



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2025 – 08:01 pm BST

PDB ID : 9R3O / pdb\_00009r3o  
Title : Structure of liver pyruvate kinase in complex with fluorescent probe 4a  
Authors : Bogucka, A.; Nilsson, O.; Grotli, M.; Hyvonen, M.  
Deposited on : 2025-05-05  
Resolution : 2.04 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

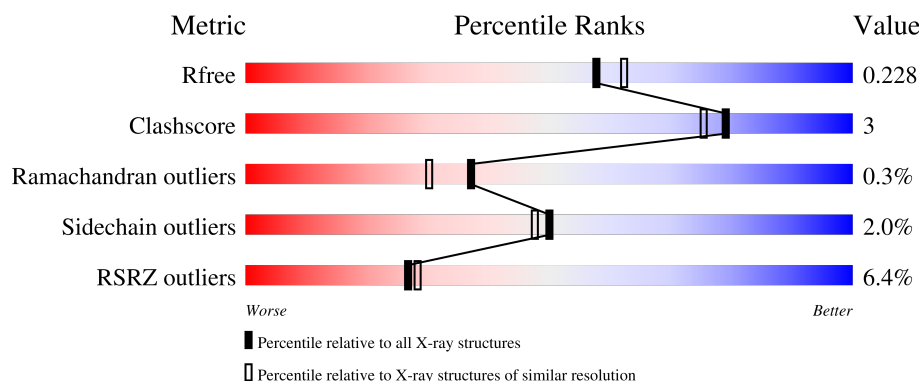
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	<div> <div>10%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>• 5%</div> </div> </div>
1	B	447	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>• •</div> </div> </div>
1	C	447	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>•</div> </div> </div>
1	D	447	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>• 5%</div> </div> </div>
1	E	447	<div> <div>13%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	447	<div><div></div><div>7%</div><div>89%</div><div>8%</div><div></div></div>
1	G	447	<div><div></div><div>2%</div><div>87%</div><div>7%</div><div>5%</div></div>
1	H	447	<div><div></div><div>4%</div><div>87%</div><div>8%</div><div>5%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28135 atoms, of which 84 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	423	Total	C	N	O	S	0	6	0
			3243	2039	586	598	20			
1	B	436	Total	C	N	O	S	0	4	0
			3329	2090	604	615	20			
1	C	427	Total	C	N	O	S	0	4	0
			3257	2045	587	606	19			
1	D	425	Total	C	N	O	S	0	6	0
			3252	2042	590	601	19			
1	E	423	Total	C	N	O	S	0	5	0
			3229	2028	583	598	20			
1	F	435	Total	C	N	O	S	0	7	0
			3335	2097	600	618	20			
1	G	423	Total	C	N	O	S	0	6	0
			3241	2036	583	603	19			
1	H	425	Total	C	N	O	S	0	4	0
			3251	2040	594	598	19			

There are 832 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	229	SER	ASP	linker	UNP P30613
A	230	GLY	LEU	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	229	SER	ASP	linker	UNP P30613
B	230	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	130	GLY	VAL	linker	UNP P30613
C	229	SER	ASP	linker	UNP P30613
C	230	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	229	SER	ASP	linker	UNP P30613
D	230	GLY	LEU	linker	UNP P30613
E	-1	GLY	-	expression tag	UNP P30613
E	0	SER	-	expression tag	UNP P30613
E	12	ASP	SER	conflict	UNP P30613
E	?	-	GLU	deletion	UNP P30613
E	?	-	ILE	deletion	UNP P30613
E	?	-	ARG	deletion	UNP P30613
E	?	-	THR	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	ILE	deletion	UNP P30613
E	?	-	LEU	deletion	UNP P30613
E	?	-	GLN	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	?	-	GLU	deletion	UNP P30613
E	?	-	SER	deletion	UNP P30613
E	?	-	GLU	deletion	UNP P30613

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	130	GLY	VAL	linker	UNP P30613
E	229	SER	ASP	linker	UNP P30613
E	230	GLY	LEU	linker	UNP P30613
F	-1	GLY	-	expression tag	UNP P30613
F	0	SER	-	expression tag	UNP P30613
F	12	ASP	SER	conflict	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	ILE	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	THR	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	ILE	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	GLN	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	SER	deletion	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	LYS	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	SER	deletion	UNP P30613
F	?	-	GLN	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	THR	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	ASP	deletion	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	?	-	ALA	deletion	UNP P30613
F	?	-	PHE	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	THR	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	ASN	deletion	UNP P30613

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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	ASN	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	SER	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	LYS	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	ASN	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	ALA	deletion	UNP P30613
F	?	-	GLN	deletion	UNP P30613
F	130	GLY	VAL	linker	UNP P30613
F	229	SER	ASP	linker	UNP P30613
F	230	GLY	LEU	linker	UNP P30613
G	-1	GLY	-	expression tag	UNP P30613
G	0	SER	-	expression tag	UNP P30613
G	12	ASP	SER	conflict	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	ARG	deletion	UNP P30613
G	?	-	THR	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	GLN	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	SER	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613

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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	ILE	deletion	UNP P30613
G	?	-	ASP	deletion	UNP P30613
G	?	-	ASP	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	SER	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	GLN	deletion	UNP P30613
G	?	-	LYS	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	THR	deletion	UNP P30613
G	?	-	GLN	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	ASN	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	SER	deletion	UNP P30613
G	?	-	ARG	deletion	UNP P30613
G	?	-	LYS	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	ASN	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	ALA	deletion	UNP P30613
G	?	-	GLN	deletion	UNP P30613
G	130	GLY	VAL	linker	UNP P30613
G	229	SER	ASP	linker	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
G	230	GLY	LEU	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	GLN	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LYS	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	GLN	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	ALA	deletion	UNP P30613
H	?	-	PHE	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	ALA	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613

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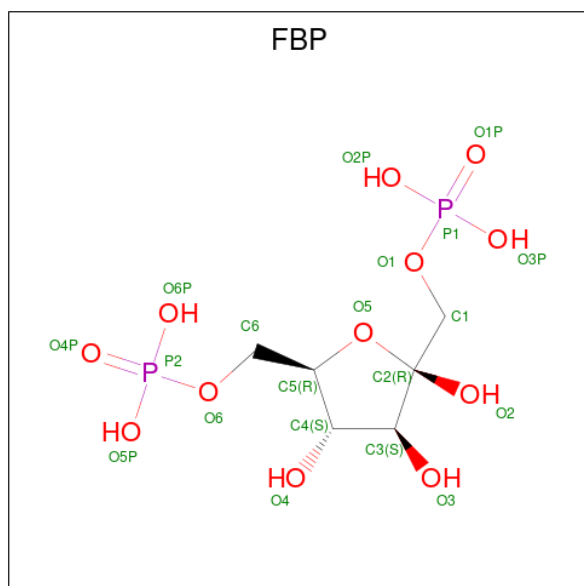
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	THR	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	TRP	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	TYR	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	ILE	deletion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

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLU	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	LYS	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	ALA	deletion	UNP P30613
H	?	-	GLN	deletion	UNP P30613
H	130	GLY	VAL	linker	UNP P30613
H	229	SER	ASP	linker	UNP P30613
H	230	GLY	LEU	linker	UNP P30613

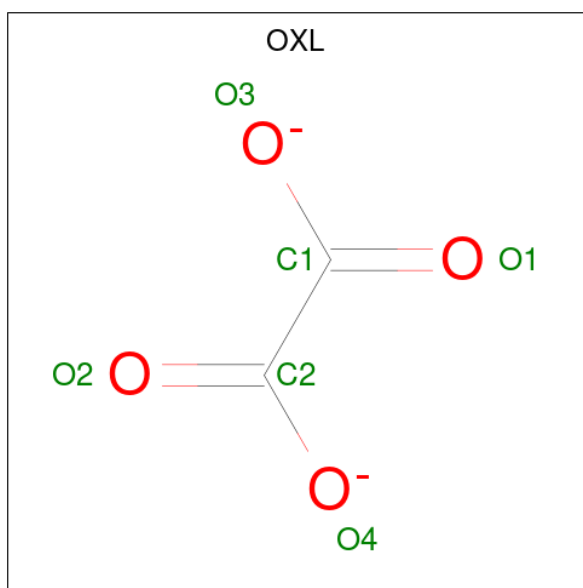
- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 20 6 12 2	0	0
2	B	1	Total C O P 20 6 12 2	0	0
2	C	1	Total C O P 20 6 12 2	0	0
2	D	1	Total C O P 20 6 12 2	0	0
2	E	1	Total C O P 20 6 12 2	0	0
2	F	1	Total C O P 20 6 12 2	0	0
2	G	1	Total C O P 20 6 12 2	0	0
2	H	1	Total C O P 20 6 12 2	0	0

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula:  $C_2O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

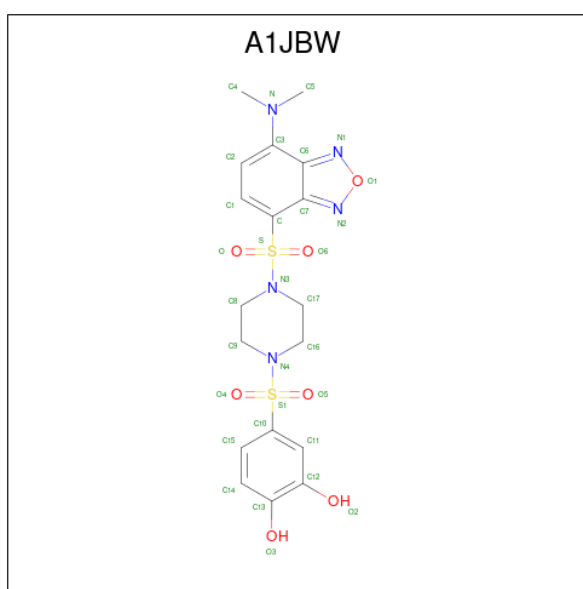
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	C	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		
5	E	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total K 1 1	0	0
5	G	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0

- Molecule 6 is 4-[4-[[7-(dimethylamino)-2,1,3-benzoxadiazol-4-yl]sulfonyl]piperazin-1-yl]sulfonylbenzene-1,2-diol (CCD ID: A1JBW) (formula: C<sub>18</sub>H<sub>21</sub>N<sub>5</sub>O<sub>7</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total 53	C 18	H 21	N 5	O 7	S 2	21	0
6	D	1	Total 53	C 18	H 21	N 5	O 7	S 2	21	0
6	G	1	Total 53	C 18	H 21	N 5	O 7	S 2	21	0
6	H	1	Total 53	C 18	H 21	N 5	O 7	S 2	21	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	125	Total O 125 125	0	0

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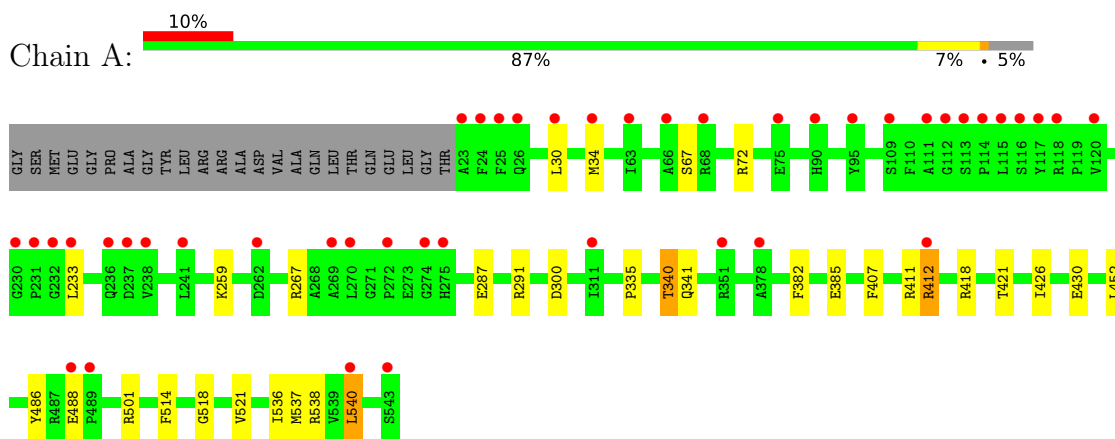
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	186	Total 186	O 186	0	0
7	C	217	Total 217	O 217	0	0
7	D	246	Total 246	O 246	0	0
7	E	149	Total 149	O 149	0	0
7	F	153	Total 153	O 153	0	0
7	G	243	Total 243	O 243	0	0
7	H	243	Total 243	O 243	0	0

