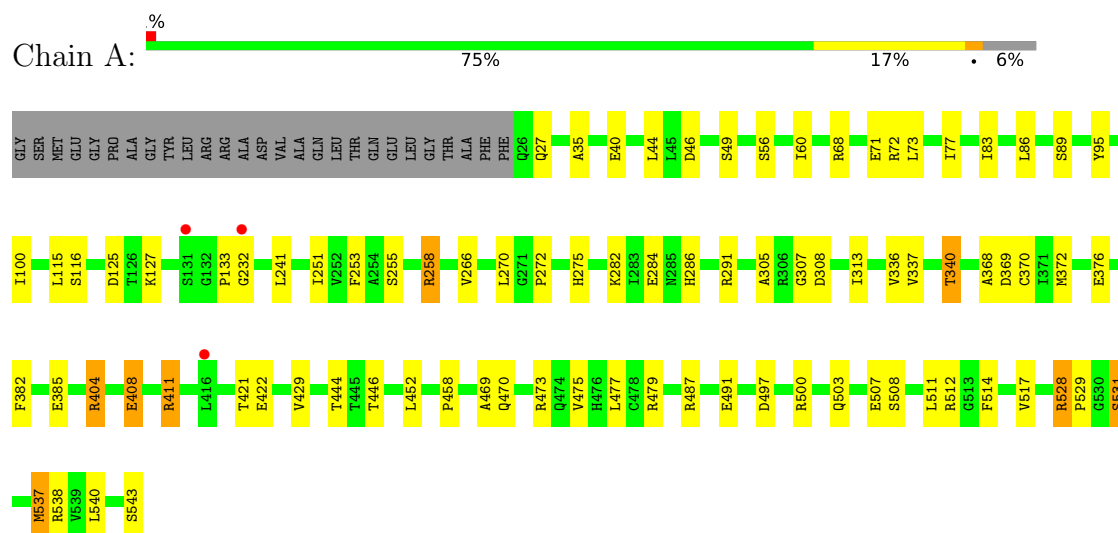
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	74	Total	O	0	0
			74	74		
4	C	30	Total	O	0	0
			30	30		
4	D	26	Total	O	0	0
			26	26		

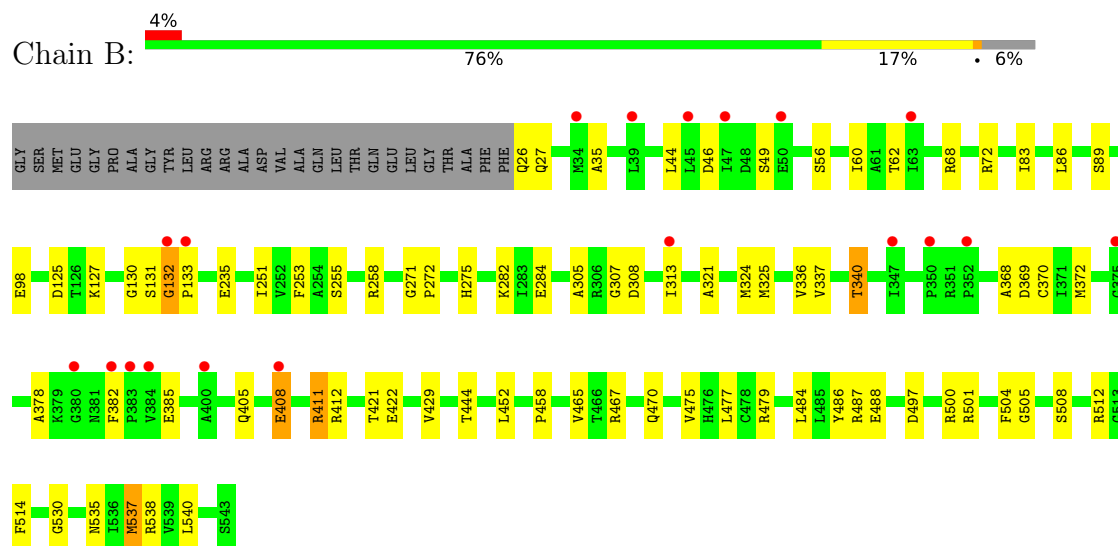
### 3 Residue-property plots [i](#)

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.

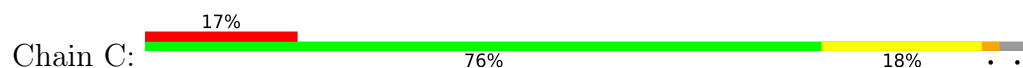
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

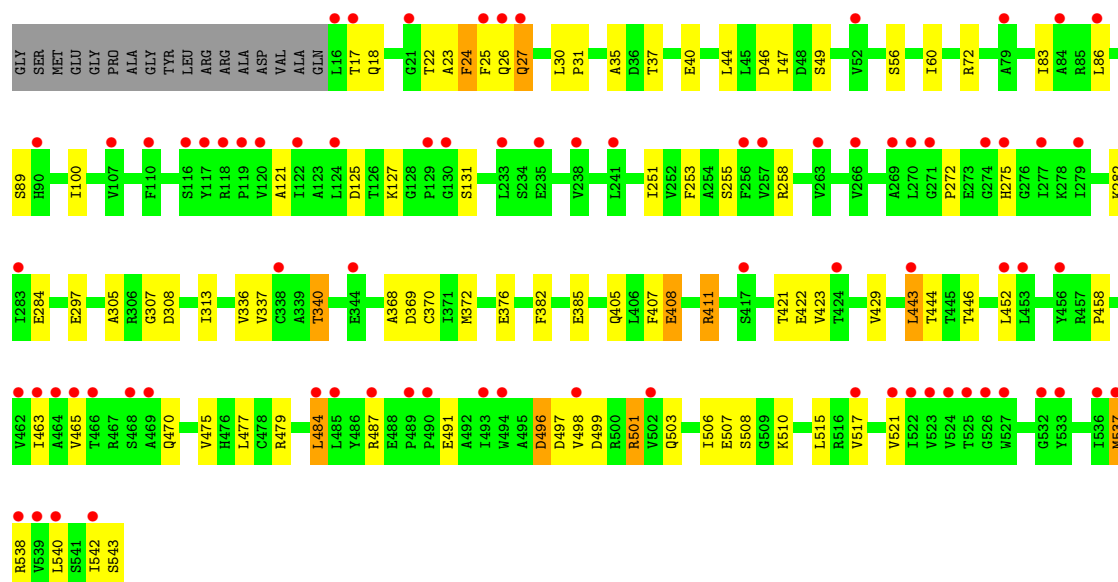


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

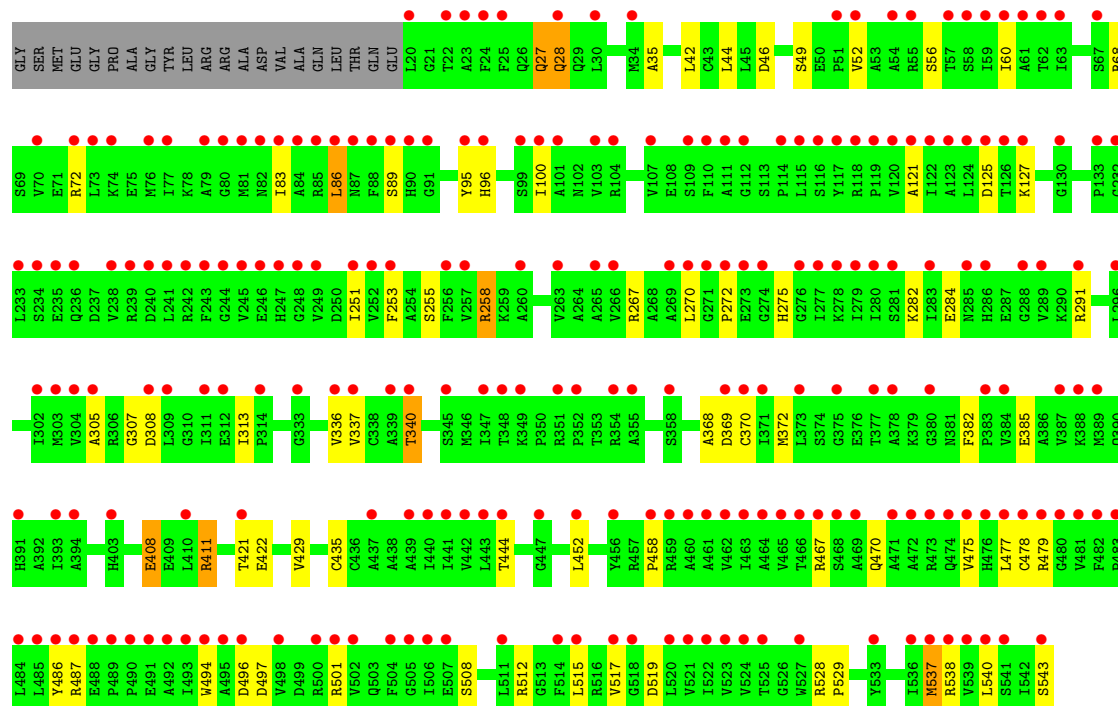
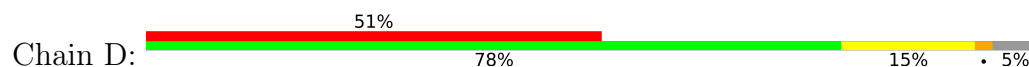


