



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 11:24 PM UTC

PDB ID : 9RFT / pdb\_00009rft  
Title : Structure of liver pyruvate kinase in complex with Liver pyruvate kinase in complex with fluorescent probe II  
Authors : Bogucka, A.; Nilsson, O.; Grotli, M.; Hyvonen, M.  
Deposited on : 2025-06-04  
Resolution : 2.27 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:

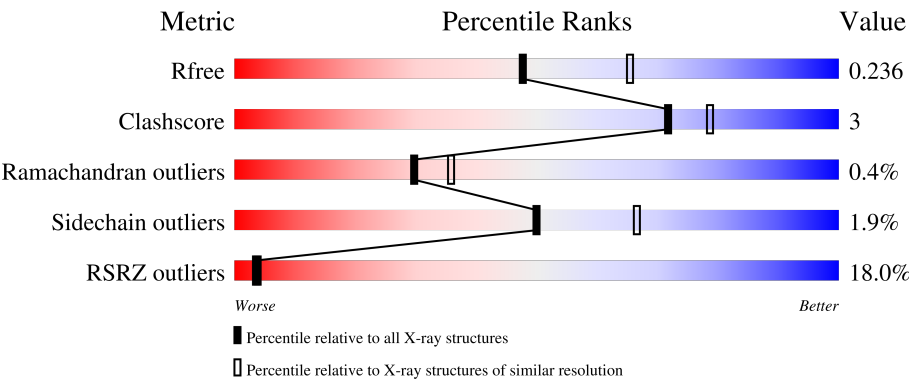
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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>41%</div><div><div></div><div></div><div></div><div></div></div><div>85%9%5%</div></div>
1	B	447	<div><div>33%</div><div><div></div><div></div><div></div><div></div></div><div>89%8%..</div></div>
1	C	447	<div><div>14%</div><div><div></div><div></div><div></div><div></div></div><div>85%9%..</div></div>
1	D	447	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>86%8%5%</div></div>
1	E	447	<div><div>26%</div><div><div></div><div></div><div></div><div></div></div><div>86%8%5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	502	-	X	-	-
3	OXL	B	502	-	X	-	-
3	OXL	C	503	-	X	-	-
3	OXL	D	502	-	X	-	-
3	OXL	E	502	-	X	-	-
3	OXL	G	502	-	X	-	-
3	OXL	H	502	-	X	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28404 atoms, of which 76 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
			3231	2030	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	131	SER	ASP	linker	UNP P30613
A	132	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	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

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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	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
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	131	SER	ASP	linker	UNP P30613
D	132	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	131	SER	ASP	linker	UNP P30613
E	132	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	131	SER	ASP	linker	UNP P30613
F	132	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	131	SER	ASP	linker	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
G	132	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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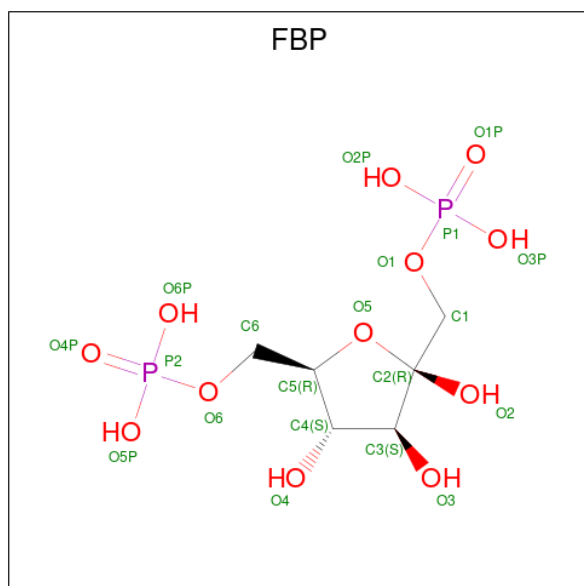
Chain	Residue	Modelled	Actual	Comment	Reference
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H	?	-	VAL	deletion	UNP P30613
H	?	-	TRP	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	TYR	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	ASN	deletion	UNP 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	131	SER	ASP	linker	UNP P30613
H	132	GLY	LEU	linker	UNP P30613

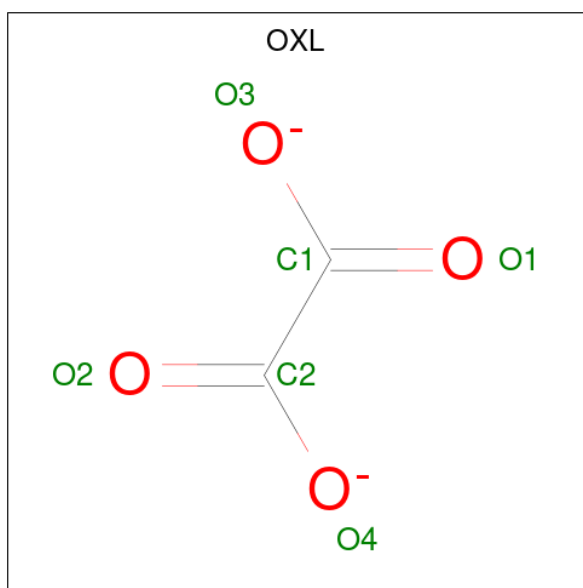
- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).





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

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

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

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

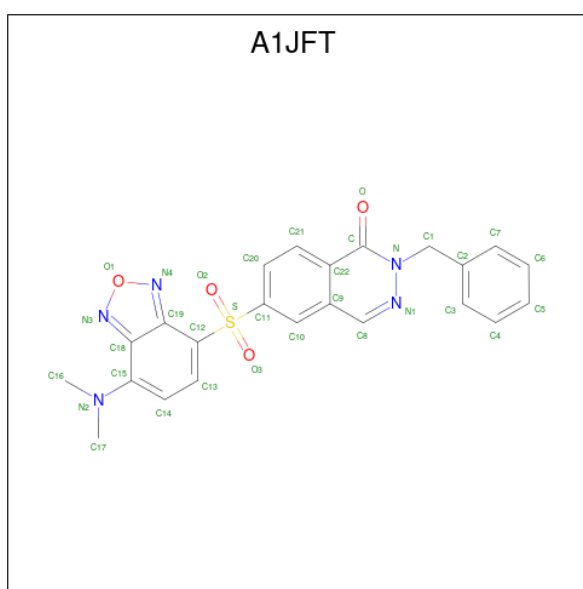
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	E	1	Total K 1 1	0	0

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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 6-[[7-(dimethylamino)-2,1,3-benzoxadiazol-4-yl]sulfonyl]-2-(phenylmethyl)phthalazin-1-one (CCD ID: A1JFT) (formula: C<sub>23</sub>H<sub>19</sub>N<sub>5</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 52	C 23	H 19	N 5	O 4	S 1	19	0
6	C	1	Total 52	C 23	H 19	N 5	O 4	S 1	19	0
6	E	1	Total 52	C 23	H 19	N 5	O 4	S 1	19	0
6	F	1	Total 52	C 23	H 19	N 5	O 4	S 1	19	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	104	Total O 104 104	0	0

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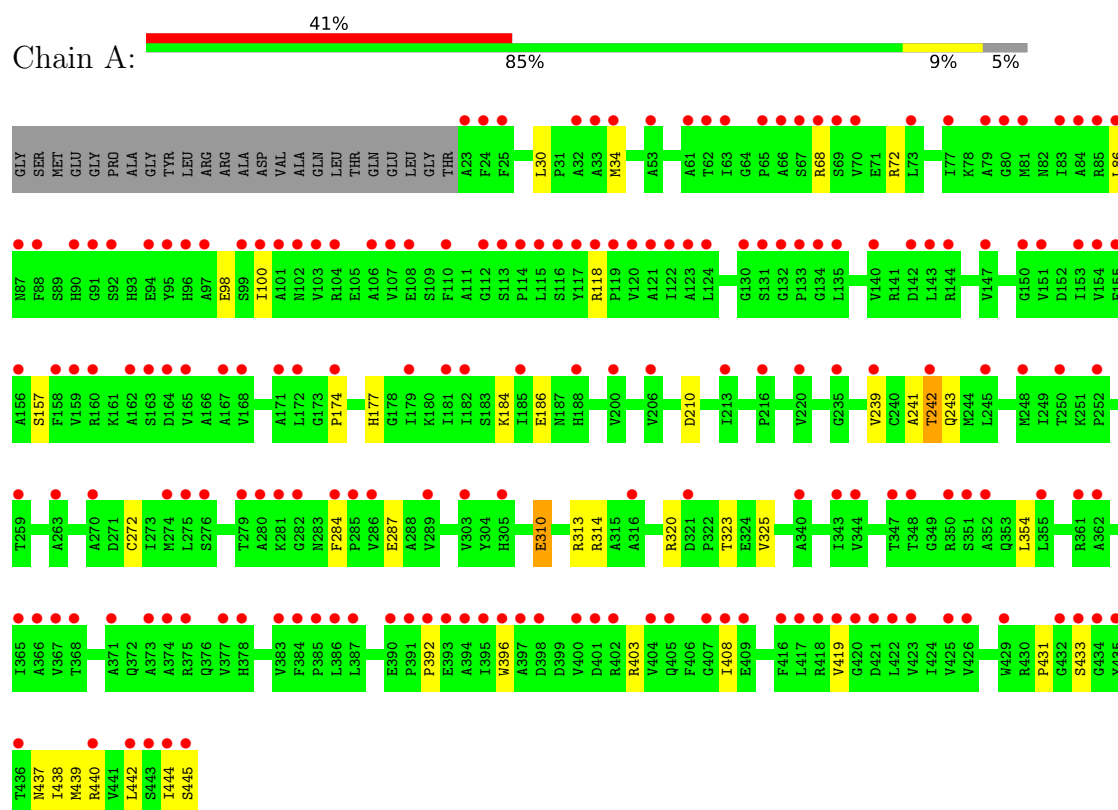
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	115	Total 115	O 115	0	0
7	C	256	Total 256	O 256	0	0
7	D	305	Total 305	O 305	0	0
7	E	143	Total 143	O 143	0	0
7	F	234	Total 234	O 234	0	0
7	G	300	Total 300	O 300	0	0
7	H	376	Total 376	O 376	0	0

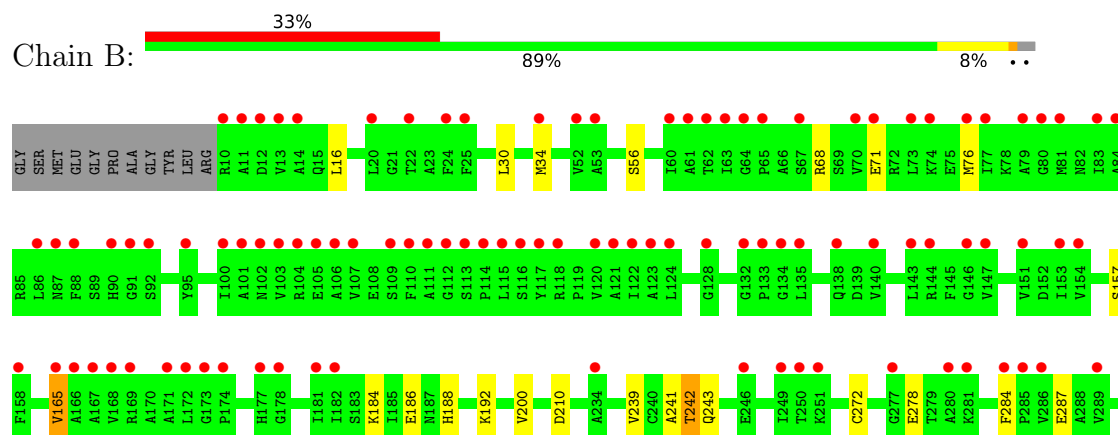
### 3 Residue-property plots [i](#)

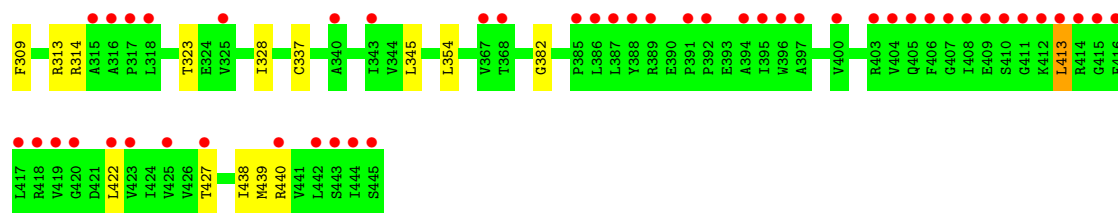
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

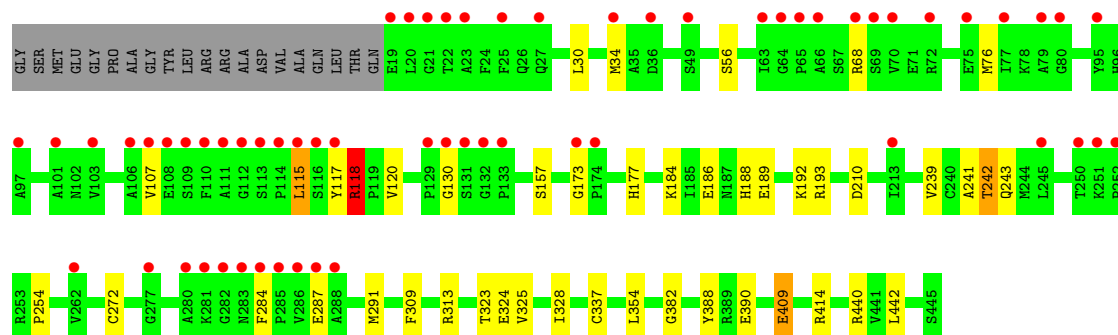
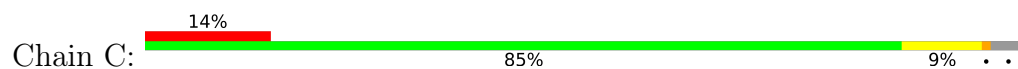


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

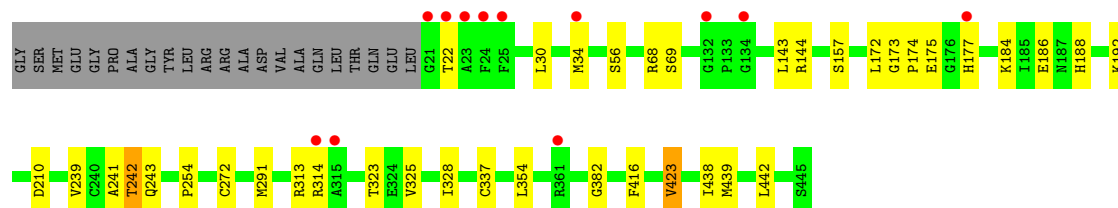
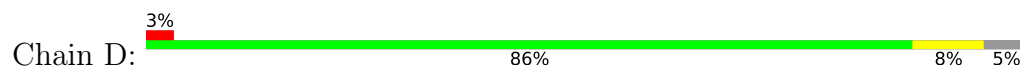