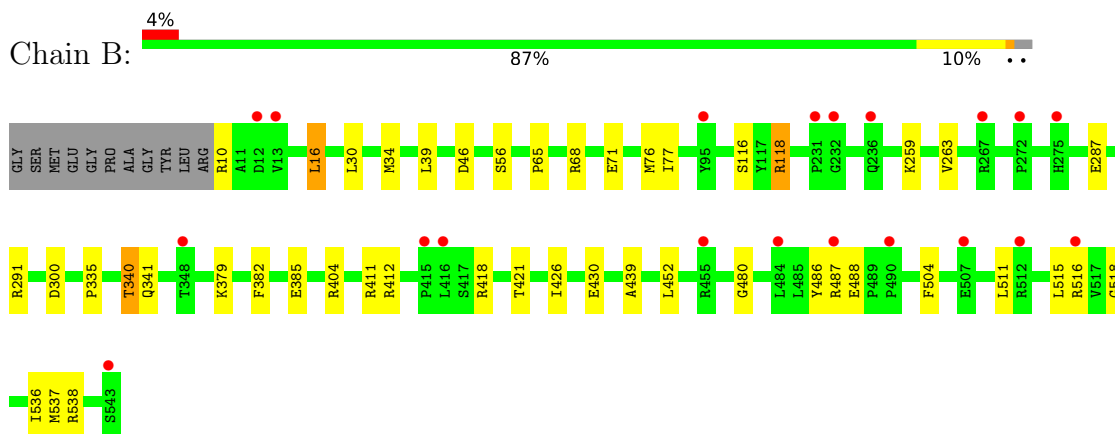
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

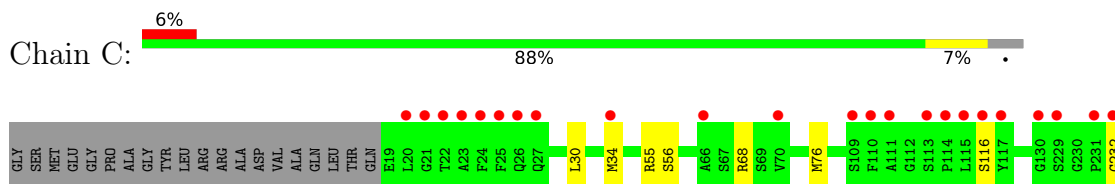
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

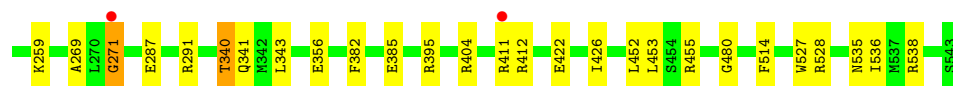


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

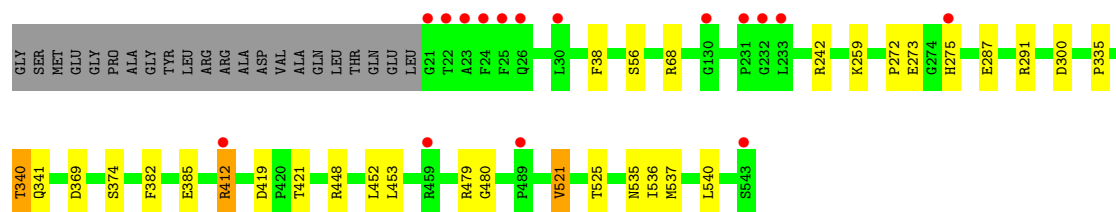
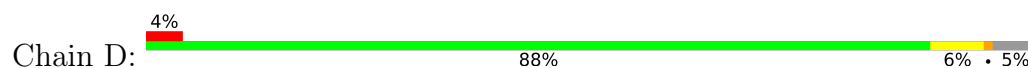


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

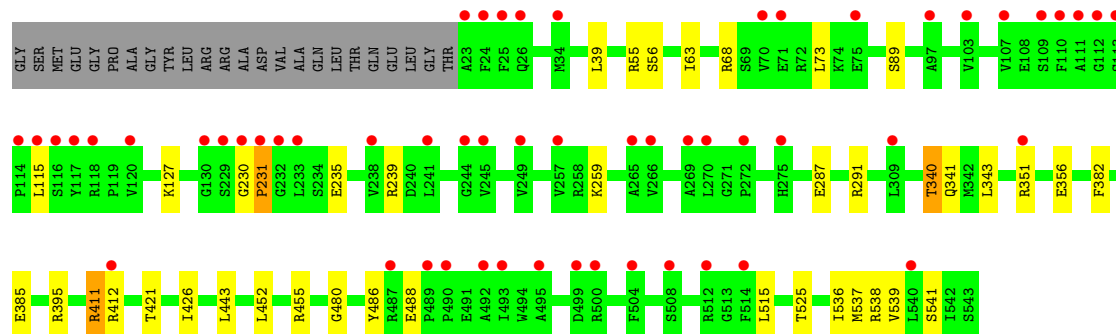
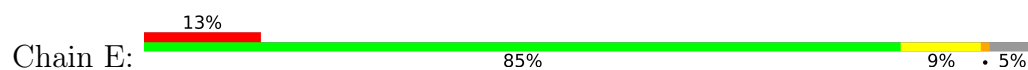




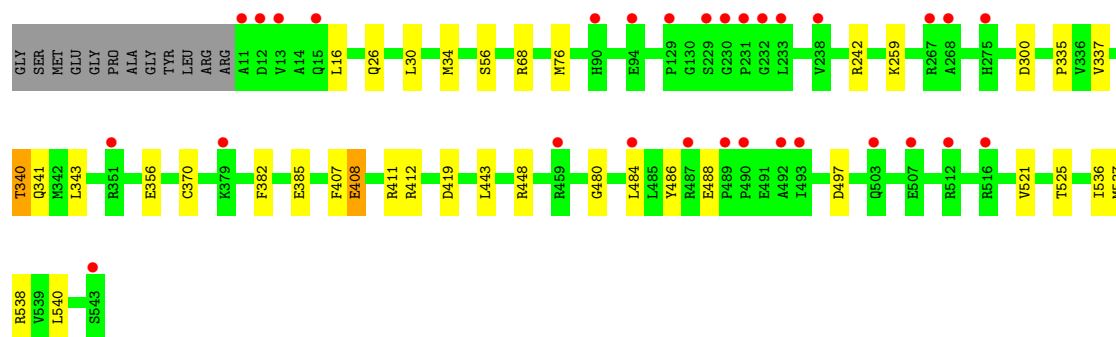
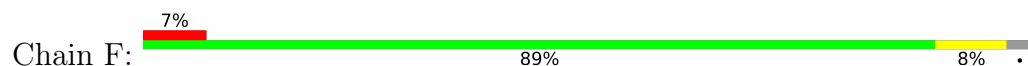
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



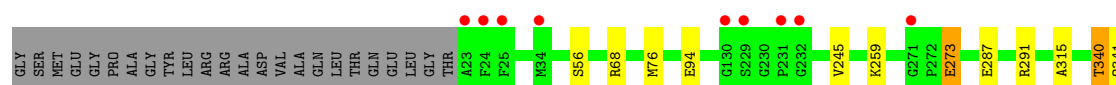
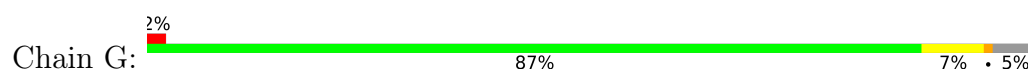
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

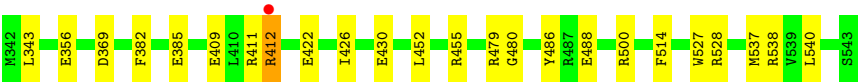


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

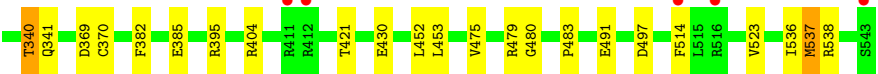
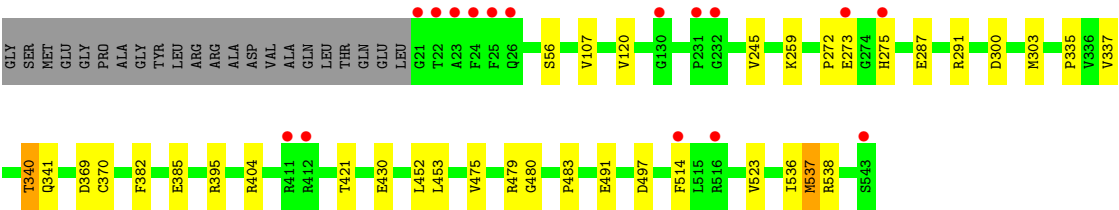
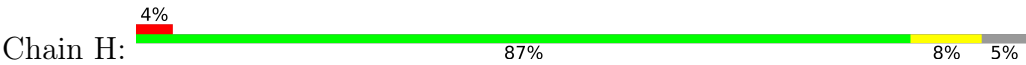


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR





● 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, $\alpha$ , $\beta$ , $\gamma$	206.88Å 112.00Å 188.13Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	188.03 – 2.04 188.03 – 2.04	Depositor EDS
% Data completeness (in resolution range)	60.8 (188.03-2.04) 60.8 (188.03-2.04)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.05Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.206 , 0.240 0.197 , 0.228	Depositor DCC
$R_{free}$ test set	8407 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4813e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, MG, OXL, A1JBW, K

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	0/3316	1.03	1/4484 (0.0%)
1	B	0.73	0/3396	1.04	3/4592 (0.1%)
1	C	0.77	0/3324	1.06	3/4495 (0.1%)
1	D	0.77	1/3326 (0.0%)	1.05	4/4497 (0.1%)
1	E	0.70	0/3298	1.03	5/4458 (0.1%)
1	F	0.71	0/3411	1.04	3/4613 (0.1%)
1	G	0.76	0/3314	1.04	1/4481 (0.0%)
1	H	0.77	1/3316 (0.0%)	1.05	3/4483 (0.1%)
All	All	0.74	2/26701 (0.0%)	1.04	23/36103 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	374	SER	CA-C	6.84	1.55	1.52
1	H	303	MET	SD-CE	-5.55	1.65	1.79

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	231	PRO	N-CA-CB	8.28	111.95	103.25
1	E	230	GLY	CA-C-N	7.29	128.96	119.84
1	E	230	GLY	C-N-CA	7.29	128.96	119.84
1	G	514	PHE	CA-CB-CG	7.17	120.97	113.80
1	H	514	PHE	CA-CB-CG	6.21	120.01	113.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3243	0	3307	20	0
1	B	3329	0	3394	23	0
1	C	3257	0	3308	18	0
1	D	3252	0	3310	16	0
1	E	3229	0	3283	19	0
1	F	3335	0	3404	17	0
1	G	3241	0	3293	20	0
1	H	3251	0	3306	22	0
2	A	20	0	10	1	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	C	32	21	0	0	0
6	D	32	21	0	2	0
6	G	32	21	0	2	0
6	H	32	21	0	0	0
7	A	125	0	0	0	0
7	B	186	0	0	2	0
7	C	217	0	0	1	0
7	D	246	0	0	1	0
7	E	149	0	0	0	0
7	F	153	0	0	1	0
7	G	243	0	0	0	0
7	H	243	0	0	1	0
All	All	28051	84	26685	138	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 3.