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR





• Molecule 1: Isoform L-type of Pyruvate kinase PKLR





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.12Å 113.03Å 140.30Å 90.00° 132.05° 90.00°	Depositor
Resolution (Å)	28.32 – 2.58 28.32 – 2.58	Depositor EDS
% Data completeness (in resolution range)	52.3 (28.32-2.58) 52.2 (28.32-2.58)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.57Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.241 , 0.291 0.237 , 0.285	Depositor DCC
$R_{free}$ test set	1710 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1JB2, FBP

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	0.72	0/3241	1.14	2/4384 (0.0%)
1	B	0.69	0/3246	1.13	2/4390 (0.0%)
1	C	0.66	0/3330	1.12	4/4504 (0.1%)
1	D	0.63	0/3303	1.09	2/4467 (0.0%)
All	All	0.68	0/13120	1.12	10/17745 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	496	ASP	CA-CB-CG	6.95	119.55	112.60
1	B	132	GLY	N-CA-C	6.07	124.72	112.34
1	A	514	PHE	CA-CB-CG	5.80	119.60	113.80
1	B	514	PHE	CA-CB-CG	5.63	119.43	113.80
1	D	496	ASP	CA-C-N	5.60	128.04	120.65
1	D	496	ASP	C-N-CA	5.60	128.04	120.65
1	C	501	ARG	CA-C-N	5.36	127.31	120.56
1	C	501	ARG	C-N-CA	5.36	127.31	120.56
1	A	71	GLU	CB-CG-CD	5.30	121.61	112.60
1	C	24	PHE	N-CA-C	-5.07	103.84	110.53

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3185	0	3238	46	0
1	B	3190	0	3246	40	0
1	C	3269	0	3315	48	0
1	D	3242	0	3296	47	0
2	A	20	0	10	1	0
2	B	20	0	10	3	0
2	C	20	0	10	2	0
2	D	20	0	10	4	0
3	C	38	24	0	2	0
3	D	38	24	0	1	0
4	A	109	0	0	0	0
4	B	74	0	0	0	0
4	C	30	0	0	0	0
4	D	26	0	0	1	0
All	All	13281	48	13135	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (173) 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:B:272:PRO:HA	1:B:275:HIS:CE1	2.03	0.94
1:D:60:ILE:HB	1:D:372:MET:HG3	1.52	0.91
1:B:60:ILE:HB	1:B:372:MET:HG3	1.53	0.88
1:A:60:ILE:HB	1:A:372:MET:HG3	1.56	0.86
1:C:60:ILE:HB	1:C:372:MET:HG3	1.56	0.86
1:C:537[B]:MET:HE3	1:D:537:MET:HG2	1.73	0.69
1:D:444:THR:HA	2:D:601:FBP:H61	1.77	0.67
1:A:444:THR:HA	2:A:601:FBP:H61	1.77	0.66
1:B:508:SER:O	1:B:512:ARG:HG3	1.94	0.66
1:B:501:ARG:NH1	2:B:601:FBP:O2P	2.31	0.62
1:D:501:ARG:NH2	2:D:601:FBP:O3P	2.32	0.61
1:B:465:VAL:HG22	1:B:484:LEU:HD12	1.82	0.60
1:A:89:SER:HA	1:A:127:LYS:HG3	1.83	0.60
1:C:517:VAL:HG13	1:C:543:SER:HB3	1.82	0.60
1:A:284:GLU:HG2	1:A:305:ALA:HB3	1.82	0.60
1:B:284:GLU:HG2	1:B:305:ALA:HB3	1.84	0.60
1:C:35:ALA:HB1	1:C:40:GLU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLU:HG2	1:C:305:ALA:HB3	1.82	0.60
1:A:86:LEU:HD21	1:A:100:ILE:HG13	1.84	0.59
1:D:517:VAL:HG13	1:D:543:SER:HB3	1.84	0.58
1:A:284:GLU:OE2	1:A:308:ASP:OD2	2.21	0.58
1:A:115:LEU:HB3	1:A:511:LEU:HD21	1.86	0.58
1:D:284:GLU:HG2	1:D:305:ALA:HB3	1.84	0.58
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.85	0.57
1:D:497:ASP:O	1:D:501:ARG:HG3	2.04	0.57
1:B:284:GLU:OE2	1:B:308:ASP:OD2	2.22	0.57
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.87	0.57
1:D:86:LEU:HD12	1:D:96:HIS:ND1	2.20	0.57
1:C:503:GLN:O	1:C:507:GLU:HG2	2.05	0.57
1:B:132:GLY:H	1:B:133:PRO:HD2	1.70	0.56
1:C:284:GLU:OE2	1:C:308:ASP:OD2	2.24	0.56
1:D:382:PHE:HB3	1:D:385:GLU:HB2	1.87	0.56
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.86	0.55
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.87	0.55
1:D:89:SER:HA	1:D:127:LYS:HG3	1.88	0.55
1:A:404:ARG:HH11	1:B:412:ARG:NH1	2.05	0.55
1:B:89:SER:HA	1:B:127:LYS:HG3	1.89	0.55
1:A:73:LEU:O	1:A:77:ILE:HG13	2.06	0.55
1:D:467:ARG:HH21	1:D:486:TYR:HE2	1.54	0.54
1:A:68:ARG:NH2	1:A:95:TYR:O	2.39	0.54
1:D:284:GLU:OE2	1:D:308:ASP:OD2	2.26	0.54
1:A:537:MET:HG3	1:B:537:MET:HG3	1.90	0.54
1:C:515:LEU:HD22	1:C:542:ILE:HG13	1.88	0.53
1:C:89:SER:HA	1:C:127:LYS:HG3	1.88	0.53
1:C:272:PRO:HA	1:C:275:HIS:NE2	2.23	0.53
1:A:35:ALA:HB1	1:A:40:GLU:HB3	1.90	0.53
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.23	0.53
1:D:272:PRO:HA	1:D:275:HIS:NE2	2.24	0.52
1:C:251:ILE:HG12	1:C:477:LEU:HD11	1.91	0.52
1:B:486:TYR:CZ	1:B:488:GLU:HB2	2.44	0.52
1:D:251:ILE:HG12	1:D:477:LEU:HD11	1.91	0.52
1:A:422:GLU:HG2	1:A:452:LEU:HD13	1.92	0.52
1:D:337:VAL:HG22	1:D:370:CYS:HB2	1.92	0.52
1:B:251:ILE:HG12	1:B:477:LEU:HD11	1.91	0.52
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.92	0.52
1:C:422:GLU:HG2	1:C:452:LEU:HD13	1.92	0.51
1:A:429:VAL:HG13	1:A:458:PRO:HB3	1.92	0.51
1:B:68:ARG:HH22	1:B:98:GLU:HB3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:SER:HB3	1:A:511:LEU:HD11	1.93	0.51
1:D:429:VAL:HG13	1:D:458:PRO:HB3	1.93	0.51
1:B:444:THR:HA	2:B:601:FBP:H61	1.92	0.51
1:D:422:GLU:HG2	1:D:452:LEU:HD13	1.93	0.51
1:A:251:ILE:HG12	1:A:477:LEU:HD11	1.92	0.50
1:C:405:GLN:HB3	3:C:601:A1JB2:O	2.10	0.50
1:A:115:LEU:CB	1:A:511:LEU:HD21	2.42	0.50
1:C:491:GLU:HB2	1:C:497:ASP:HB2	1.94	0.50
1:D:267:ARG:HA	1:D:270:LEU:HD12	1.94	0.50
1:C:37:THR:OG1	1:C:40:GLU:HB2	2.12	0.50
1:C:307:GLY:CA	1:C:340:THR:HG21	2.42	0.50
1:C:337:VAL:HG22	1:C:370:CYS:HB2	1.93	0.49
1:D:307:GLY:CA	1:D:340:THR:HG21	2.42	0.49
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.94	0.49
1:B:486:TYR:OH	1:B:500:ARG:HG3	2.12	0.49
1:B:255:SER:HA	1:B:282:LYS:HD3	1.95	0.49
1:B:307:GLY:CA	1:B:340:THR:HG21	2.42	0.48
1:A:115:LEU:HB3	1:A:511:LEU:CD2	2.43	0.48
1:D:494:TRP:NE1	1:D:529:PRO:HB3	2.29	0.48
1:D:27:GLN:HA	4:D:711:HOH:O	2.13	0.48
1:C:125:ASP:HA	1:C:253:PHE:HB2	1.96	0.47
1:D:68:ARG:NH1	1:D:95:TYR:CE1	2.83	0.47
1:A:255:SER:HA	1:A:282:LYS:HD3	1.96	0.47
1:D:255:SER:HA	1:D:282:LYS:HD3	1.96	0.47
1:D:508:SER:O	1:D:512:ARG:HG3	2.15	0.47
1:A:307:GLY:CA	1:A:340:THR:HG21	2.45	0.47
1:A:408:GLU:HG2	1:A:411:ARG:HH21	1.79	0.47
1:B:429:VAL:HG13	1:B:458:PRO:HB3	1.96	0.47
1:A:241:LEU:HD22	1:A:270:LEU:HD21	1.96	0.47
1:C:255:SER:HA	1:C:282:LYS:HD3	1.96	0.47
1:A:286:HIS:CD2	1:C:47:ILE:HD12	2.50	0.47
1:A:508:SER:O	1:A:512:ARG:HG3	2.14	0.46
1:B:369:ASP:HA	1:B:479:ARG:HB2	1.98	0.46
1:B:405:GLN:HB3	3:D:602:A1JB2:O	2.15	0.46
1:C:498:VAL:HG22	1:C:501:ARG:HH21	1.80	0.46
1:C:429:VAL:HG13	1:C:458:PRO:HB3	1.97	0.46
1:C:24:PHE:O	1:C:25:PHE:HB2	2.16	0.46
1:D:369:ASP:HA	1:D:479:ARG:HB2	1.98	0.46
1:A:125:ASP:HA	1:A:253:PHE:HB2	1.97	0.46
1:A:369:ASP:HA	1:A:479:ARG:HB2	1.97	0.46
1:C:408:GLU:HG2	1:C:411:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.97	0.45
1:B:272:PRO:HA	1:B:275:HIS:NE2	2.29	0.45
1:D:125:ASP:HA	1:D:253:PHE:HB2	1.98	0.45
1:A:266:VAL:O	1:A:270:LEU:HG	2.16	0.45
1:C:369:ASP:HA	1:C:479:ARG:HB2	1.98	0.45
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.98	0.45
1:D:96:HIS:O	1:D:100:ILE:HG13	2.17	0.45
1:C:503:GLN:HA	1:C:506:ILE:HD12	1.99	0.45
1:A:286:HIS:CD2	1:C:47:ILE:CD1	3.00	0.45
1:B:125:ASP:HA	1:B:253:PHE:HB2	1.98	0.45
1:C:443:LEU:HD12	1:C:465:VAL:HB	1.99	0.44
1:D:467:ARG:NH2	1:D:486:TYR:HE2	2.15	0.44
1:C:23:ALA:O	1:C:27:GLN:HG3	2.18	0.44
1:C:510:LYS:NZ	1:C:543:SER:HB2	2.32	0.44
1:C:537[A]:MET:HG3	1:D:537:MET:HG3	1.99	0.44
1:D:68:ARG:NH1	1:D:95:TYR:CD1	2.85	0.44
1:C:272:PRO:HA	1:C:275:HIS:CE1	2.53	0.44
1:A:446:THR:HG23	1:A:531:SER:OG	2.18	0.44
1:D:408:GLU:HG2	1:D:411:ARG:HH21	1.83	0.44
1:C:46:ASP:HB3	1:C:49:SER:HB2	1.99	0.44
1:C:336:VAL:HG13	1:C:368:ALA:HA	1.99	0.44
1:B:46:ASP:HB3	1:B:49:SER:HB2	2.01	0.43
1:C:60:ILE:HG12	1:C:83:ILE:HB	2.01	0.43
1:A:528:ARG:HD3	1:A:529:PRO:O	2.17	0.43
1:C:515:LEU:HD21	1:C:521:VAL:CG1	2.48	0.43
1:D:28:GLN:HG2	1:D:52:VAL:HG22	1.99	0.43
1:D:60:ILE:HG12	1:D:83:ILE:HB	2.00	0.43
1:D:272:PRO:HA	1:D:275:HIS:CE1	2.54	0.43
1:C:421:THR:HG22	1:C:452:LEU:HD12	2.00	0.43
1:B:408:GLU:HG2	1:B:411:ARG:HH21	1.84	0.43
1:C:463:ILE:HG23	1:C:484:LEU:HD21	2.01	0.43
1:D:501:ARG:HH22	2:D:601:FBP:P1	2.42	0.43
1:B:467:ARG:HH22	1:B:497:ASP:CG	2.26	0.43
1:A:336:VAL:HG13	1:A:368:ALA:HA	2.00	0.43
1:D:444:THR:OG1	2:D:601:FBP:O4P	2.29	0.42
1:A:60:ILE:HG12	1:A:83:ILE:HB	2.00	0.42
1:A:491:GLU:HB2	1:A:497:ASP:HB2	2.01	0.42
1:B:56:SER:HB3	1:B:479:ARG:HG2	2.00	0.42
1:A:35:ALA:HB2	1:A:44:LEU:HD12	2.02	0.42
1:C:446:THR:OG1	2:C:602:FBP:O5P	2.30	0.42
1:D:46:ASP:HB3	1:D:49:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:LEU:CD1	1:B:505:GLY:HA2	2.49	0.42
1:C:423:VAL:HG21	1:D:435:CYS:HB3	2.02	0.42
1:A:46:ASP:HB3	1:A:49:SER:HB2	2.02	0.42
1:C:56:SER:HB3	1:C:479:ARG:HG2	2.02	0.42
1:B:35:ALA:HB2	1:B:44:LEU:HD12	2.02	0.41
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.55	0.41
1:A:469:ALA:O	1:A:473:ARG:HG3	2.20	0.41
1:B:60:ILE:HG12	1:B:83:ILE:HB	2.02	0.41
1:C:444:THR:OG1	2:C:602:FBP:O4P	2.27	0.41
1:A:56:SER:HB3	1:A:479:ARG:HG2	2.02	0.41
1:B:324:MET:HA	1:D:42:LEU:O	2.20	0.41
1:A:503:GLN:O	1:A:507:GLU:HG2	2.20	0.41
1:B:336:VAL:HG13	1:B:368:ALA:HA	2.02	0.41
3:C:601:A1JB2:N4	3:C:601:A1JB2:C17	2.83	0.41
1:B:501:ARG:O	1:B:504:PHE:HB3	2.21	0.41
1:D:56:SER:HB3	1:D:479:ARG:HG2	2.02	0.41
1:A:258:ARG:O	1:A:291:ARG:HD3	2.21	0.41
1:D:35:ALA:HB2	1:D:44:LEU:HD12	2.03	0.41
1:D:258:ARG:O	1:D:291:ARG:HD3	2.21	0.41
1:B:372:MET:HE2	1:B:372:MET:HB3	1.97	0.41
1:C:30:LEU:N	1:C:31:PRO:HD2	2.35	0.41
1:C:83:ILE:HG12	1:C:121:ALA:HB3	2.03	0.41
1:C:407:PHE:CE2	1:C:411:ARG:NH1	2.89	0.41
1:D:336:VAL:HG13	1:D:368:ALA:HA	2.01	0.41
1:D:467:ARG:NH2	1:D:486:TYR:CE2	2.89	0.41
1:B:321:ALA:O	1:B:325:MET:HG3	2.21	0.41
1:C:35:ALA:HB2	1:C:44:LEU:HD12	2.02	0.40
1:A:286:HIS:HD2	1:C:47:ILE:HD12	1.85	0.40
1:B:421:THR:HG22	1:B:452:LEU:HD12	2.02	0.40
1:D:83:ILE:HG12	1:D:121:ALA:HB3	2.03	0.40
1:B:62:THR:HG22	1:B:378:ALA:HB2	2.04	0.40
1:B:530:GLY:O	2:B:601:FBP:O4	2.37	0.40
1:D:267:ARG:HD3	1:D:270:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