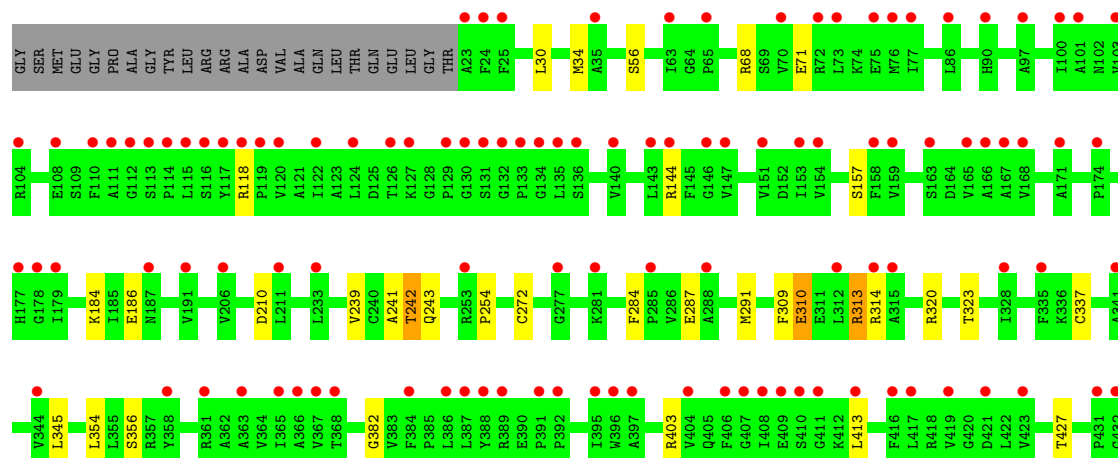
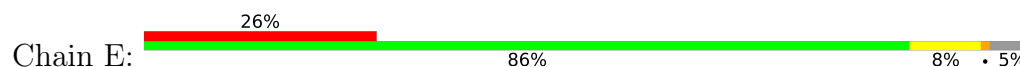
● Molecule 1: Isoform L-type of Pyruvate kinase PKLR

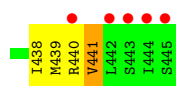


● Molecule 1: Isoform L-type of Pyruvate kinase PKLR

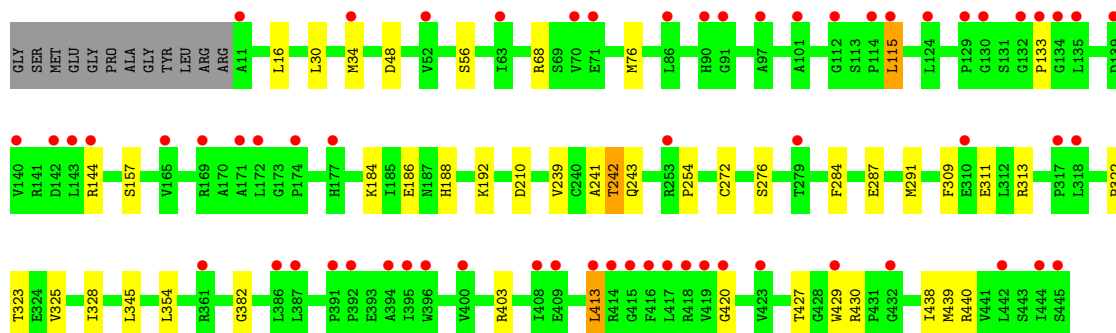
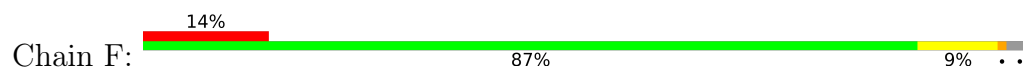


● Molecule 1: Isoform L-type of Pyruvate kinase PKLR

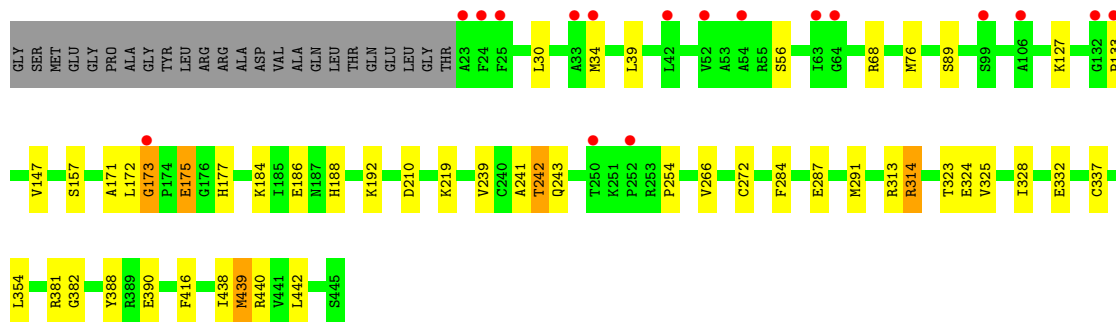
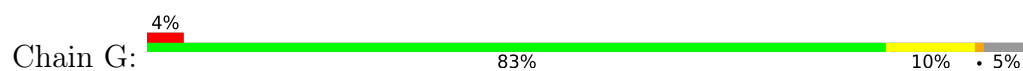




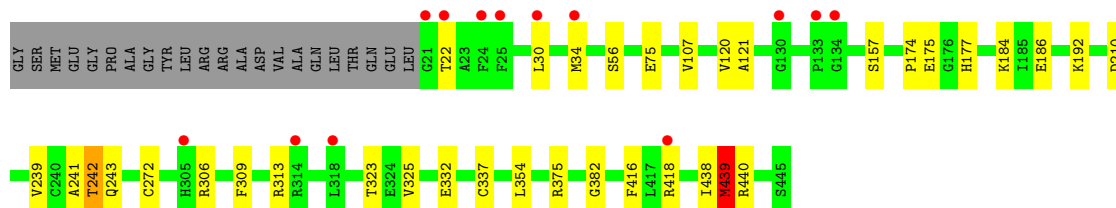
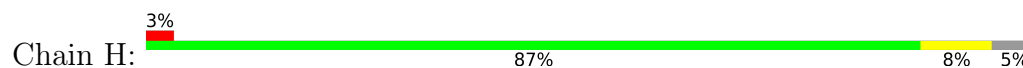
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



- 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, $\alpha$ , $\beta$ , $\gamma$	207.92Å 112.97Å 188.56Å 90.00° 91.44° 90.00°	Depositor
Resolution (Å)	188.50 – 2.27 188.50 – 2.27	Depositor EDS
% Data completeness (in resolution range)	66.2 (188.50-2.27) 66.2 (188.50-2.27)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.210 , 0.245 0.203 , 0.236	Depositor DCC
$R_{free}$ test set	6787 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	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 75.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1410e-06. 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: A1JFT, FBP, OXL, MG, 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	0.67	0/3316	1.05	2/4484 (0.0%)
1	B	0.65	0/3396	1.04	2/4592 (0.0%)
1	C	0.73	0/3324	1.05	3/4495 (0.1%)
1	D	0.73	0/3326	1.03	3/4497 (0.1%)
1	E	0.65	0/3301	1.04	2/4463 (0.0%)
1	F	0.70	1/3411 (0.0%)	1.04	2/4613 (0.0%)
1	G	0.74	1/3314 (0.0%)	1.04	5/4481 (0.1%)
1	H	0.76	1/3316 (0.0%)	1.05	3/4483 (0.1%)
All	All	0.70	3/26704 (0.0%)	1.04	22/36108 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	439	MET	SD-CE	-6.09	1.64	1.79
1	H	439	MET	SD-CE	-5.56	1.65	1.79
1	F	276	SER	CA-C	5.38	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	172	LEU	CA-C-N	5.81	130.99	121.87
1	G	172	LEU	C-N-CA	5.81	130.99	121.87
1	C	409	GLU	CB-CG-CD	5.47	121.89	112.60
1	G	416	PHE	CA-CB-CG	5.38	119.18	113.80
1	H	416	PHE	CA-CB-CG	5.33	119.13	113.80
1	D	416	PHE	CA-CB-CG	5.32	119.12	113.80
1	C	241	ALA	CA-C-N	5.30	131.66	121.54
1	C	241	ALA	C-N-CA	5.30	131.66	121.54
1	H	241	ALA	CA-C-N	5.29	131.65	121.54
1	H	241	ALA	C-N-CA	5.29	131.65	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	241	ALA	CA-C-N	5.23	131.53	121.54
1	D	241	ALA	C-N-CA	5.23	131.53	121.54
1	B	241	ALA	CA-C-N	5.21	131.49	121.54
1	B	241	ALA	C-N-CA	5.21	131.49	121.54
1	E	241	ALA	CA-C-N	5.17	131.41	121.54
1	E	241	ALA	C-N-CA	5.17	131.41	121.54
1	F	241	ALA	CA-C-N	5.15	131.38	121.54
1	F	241	ALA	C-N-CA	5.15	131.38	121.54
1	G	241	ALA	CA-C-N	5.11	131.30	121.54
1	G	241	ALA	C-N-CA	5.11	131.30	121.54
1	A	241	ALA	CA-C-N	5.07	131.22	121.54
1	A	241	ALA	C-N-CA	5.07	131.22	121.54