The worst 5 of 138 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.60	0.84
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.61	0.81
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.64	0.80
1:E:411:ARG:HG2	1:E:426:ILE:HD11	1.67	0.75
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.68	0.74

There are no symmetry-related clashes.

## 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	427/447 (96%)	422 (99%)	4 (1%)	1 (0%)	44	38
1	B	438/447 (98%)	433 (99%)	4 (1%)	1 (0%)	44	38
1	C	429/447 (96%)	419 (98%)	8 (2%)	2 (0%)	25	17
1	D	429/447 (96%)	423 (99%)	5 (1%)	1 (0%)	44	38
1	E	426/447 (95%)	420 (99%)	4 (1%)	2 (0%)	25	17
1	F	440/447 (98%)	434 (99%)	5 (1%)	1 (0%)	44	38
1	G	427/447 (96%)	418 (98%)	8 (2%)	1 (0%)	44	38
1	H	427/447 (96%)	421 (99%)	5 (1%)	1 (0%)	44	38
All	All	3443/3576 (96%)	3390 (98%)	43 (1%)	10 (0%)	37	30

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	231	PRO
1	C	271	GLY
1	A	340	THR
1	B	340	THR
1	C	340	THR

### 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	341/352 (97%)	335 (98%)	6 (2%)	54	52
1	B	349/352 (99%)	335 (96%)	14 (4%)	27	21
1	C	342/352 (97%)	336 (98%)	6 (2%)	54	52
1	D	342/352 (97%)	335 (98%)	7 (2%)	50	47
1	E	339/352 (96%)	329 (97%)	10 (3%)	37	32
1	F	351/352 (100%)	341 (97%)	10 (3%)	38	34
1	G	341/352 (97%)	332 (97%)	9 (3%)	41	36
1	H	340/352 (97%)	337 (99%)	3 (1%)	75	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2745/2816 (98%)	2680 (98%)	65 (2%)	50 40

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	259	LYS
1	G	412	ARG
1	C	259	LYS
1	C	116	SER
1	G	500	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	390	GLN
1	H	405	GLN
1	D	535	ASN
1	F	390	GLN
1	F	405	GLN

### 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](#)

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OXL	C	603	4	5,5,5	1.88	2 (40%)	6,6,6	1.16	1 (16%)
3	OXL	G	602	4	5,5,5	2.11	2 (40%)	6,6,6	0.78	0
3	OXL	F	602	4	5,5,5	1.86	2 (40%)	6,6,6	1.35	1 (16%)
2	FBP	G	601	-	18,20,20	0.53	0	23,32,32	0.70	0
3	OXL	B	602	4	5,5,5	2.10	2 (40%)	6,6,6	1.02	0
6	A1JBW	C	601	-	33,35,35	0.62	1 (3%)	45,54,54	0.70	1 (2%)
6	A1JBW	H	605	-	33,35,35	0.72	1 (3%)	45,54,54	1.16	6 (13%)
3	OXL	E	602	4	5,5,5	1.92	2 (40%)	6,6,6	1.28	1 (16%)
2	FBP	A	601	-	18,20,20	0.57	0	23,32,32	0.70	1 (4%)
3	OXL	D	602	4	5,5,5	2.28	2 (40%)	6,6,6	1.16	0
2	FBP	E	601	-	18,20,20	0.47	0	23,32,32	0.77	1 (4%)
2	FBP	H	601	-	18,20,20	0.57	0	23,32,32	0.76	1 (4%)
3	OXL	A	602	4	5,5,5	1.74	1 (20%)	6,6,6	1.60	2 (33%)
2	FBP	B	601	-	18,20,20	0.43	0	23,32,32	0.83	1 (4%)
2	FBP	D	601	-	18,20,20	0.49	0	23,32,32	1.02	2 (8%)
2	FBP	F	601	-	18,20,20	0.35	0	23,32,32	0.67	0
3	OXL	H	602	4	5,5,5	1.64	2 (40%)	6,6,6	1.30	1 (16%)
6	A1JBW	D	605	-	33,35,35	0.73	1 (3%)	45,54,54	1.08	3 (6%)
6	A1JBW	G	605	-	33,35,35	0.69	1 (3%)	45,54,54	0.98	6 (13%)
2	FBP	C	602	-	18,20,20	0.61	0	23,32,32	1.12	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	C	603	4	-	0/4/4/4	-
3	OXL	G	602	4	-	0/4/4/4	-
3	OXL	F	602	4	-	0/4/4/4	-
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	0/4/4/4	-
6	A1JBW	C	601	-	-	17/28/38/38	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1JBW	H	605	-	-	13/28/38/38	0/4/4/4
3	OXL	E	602	4	-	0/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	4	-	0/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	4	-	0/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	0/4/4/4	-
6	A1JBW	D	605	-	-	8/28/38/38	1/4/4/4
6	A1JBW	G	605	-	-	15/28/38/38	1/4/4/4
2	FBP	C	602	-	-	2/13/32/32	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	OXL	O2-C2	4.04	1.33	1.22
3	B	602	OXL	O2-C2	3.93	1.33	1.22
3	D	602	OXL	O2-C2	3.90	1.33	1.22
3	C	603	OXL	O2-C2	3.52	1.32	1.22
3	F	602	OXL	O2-C2	3.33	1.31	1.22

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FBP	O6-P2-O4P	3.51	116.32	106.47
6	H	605	A1JBW	C16-C17-N3	3.19	111.35	108.91
6	H	605	A1JBW	C17-C16-N4	3.15	111.32	108.91
6	D	605	A1JBW	C16-C17-N3	3.06	111.25	108.91
3	A	602	OXL	O4-C2-C1	2.99	122.04	113.16

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	602	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6

All (2) ring outliers are listed below:

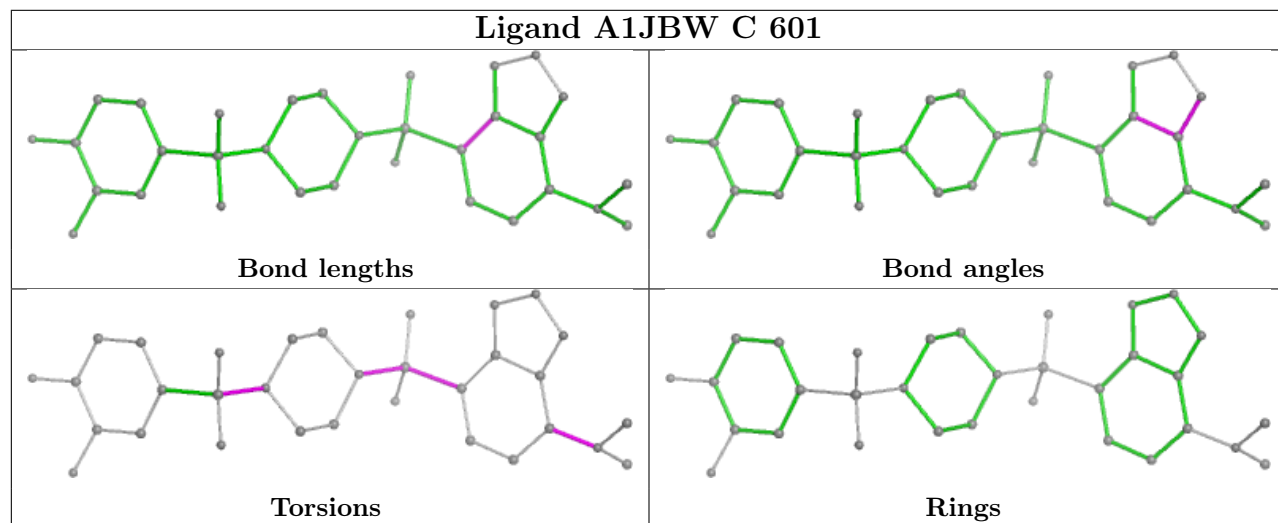
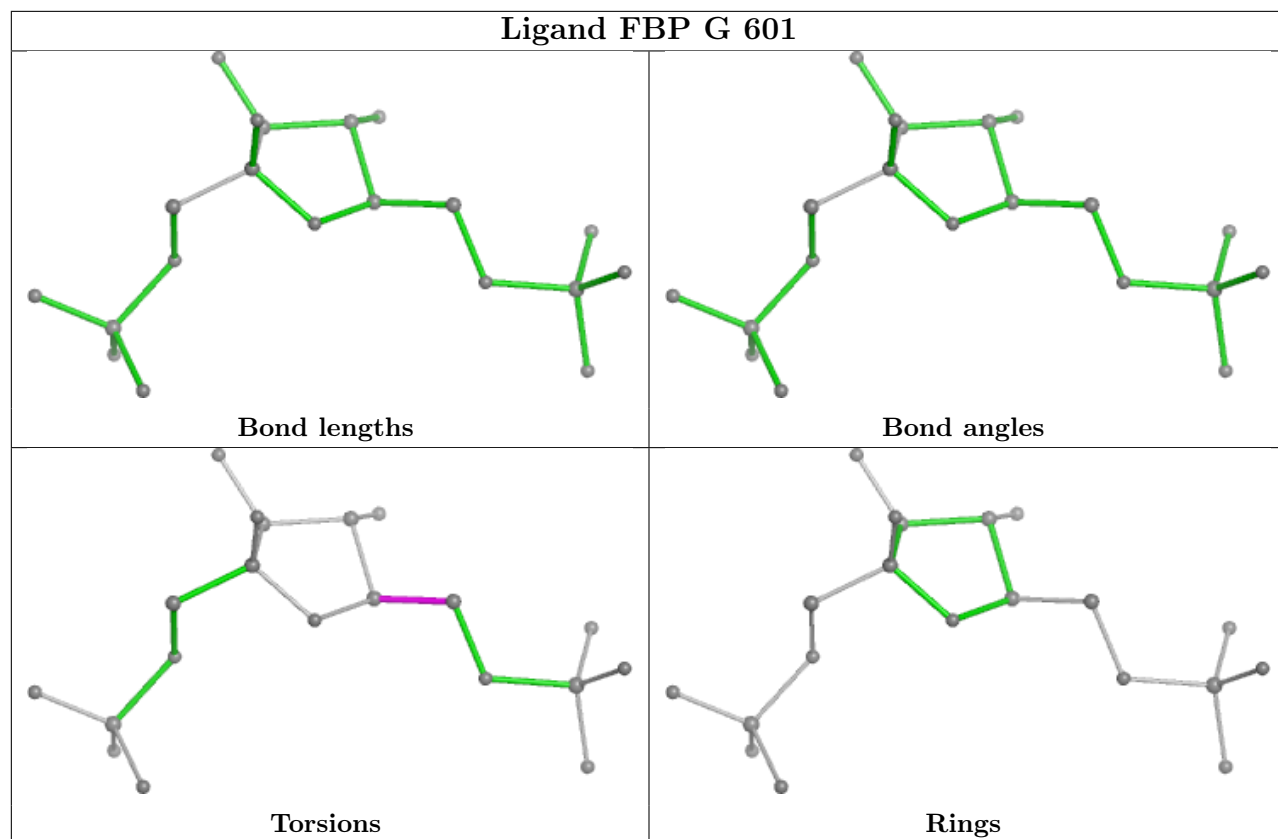
Mol	Chain	Res	Type	Atoms
6	D	605	A1JBW	C16-C17-C8-C9-N3-N4
6	G	605	A1JBW	C16-C17-C8-C9-N3-N4