## 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	419/447 (94%)	406 (97%)	10 (2%)	3 (1%)	19	36
1	B	419/447 (94%)	407 (97%)	7 (2%)	5 (1%)	11	23
1	C	430/447 (96%)	420 (98%)	9 (2%)	1 (0%)	44	64
1	D	426/447 (95%)	415 (97%)	9 (2%)	2 (0%)	25	45
All	All	1694/1788 (95%)	1648 (97%)	35 (2%)	11 (1%)	19	41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	GLY
1	A	133	PRO
1	B	131	SER
1	B	130	GLY
1	A	340	THR
1	B	340	THR
1	B	535	ASN
1	C	340	THR
1	D	340	THR
1	D	519	ASP
1	B	271	GLY

### 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	334/352 (95%)	317 (95%)	17 (5%)	20	40
1	B	334/352 (95%)	318 (95%)	16 (5%)	21	42
1	C	342/352 (97%)	315 (92%)	27 (8%)	10	20
1	D	339/352 (96%)	322 (95%)	17 (5%)	20	41
All	All	1349/1408 (96%)	1272 (94%)	77 (6%)	17	35

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	72	ARG
1	A	258	ARG
1	A	313	ILE
1	A	376	GLU
1	A	404	ARG
1	A	408	GLU
1	A	411	ARG
1	A	470	GLN
1	A	475	VAL
1	A	487	ARG
1	A	500	ARG
1	A	528	ARG
1	A	531	SER
1	A	537	MET
1	A	538	ARG
1	A	540	LEU
1	B	26	GLN
1	B	27	GLN
1	B	72	ARG
1	B	86	LEU
1	B	235	GLU
1	B	258	ARG
1	B	313	ILE
1	B	408	GLU
1	B	411	ARG
1	B	422	GLU
1	B	470	GLN
1	B	475	VAL
1	B	487	ARG
1	B	537	MET
1	B	538	ARG
1	B	540	LEU

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Mol	Chain	Res	Type
1	C	17	THR
1	C	18	GLN
1	C	22	THR
1	C	26	GLN
1	C	27	GLN
1	C	72	ARG
1	C	86	LEU
1	C	100	ILE
1	C	131	SER
1	C	258	ARG
1	C	297	GLU
1	C	313	ILE
1	C	376	GLU
1	C	408	GLU
1	C	411	ARG
1	C	443	LEU
1	C	470	GLN
1	C	475	VAL
1	C	484	LEU
1	C	487	ARG
1	C	496	ASP
1	C	499	ASP
1	C	508	SER
1	C	537[A]	MET
1	C	537[B]	MET
1	C	538	ARG
1	C	540	LEU
1	D	27	GLN
1	D	28	GLN
1	D	72	ARG
1	D	86	LEU
1	D	258	ARG
1	D	313	ILE
1	D	408	GLU
1	D	411	ARG
1	D	470	GLN
1	D	475	VAL
1	D	478	CYS
1	D	487	ARG
1	D	515	LEU
1	D	528	ARG
1	D	537	MET