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	3243	0	3308	23	0
1	B	3329	0	3394	26	1
1	C	3257	0	3308	27	0
1	D	3252	0	3310	20	0
1	E	3231	0	3289	21	0
1	F	3335	0	3404	28	0
1	G	3241	0	3293	31	0
1	H	3251	0	3306	24	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	1	0
2	F	20	0	10	1	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	B	33	19	0	0	0
6	C	33	19	0	0	0
6	E	33	19	0	1	0
6	F	33	19	0	2	0
7	A	104	0	0	1	0
7	B	115	0	0	1	0
7	C	256	0	0	1	0
7	D	305	0	0	1	0
7	E	143	0	0	0	0
7	F	234	0	0	1	0
7	G	300	0	0	1	0
7	H	376	0	0	1	0
All	All	28328	76	26692	173	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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:C:324[A]:GLU:HG3	1:C:354:LEU:HD13	1.60	0.82
1:E:310:GLU:OE2	1:F:313:ARG:NH2	2.13	0.81
1:G:324[A]:GLU:HG3	1:G:354:LEU:HD13	1.64	0.79
1:C:313:ARG:HG3	1:C:328:ILE:HD11	1.66	0.78
1:A:310:GLU:OE2	1:B:313:ARG:NH2	2.17	0.76
1:E:441:VAL:HG22	1:F:322:PRO:HB3	1.72	0.71
1:C:440:ARG:HD3	7:C:637:HOH:O	1.92	0.68
1:G:440:ARG:HG2	1:H:438:ILE:HG12	1.75	0.67
1:G:313:ARG:HG2	1:G:328:ILE:HD11	1.78	0.66
1:A:320[A]:ARG:HG3	1:B:16:LEU:HD11	1.77	0.66
1:G:438:ILE:HG12	1:H:440[A]:ARG:HG2	1.79	0.64
1:H:56:SER:HB2	1:H:382:GLY:HA2	1.80	0.64
1:E:320:ARG:NH2	1:F:420:GLY:O	2.31	0.64
1:G:323:THR:HG22	1:G:354:LEU:HD12	1.81	0.62
1:C:440:ARG:HG2	1:D:438:ILE:HG12	1.81	0.62
1:A:438:ILE:HG12	1:B:440:ARG:HG2	1.81	0.61
1:H:75:GLU:HG3	7:H:921:HOH:O	2.00	0.61
1:A:174:PRO:HA	1:A:177:HIS:NE2	2.16	0.61
1:B:56:SER:HB2	1:B:382:GLY:HA2	1.83	0.61
1:C:242:THR:HG22	1:C:243:GLN:HG3	1.84	0.60
1:G:173:GLY:O	1:G:177:HIS:CE1	2.55	0.59
1:A:440:ARG:HG2	1:B:438:ILE:HG12	1.84	0.59
1:F:56:SER:HB2	1:F:382:GLY:HA2	1.84	0.59
1:D:174:PRO:HA	1:D:177[A]:HIS:CE1	2.38	0.59
1:E:441:VAL:CG2	1:F:322:PRO:HB3	2.32	0.59
1:G:242:THR:HG22	1:G:243:GLN:HG3	1.85	0.59
1:E:309:PHE:O	1:E:313:ARG:HB2	2.03	0.58
1:D:242:THR:HG22	1:D:243:GLN:HG3	1.85	0.58
1:E:440:ARG:HG2	1:F:438:ILE:HG12	1.85	0.58
1:H:174:PRO:HA	1:H:177[A]:HIS:CE1	2.38	0.58
1:A:242:THR:HG22	1:A:243:GLN:HG3	1.86	0.57
1:B:242:THR:HG22	1:B:243:GLN:HG3	1.86	0.57
1:E:242:THR:HG22	1:E:243:GLN:HG3	1.86	0.57
1:E:438:ILE:HG12	1:F:440:ARG:HG2	1.87	0.56
1:F:313:ARG:HG2	1:F:328:ILE:HD11	1.87	0.56
1:C:323:THR:HG22	1:C:354:LEU:HD12	1.87	0.56
1:G:89:SER:HA	1:G:127:LYS:HG3	1.86	0.56
1:F:284:PHE:HB3	1:F:287:GLU:HB2	1.87	0.56
1:E:56:SER:HB2	1:E:382:GLY:HA2	1.87	0.56
1:C:56:SER:HB2	1:C:382:GLY:HA2	1.86	0.55
1:E:320:ARG:HG3	1:F:16:LEU:HD11	1.88	0.55
1:G:314:ARG:CZ	1:H:306:ARG:HD3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:NH1	2:A:501:FBP:O2P	2.29	0.55
1:B:313:ARG:HG2	1:B:328:ILE:HD11	1.88	0.55
1:B:71:GLU:H	1:B:71:GLU:CD	2.14	0.54
1:D:56:SER:HB2	1:D:382:GLY:HA2	1.88	0.54
1:A:396:TRP:NE1	1:A:431:PRO:HG3	2.22	0.54
1:D:313:ARG:HG2	1:D:328:ILE:HD11	1.90	0.54
1:F:345:LEU:HD22	1:F:427:THR:HG22	1.89	0.54
1:G:439:MET:HE3	1:H:439:MET:HG2	1.90	0.54
1:H:309:PHE:O	1:H:313:ARG:HG3	2.07	0.54
1:C:117:TYR:O	1:C:118:ARG:HB2	2.09	0.53
1:G:219:LYS:NZ	7:G:604:HOH:O	2.41	0.53
1:A:284:PHE:HB3	1:A:287:GLU:HB2	1.90	0.53
1:G:171:ALA:C	1:G:173:GLY:H	2.15	0.53
1:H:242:THR:HG22	1:H:243:GLN:HG3	1.90	0.53
1:E:345:LEU:HD13	1:E:427:THR:HG22	1.91	0.52
1:F:242:THR:HG22	1:F:243:GLN:HG3	1.91	0.52
1:H:309:PHE:CE2	1:H:313:ARG:HD3	2.45	0.52
1:B:284:PHE:HB3	1:B:287:GLU:HB2	1.91	0.52
1:H:323:THR:HG22	1:H:354:LEU:HD12	1.93	0.51
1:G:337:CYS:HB3	1:H:325:VAL:HG21	1.91	0.51
1:A:419:VAL:HG22	1:A:445:SER:HB3	1.91	0.51
1:B:309:PHE:CE2	1:B:313:ARG:NH1	2.77	0.51
1:B:309:PHE:CD2	1:B:313:ARG:NH1	2.79	0.51
1:F:309:PHE:CD2	1:F:313:ARG:NH1	2.79	0.50
1:H:56:SER:HB2	1:H:382:GLY:CA	2.41	0.50
1:G:56:SER:HB2	1:G:382:GLY:HA2	1.93	0.50
1:G:284:PHE:HB3	1:G:287:GLU:HB2	1.91	0.50
1:A:392:PRO:HD3	7:A:699:HOH:O	2.10	0.50
1:F:309:PHE:CE2	1:F:313:ARG:NH1	2.79	0.49
1:C:107:VAL:HG21	1:C:120:VAL:HB	1.94	0.49
1:A:30:LEU:O	1:A:34:MET:HG2	2.13	0.49
1:C:388:TYR:CZ	1:C:390:GLU:HB2	2.47	0.49
1:C:173:GLY:O	1:C:177:HIS:CE1	2.65	0.49
1:E:403:ARG:NH1	2:E:501:FBP:O3P	2.44	0.49
1:F:30:LEU:O	1:F:34:MET:HG2	2.13	0.49
1:F:323:THR:HG22	1:F:354:LEU:HD12	1.95	0.49
1:G:332[B]:GLU:OE2	1:H:332:GLU:OE1	2.31	0.48
1:A:68:ARG:HH22	1:A:98:GLU:HB3	1.78	0.48
1:B:165:VAL:HG11	1:B:200:VAL:HG23	1.95	0.48
1:B:165:VAL:HG21	1:B:200:VAL:HG23	1.95	0.48
1:B:56:SER:HB2	1:B:382:GLY:CA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:GLU:OE1	6:F:505:A1JFT:O1	2.32	0.48
1:C:30:LEU:O	1:C:34:MET:HG2	2.13	0.48
1:B:345:LEU:HD13	1:B:427:THR:HG22	1.95	0.48
1:B:30:LEU:O	1:B:34:MET:HG2	2.14	0.48
1:E:323:THR:HG22	1:E:354:LEU:HD12	1.96	0.48
1:A:320[B]:ARG:HG2	1:B:422:LEU:HD12	1.96	0.47
1:C:115:LEU:HD21	1:C:409:GLU:HB3	1.97	0.47
1:E:284:PHE:HB3	1:E:287:GLU:HB2	1.96	0.47
1:H:30:LEU:O	1:H:34:MET:HG2	2.15	0.47
1:D:423:VAL:HG12	1:D:442:LEU:HB3	1.96	0.47
1:F:56:SER:HB2	1:F:382:GLY:CA	2.45	0.47
1:G:254:PRO:HG3	1:G:291:MET:HG2	1.96	0.47
1:G:332[A]:GLU:OE1	1:H:332:GLU:OE1	2.33	0.47
1:G:30:LEU:O	1:G:34:MET:HG2	2.14	0.47
1:G:266:VAL:O	1:G:381:ARG:NH1	2.47	0.46
1:E:239:VAL:HG22	1:E:272:CYS:HB2	1.97	0.46
1:G:323:THR:CG2	1:G:354:LEU:HD12	2.45	0.46
1:C:56:SER:HB2	1:C:382:GLY:CA	2.45	0.46
1:D:143:LEU:HD22	1:D:172:LEU:HD21	1.97	0.46
6:E:505:A1JFT:C16	1:G:39:LEU:HD13	2.46	0.46
1:H:121:ALA:HB2	1:H:375:ARG:O	2.16	0.46
1:A:239:VAL:HG22	1:A:272:CYS:HB2	1.97	0.46
1:C:157:SER:HA	1:C:184:LYS:HD3	1.98	0.46
1:C:313:ARG:HH12	1:D:313:ARG:NH2	2.14	0.45
1:G:157:SER:HA	1:G:184:LYS:HD3	1.97	0.45
1:G:388:TYR:CZ	1:G:390:GLU:HB2	2.51	0.45
1:D:30:LEU:O	1:D:34:MET:HG3	2.16	0.45
1:F:115:LEU:HD22	1:F:413:LEU:HG	1.98	0.45
1:B:71:GLU:HG3	7:B:667:HOH:O	2.15	0.45
1:C:284:PHE:HB3	1:C:287:GLU:HB2	1.99	0.45
1:A:157:SER:HA	1:A:184:LYS:HD3	1.99	0.45
1:A:323:THR:HG22	1:A:354:LEU:HD12	1.97	0.45
1:G:147:VAL:HG11	1:G:175:GLU:HG2	1.98	0.45
1:D:56:SER:HB2	1:D:382:GLY:CA	2.47	0.45
1:D:323:THR:HG22	1:D:354:LEU:HD12	1.99	0.45
1:E:157:SER:HA	1:E:184:LYS:HD3	1.98	0.45
1:D:175:GLU:HB2	7:D:634:HOH:O	2.17	0.44
1:G:56:SER:CB	1:G:382:GLY:HA2	2.48	0.44
1:E:254:PRO:HG3	1:E:291:MET:HG2	2.00	0.44
1:C:239:VAL:HG22	1:C:272:CYS:HB2	1.99	0.44
1:B:239:VAL:HG22	1:B:272:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:VAL:HG22	1:F:272:CYS:HB2	1.99	0.44
1:A:396:TRP:CE2	1:A:431:PRO:HG3	2.53	0.43
1:B:323:THR:HG22	1:B:354:LEU:HD12	2.00	0.43
1:C:186:GLU:HB3	1:C:210:ASP:HB2	2.00	0.43
1:D:157:SER:HA	1:D:184:LYS:HD3	2.00	0.43
1:A:325:VAL:HG21	1:B:337:CYS:HB3	1.99	0.43
1:B:186:GLU:HB3	1:B:210:ASP:HB2	2.01	0.43
1:C:188:HIS:CE1	1:C:192:LYS:HG3	2.54	0.43
1:B:157:SER:HA	1:B:184:LYS:HD3	2.00	0.43
1:G:239:VAL:HG22	1:G:272:CYS:HB2	2.01	0.43
1:C:388:TYR:CE2	1:C:390:GLU:HB2	2.54	0.43
1:F:403:ARG:NH1	2:F:501:FBP:O2P	2.28	0.43
1:A:186:GLU:HB3	1:A:210:ASP:HB2	2.01	0.42
1:D:239:VAL:HG22	1:D:272:CYS:HB2	2.01	0.42
1:F:157:SER:HA	1:F:184:LYS:HD3	2.00	0.42
1:G:56:SER:HB2	1:G:382:GLY:CA	2.49	0.42
1:D:144[A]:ARG:HH22	1:D:173:GLY:HA3	1.84	0.42
1:E:30:LEU:O	1:E:34:MET:HG3	2.20	0.42
1:H:239:VAL:HG22	1:H:272:CYS:HB2	2.02	0.42
1:C:189:GLU:HG2	1:C:193:ARG:HD2	2.00	0.42
1:D:186:GLU:HB3	1:D:210:ASP:HB2	2.01	0.42
1:H:157:SER:HA	1:H:184:LYS:HD3	2.00	0.42
1:D:188:HIS:CE1	1:D:192:LYS:HG3	2.55	0.42
1:G:188:HIS:CE1	1:G:192:LYS:HG3	2.55	0.42
1:B:71:GLU:CD	1:B:71:GLU:N	2.77	0.42
1:F:48:ASP:OD2	1:H:192:LYS:HE2	2.20	0.42
1:C:309:PHE:O	1:C:313:ARG:HB2	2.20	0.41
1:E:56:SER:HB2	1:E:382:GLY:CA	2.48	0.41
1:D:254:PRO:HG3	1:D:291:MET:HG2	2.02	0.41
1:H:121:ALA:HA	1:H:375:ARG:HB3	2.00	0.41
1:F:186:GLU:HB3	1:F:210:ASP:HB2	2.01	0.41
1:F:254:PRO:HG3	1:F:291:MET:HG2	2.02	0.41
1:F:429:TRP:CE2	1:F:430:ARG:HG2	2.55	0.41
6:F:505:A1JFT:O3	7:F:601:HOH:O	2.20	0.41
1:B:188:HIS:CE1	1:B:192:LYS:HG3	2.56	0.41
1:C:117:TYR:H	1:C:414:ARG:NH2	2.18	0.41
1:C:254:PRO:HG3	1:C:291:MET:HG2	2.02	0.41
1:F:188:HIS:CE1	1:F:192:LYS:HG3	2.56	0.41
1:A:408:ILE:HG23	1:A:444:ILE:HD12	2.03	0.41
1:E:186:GLU:HB3	1:E:210:ASP:HB2	2.02	0.41
1:G:186:GLU:HB3	1:G:210:ASP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD21	1:A:100:ILE:HG13	2.03	0.41
1:H:186:GLU:HB3	1:H:210:ASP:HB2	2.03	0.41
1:G:325:VAL:HG21	1:H:337:CYS:HB3	2.01	0.41
1:C:337:CYS:HB3	1:D:325:VAL:HG21	2.02	0.40
1:H:107:VAL:HG21	1:H:120:VAL:HB	2.03	0.40
1:C:325:VAL:HG21	1:D:337:CYS:HB3	2.02	0.40
1:E:337:CYS:HB3	1:F:325:VAL:HG21	2.03	0.40
1:A:313:ARG:HH21	1:B:313:ARG:HH22	1.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LEU:O	1:B:413:LEU:O[2_555]	2.07	0.13

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/447 (96%)	419 (98%)	6 (1%)	2 (0%)	24	29
1	B	438/447 (98%)	431 (98%)	6 (1%)	1 (0%)	43	53
1	C	429/447 (96%)	417 (97%)	9 (2%)	3 (1%)	18	21
1	D	429/447 (96%)	423 (99%)	5 (1%)	1 (0%)	43	53
1	E	426/447 (95%)	420 (99%)	5 (1%)	1 (0%)	43	53
1	F	440/447 (98%)	432 (98%)	6 (1%)	2 (0%)	24	29
1	G	427/447 (96%)	417 (98%)	7 (2%)	3 (1%)	18	21
1	H	427/447 (96%)	421 (99%)	5 (1%)	1 (0%)	43	53
All	All	3443/3576 (96%)	3380 (98%)	49 (1%)	14 (0%)	30	36



All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	118	ARG
1	C	130	GLY
1	F	133	PRO
1	G	173	GLY
1	A	242	THR
1	C	242	THR
1	D	242	THR
1	E	242	THR
1	G	242	THR
1	A	437	ASN
1	B	242	THR
1	F	242	THR
1	H	242	THR
1	G	133	PRO

### 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%)	333 (98%)	8 (2%)	44	60
1	B	349/352 (99%)	340 (97%)	9 (3%)	40	56
1	C	342/352 (97%)	336 (98%)	6 (2%)	51	68
1	D	342/352 (97%)	336 (98%)	6 (2%)	51	68
1	E	340/352 (97%)	327 (96%)	13 (4%)	29	42
1	F	351/352 (100%)	343 (98%)	8 (2%)	44	60
1	G	341/352 (97%)	335 (98%)	6 (2%)	51	68
1	H	340/352 (97%)	336 (99%)	4 (1%)	63	77
All	All	2746/2816 (98%)	2686 (98%)	60 (2%)	50	62

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	118	ARG
1	A	310	GLU
1	A	314	ARG
1	A	433	SER
1	A	439[A]	MET
1	A	439[B]	MET
1	A	442	LEU
1	B	68	ARG
1	B	76[A]	MET
1	B	76[B]	MET
1	B	165	VAL
1	B	278	GLU
1	B	314	ARG
1	B	413	LEU
1	B	439[A]	MET
1	B	439[B]	MET
1	C	68	ARG
1	C	76[A]	MET
1	C	76[B]	MET
1	C	115	LEU
1	C	118	ARG
1	C	442	LEU
1	D	22	THR
1	D	68	ARG
1	D	69	SER
1	D	314	ARG
1	D	423	VAL
1	D	439	MET
1	E	68	ARG
1	E	71	GLU
1	E	118	ARG
1	E	144	ARG
1	E	310	GLU
1	E	313	ARG
1	E	314	ARG
1	E	356[A]	SER
1	E	356[B]	SER
1	E	413	LEU
1	E	439[A]	MET
1	E	439[B]	MET
1	E	441	VAL
1	F	68	ARG

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Mol	Chain	Res	Type
1	F	76[A]	MET
1	F	76[B]	MET
1	F	115	LEU
1	F	144	ARG
1	F	413	LEU
1	F	439[A]	MET
1	F	439[B]	MET
1	G	68	ARG
1	G	76[A]	MET
1	G	76[B]	MET
1	G	175	GLU
1	G	314	ARG
1	G	442	LEU
1	H	22	THR
1	H	175	GLU
1	H	418	ARG
1	H	439	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	90	HIS
1	B	27	GLN
1	B	90	HIS
1	C	27	GLN
1	C	90	HIS
1	C	177	HIS
1	D	27	GLN
1	D	90	HIS
1	E	27	GLN
1	E	90	HIS
1	E	305	HIS
1	F	27	GLN
1	F	90	HIS
1	G	27	GLN
1	G	90	HIS
1	G	177	HIS
1	G	305	HIS
1	H	27	GLN
1	H	90	HIS
1	H	292	GLN

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Mol	Chain	Res	Type
1	H	305	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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$
2	FBP	D	501	-	18,20,20	0.66	0	21,32,32	0.91	1 (4%)
3	OXL	F	502	4	5,5,5	2.20	2 (40%)	6,6,6	2.11	3 (50%)
2	FBP	G	501	-	18,20,20	0.40	0	21,32,32	0.94	1 (4%)
6	A1JFT	F	505	-	37,37,37	1.07	4 (10%)	47,55,55	1.24	4 (8%)
6	A1JFT	E	505	-	37,37,37	1.10	4 (10%)	47,55,55	1.24	4 (8%)
3	OXL	B	502	4	5,5,5	2.20	2 (40%)	6,6,6	1.70	2 (33%)
3	OXL	D	502	4	5,5,5	2.35	3 (60%)	6,6,6	2.29	2 (33%)
6	A1JFT	C	501	-	37,37,37	1.07	4 (10%)	47,55,55	1.25	4 (8%)
2	FBP	B	501	-	18,20,20	0.54	0	21,32,32	0.79	1 (4%)
3	OXL	E	502	4	5,5,5	2.17	2 (40%)	6,6,6	1.78	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FBP	E	501	-	18,20,20	0.41	0	21,32,32	0.70	0
3	OXL	A	502	4	5,5,5	2.16	2 (40%)	6,6,6	1.73	1 (16%)
2	FBP	C	502	-	18,20,20	0.46	0	21,32,32	0.88	1 (4%)
2	FBP	F	501	-	18,20,20	0.36	0	21,32,32	0.69	0
2	FBP	A	501	-	18,20,20	0.37	0	21,32,32	0.73	0
3	OXL	H	502	4	5,5,5	2.06	2 (40%)	6,6,6	2.00	2 (33%)
3	OXL	C	503	4	5,5,5	2.17	2 (40%)	6,6,6	2.07	3 (50%)
3	OXL	G	502	4	5,5,5	2.11	2 (40%)	6,6,6	2.25	2 (33%)
6	A1JFT	B	505	-	37,37,37	1.01	4 (10%)	47,55,55	1.25	3 (6%)
2	FBP	H	501	-	18,20,20	0.81	1 (5%)	21,32,32	0.78	0