3 monomers are involved in 5 short contacts:

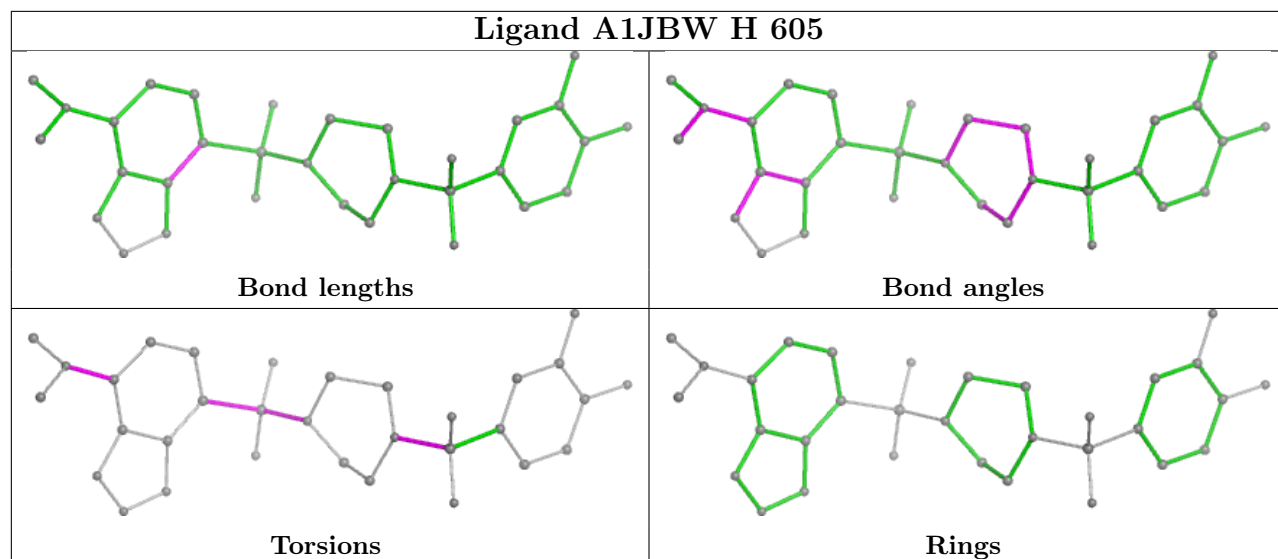
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FBP	1	0
6	D	605	A1JBW	2	0
6	G	605	A1JBW	2	0

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.

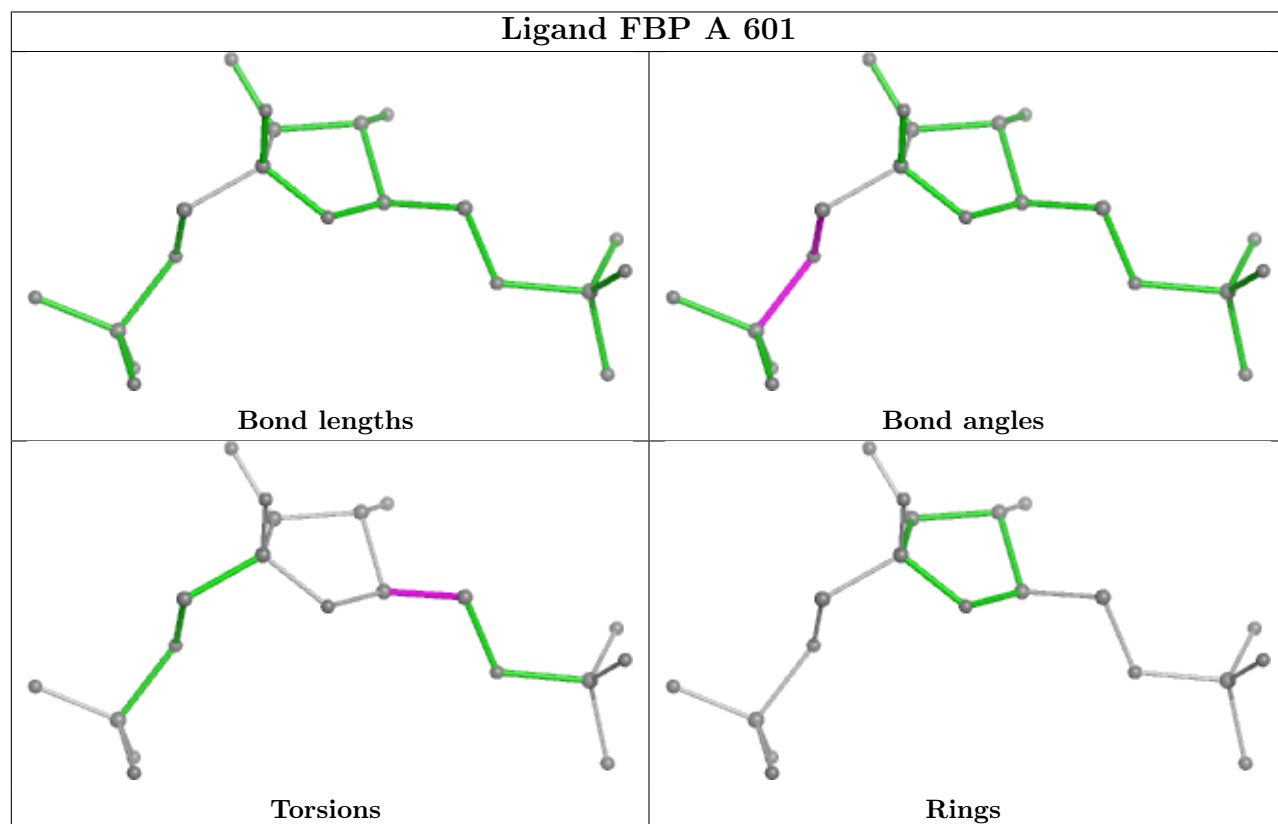


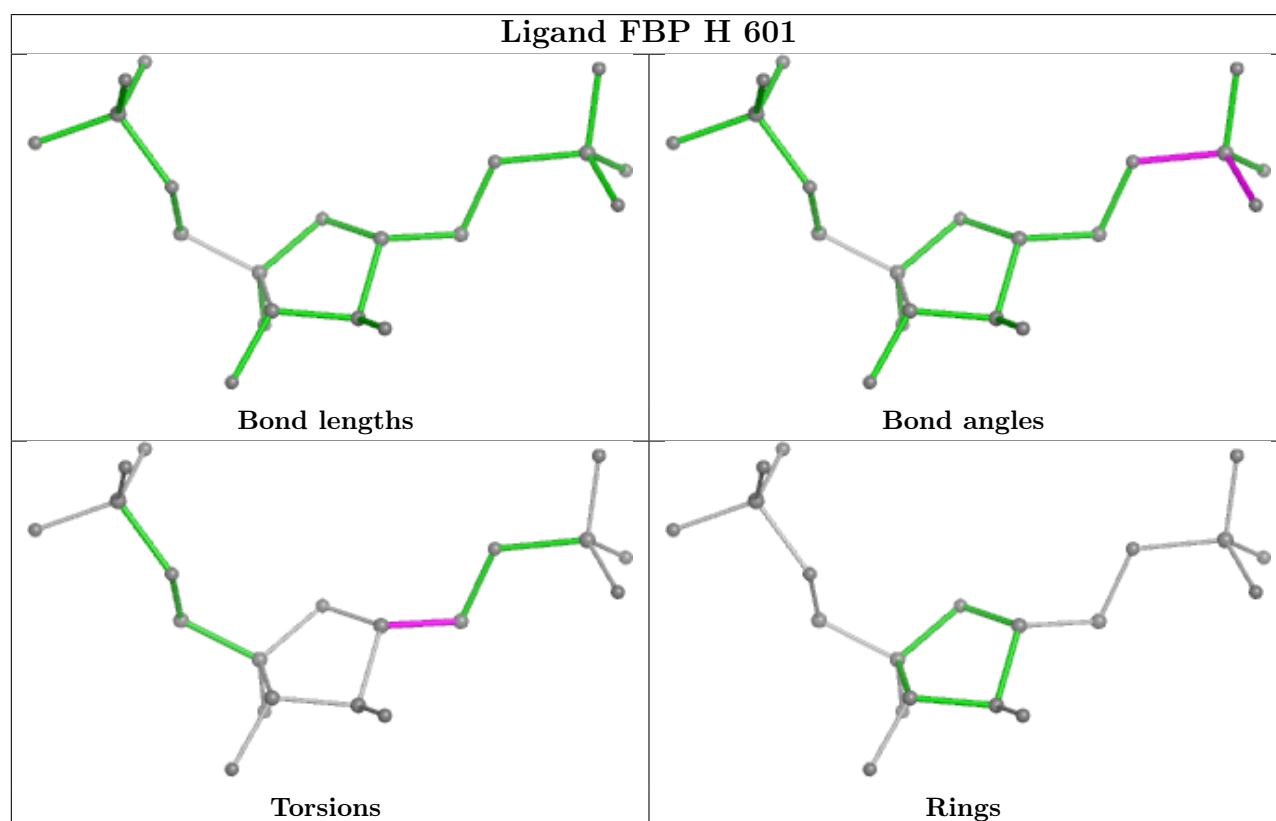
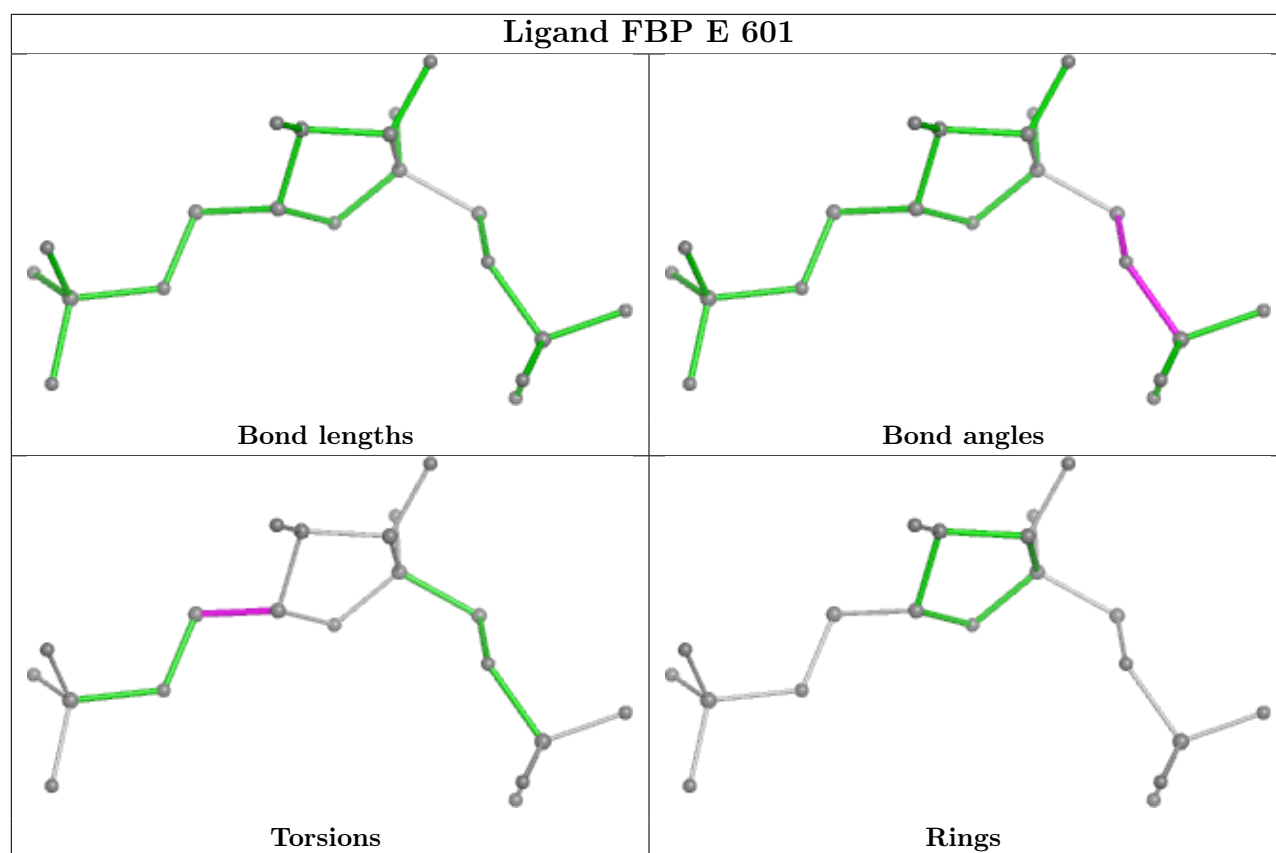