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Mol	Chain	Res	Type
1	D	538	ARG
1	D	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	286	HIS
1	A	403	HIS
1	A	503	GLN
1	B	26	GLN
1	B	27	GLN
1	B	403	HIS
1	B	535	ASN
1	C	18	GLN
1	C	27	GLN
1	C	403	HIS
1	D	26	GLN
1	D	403	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](#)

6 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	FBP	D	601	-	18,20,20	0.39	0	23,32,32	0.82	1 (4%)
2	FBP	B	601	-	18,20,20	0.44	0	23,32,32	1.01	1 (4%)
3	A1JB2	D	602	-	40,42,42	0.57	1 (2%)	54,64,64	0.65	1 (1%)
2	FBP	C	602	-	18,20,20	0.42	0	23,32,32	0.93	1 (4%)
2	FBP	A	601	-	18,20,20	0.55	0	23,32,32	0.98	2 (8%)
3	A1JB2	C	601	-	40,42,42	0.62	1 (2%)	54,64,64	0.65	1 (1%)

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
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	601	-	-	5/13/32/32	0/1/1/1
3	A1JB2	D	602	-	-	14/32/42/42	0/5/5/5
2	FBP	C	602	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	11/13/32/32	0/1/1/1
3	A1JB2	C	601	-	-	16/32/42/42	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	A1JB2	C13-C20	-2.88	1.40	1.42
3	D	602	A1JB2	C13-C20	-2.74	1.40	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	FBP	P1-O1-C1	3.30	127.38	118.30
2	A	601	FBP	P1-O1-C1	2.88	126.22	118.30
2	B	601	FBP	P1-O1-C1	2.85	126.15	118.30
2	A	601	FBP	O1-P1-O1P	2.72	114.10	106.47
2	D	601	FBP	P1-O1-C1	2.51	125.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	A1JB2	C17-N3-C16	2.25	120.81	114.12
3	C	601	A1JB2	C17-N3-C16	2.23	120.76	114.12

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C1-O1-P1-O1P
2	A	601	FBP	C1-O1-P1-O2P
2	A	601	FBP	C1-O1-P1-O3P
2	A	601	FBP	O1-C1-C2-C3
2	A	601	FBP	O1-C1-C2-O5
2	A	601	FBP	C6-O6-P2-O4P
2	A	601	FBP	C6-O6-P2-O5P
2	A	601	FBP	C6-O6-P2-O6P
2	B	601	FBP	C1-O1-P1-O1P
2	B	601	FBP	C1-O1-P1-O2P
2	B	601	FBP	C1-O1-P1-O3P
2	B	601	FBP	C4-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	602	FBP	C4-C5-C6-O6
3	D	602	A1JB2	C12-N2-S1-O5
3	C	601	A1JB2	C11-N1-S-O6
3	C	601	A1JB2	C11-N1-S-C
3	C	601	A1JB2	C12-N2-S1-O5
3	D	602	A1JB2	C11-N1-S-O6
3	D	602	A1JB2	C11-N1-S-C
3	C	601	A1JB2	C12-N2-S1-C13
3	D	602	A1JB2	C12-N2-S1-C13
3	D	602	A1JB2	C11-N1-S-O
2	A	601	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
3	C	601	A1JB2	C11-N1-S-O
2	C	602	FBP	O5-C5-C6-O6
3	C	601	A1JB2	C19-C16-N3-C17
3	C	601	A1JB2	C12-N2-S1-O4
3	C	601	A1JB2	C15-C16-N3-C17
3	D	602	A1JB2	C12-N2-S1-O4
3	D	602	A1JB2	C22-N1-S-O
3	C	601	A1JB2	C22-N1-S-O
3	D	602	A1JB2	C22-N1-S-O6
3	C	601	A1JB2	C22-N1-S-O6

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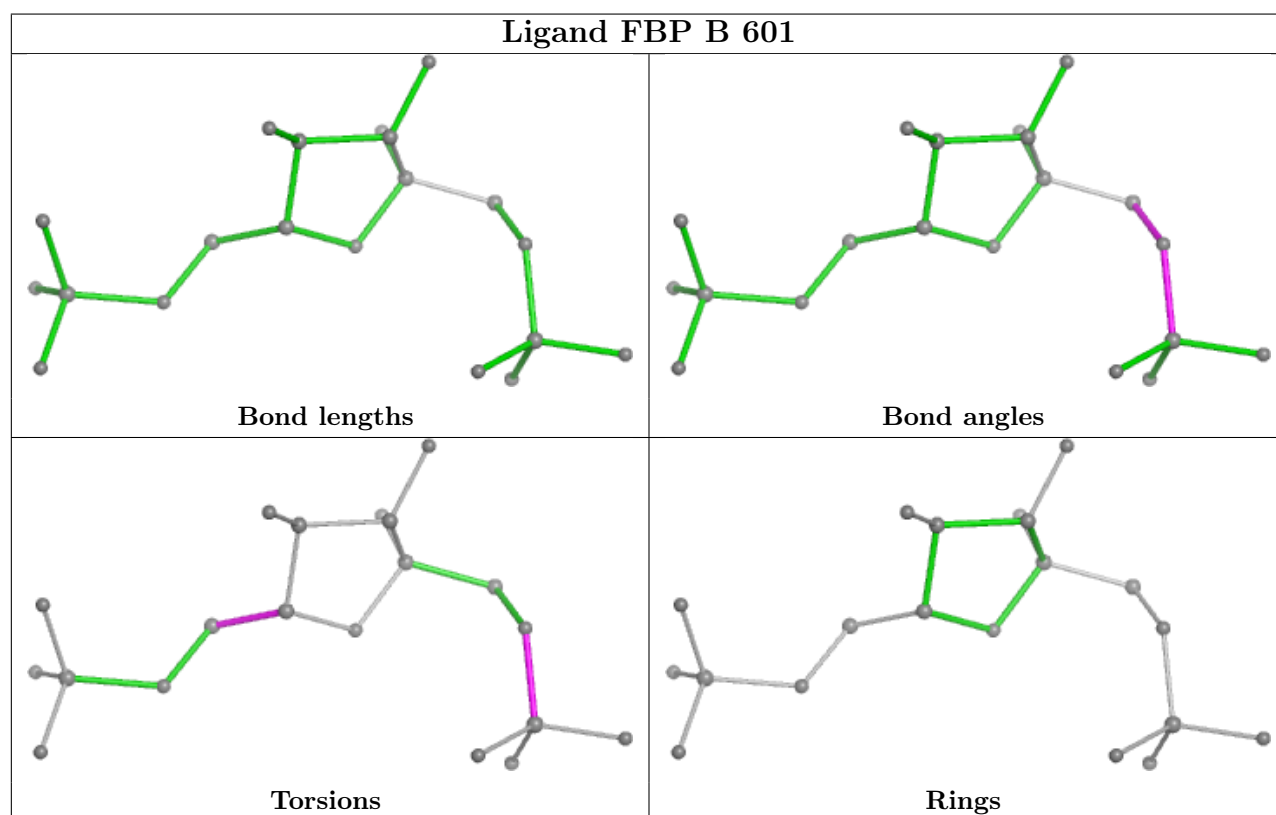
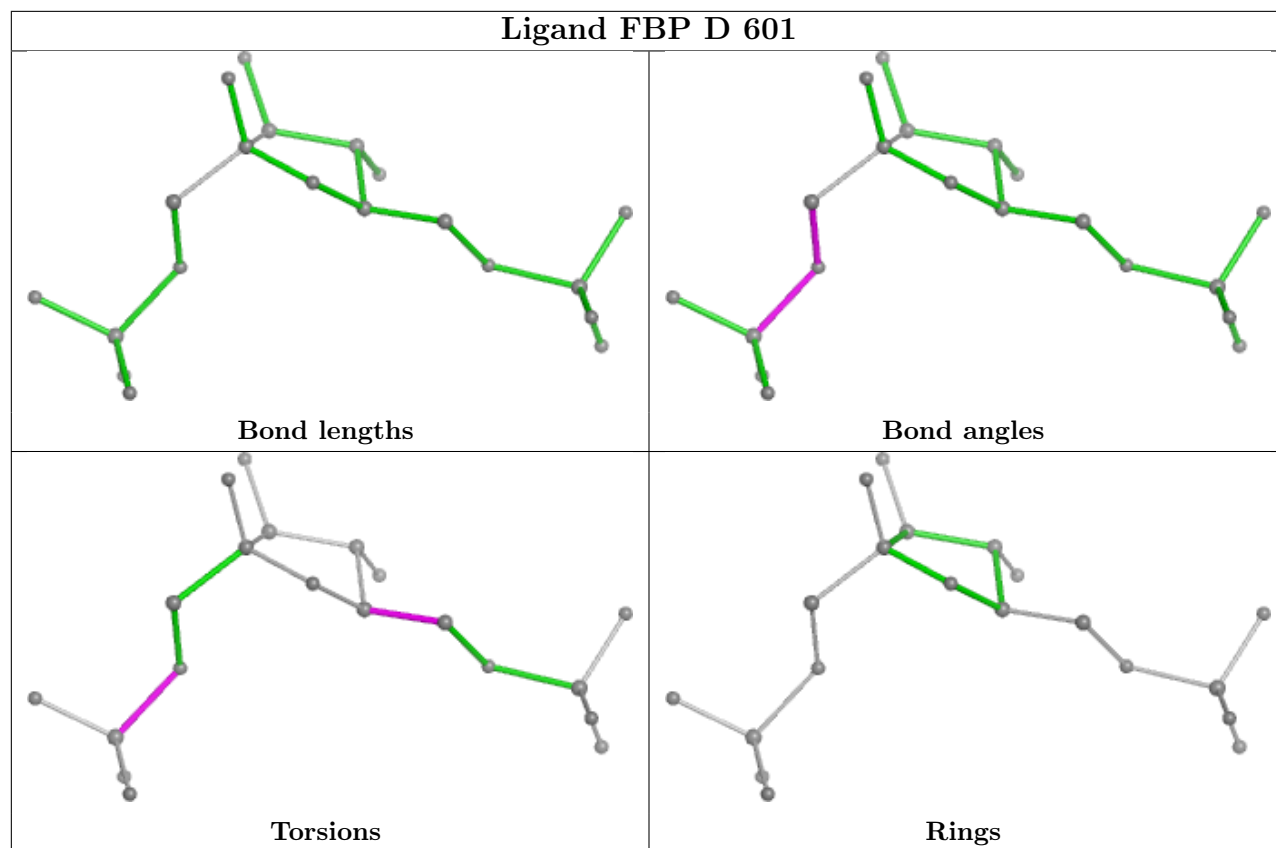
Mol	Chain	Res	Type	Atoms
3	C	601	A1JB2	C20-C13-S1-O4
3	D	602	A1JB2	C20-C13-S1-O4
3	D	602	A1JB2	C22-N1-S-C
3	C	601	A1JB2	C21-N2-S1-O4
3	D	602	A1JB2	C21-N2-S1-O4
3	C	601	A1JB2	C21-N2-S1-O5
3	D	602	A1JB2	C21-N2-S1-O5
2	A	601	FBP	O1-C1-C2-O2
3	C	601	A1JB2	C22-N1-S-C
3	D	602	A1JB2	C-C1-C2-C3
2	D	601	FBP	O5-C5-C6-O6
3	C	601	A1JB2	C7-C1-C2-C3
3	D	602	A1JB2	C7-C1-C2-C3
3	C	601	A1JB2	C-C1-C2-C3
2	D	601	FBP	C1-O1-P1-O3P