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	501	-	-	2/13/32/32	0/1/1/1
3	OXL	F	502	4	-	0/4/4/4	-
2	FBP	G	501	-	-	2/13/32/32	0/1/1/1
6	A1JFT	F	505	-	-	0/20/20/20	0/5/5/5
6	A1JFT	E	505	-	-	0/20/20/20	0/5/5/5
3	OXL	B	502	4	-	4/4/4/4	-
3	OXL	D	502	4	-	4/4/4/4	-
6	A1JFT	C	501	-	-	0/20/20/20	0/5/5/5
2	FBP	B	501	-	-	4/13/32/32	0/1/1/1
3	OXL	E	502	4	-	4/4/4/4	-
2	FBP	E	501	-	-	2/13/32/32	0/1/1/1
3	OXL	A	502	4	-	4/4/4/4	-
2	FBP	C	502	-	-	2/13/32/32	0/1/1/1
2	FBP	F	501	-	-	2/13/32/32	0/1/1/1
2	FBP	A	501	-	-	2/13/32/32	0/1/1/1
3	OXL	H	502	4	-	4/4/4/4	-
3	OXL	C	503	4	-	4/4/4/4	-
3	OXL	G	502	4	-	4/4/4/4	-
6	A1JFT	B	505	-	-	0/20/20/20	0/5/5/5
2	FBP	H	501	-	-	2/13/32/32	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	OXL	O2-C2	4.09	1.32	1.22
6	E	505	A1JFT	C18-N3	3.91	1.37	1.31
3	A	502	OXL	O2-C2	3.80	1.31	1.22
3	F	502	OXL	O2-C2	3.79	1.31	1.22
3	G	502	OXL	O2-C2	3.73	1.31	1.22
6	F	505	A1JFT	C18-N3	3.64	1.37	1.31
3	C	503	OXL	O2-C2	3.62	1.31	1.22
3	D	502	OXL	O2-C2	3.60	1.31	1.22
3	H	502	OXL	O2-C2	3.45	1.31	1.22
3	E	502	OXL	O2-C2	3.43	1.31	1.22
6	C	501	A1JFT	C18-N3	3.43	1.36	1.31
6	B	505	A1JFT	C18-N3	3.15	1.36	1.31
6	C	501	A1JFT	C19-N4	3.07	1.36	1.31
6	F	505	A1JFT	C19-N4	3.06	1.36	1.31
3	E	502	OXL	O4-C2	-3.01	1.22	1.30
3	D	502	OXL	O4-C2	-2.99	1.22	1.30
6	C	501	A1JFT	O1-N3	-2.93	1.32	1.39
3	G	502	OXL	O4-C2	-2.81	1.22	1.30
6	E	505	A1JFT	C12-C19	-2.79	1.40	1.42
3	B	502	OXL	O4-C2	-2.74	1.23	1.30
6	E	505	A1JFT	O1-N3	-2.73	1.33	1.39
6	B	505	A1JFT	O1-N3	-2.71	1.33	1.39
6	F	505	A1JFT	O1-N3	-2.69	1.33	1.39
3	H	502	OXL	O4-C2	-2.66	1.23	1.30
6	B	505	A1JFT	C12-C19	-2.64	1.41	1.42
3	A	502	OXL	O4-C2	-2.56	1.23	1.30
3	C	503	OXL	O4-C2	-2.54	1.23	1.30
6	B	505	A1JFT	C19-N4	2.53	1.35	1.31
3	F	502	OXL	O4-C2	-2.50	1.23	1.30
6	F	505	A1JFT	C12-C19	-2.44	1.41	1.42
6	E	505	A1JFT	C19-N4	2.37	1.35	1.31
3	D	502	OXL	C2-C1	2.29	1.58	1.54
2	H	501	FBP	P1-O1	-2.29	1.53	1.60
6	C	501	A1JFT	C12-C19	-2.22	1.41	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	501	A1JFT	C12-C19-C18	-5.16	117.75	121.86
6	E	505	A1JFT	C12-C19-C18	-5.02	117.85	121.86
6	B	505	A1JFT	C12-C19-C18	-5.01	117.86	121.86
6	F	505	A1JFT	C12-C19-C18	-4.99	117.88	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	505	A1JFT	C13-C14-C15	4.78	121.01	116.82
6	F	505	A1JFT	C13-C14-C15	4.74	120.97	116.82
6	C	501	A1JFT	C13-C14-C15	4.61	120.86	116.82
6	E	505	A1JFT	C13-C14-C15	4.61	120.86	116.82
3	H	502	OXL	O4-C2-C1	3.99	120.57	112.83
3	F	502	OXL	O4-C2-C1	3.96	120.52	112.83
3	C	503	OXL	O4-C2-C1	3.95	120.50	112.83
3	D	502	OXL	O4-C2-C1	3.63	119.86	112.83
3	D	502	OXL	O3-C1-C2	3.60	119.82	112.83
3	G	502	OXL	O4-C2-C1	3.48	119.58	112.83
3	A	502	OXL	O4-C2-C1	3.39	119.40	112.83
3	E	502	OXL	O4-C2-C1	3.38	119.39	112.83
3	G	502	OXL	O3-C1-C2	3.38	119.39	112.83
2	D	501	FBP	O6-P2-O4P	3.22	115.14	106.44
3	B	502	OXL	O4-C2-C1	3.01	118.67	112.83
6	E	505	A1JFT	C17-N2-C15	2.62	123.28	115.16
3	F	502	OXL	O3-C1-C2	2.50	117.67	112.83
6	F	505	A1JFT	C17-N2-C15	2.32	122.36	115.16
3	H	502	OXL	O2-C2-C1	-2.31	115.82	120.63
3	B	502	OXL	O3-C1-C2	2.30	117.29	112.83
3	C	503	OXL	O3-C1-C2	2.30	117.29	112.83
2	G	501	FBP	O3-C3-C4	2.29	121.31	113.25
2	B	501	FBP	O6-P2-O4P	2.28	112.59	106.44
3	E	502	OXL	O3-C1-C2	2.25	117.19	112.83
6	C	501	A1JFT	C17-N2-C15	2.24	122.11	115.16
2	C	502	FBP	O6-P2-O4P	2.23	112.47	106.44
6	B	505	A1JFT	C17-N2-C15	2.20	122.00	115.16
6	C	501	A1JFT	O1-N3-C18	2.15	108.22	105.65
3	C	503	OXL	O2-C2-C1	-2.12	116.22	120.63
6	E	505	A1JFT	O1-N3-C18	2.07	108.12	105.65
3	F	502	OXL	O2-C2-C1	-2.03	116.41	120.63
6	F	505	A1JFT	O1-N3-C18	2.01	108.05	105.65

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	FBP	C4-C5-C6-O6
2	C	502	FBP	C4-C5-C6-O6
2	D	501	FBP	C4-C5-C6-O6
2	E	501	FBP	C4-C5-C6-O6
2	F	501	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	G	501	FBP	C4-C5-C6-O6
2	H	501	FBP	C4-C5-C6-O6
2	A	501	FBP	O5-C5-C6-O6
2	E	501	FBP	O5-C5-C6-O6
2	F	501	FBP	O5-C5-C6-O6
2	A	501	FBP	C4-C5-C6-O6
2	B	501	FBP	O5-C5-C6-O6
2	C	502	FBP	O5-C5-C6-O6
2	G	501	FBP	O5-C5-C6-O6
2	H	501	FBP	O5-C5-C6-O6
2	D	501	FBP	O5-C5-C6-O6
3	A	502	OXL	O3-C1-C2-O4
3	E	502	OXL	O3-C1-C2-O4
3	B	502	OXL	O3-C1-C2-O4
3	C	503	OXL	O3-C1-C2-O4
3	G	502	OXL	O3-C1-C2-O4
3	A	502	OXL	O1-C1-C2-O2
3	E	502	OXL	O1-C1-C2-O2
3	D	502	OXL	O3-C1-C2-O4
3	H	502	OXL	O3-C1-C2-O4
3	B	502	OXL	O1-C1-C2-O2
3	C	503	OXL	O1-C1-C2-O2
3	D	502	OXL	O1-C1-C2-O2
3	G	502	OXL	O1-C1-C2-O2
3	H	502	OXL	O1-C1-C2-O2
2	B	501	FBP	C1-O1-P1-O1P
3	A	502	OXL	O1-C1-C2-O4
3	A	502	OXL	O3-C1-C2-O2
3	B	502	OXL	O1-C1-C2-O4
3	B	502	OXL	O3-C1-C2-O2
3	C	503	OXL	O1-C1-C2-O4
3	D	502	OXL	O3-C1-C2-O2
3	E	502	OXL	O1-C1-C2-O4
3	E	502	OXL	O3-C1-C2-O2
3	G	502	OXL	O1-C1-C2-O4
3	G	502	OXL	O3-C1-C2-O2
3	C	503	OXL	O3-C1-C2-O2
3	D	502	OXL	O1-C1-C2-O4
3	H	502	OXL	O1-C1-C2-O4
3	H	502	OXL	O3-C1-C2-O2
2	B	501	FBP	C1-O1-P1-O2P

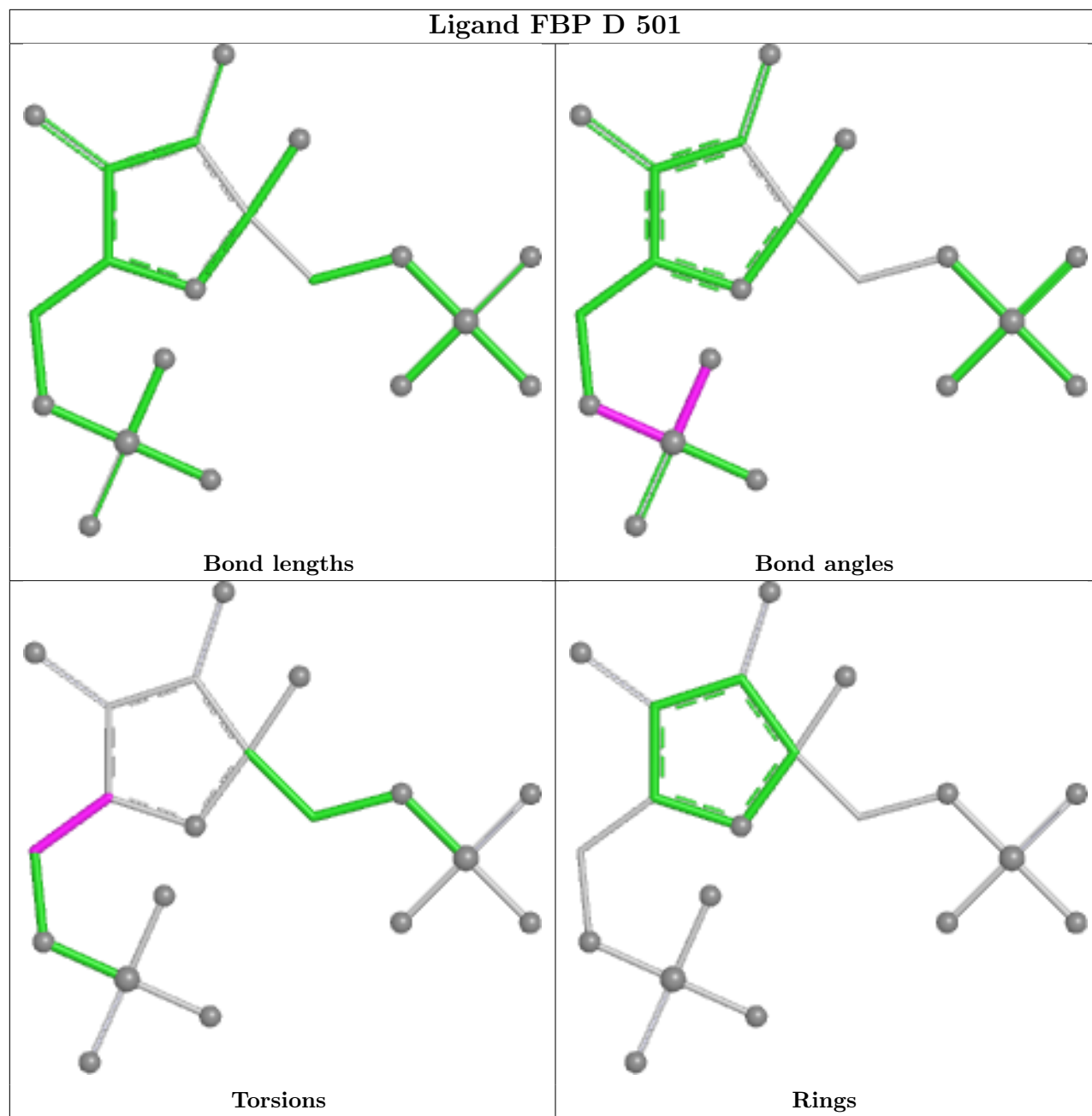
There are no ring outliers.