## Ligand A1JBW H 605

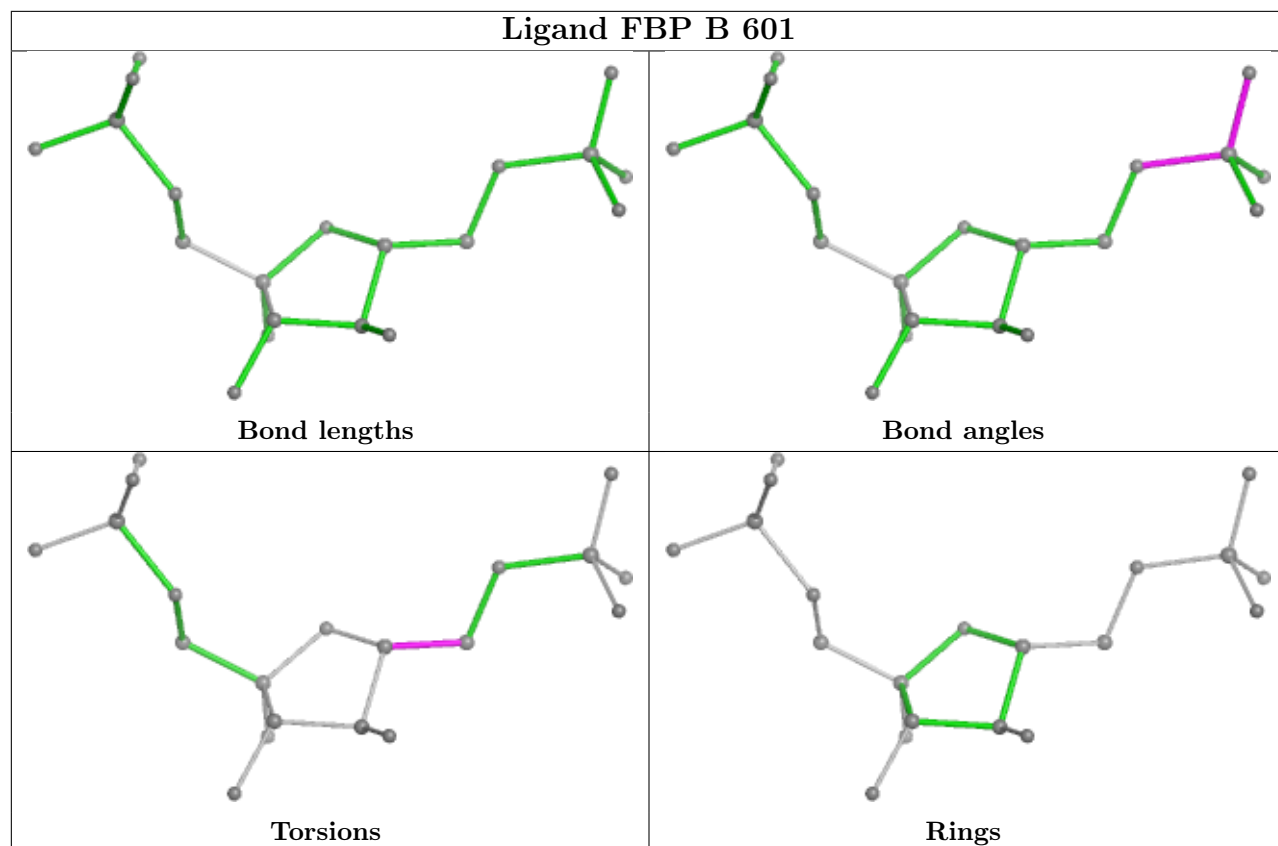


## Ligand FBP A 601

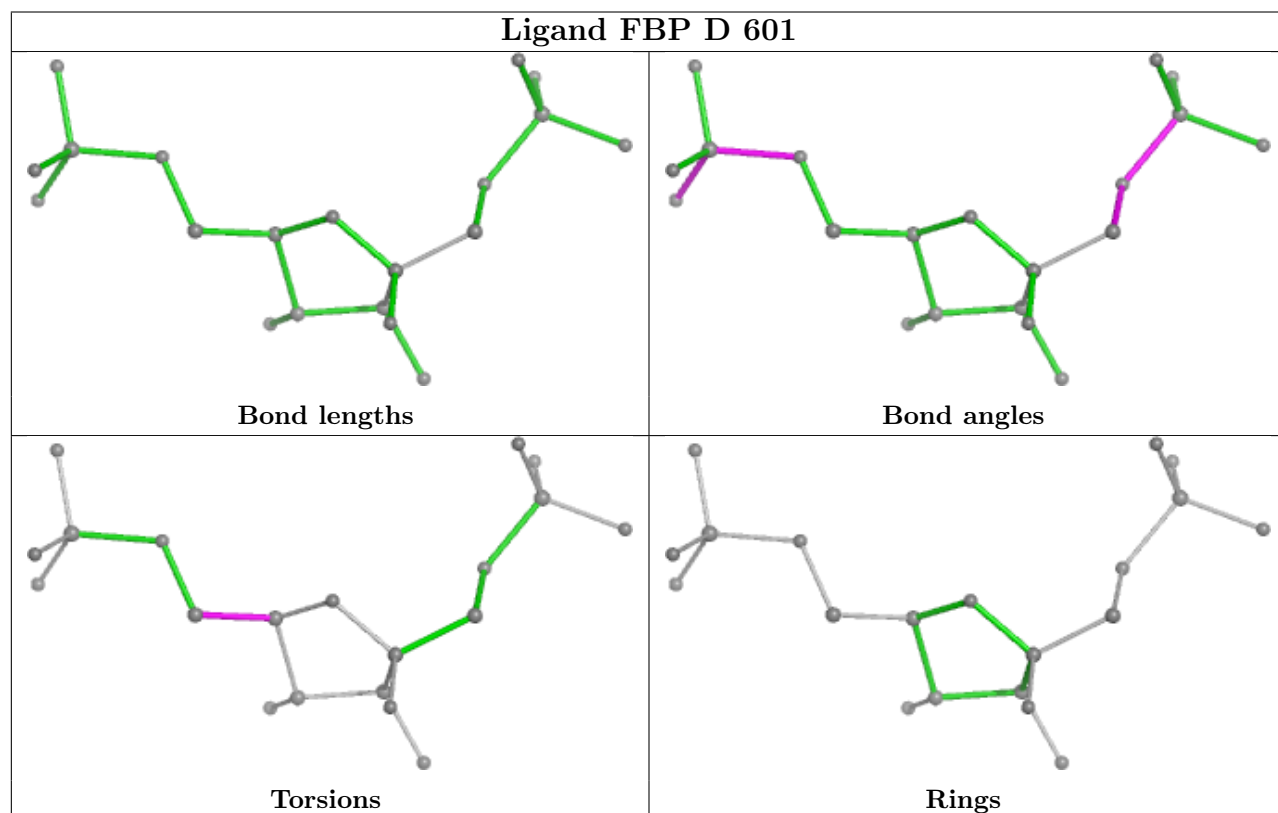




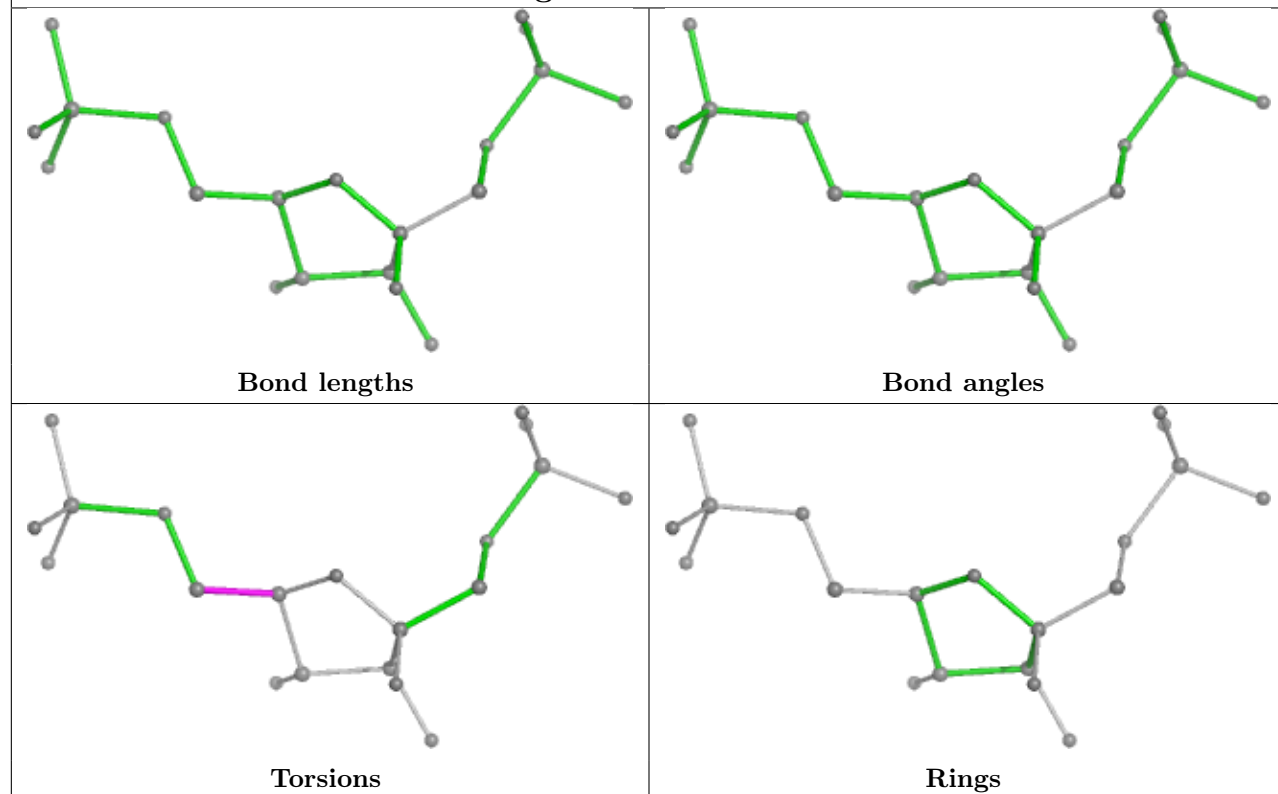
## Ligand FBP B 601



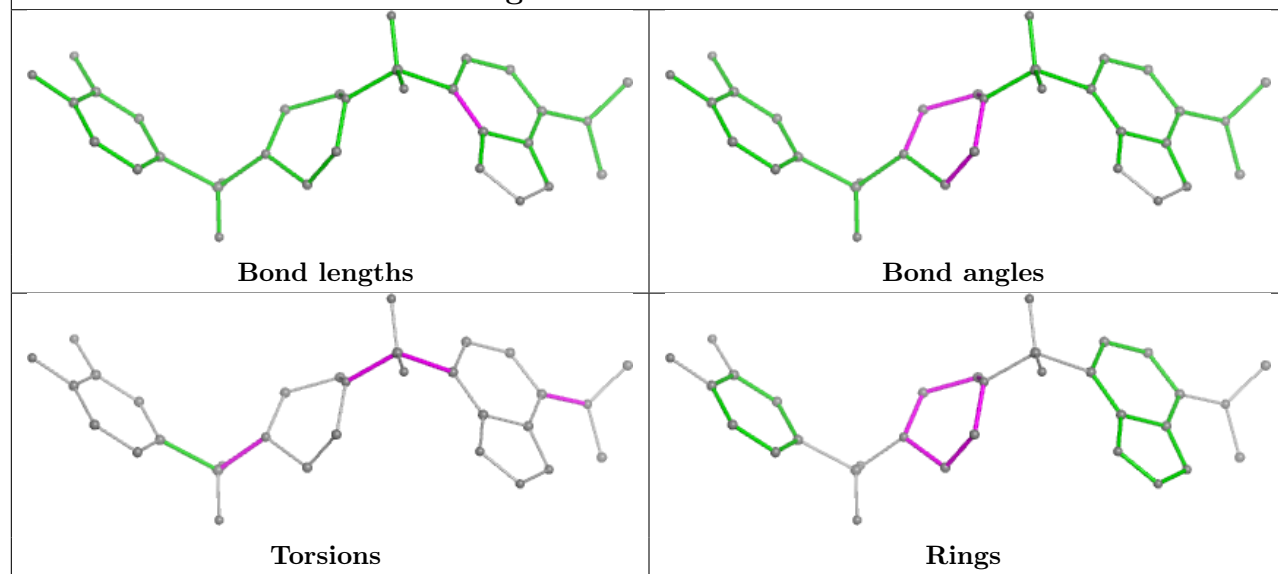
## Ligand FBP D 601

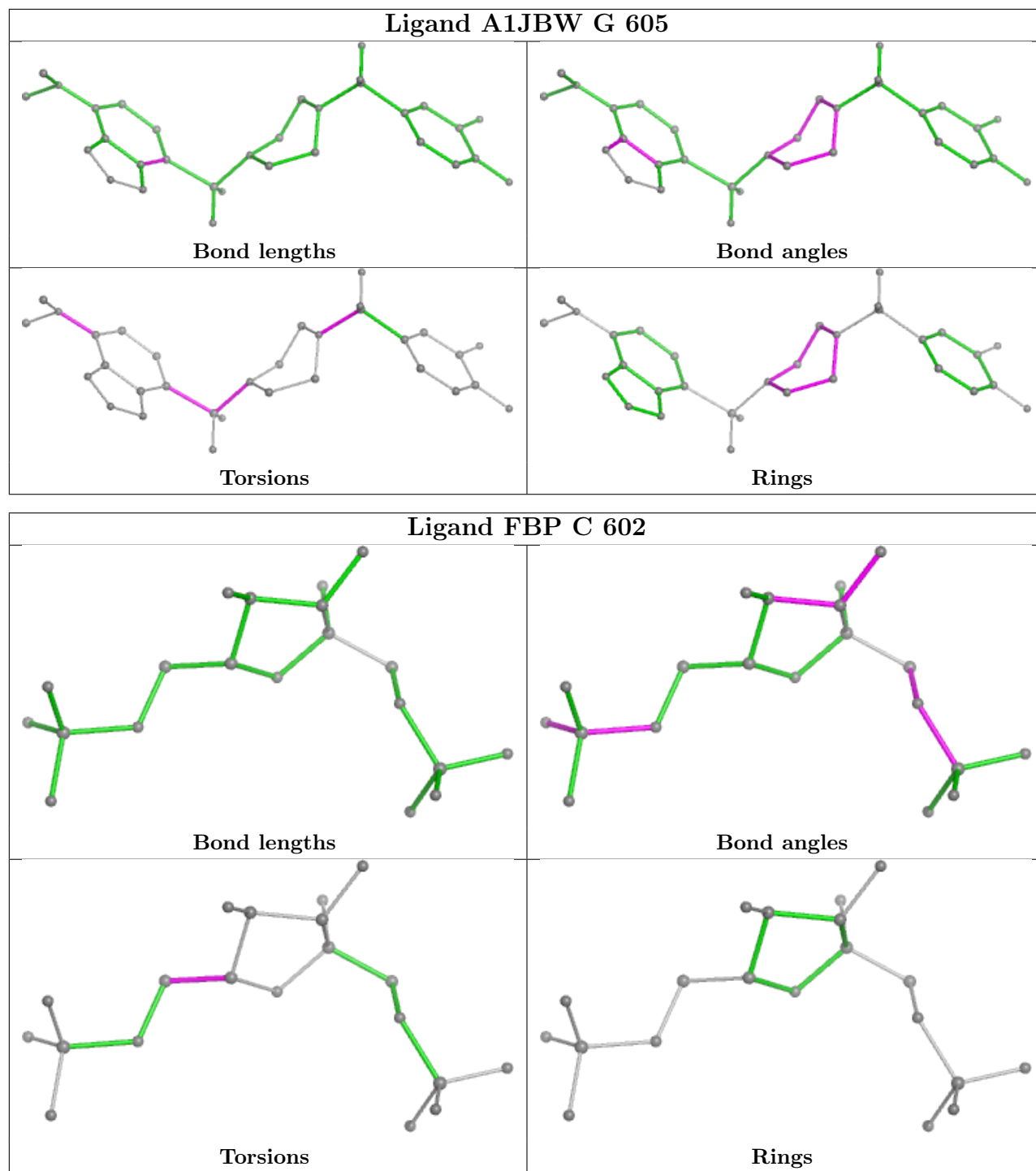


## Ligand FBP F 601



## Ligand A1JBW D 605





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	423/447 (94%)	0.78	44 (10%)	13 13	20, 41, 71, 92	6 (1%)
1	B	436/447 (97%)	0.37	20 (4%)	38 40	17, 34, 59, 77	4 (0%)
1	C	427/447 (95%)	0.23	25 (5%)	29 31	15, 31, 58, 99	4 (0%)
1	D	425/447 (95%)	-0.06	16 (3%)	44 46	12, 25, 50, 97	6 (1%)
1	E	423/447 (94%)	0.82	56 (13%)	8 8	19, 40, 72, 83	5 (1%)
1	F	435/447 (97%)	0.49	30 (6%)	24 26	20, 36, 63, 86	7 (1%)
1	G	423/447 (94%)	-0.06	10 (2%)	59 61	14, 27, 46, 68	7 (1%)
1	H	425/447 (95%)	-0.08	16 (3%)	44 46	13, 26, 49, 79	4 (0%)
All	All	3417/3576 (95%)	0.31	217 (6%)	27 28	12, 33, 62, 99	43 (1%)

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	PHE	7.5
1	E	114	PRO	7.5
1	D	25	PHE	7.1
1	G	25	PHE	6.5
1	E	115	LEU	6.5

### 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 ⓘ

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.

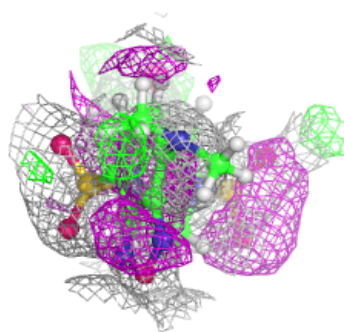
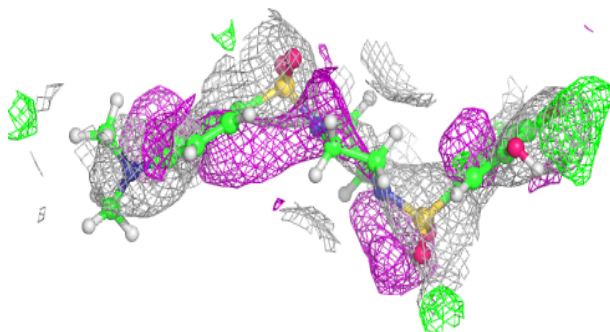
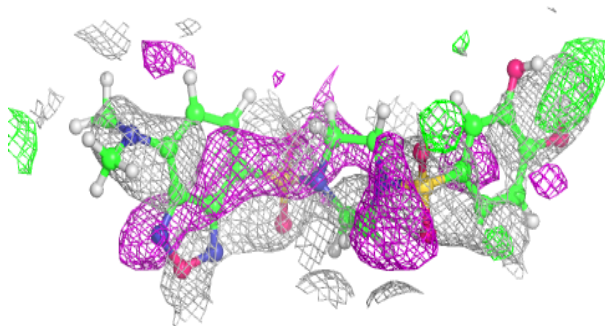
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	A1JBW	H	605	32/32	0.76	0.27	90,92,92,92	21
6	A1JBW	G	605	32/32	0.78	0.25	89,92,93,93	21