There are no ring outliers.

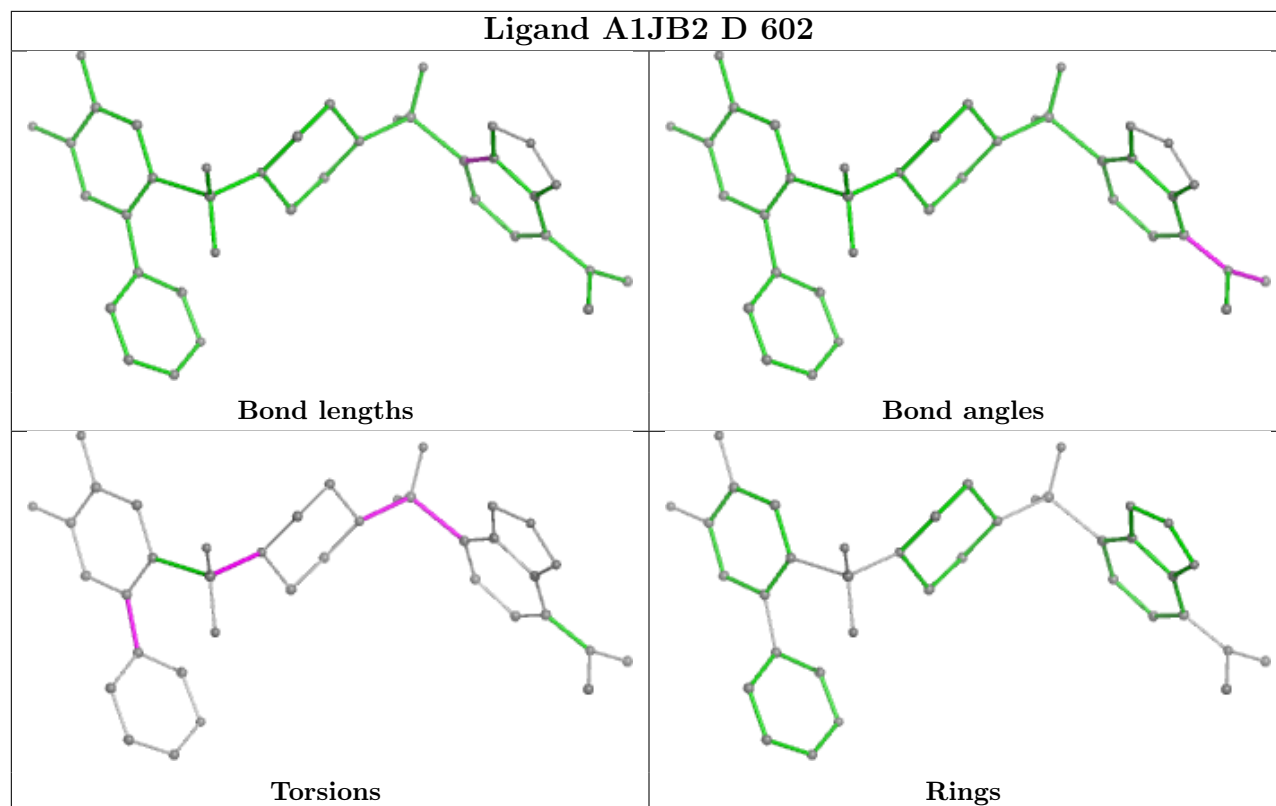
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	FBP	4	0
2	B	601	FBP	3	0
3	D	602	A1JB2	1	0
2	C	602	FBP	2	0
2	A	601	FBP	1	0
3	C	601	A1JB2	2	0

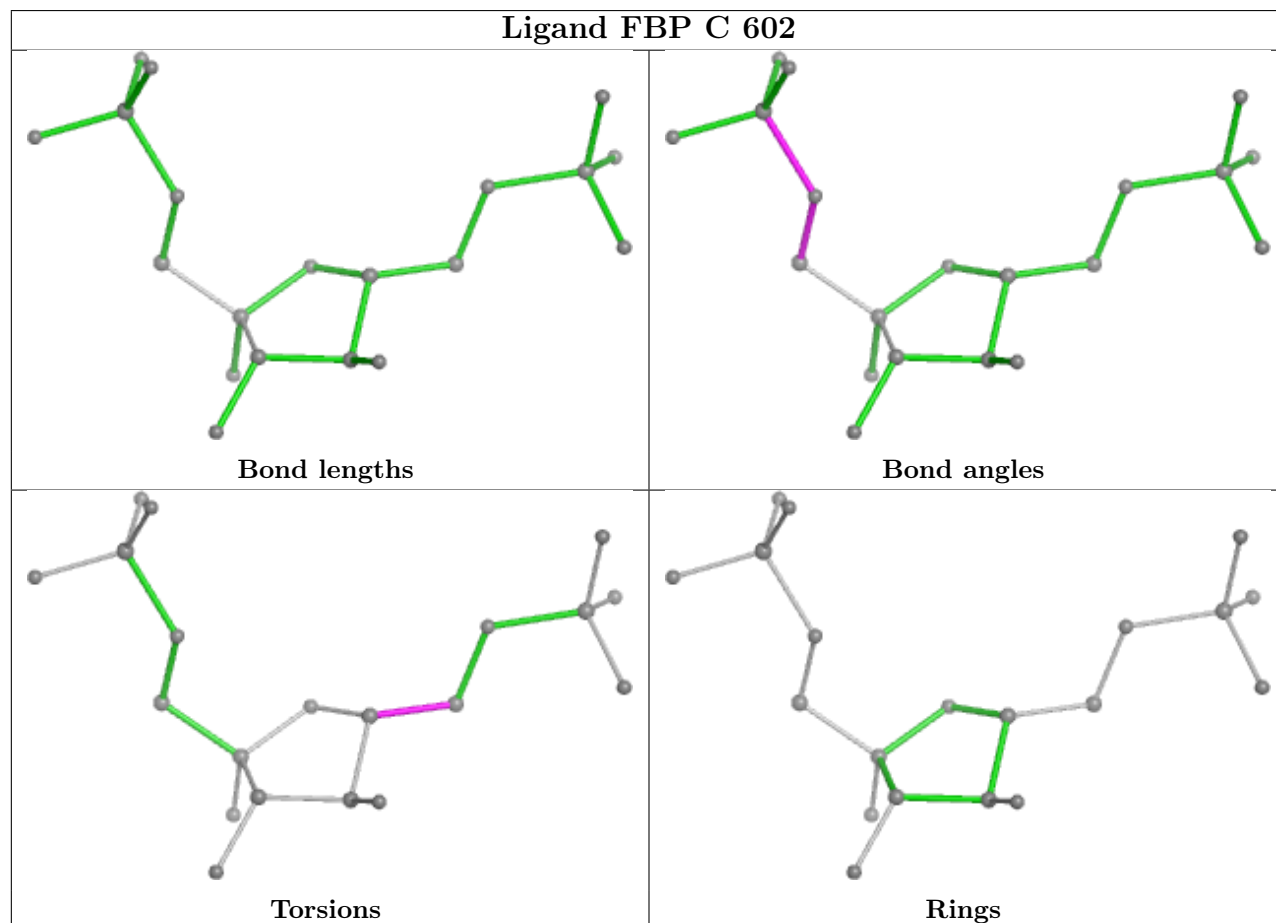
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