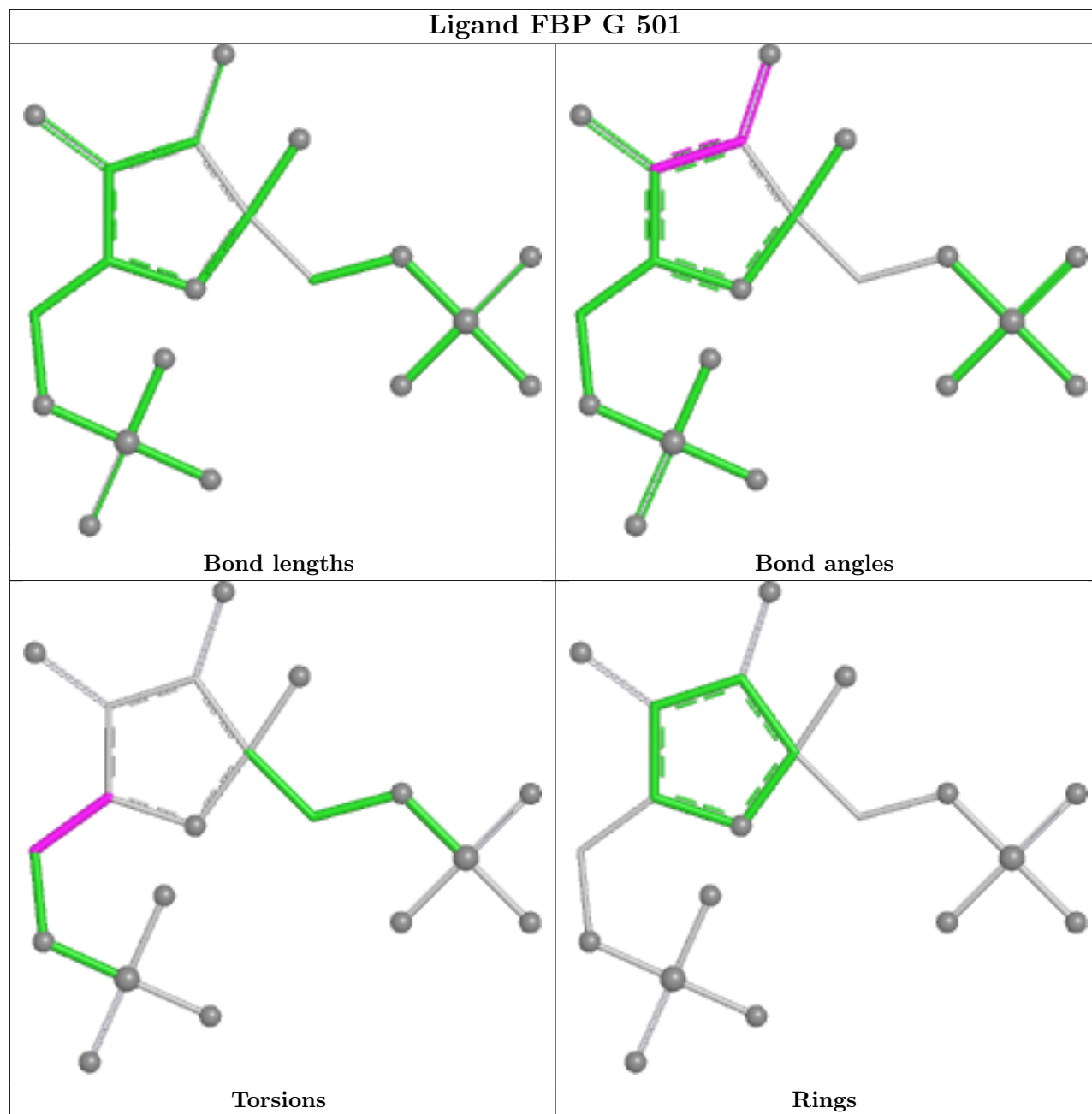


5 monomers are involved in 6 short contacts:

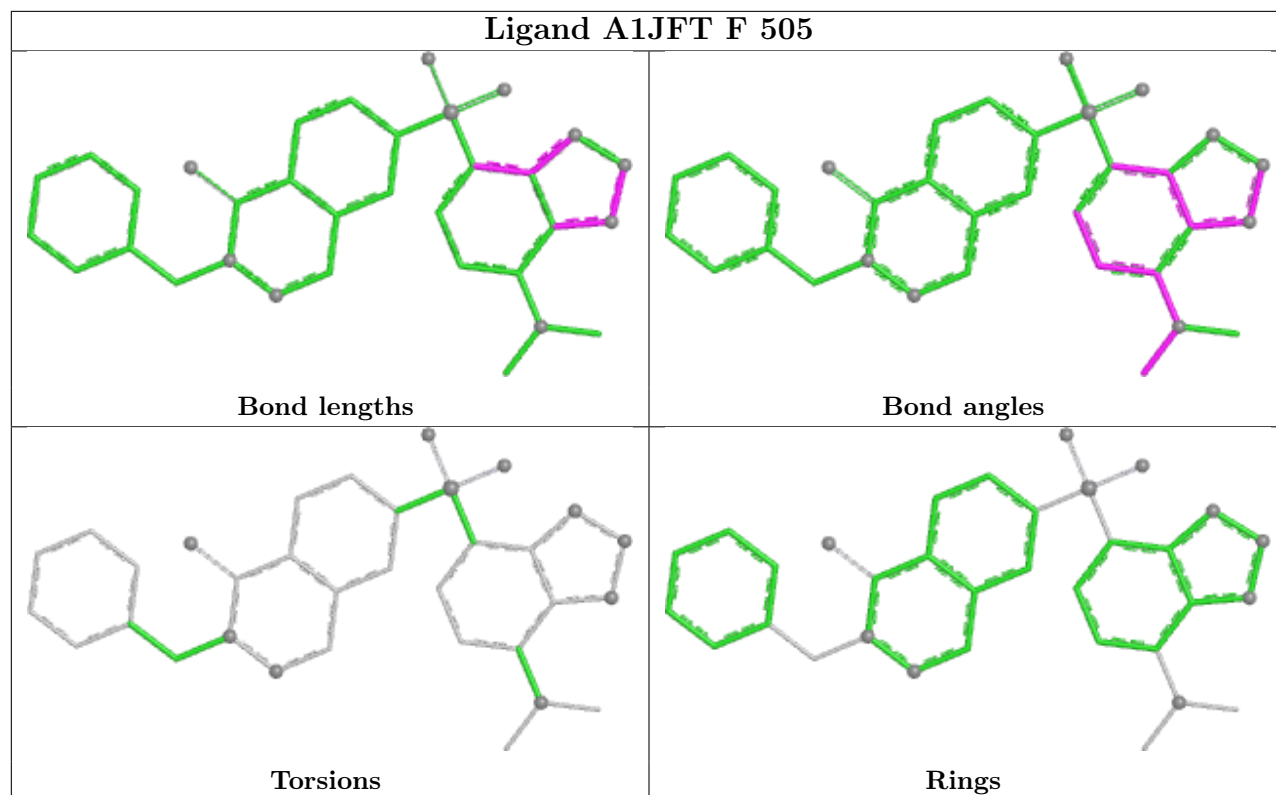
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	505	A1JFT	2	0
6	E	505	A1JFT	1	0
2	E	501	FBP	1	0
2	F	501	FBP	1	0
2	A	501	FBP	1	0

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.