6	A1JBW	D	605	32/32	0.78	0.24	74,77,79,81	21
3	OXL	A	602	6/6	0.86	0.12	48,49,50,50	0
3	OXL	E	602	6/6	0.86	0.14	56,56,57,57	0
6	A1JBW	C	601	32/32	0.86	0.18	63,68,68,68	21
3	OXL	B	602	6/6	0.89	0.10	36,37,38,39	0
3	OXL	C	603	6/6	0.91	0.09	45,46,46,46	0
3	OXL	F	602	6/6	0.91	0.12	61,61,62,62	0
4	MG	F	603	1/1	0.93	0.14	35,35,35,35	0
2	FBP	E	601	20/20	0.94	0.08	33,34,37,38	0
5	K	B	604	1/1	0.94	0.07	53,53,53,53	0
3	OXL	G	602	6/6	0.94	0.07	30,31,31,31	0
3	OXL	D	602	6/6	0.95	0.11	28,29,30,31	0
2	FBP	A	601	20/20	0.95	0.07	33,34,35,36	0
3	OXL	H	602	6/6	0.95	0.08	32,33,34,34	0
2	FBP	B	601	20/20	0.96	0.06	27,30,32,32	0
2	FBP	F	601	20/20	0.96	0.07	29,34,37,37	0
4	MG	A	603	1/1	0.96	0.13	37,37,37,37	0
4	MG	B	603	1/1	0.97	0.11	30,30,30,30	0
5	K	A	604	1/1	0.97	0.06	54,54,54,54	0
4	MG	E	603	1/1	0.97	0.12	34,34,34,34	0
5	K	E	604	1/1	0.97	0.06	56,56,56,56	0
5	K	F	604	1/1	0.98	0.05	57,57,57,57	0
5	K	G	604	1/1	0.98	0.07	35,35,35,35	0
5	K	H	604	1/1	0.98	0.03	33,33,33,33	0
2	FBP	C	602	20/20	0.98	0.04	18,19,24,25	0
2	FBP	D	601	20/20	0.98	0.05	19,20,24,24	0
5	K	C	605	1/1	0.98	0.05	41,41,41,41	0
2	FBP	H	601	20/20	0.98	0.05	18,20,23,24	0
2	FBP	G	601	20/20	0.99	0.04	18,19,21,21	0
4	MG	C	604	1/1	0.99	0.05	26,26,26,26	0
4	MG	H	603	1/1	0.99	0.05	16,16,16,16	0
5	K	D	604	1/1	0.99	0.02	30,30,30,30	0
4	MG	G	603	1/1	1.00	0.06	15,15,15,15	0
4	MG	D	603	1/1	1.00	0.05	19,19,19,19	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.