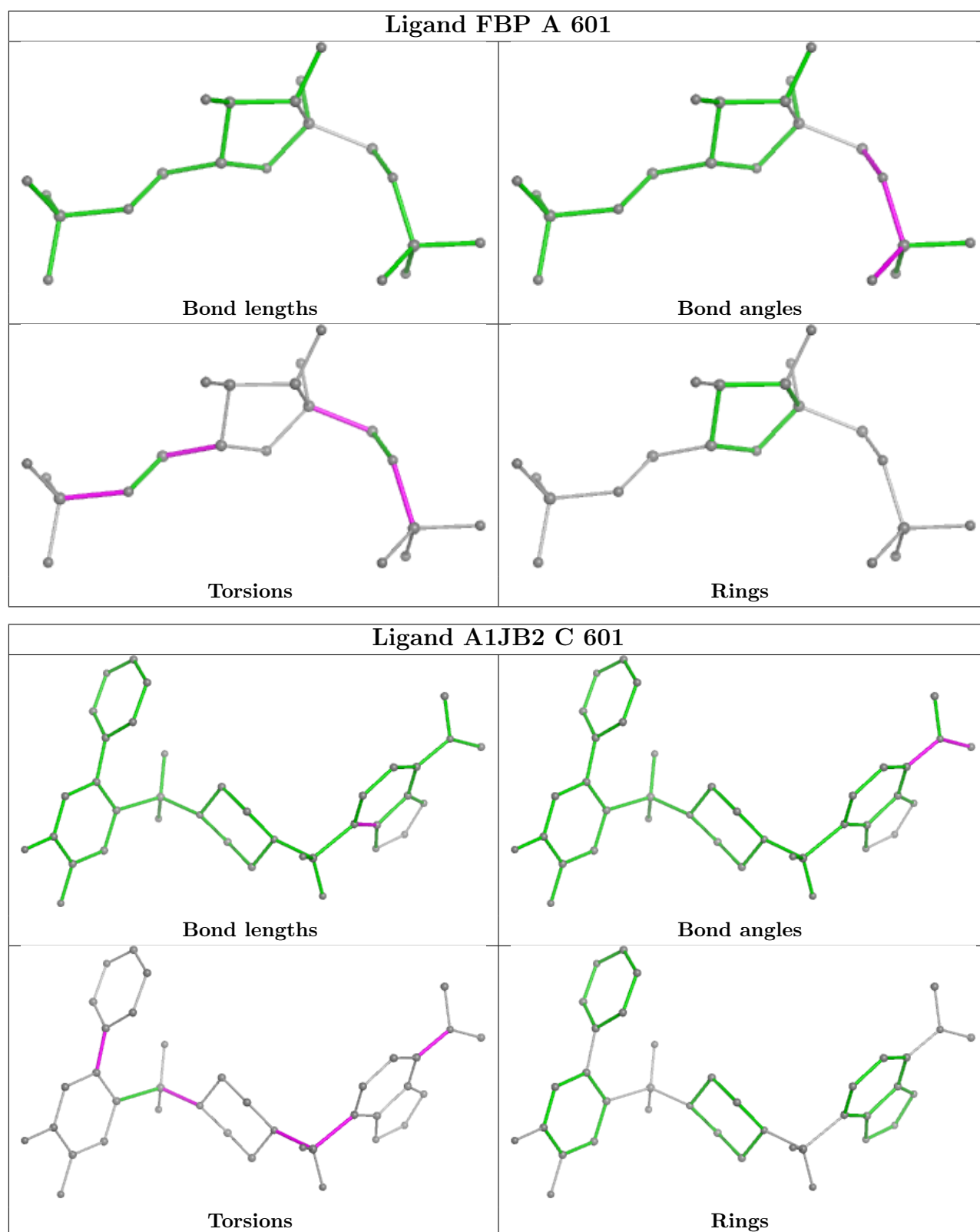
## Ligand A1JB2 D 602



## Ligand FBP C 602







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	420/447 (93%)	-0.10	3 (0%) 84 82	9, 25, 53, 72	1 (0%)
1	B	420/447 (93%)	0.39	19 (4%) 39 34	9, 39, 68, 81	1 (0%)
1	C	430/447 (96%)	1.07	78 (18%) 4 4	18, 60, 89, 107	2 (0%)
1	D	426/447 (95%)	2.24	230 (53%) 0 0	34, 86, 120, 133	2 (0%)
All	All	1696/1788 (94%)	0.91	330 (19%) 4 3	9, 50, 105, 133	6 (0%)