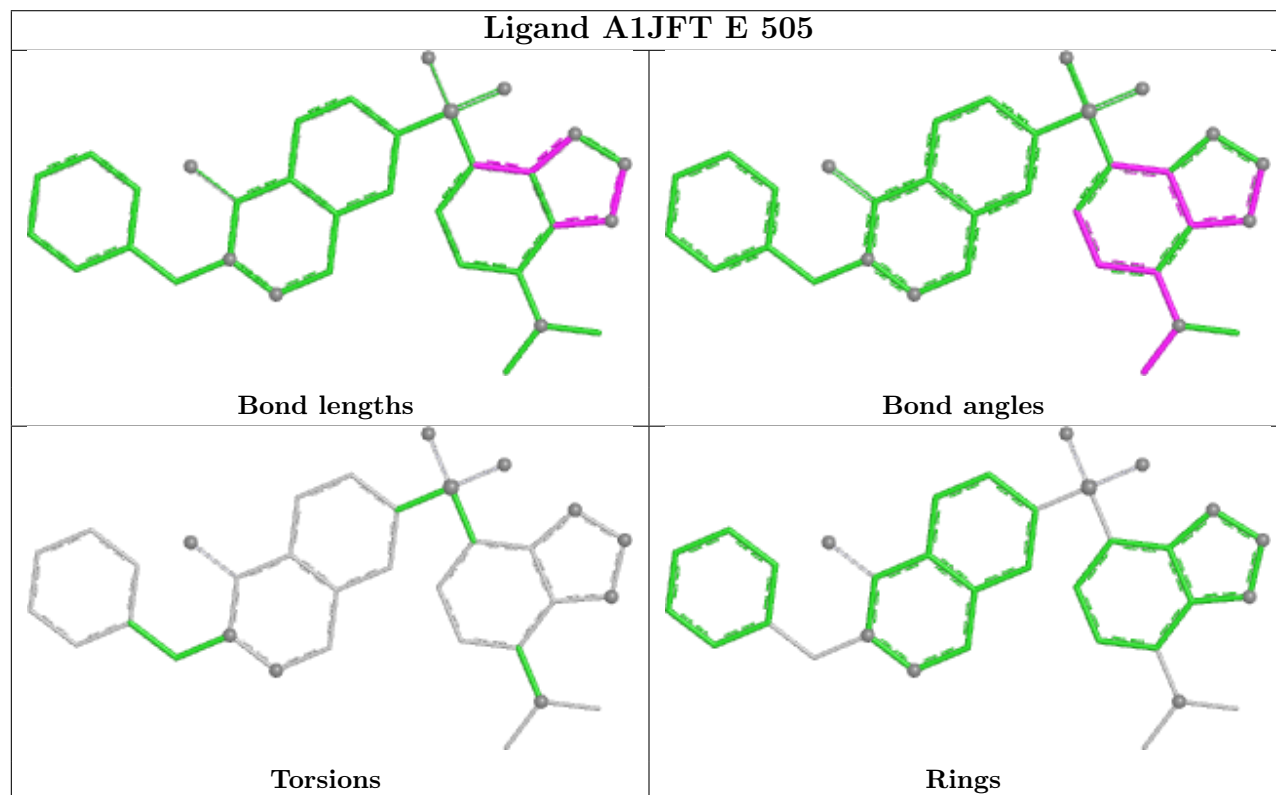


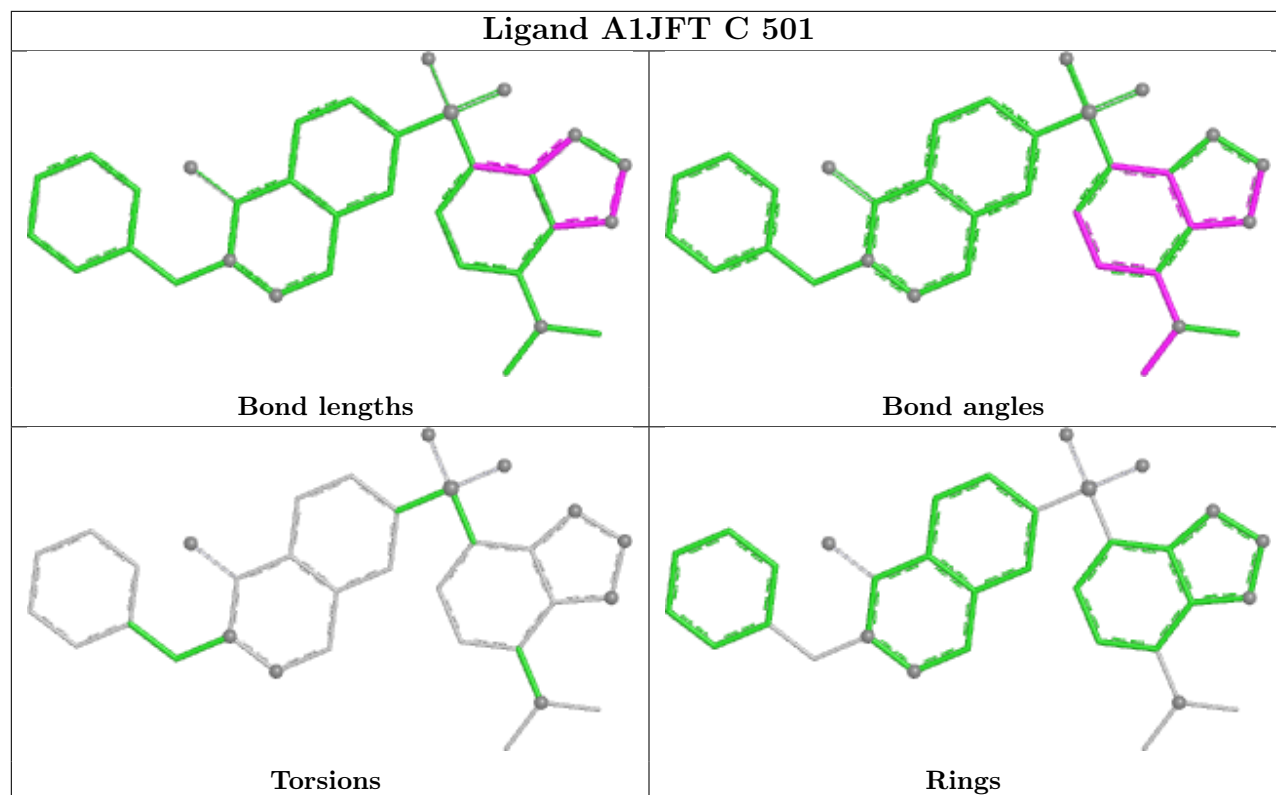


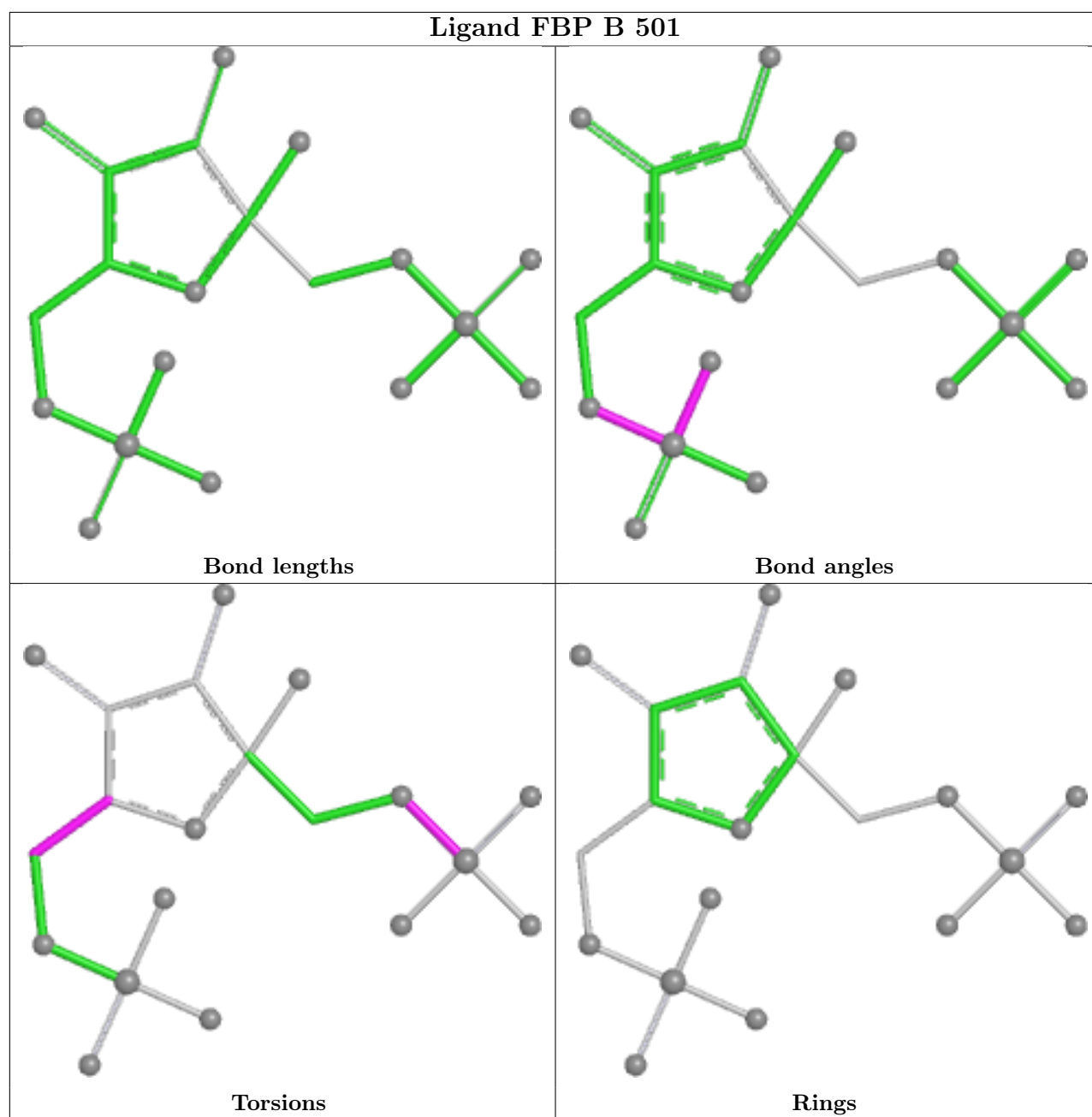
## Ligand A1JFT F 505



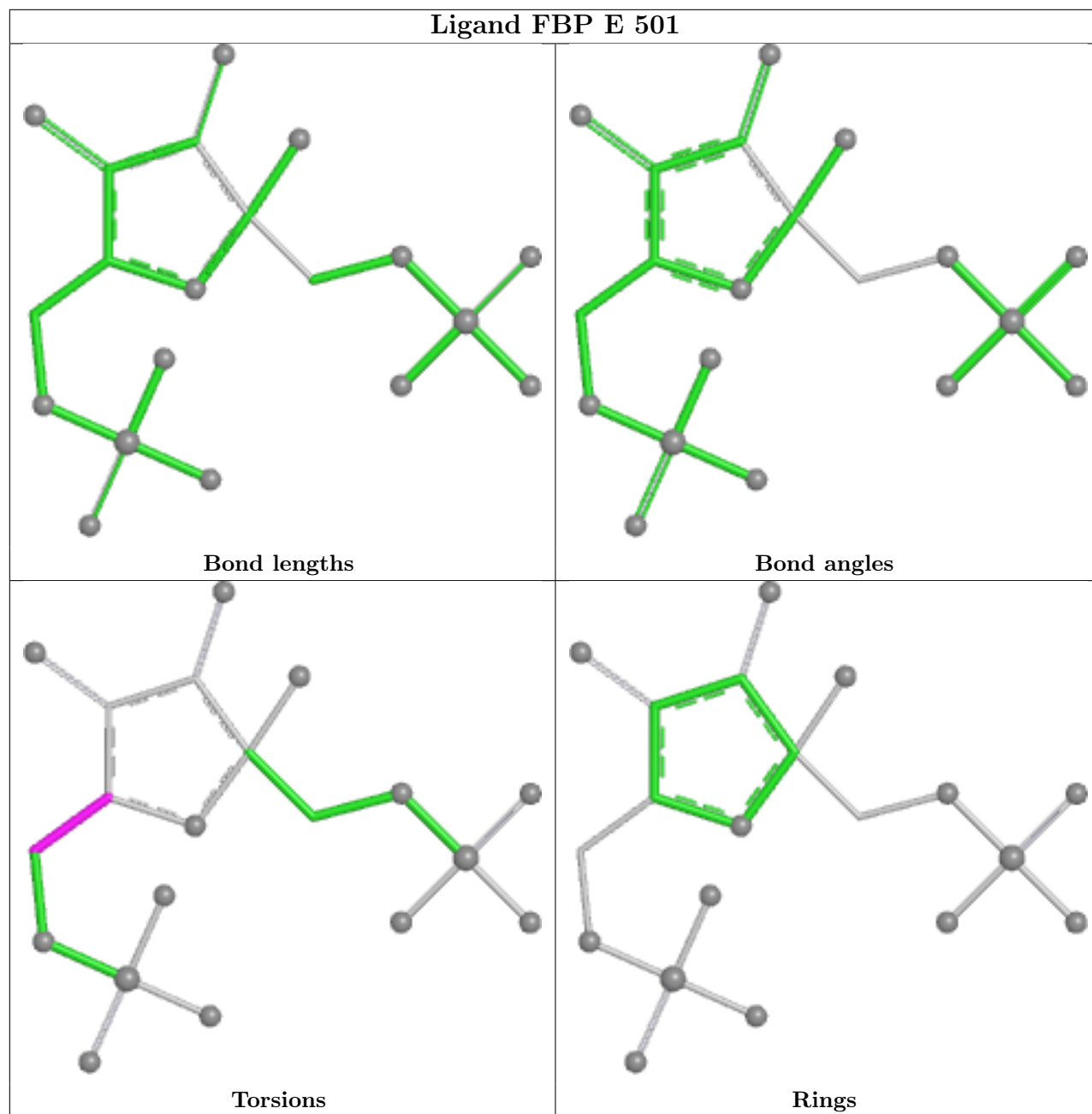
## Ligand A1JFT E 505

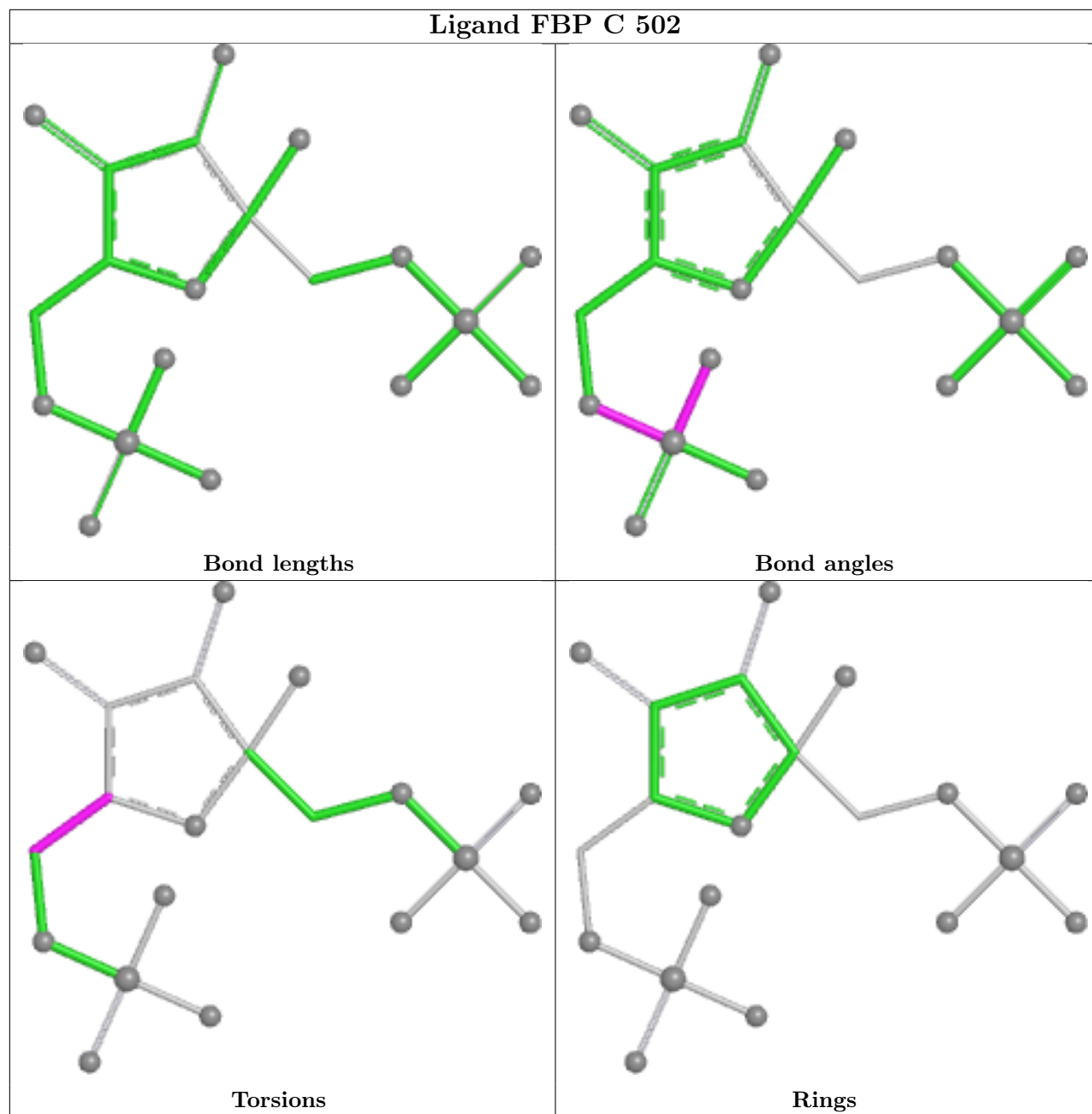






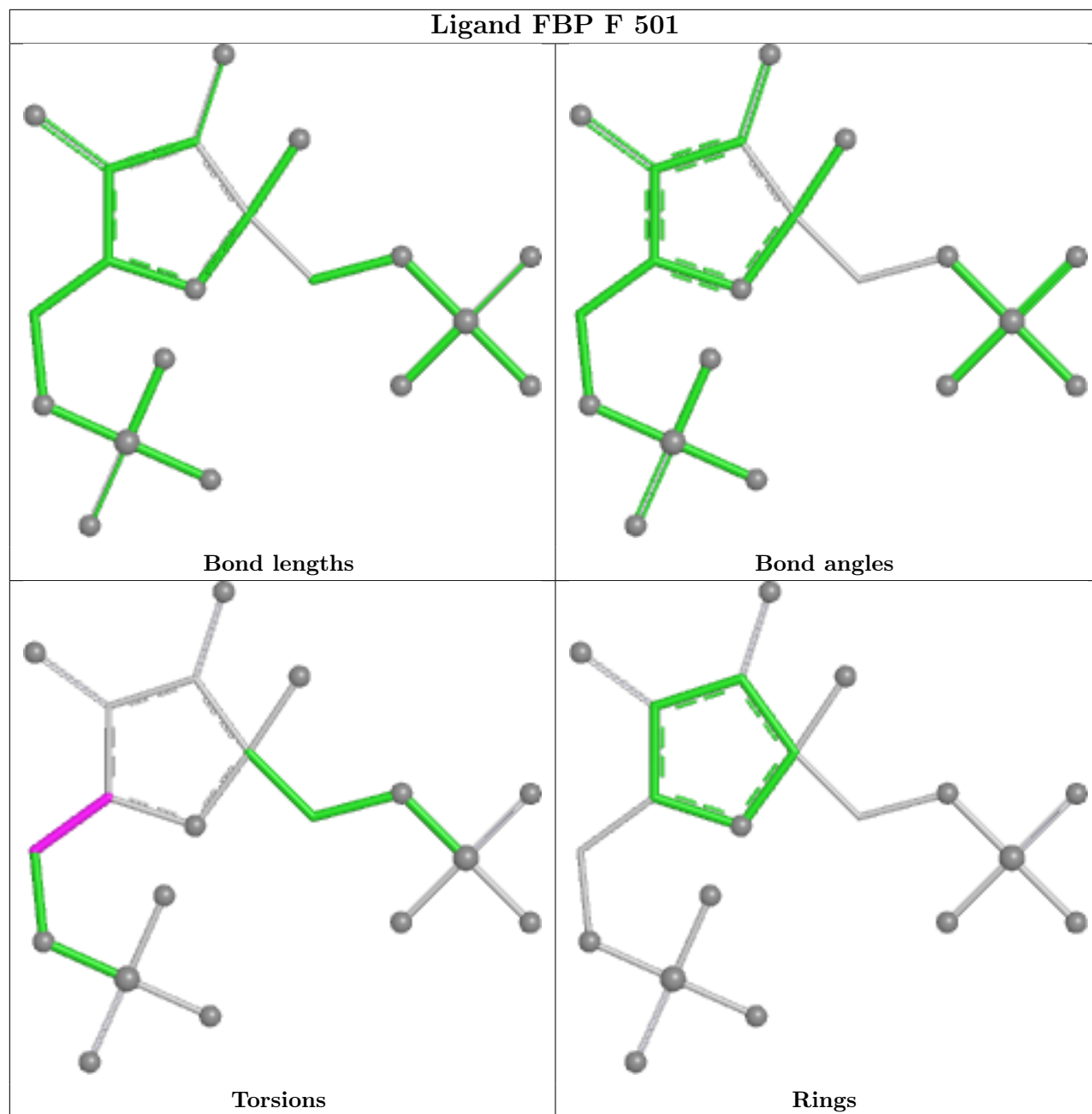
## Ligand FBP E 501

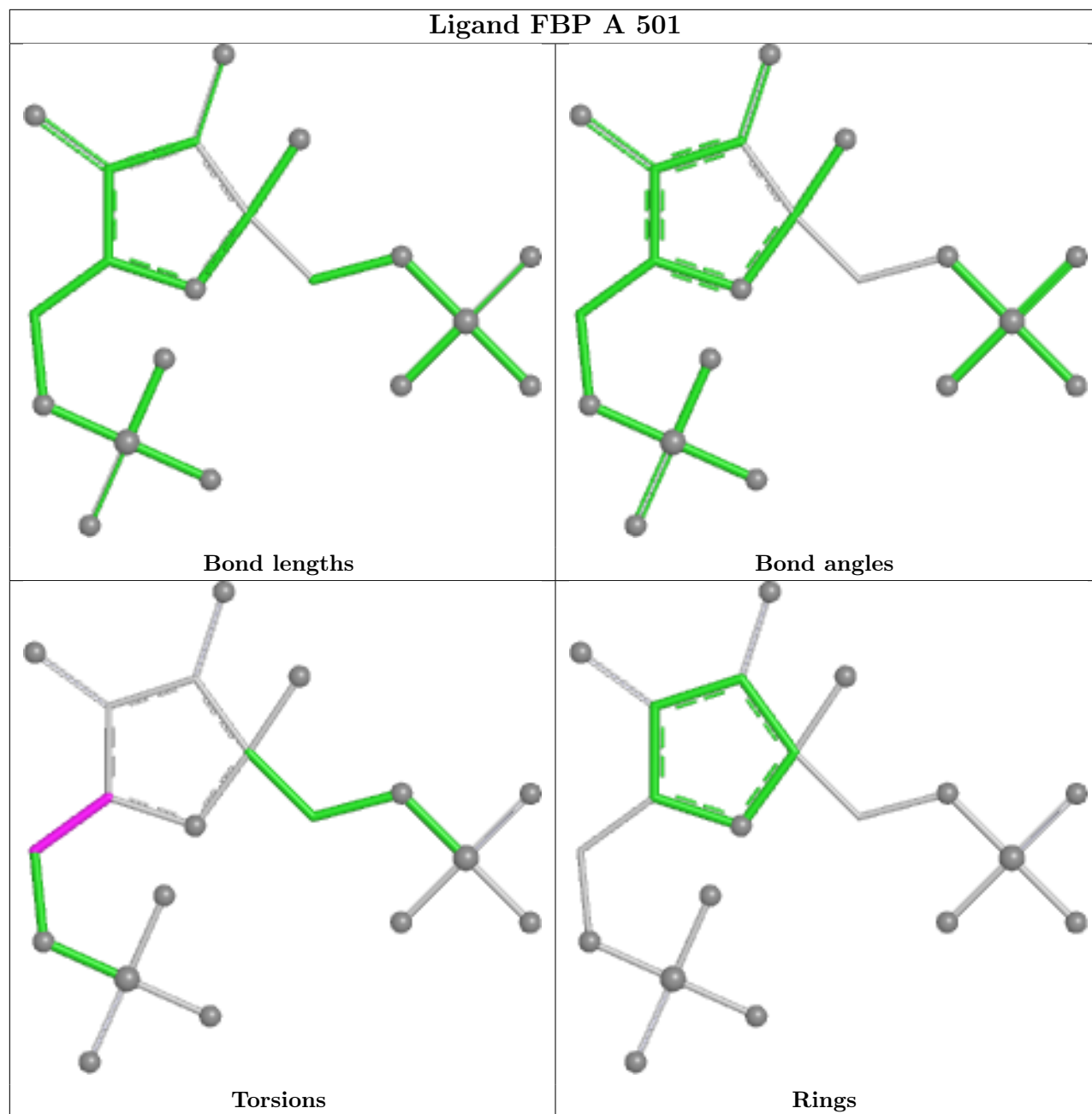


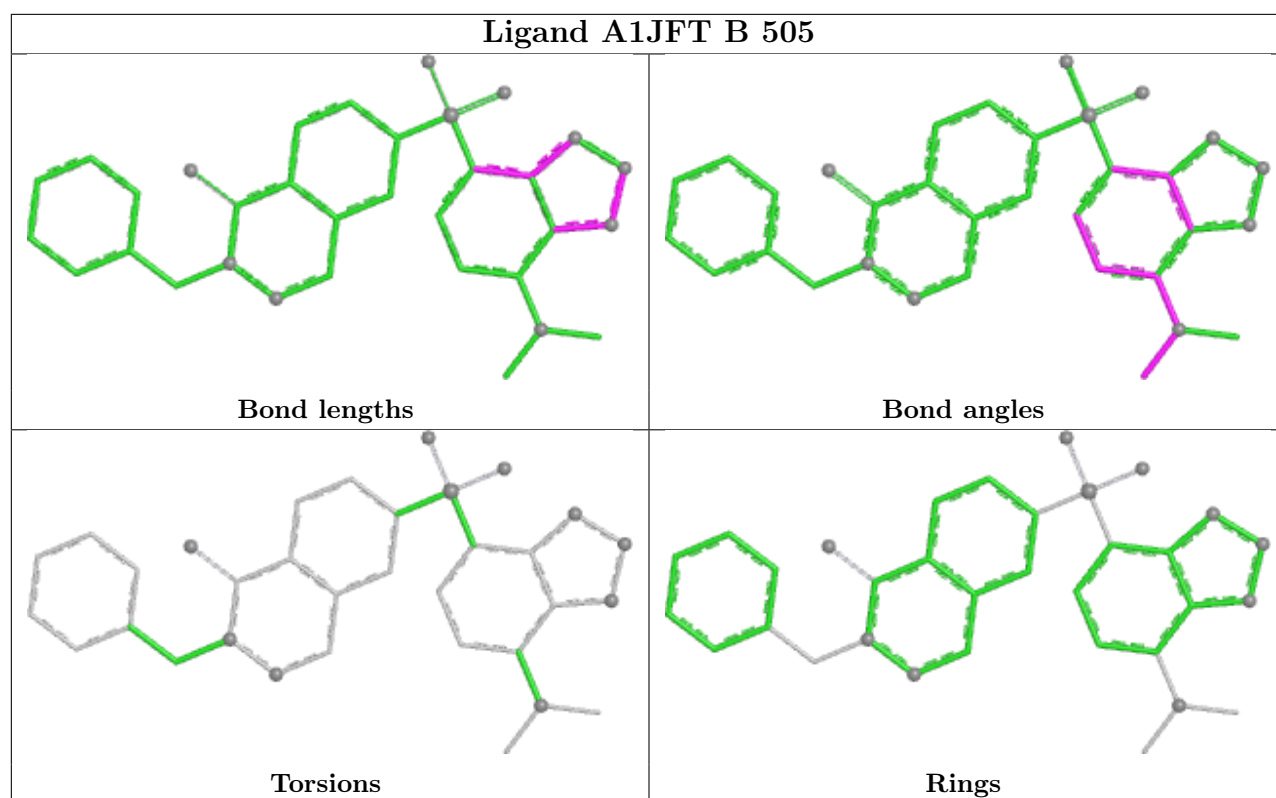


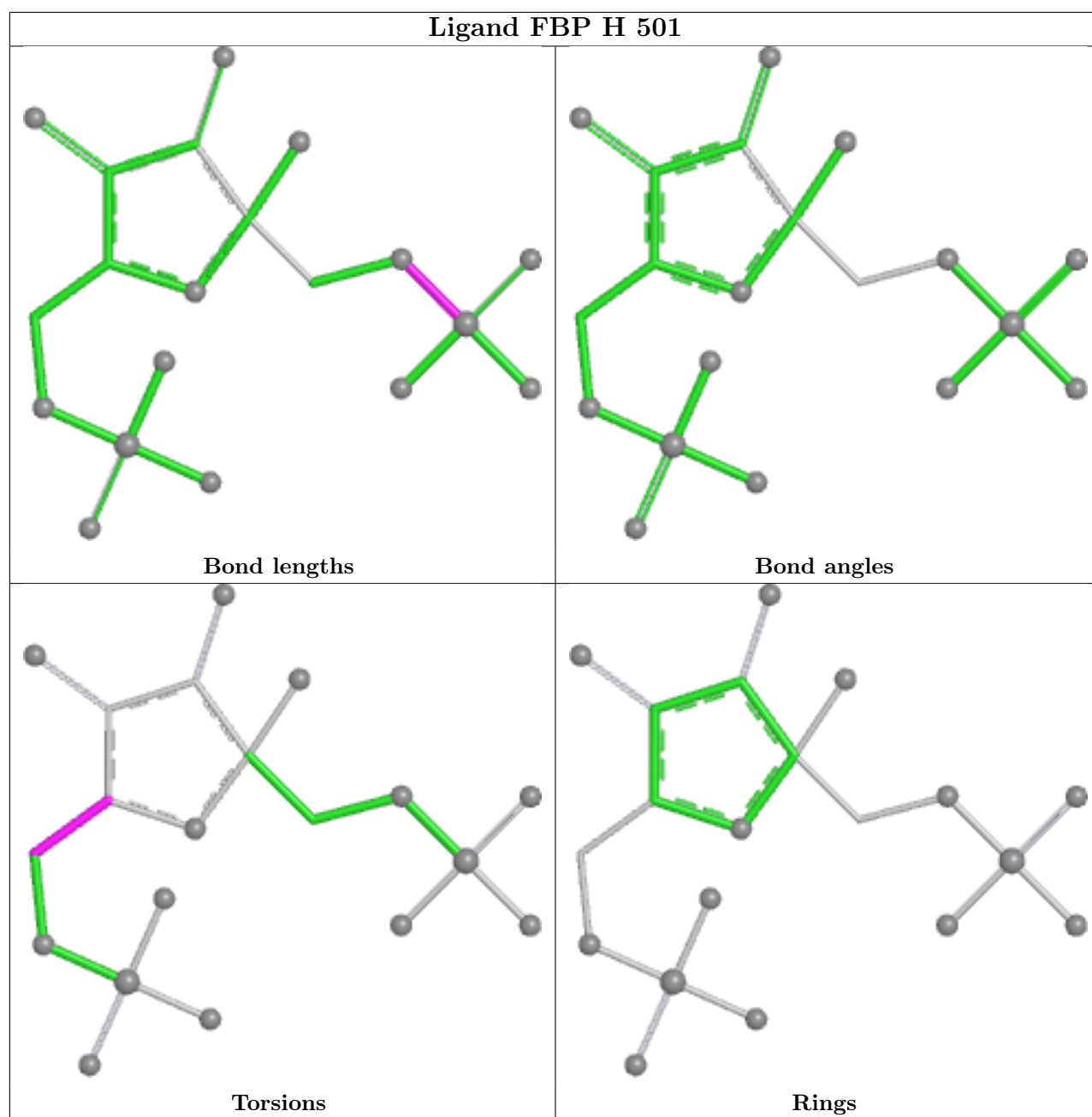


## Ligand FBP F 501









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	2.02	185 (43%) 0 0	39, 80, 111, 120	6 (1%)
1	B	436/447 (97%)	1.58	148 (33%) 1 1	37, 69, 108, 118	4 (0%)
1	C	427/447 (95%)	0.77	61 (14%) 6 6	25, 52, 84, 125	4 (0%)
1	D	425/447 (95%)	0.04	12 (2%) 55 56	18, 38, 62, 104	6 (1%)
1	E	423/447 (94%)	1.53	117 (27%) 1 1	31, 68, 104, 126	5 (1%)
1	F	435/447 (97%)	0.89	62 (14%) 6 6	32, 55, 88, 107	7 (1%)
1	G	423/447 (94%)	0.30	17 (4%) 42 44	24, 46, 66, 89	7 (1%)
1	H	425/447 (95%)	-0.09	13 (3%) 51 53	18, 35, 59, 100	4 (0%)
All	All	3417/3576 (95%)	0.88	615 (17%) 3 4	18, 55, 102, 126	43 (1%)