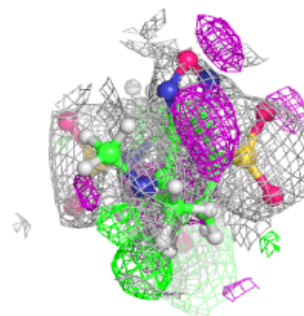
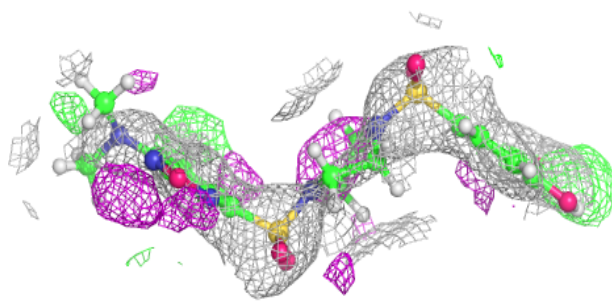
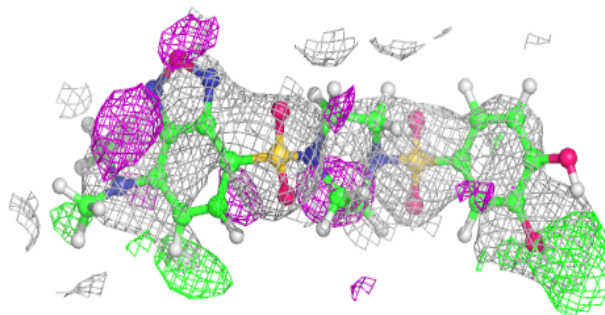
**Electron density around A1JBW H 605:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

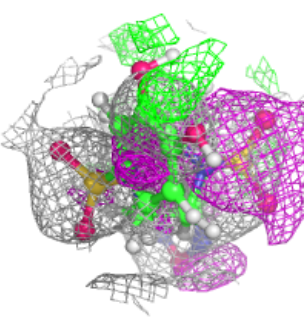
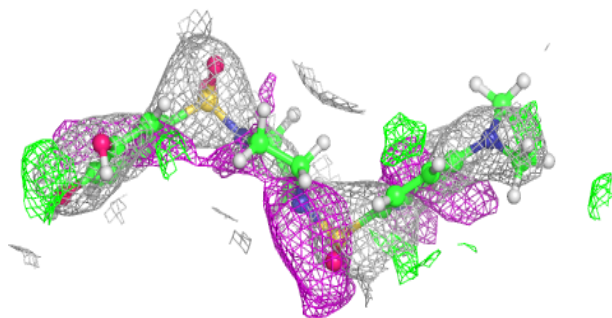
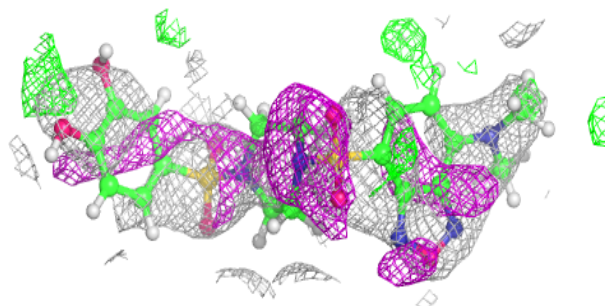


**Electron density around A1JBW G 605:**

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

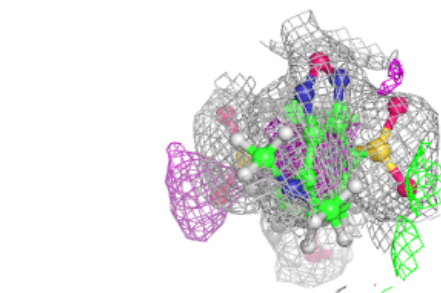
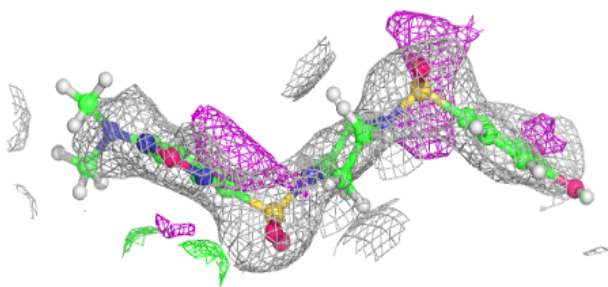
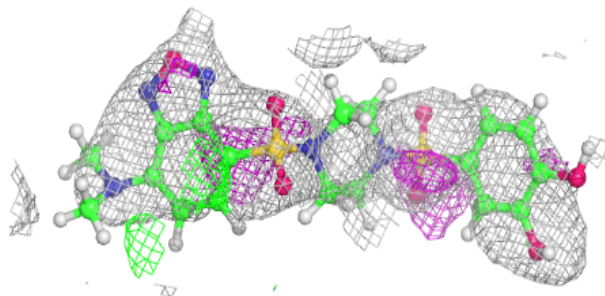
**Electron density around A1JBW D 605:**

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

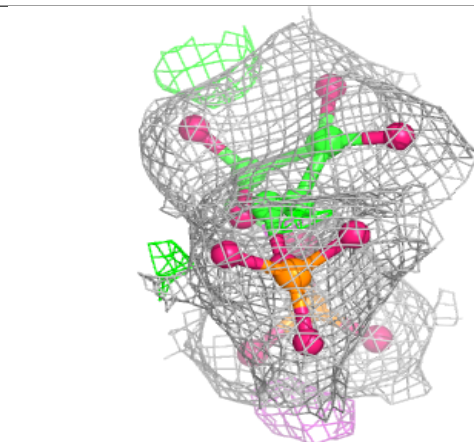
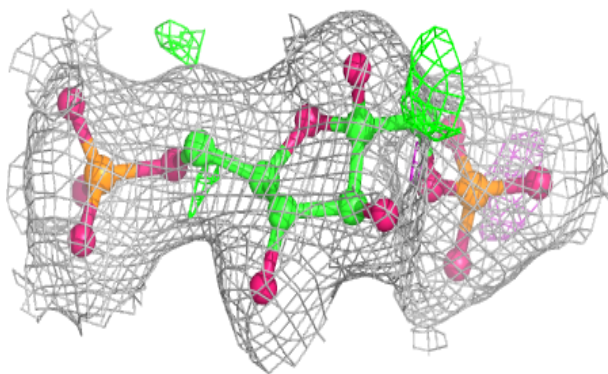
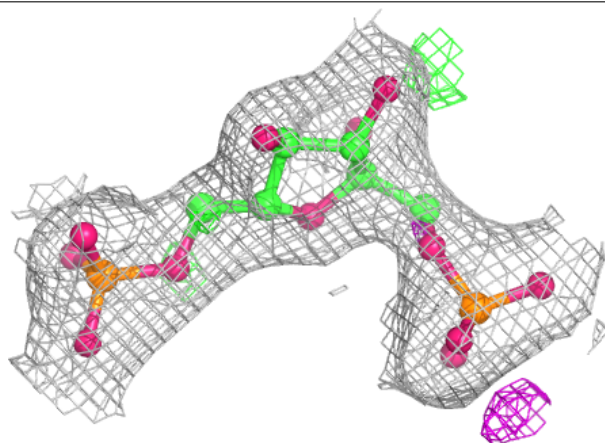


**Electron density around A1JBW C 601:**

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

**Electron density around FBP E 601:**

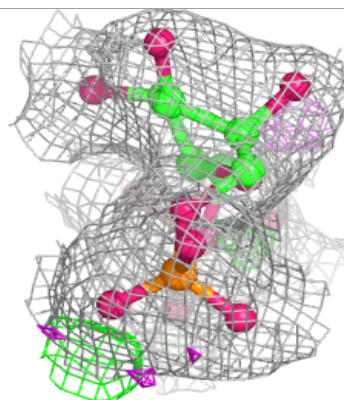
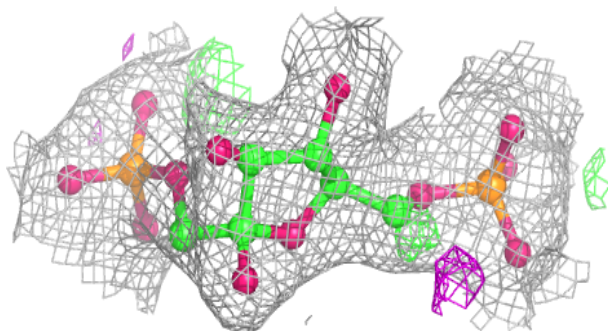
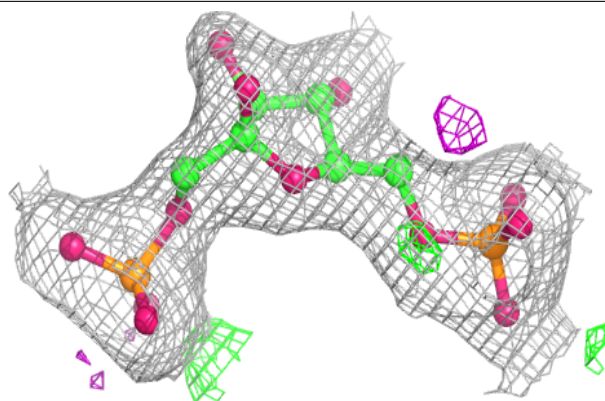
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



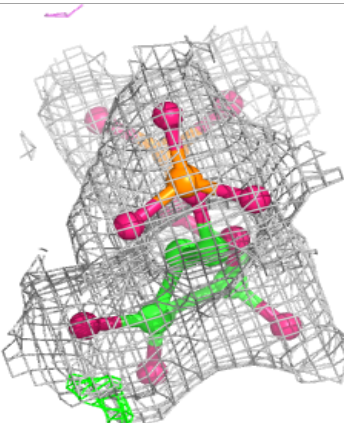
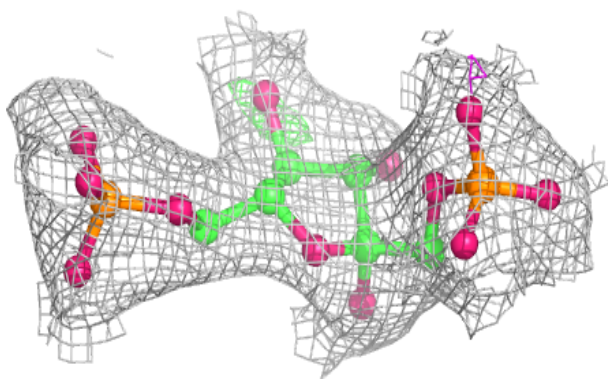
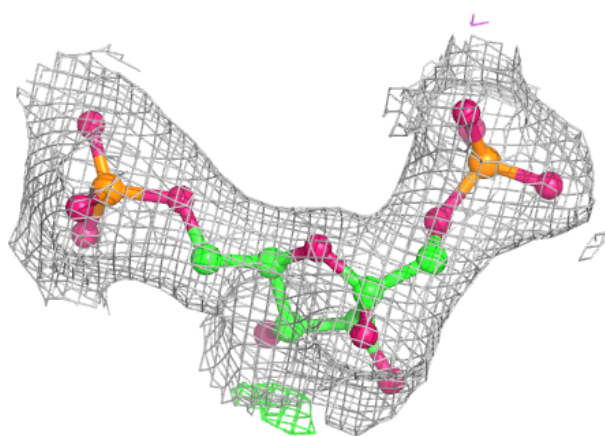