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	LEU	7.3
1	D	241	LEU	6.3
1	D	249	VAL	5.7
1	D	485	LEU	5.6
1	D	120	VAL	5.3
1	D	122	ILE	5.3
1	D	538	ARG	5.2
1	D	484	LEU	4.9
1	D	482	PHE	4.9
1	D	110	PHE	4.8
1	D	114	PRO	4.8
1	D	79	ALA	4.8
1	D	461	ALA	4.8
1	D	77	ILE	4.8
1	C	16	LEU	4.7
1	C	233	LEU	4.7
1	D	465	VAL	4.7
1	D	251	ILE	4.7
1	D	281	SER	4.5
1	D	523	VAL	4.4
1	D	121	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	233	LEU	4.4
1	D	283	ILE	4.3
1	C	266	VAL	4.3
1	D	478	CYS	4.3
1	D	515	LEU	4.3
1	D	514	PHE	4.2
1	D	245	VAL	4.2
1	D	257	VAL	4.2
1	D	80	GLY	4.2
1	D	378	ALA	4.1
1	D	486	TYR	4.1
1	D	289	VAL	4.0
1	D	471	ALA	4.0
1	D	304	VAL	4.0
1	D	475	VAL	4.0
1	D	521	VAL	4.0
1	D	115	LEU	4.0
1	D	541	SER	4.0
1	D	502	VAL	4.0
1	D	280	ILE	3.9
1	D	462	VAL	3.9
1	D	100	ILE	3.9
1	D	539	VAL	3.9
1	D	20	LEU	3.9
1	D	266	VAL	3.8
1	D	452	LEU	3.8
1	D	525	THR	3.8
1	C	525	THR	3.8
1	D	537	MET	3.8
1	D	60	ILE	3.8
1	D	63	ILE	3.8
1	D	103	VAL	3.7
1	D	88	PHE	3.7
1	D	277	ILE	3.7
1	D	383	PRO	3.7
1	D	238	VAL	3.7
1	D	442	VAL	3.7
1	D	373	LEU	3.6
1	D	490	PRO	3.6
1	D	481	VAL	3.6
1	D	464	ALA	3.6
1	D	118	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	466	THR	3.6
1	D	380	GLY	3.6
1	C	540	LEU	3.5
1	D	480	GLY	3.5
1	D	111	ALA	3.5
1	D	441	ILE	3.5
1	D	253	PHE	3.5
1	D	377	THR	3.5
1	D	260	ALA	3.5
1	C	494	TRP	3.5
1	D	375	GLY	3.5
1	D	59	ILE	3.5
1	D	467	ARG	3.5
1	D	28	GLN	3.5
1	D	133	PRO	3.4
1	D	123	ALA	3.4
1	D	285	ASN	3.4
1	D	463	ILE	3.4
1	C	498	VAL	3.4
1	D	270	LEU	3.3
1	D	74	LYS	3.3
1	D	81	MET	3.3
1	D	244	GLY	3.3
1	D	469	ALA	3.3
1	D	305	ALA	3.3
1	D	23	ALA	3.2
1	D	82	ASN	3.2
1	B	350	PRO	3.2
1	D	286	HIS	3.2
1	D	336	VAL	3.2
1	D	355	ALA	3.2
1	D	543	SER	3.2
1	D	440	ILE	3.2
1	D	460	ALA	3.2
1	D	488	GLU	3.2
1	D	24	PHE	3.2
1	D	505	GLY	3.1
1	D	86	LEU	3.1
1	D	540	LEU	3.1
1	D	107	VAL	3.1
1	D	252	VAL	3.1
1	D	232	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	302	ILE	3.1
1	C	122	ILE	3.1
1	D	522	ILE	3.1
1	D	439	ALA	3.1
1	D	351	ARG	3.1
1	D	109	SER	3.1
1	C	270	LEU	3.0
1	D	73	LEU	3.0
1	C	21	GLY	3.0
1	D	272	PRO	3.0
1	D	52	VAL	3.0
1	D	127	LYS	3.0
1	C	464	ALA	3.0
1	D	520	LEU	3.0
1	D	25	PHE	3.0
1	D	314	PRO	3.0
1	C	533	TYR	3.0
1	D	296	LEU	3.0
1	C	130	GLY	3.0
1	D	493	ILE	3.0
1	C	118	ARG	3.0
1	D	498	VAL	3.0
1	C	17	THR	3.0
1	D	500	ARG	2.9
1	D	22	THR	2.9
1	D	340	THR	2.9
1	C	274	GLY	2.9
1	D	83	ILE	2.9
1	D	501	ARG	2.9
1	D	384	VAL	2.9
1	B	63	ILE	2.9
1	D	389	MET	2.9
1	D	311	ILE	2.9
1	D	58	SER	2.9
1	D	265	ALA	2.9
1	C	279	ILE	2.8
1	C	522	ILE	2.8
1	B	380	GLY	2.8
1	C	489	PRO	2.8
1	D	234	SER	2.8
1	B	384	VAL	2.8
1	D	279	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	382	PHE	2.8
1	D	504	PHE	2.8
1	C	465	VAL	2.8
1	D	70	VAL	2.8
1	D	61	ALA	2.8
1	D	492	ALA	2.8
1	D	256	PHE	2.8
1	D	308	ASP	2.7
1	D	309	LEU	2.7
1	C	90	HIS	2.7
1	C	490	PRO	2.7
1	D	96	HIS	2.7
1	D	403	HIS	2.7
1	C	110	PHE	2.7
1	C	443	LEU	2.7
1	D	269	ALA	2.7
1	D	495	ALA	2.7
1	B	47	ILE	2.7
1	B	383	PRO	2.7
1	D	119	PRO	2.7
1	D	337	VAL	2.7
1	C	79	ALA	2.7
1	D	30	LEU	2.7
1	D	84	ALA	2.7
1	D	394	ALA	2.7
1	D	247	HIS	2.7
1	B	313	ILE	2.7
1	C	527	TRP	2.7
1	D	130	GLY	2.7
1	D	459	ARG	2.6
1	D	371	ILE	2.6
1	C	271	GLY	2.6
1	D	248	GLY	2.6
1	D	479	ARG	2.6
1	D	126	THR	2.6
1	D	458	PRO	2.6
1	D	87	ASN	2.6
1	B	39	LEU	2.6
1	C	417	SER	2.6
1	C	536	ILE	2.6
1	D	62	THR	2.6
1	D	421	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	288	GLY	2.6
1	C	537[A]	MET	2.6
1	C	269	ALA	2.6
1	C	463	ILE	2.6
1	D	536	ILE	2.6
1	D	91	GLY	2.6
1	D	303	MET	2.6
1	C	517	VAL	2.5
1	D	263	VAL	2.5
1	D	391	HIS	2.5
1	D	489	PRO	2.5
1	D	240	ASP	2.5
1	D	348	THR	2.5
1	D	236	GLN	2.5
1	D	76	MET	2.5
1	C	485	LEU	2.5
1	D	387	VAL	2.5
1	C	86	LEU	2.5
1	A	131	SER	2.5
1	C	119	PRO	2.5
1	D	99	SER	2.5
1	D	112	GLY	2.5
1	C	124	LEU	2.5
1	C	502	VAL	2.5
1	D	524	VAL	2.5
1	C	84	ALA	2.5
1	C	129	PRO	2.5
1	D	483	PRO	2.5
1	D	527	TRP	2.5
1	D	491	GLU	2.5
1	D	95	TYR	2.5
1	D	117	TYR	2.5
1	D	278	LYS	2.4
1	D	388	LYS	2.4
1	A	232	GLY	2.4
1	D	90	HIS	2.4
1	C	107	VAL	2.4
1	D	101	ALA	2.4
1	D	246	GLU	2.4
1	D	85	ARG	2.4
1	D	116	SER	2.4
1	D	239	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	347	ILE	2.4
1	C	26	GLN	2.4
1	C	493	ILE	2.4
1	D	494	TRP	2.4
1	C	484	LEU	2.4
1	D	456	TYR	2.4
1	D	34	MET	2.4
1	D	235	GLU	2.4
1	C	27	GLN	2.4
1	C	469	ALA	2.4
1	D	473	ARG	2.3
1	D	89	SER	2.3
1	D	345	SER	2.3
1	D	444	THR	2.3
1	A	416	LEU	2.3
1	D	443	LEU	2.3
1	D	476	HIS	2.3
1	D	243	PHE	2.3
1	B	408	GLU	2.3
1	C	539	VAL	2.3
1	C	542	ILE	2.3
1	D	67	SER	2.3
1	D	447	GLY	2.3
1	B	352	PRO	2.3
1	C	524	VAL	2.3
1	D	437	ALA	2.3
1	C	532	GLY	2.3
1	D	55	ARG	2.3
1	D	487	ARG	2.3
1	C	257	VAL	2.3
1	D	347	ILE	2.2
1	D	533	TYR	2.2
1	D	370	CYS	2.2
1	D	518	GLY	2.2
1	C	468	SER	2.2
1	D	352	PRO	2.2
1	C	277	ILE	2.2
1	C	521	VAL	2.2
1	D	506	ILE	2.2
1	D	333	GLY	2.2
1	C	52	VAL	2.2
1	C	462	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	349	LYS	2.2
1	D	477	LEU	2.2
1	B	34	MET	2.2
1	C	538	ARG	2.2
1	D	104	ARG	2.2
1	D	393	ILE	2.2
1	C	523	VAL	2.2
1	C	275	HIS	2.2
1	C	526	GLY	2.1
1	C	424	THR	2.1
1	C	466	THR	2.1
1	D	468	SER	2.1
1	B	50	GLU	2.1
1	D	474	GLN	2.1
1	C	238	VAL	2.1
1	C	452	LEU	2.1
1	D	472	ALA	2.1
1	C	117	TYR	2.1
1	C	456	TYR	2.1
1	C	487	ARG	2.1
1	D	274	GLY	2.1
1	D	276	GLY	2.1
1	C	25	PHE	2.1
1	C	116	SER	2.1
1	C	338	CYS	2.1
1	D	369	ASP	2.1
1	C	283	ILE	2.1
1	C	263	VAL	2.1
1	B	400	ALA	2.1
1	C	453	LEU	2.1
1	D	242	ARG	2.1
1	D	291	ARG	2.1
1	B	133	PRO	2.1
1	D	51	PRO	2.1
1	D	125	ASP	2.1
1	D	496	ASP	2.1
1	C	120	VAL	2.1
1	D	511	LEU	2.1
1	D	271	GLY	2.1
1	D	57	THR	2.1
1	C	344	GLU	2.1
1	D	312	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	354	ARG	2.0
1	D	339	ALA	2.0
1	B	132	GLY	2.0
1	B	375	GLY	2.0
1	C	256	PHE	2.0
1	B	45	LEU	2.0
1	C	241	LEU	2.0
1	D	72	ARG	2.0
1	D	410	LEU	2.0
1	D	517	VAL	2.0
1	D	54	ALA	2.0
1	C	235	GLU	2.0
1	D	273	GLU	2.0
1	D	507	GLU	2.0
1	D	358	SER	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 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, 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.

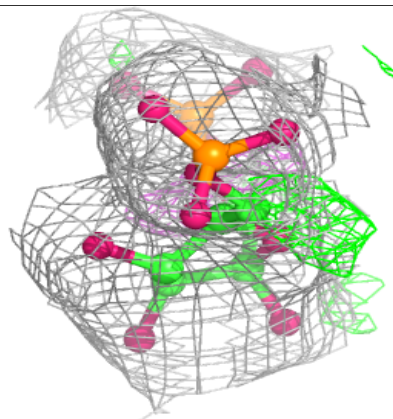
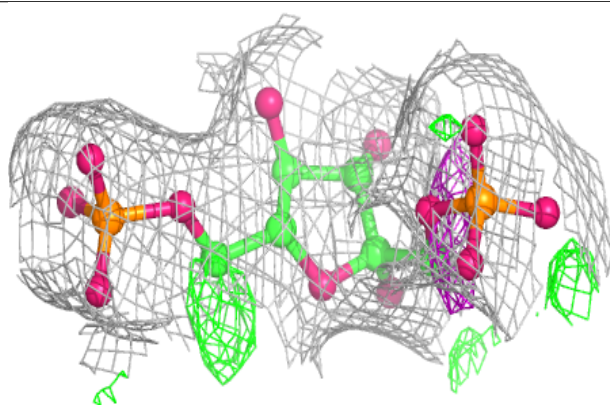
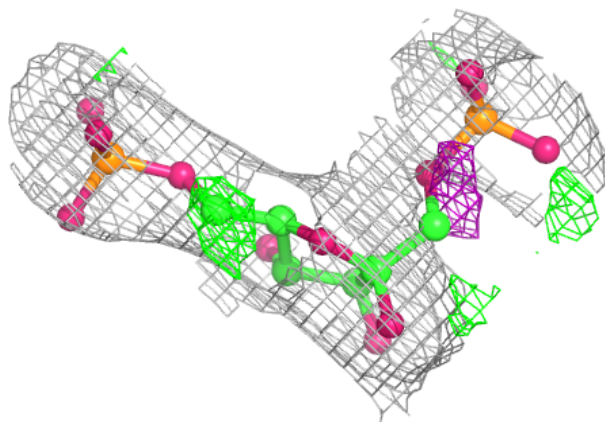
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FBP	D	601	20/20	0.74	0.15	85,86,87,87	0
2	FBP	C	602	20/20	0.82	0.13	79,81,84,84	0
3	A1JB2	C	601	38/38	0.91	0.14	68,70,70,71	24
3	A1JB2	D	602	38/38	0.92	0.14	68,70,71,71	24
2	FBP	B	601	20/20	0.97	0.07	20,21,23,23	0
2	FBP	A	601	20/20	0.98	0.05	17,21,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