**Electron density around FBP A 601:**

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

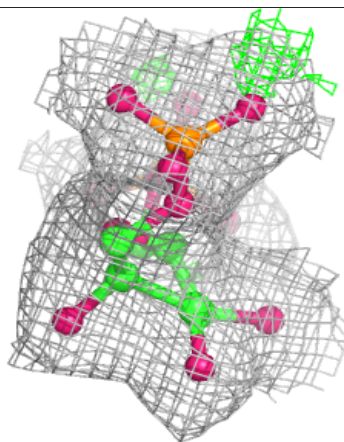
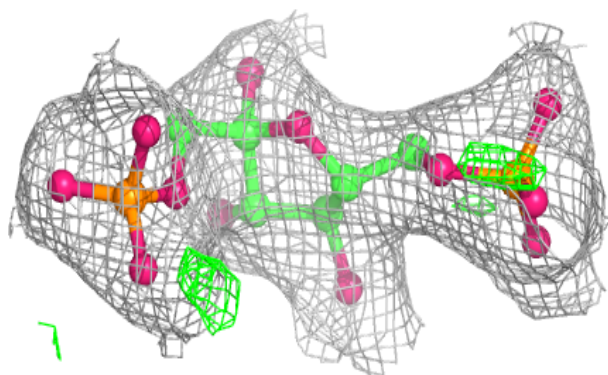
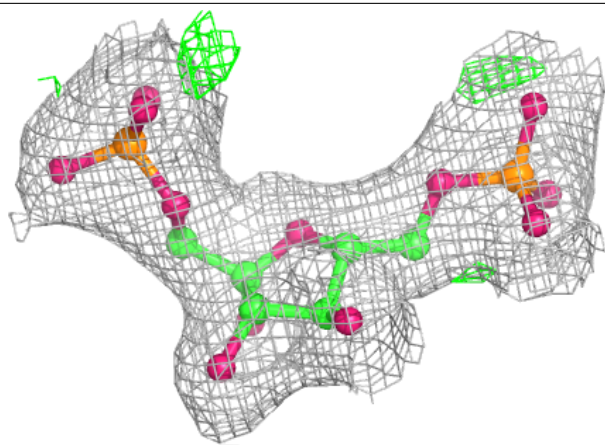
**Electron density around FBP B 601:**

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

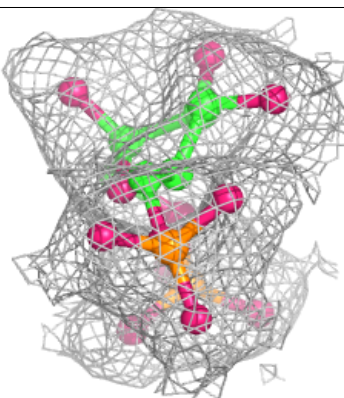
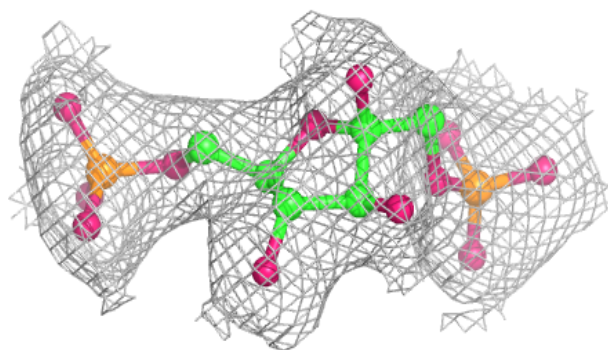
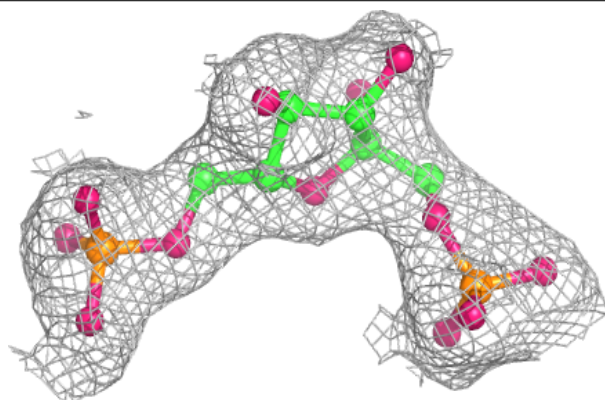


**Electron density around FBP F 601:**

$2mF_o-DF_c$  (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:**

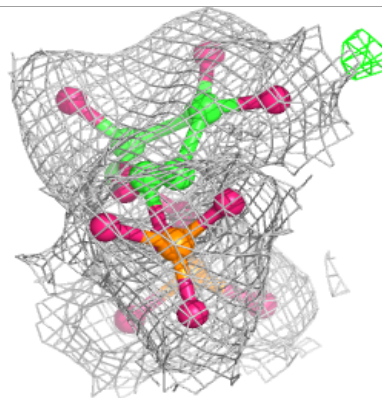
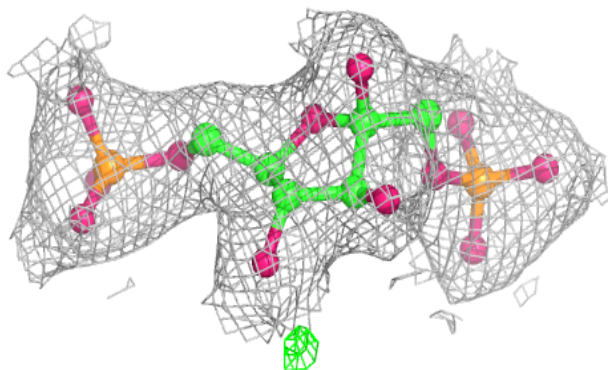
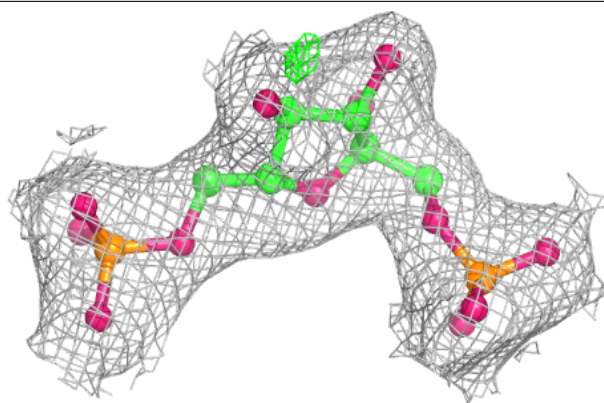
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



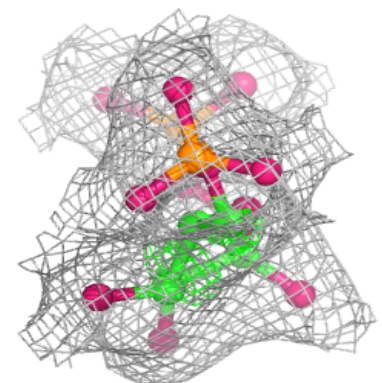
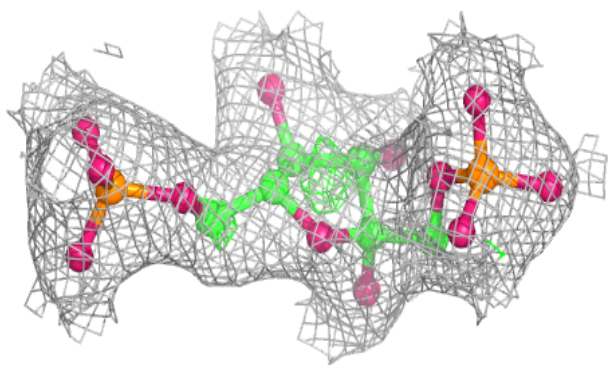
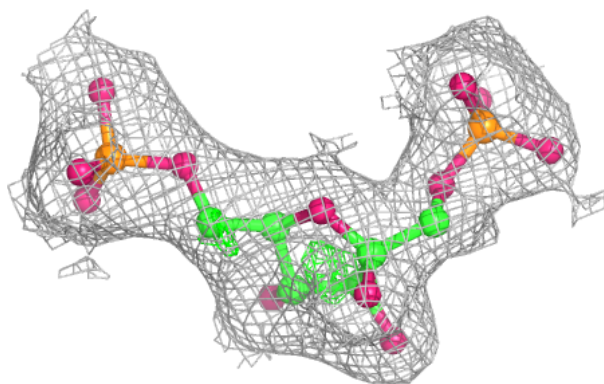


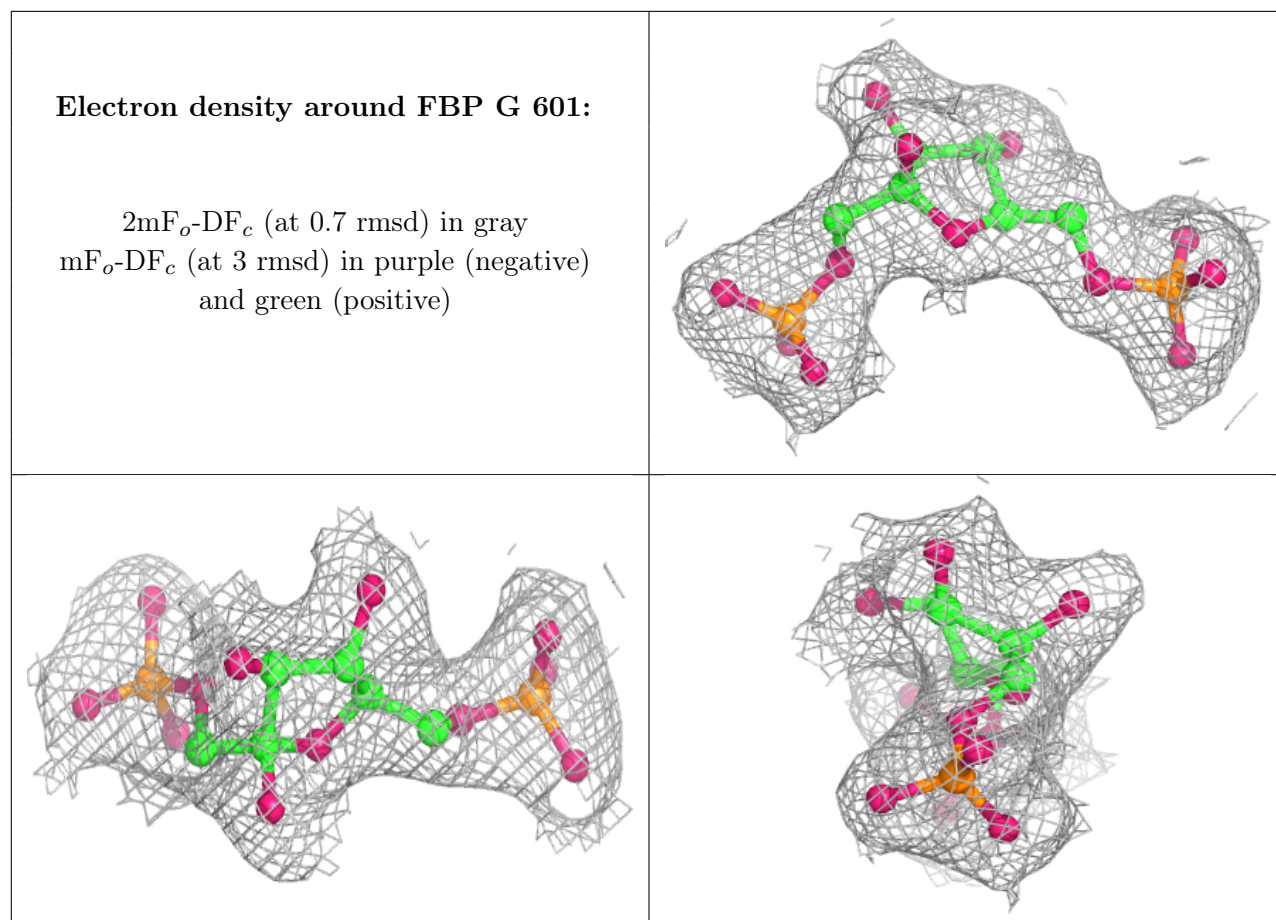
**Electron density around FBP D 601:**

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

**Electron density around FBP H 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.