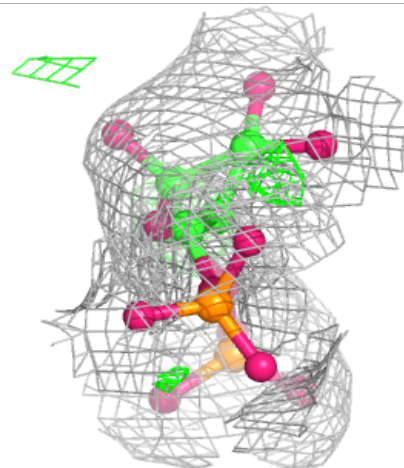
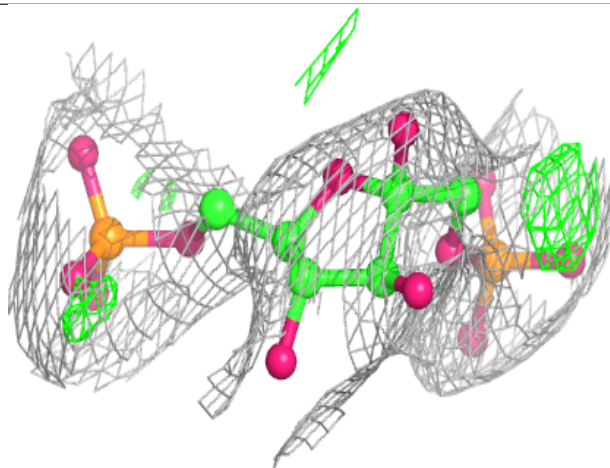
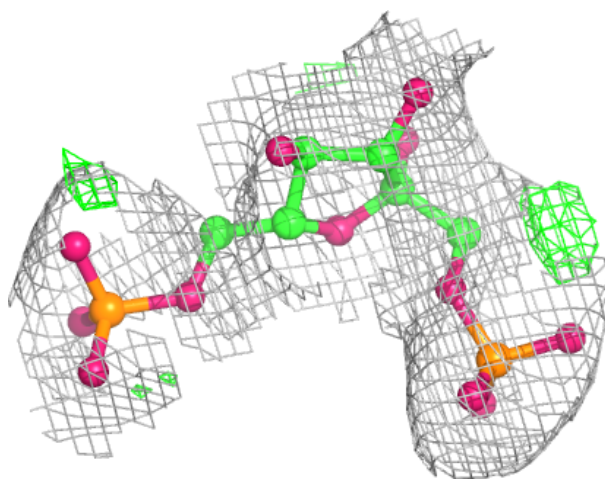
**Electron density around FBP D 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



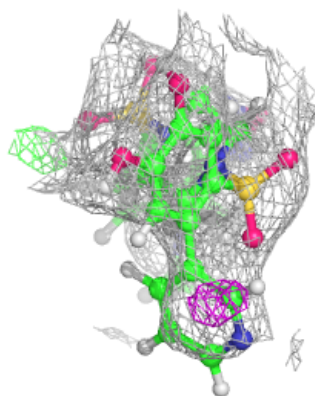
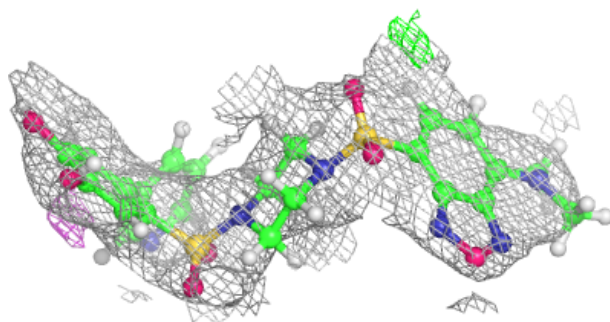
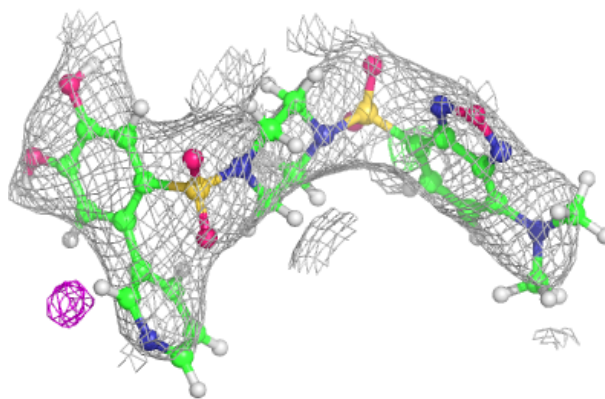
**Electron density around FBP C 602:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

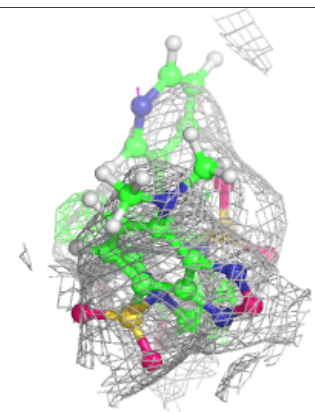
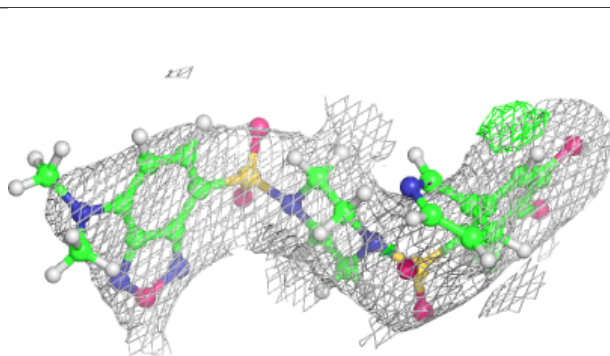
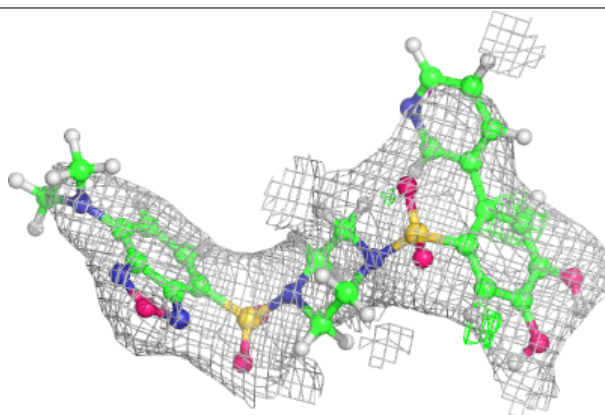


**Electron density around A1JB2 C 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around A1JB2 D 602:**

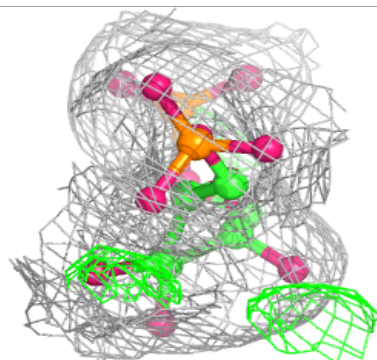
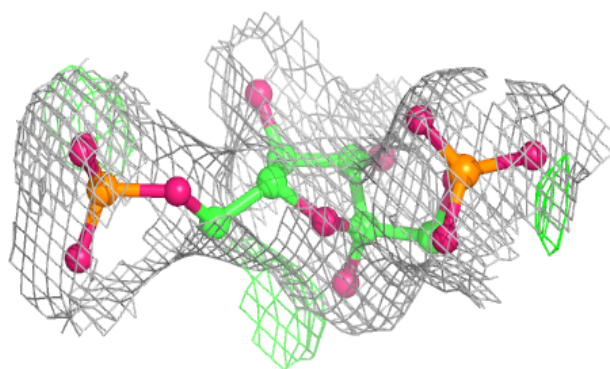
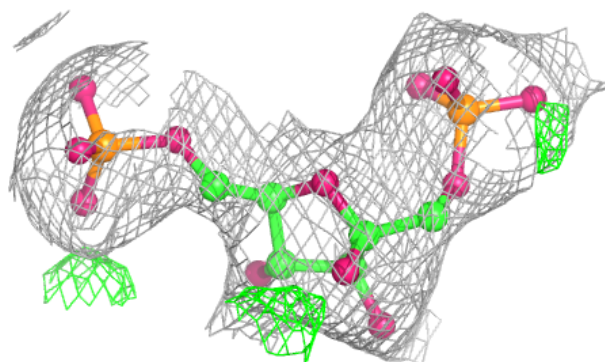
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



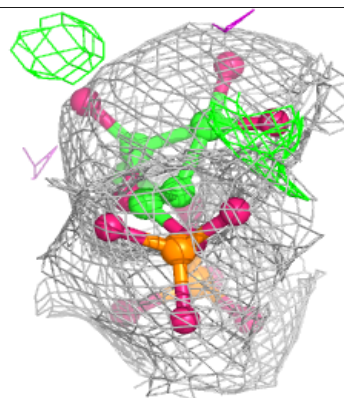
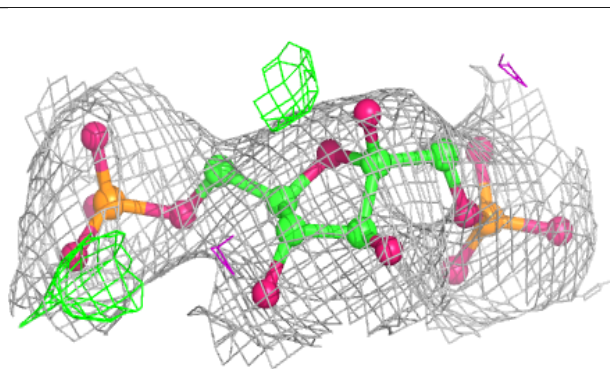
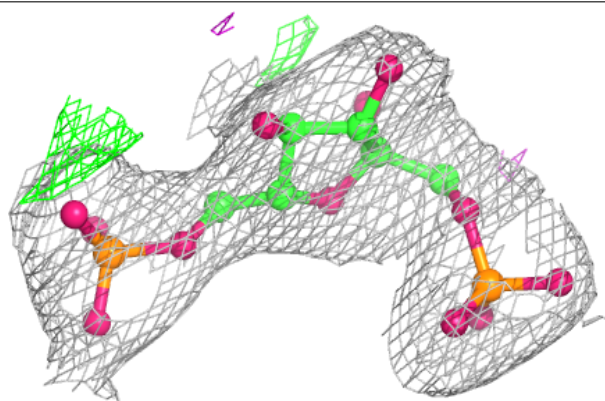


**Electron density around FBP B 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FBP A 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.