All (615) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	PHE	7.8
1	A	392	PRO	7.3
1	B	413	LEU	6.6
1	A	445	SER	6.6
1	A	390[A]	GLU	6.5
1	B	445	SER	6.4
1	E	407	GLY	6.3
1	H	21	GLY	6.2
1	A	408	ILE	6.1
1	D	21	GLY	5.8
1	B	419	VAL	5.8
1	A	365	ILE	5.8
1	A	404	VAL	5.7
1	A	63	ILE	5.7
1	D	25	PHE	5.7
1	A	391	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	442	LEU	5.5
1	E	133	PRO	5.5
1	B	115	LEU	5.5
1	E	444	ILE	5.5
1	A	115	LEU	5.4
1	E	23	ALA	5.4
1	A	343	ILE	5.4
1	F	418	ARG	5.3
1	A	114	PRO	5.1
1	A	367	VAL	5.0
1	E	114	PRO	5.0
1	B	250	THR	4.9
1	A	25	PHE	4.9
1	C	111	ALA	4.9
1	A	133	PRO	4.9
1	E	404	VAL	4.9
1	A	279	THR	4.8
1	A	84	ALA	4.7
1	A	366	ALA	4.7
1	H	25	PHE	4.7
1	F	133	PRO	4.7
1	F	115	LEU	4.6
1	D	24	PHE	4.6
1	F	134	GLY	4.5
1	A	386	LEU	4.5
1	B	114	PRO	4.4
1	E	387	LEU	4.3
1	F	318	LEU	4.3
1	A	434	GLY	4.3
1	C	20	LEU	4.3
1	E	115	LEU	4.3
1	A	377	VAL	4.3
1	B	88	PHE	4.3
1	A	373	ALA	4.3
1	B	340	ALA	4.3
1	B	91	GLY	4.3
1	E	151	VAL	4.2
1	A	130	GLY	4.2
1	A	394	ALA	4.2
1	A	79	ALA	4.2
1	B	318	LEU	4.1
1	E	140	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	391	PRO	4.1
1	B	111	ALA	4.1
1	E	101	ALA	4.1
1	B	134	GLY	4.1
1	A	70	VAL	4.1
1	A	387	LEU	4.0
1	A	442	LEU	4.0
1	A	432	GLY	4.0
1	A	140	VAL	4.0
1	A	151	VAL	4.0
1	G	23	ALA	4.0
1	B	169[A]	ARG	4.0
1	E	416	PHE	4.0
1	A	143	LEU	4.0
1	E	134	GLY	4.0
1	A	398	ASP	4.0
1	A	280	ALA	4.0
1	E	111	ALA	4.0
1	A	433	SER	4.0
1	B	133	PRO	3.9
1	A	409	GLU	3.9
1	B	116	SER	3.9
1	B	418	ARG	3.9
1	E	366	ALA	3.9
1	A	395	ILE	3.9
1	C	64	GLY	3.9
1	G	25	PHE	3.8
1	B	444	ILE	3.8
1	B	52	VAL	3.8
1	C	66	ALA	3.8
1	F	416	PHE	3.8
1	C	75	GLU	3.8
1	B	404	VAL	3.8
1	F	413	LEU	3.8
1	A	282	GLY	3.8
1	B	73	LEU	3.8
1	E	120	VAL	3.8
1	A	347	THR	3.7
1	C	36	ASP	3.7
1	E	445	SER	3.7
1	B	25	PHE	3.7
1	A	86	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	277	GLY	3.7
1	E	25	PHE	3.7
1	F	395	ILE	3.7
1	B	61	ALA	3.7
1	B	392	PRO	3.7
1	B	395	ILE	3.6
1	A	23	ALA	3.6
1	A	181	ILE	3.6
1	B	284	PHE	3.6
1	A	425	VAL	3.6
1	C	70	VAL	3.6
1	A	235	GLY	3.6
1	B	110	PHE	3.6
1	D	22	THR	3.6
1	E	159	VAL	3.6
1	A	34	MET	3.5
1	E	443[A]	SER	3.5
1	H	24	PHE	3.5
1	C	22	THR	3.5
1	A	165	VAL	3.5
1	A	405	GLN	3.5
1	B	414	ARG	3.5
1	E	168	VAL	3.5
1	A	162	ALA	3.5
1	A	167	ALA	3.5
1	A	213	ILE	3.5
1	G	63	ILE	3.5
1	A	419	VAL	3.5
1	E	344	VAL	3.5
1	C	23	ALA	3.5
1	E	70	VAL	3.4
1	A	121	ALA	3.4
1	C	117	TYR	3.4
1	A	62	THR	3.4
1	B	151	VAL	3.4
1	A	61	ALA	3.4
1	A	101	ALA	3.4
1	A	263	ALA	3.4
1	A	407	GLY	3.4
1	B	387	LEU	3.4
1	E	129	PRO	3.4
1	B	70	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	417	LEU	3.4
1	E	135	LEU	3.4
1	B	416	PHE	3.4
1	E	406	PHE	3.4
1	B	138	GLN	3.4
1	C	115	LEU	3.3
1	A	158	PHE	3.3
1	A	97	ALA	3.3
1	B	397	ALA	3.3
1	F	445	SER	3.3
1	A	252	PRO	3.3
1	E	191	VAL	3.3
1	C	34	MET	3.3
1	A	124	LEU	3.3
1	B	442[A]	LEU	3.3
1	E	417	LEU	3.3
1	A	95	TYR	3.3
1	E	397	ALA	3.3
1	B	411	GLY	3.3
1	F	442[A]	LEU	3.3
1	C	108	GLU	3.3
1	A	416	PHE	3.3
1	B	280	ALA	3.2
1	E	97	ALA	3.2
1	E	177	HIS	3.2
1	F	408	ILE	3.2
1	H	22	THR	3.2
1	B	101	ALA	3.2
1	A	393	GLU	3.2
1	C	63	ILE	3.2
1	A	436	THR	3.2
1	A	110	PHE	3.2
1	C	110	PHE	3.2
1	B	107	VAL	3.2
1	B	423	VAL	3.2
1	F	400	VAL	3.2
1	A	73	LEU	3.2
1	C	25	PHE	3.2
1	A	116	SER	3.2
1	C	281	LYS	3.2
1	B	123	ALA	3.2
1	B	400	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	423	VAL	3.2
1	B	135	LEU	3.2
1	E	122	ILE	3.2
1	A	286	VAL	3.1
1	A	383	VAL	3.1
1	B	12	ASP	3.1
1	B	79	ALA	3.1
1	E	166	ALA	3.1
1	C	95	TYR	3.1
1	B	153	ILE	3.1
1	B	62	THR	3.1
1	A	443	SER	3.1
1	E	90	HIS	3.1
1	B	415	GLY	3.1
1	A	156	ALA	3.1
1	A	362	ALA	3.1
1	G	33	ALA	3.1
1	B	63	ILE	3.1
1	B	100	ILE	3.1
1	E	281	LYS	3.1
1	A	88	PHE	3.1
1	B	64	GLY	3.1
1	B	112	GLY	3.1
1	F	130	GLY	3.1
1	A	120	VAL	3.1
1	A	220	VAL	3.1
1	A	348	THR	3.1
1	F	90	HIS	3.1
1	A	171	ALA	3.1
1	C	79	ALA	3.1
1	A	159	VAL	3.1
1	C	285	PRO	3.1
1	A	396	TRP	3.0
1	E	178	GLY	3.0
1	A	397	ALA	3.0
1	B	117	TYR	3.0
1	B	396	TRP	3.0
1	C	113	SER	3.0
1	E	146	GLY	3.0
1	B	174	PRO	3.0
1	C	101	ALA	3.0
1	E	392	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	147	VAL	3.0
1	A	117	TYR	3.0
1	E	104	ARG	3.0
1	F	253	ARG	3.0
1	A	99	SER	3.0
1	H	34	MET	3.0
1	E	413	LEU	3.0
1	A	100	ILE	3.0
1	B	408	ILE	3.0
1	A	259	THR	3.0
1	C	21	GLY	3.0
1	F	91	GLY	3.0
1	C	65	PRO	3.0
1	F	391	PRO	3.0
1	A	90	HIS	2.9
1	F	52	VAL	2.9
1	C	80	GLY	2.9
1	B	24	PHE	2.9
1	E	110	PHE	2.9
1	E	143	LEU	2.9
1	B	120	VAL	2.9
1	B	281	LYS	2.9
1	B	410	SER	2.9
1	E	116	SER	2.9
1	E	130	GLY	2.9
1	A	65	PRO	2.9
1	B	124	LEU	2.9
1	E	386	LEU	2.9
1	F	169[A]	ARG	2.9
1	F	387	LEU	2.9
1	G	24	PHE	2.9
1	B	165	VAL	2.9
1	B	425	VAL	2.9
1	A	435	TYR	2.9
1	B	95	TYR	2.9
1	F	392	PRO	2.9
1	C	106	ALA	2.9
1	E	108	GLU	2.9
1	B	249	ILE	2.9
1	E	100	ILE	2.9
1	F	112	GLY	2.8
1	C	133	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	117	TYR	2.8
1	E	24	PHE	2.8
1	A	154	VAL	2.8
1	B	367	VAL	2.8
1	E	396	TRP	2.8
1	F	409	GLU	2.8
1	A	118	ARG	2.8
1	B	407	GLY	2.8
1	A	135	LEU	2.8
1	B	417	LEU	2.8
1	E	86	LEU	2.8
1	F	135	LEU	2.8
1	B	158	PHE	2.8
1	C	97	ALA	2.8
1	A	107	VAL	2.8
1	A	104	ARG	2.8
1	A	112	GLY	2.8
1	A	420	GLY	2.8
1	B	90	HIS	2.8
1	B	132	GLY	2.8
1	C	282	GLY	2.8
1	A	174	PRO	2.8
1	A	285	PRO	2.8
1	A	245	LEU	2.8
1	A	352	ALA	2.8
1	E	341	ALA	2.8
1	E	335	PHE	2.8
1	A	200	VAL	2.8
1	B	13	VAL	2.8
1	E	389	ARG	2.8
1	F	444[A]	ILE	2.8
1	H	130	GLY	2.8
1	C	114	PRO	2.8
1	G	34	MET	2.8
1	E	206	VAL	2.8
1	B	87	ASN	2.7
1	A	113	SER	2.7
1	E	410	SER	2.7
1	A	119	PRO	2.7
1	D	23	ALA	2.7
1	E	171	ALA	2.7
1	A	147	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	103	VAL	2.7
1	E	419	VAL	2.7
1	A	153	ILE	2.7
1	B	92	SER	2.7
1	C	252	PRO	2.7
1	A	53	ALA	2.7
1	A	103	VAL	2.7
1	A	400	VAL	2.7
1	E	126	THR	2.7
1	E	365	ILE	2.7
1	E	285	PRO	2.7
1	H	318	LEU	2.7
1	B	11	ALA	2.7
1	B	315	ALA	2.7
1	A	423	VAL	2.7
1	F	142	ASP	2.7
1	G	52	VAL	2.7
1	E	174	PRO	2.7
1	A	350	ARG	2.7
1	A	374	ALA	2.6
1	F	11	ALA	2.6
1	F	171	ALA	2.6
1	A	155	PHE	2.6
1	B	147	VAL	2.6
1	F	423	VAL	2.6
1	A	444	ILE	2.6
1	B	420	GLY	2.6
1	A	163	SER	2.6
1	B	285	PRO	2.6
1	C	77	ILE	2.6
1	E	408	ILE	2.6
1	E	136	SER	2.6
1	B	386	LEU	2.6
1	E	124	LEU	2.6
1	F	86	LEU	2.6
1	B	74	LYS	2.6
1	E	361	ARG	2.6
1	F	144	ARG	2.6
1	E	367	VAL	2.6
1	A	134	GLY	2.6
1	C	132	GLY	2.6
1	F	279	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	92	SER	2.6
1	B	76[A]	MET	2.6
1	E	391	PRO	2.6
1	H	133	PRO	2.6
1	C	131	SER	2.6
1	E	144	ARG	2.6
1	A	80	GLY	2.6
1	A	168	VAL	2.6
1	E	119	PRO	2.6
1	F	114	PRO	2.6
1	F	419	VAL	2.6
1	B	113	SER	2.6
1	A	172	LEU	2.6
1	A	275	LEU	2.6
1	F	417	LEU	2.6
1	C	19	GLU	2.6
1	A	429	TRP	2.6
1	B	65	PRO	2.6
1	B	178	GLY	2.6
1	B	427	THR	2.6
1	B	154	VAL	2.6
1	F	140	VAL	2.6
1	E	63	ILE	2.6
1	B	10	ARG	2.5
1	E	421	ASP	2.5
1	F	317	PRO	2.5
1	B	409	GLU	2.5
1	E	409	GLU	2.5
1	C	68	ARG	2.5
1	B	143	LEU	2.5
1	E	73	LEU	2.5
1	A	123	ALA	2.5
1	F	132	GLY	2.5
1	F	415	GLY	2.5
1	G	252	PRO	2.5
1	A	289	VAL	2.5
1	B	286	VAL	2.5
1	C	69	SER	2.5
1	E	103	VAL	2.5
1	A	281	LYS	2.5
1	B	316	ALA	2.5
1	B	146	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	165	VAL	2.5
1	F	386	LEU	2.5
1	A	216	PRO	2.5
1	A	385	PRO	2.5
1	C	129	PRO	2.5
1	B	118	ARG	2.4
1	A	351	SER	2.4
1	B	103	VAL	2.4
1	B	140	VAL	2.4
1	A	355	LEU	2.4
1	H	30	LEU	2.4
1	A	32	ALA	2.4
1	A	132	GLY	2.4
1	A	402	ARG	2.4
1	C	72	ARG	2.4
1	E	315	ALA	2.4
1	E	75	GLU	2.4
1	C	109	SER	2.4
1	E	158	PHE	2.4
1	D	177[A]	HIS	2.4
1	A	142	ASP	2.4
1	B	104	ARG	2.4
1	B	403	ARG	2.4
1	F	361	ARG	2.4
1	H	418	ARG	2.4
1	B	84	ALA	2.4
1	B	171	ALA	2.4
1	F	129	PRO	2.4
1	E	132	GLY	2.4
1	G	54	ALA	2.4
1	A	242	THR	2.4
1	A	368	THR	2.4
1	C	250	THR	2.4
1	A	276	SER	2.4
1	A	179	ILE	2.4
1	B	168	VAL	2.4
1	B	81	MET	2.4
1	B	172	LEU	2.4
1	E	314	ARG	2.4
1	B	317	PRO	2.4
1	B	14	ALA	2.4
1	C	112	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	315	ALA	2.4
1	G	250	THR	2.4
1	A	426	VAL	2.4
1	E	179	ILE	2.4
1	F	34	MET	2.4
1	F	70	VAL	2.4
1	C	245	LEU	2.4
1	D	361	ARG	2.4
1	E	118	ARG	2.4
1	E	440	ARG	2.4
1	H	314	ARG	2.4
1	B	71	GLU	2.4
1	A	164	ASP	2.3
1	F	174	PRO	2.3
1	A	106	ALA	2.3
1	B	443	SER	2.3
1	A	81	MET	2.3
1	A	248	MET	2.3
1	A	303	VAL	2.3
1	C	107	VAL	2.3
1	C	286	VAL	2.3
1	E	395	ILE	2.3
1	B	177	HIS	2.3
1	E	253	ARG	2.3
1	A	94	GLU	2.3
1	C	287	GLU	2.3
1	B	388	TYR	2.3
1	E	431	PRO	2.3
1	E	167	ALA	2.3
1	A	69	SER	2.3
1	B	67	SER	2.3
1	A	144	ARG	2.3
1	A	375	ARG	2.3
1	A	182	ILE	2.3
1	A	206	VAL	2.3
1	A	344	VAL	2.3
1	B	422	LEU	2.3
1	B	412	LYS	2.3
1	B	277	GLY	2.3
1	E	112	GLY	2.3
1	A	371	ALA	2.3
1	C	288	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	101	ALA	2.3
1	F	394	ALA	2.3
1	A	250	THR	2.3
1	B	144	ARG	2.3
1	A	122	ILE	2.3
1	C	284	PHE	2.3
1	E	312	LEU	2.3
1	A	87	ASN	2.3
1	B	80	GLY	2.3
1	B	22	THR	2.3
1	E	368	THR	2.3
1	A	131	SER	2.3
1	A	188	HIS	2.3
1	B	246	GLU	2.3
1	A	185	ILE	2.3
1	B	181	ILE	2.3
1	A	24	PHE	2.2
1	B	20	LEU	2.2
1	B	325	VAL	2.3
1	A	378	HIS	2.2
1	E	358	TYR	2.2
1	F	177	HIS	2.2
1	B	109	SER	2.2
1	E	77	ILE	2.2
1	B	86	LEU	2.2
1	E	233	LEU	2.2
1	A	440	ARG	2.2
1	A	150	GLY	2.2
1	B	128	GLY	2.2
1	C	277	GLY	2.2
1	A	316	ALA	2.2
1	B	53	ALA	2.2
1	B	251	LYS	2.2
1	B	394	ALA	2.2
1	E	363	ALA	2.2
1	F	97	ALA	2.2
1	F	396	TRP	2.2
1	A	160	ARG	2.2
1	B	389	ARG	2.2
1	C	174	PRO	2.2
1	C	173	GLY	2.2
1	D	134	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	432	GLY	2.2
1	G	173	GLY	2.2
1	B	105	GLU	2.2
1	C	27	GLN	2.2
1	B	167	ALA	2.2
1	E	113	SER	2.2
1	A	83	ILE	2.2
1	B	77	ILE	2.2
1	B	343	ILE	2.2
1	F	63	ILE	2.2
1	A	68	ARG	2.2
1	G	42	LEU	2.2
1	A	102	ASN	2.2
1	C	251	LYS	2.2
1	A	67	SER	2.2
1	B	106	ALA	2.2
1	B	166	ALA	2.2
1	B	234	ALA	2.2
1	A	361	ARG	2.1
1	D	314	ARG	2.1
1	F	414	ARG	2.1
1	B	122	ILE	2.1
1	E	328	ILE	2.1
1	C	283	ASN	2.1
1	A	108	GLU	2.1
1	E	127	LYS	2.1
1	B	385	PRO	2.1
1	H	305	HIS	2.1
1	A	33	ALA	2.1
1	C	49	SER	2.1
1	E	35	ALA	2.1
1	E	288	ALA	2.1
1	A	418	ARG	2.1
1	E	72	ARG	2.1
1	A	77	ILE	2.1
1	B	34	MET	2.1
1	E	388	TYR	2.1
1	B	182	ILE	2.1
1	C	213	ILE	2.1
1	E	153	ILE	2.1
1	E	211	LEU	2.1
1	F	124	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	401[A]	ASP	2.1
1	F	139	ASP	2.1
1	F	310	GLU	2.1
1	A	239	VAL	2.1
1	B	289	VAL	2.1
1	F	429	TRP	2.1
1	C	130	GLY	2.1
1	E	411	GLY	2.1
1	G	64	GLY	2.1
1	H	134	GLY	2.1
1	A	340	ALA	2.1
1	B	121	ALA	2.1
1	E	131	SER	2.1
1	E	163	SER	2.1
1	G	99	SER	2.1
1	G	106	ALA	2.1
1	F	71	GLU	2.1
1	A	421	ASP	2.1
1	B	60	ILE	2.1
1	F	172	LEU	2.1
1	A	96	HIS	2.1
1	E	154	VAL	2.1
1	F	165	VAL	2.1
1	A	284	PHE	2.1
1	A	91	GLY	2.1
1	B	440	ARG	2.1
1	B	368	THR	2.1
1	C	116	SER	2.1
1	A	66	ALA	2.1
1	A	270	ALA	2.1
1	G	133	PRO	2.1
1	B	406	PHE	2.1
1	D	132	GLY	2.1
1	E	432	GLY	2.1
1	F	420	GLY	2.1
1	C	280	ALA	2.0
1	D	34	MET	2.0
1	A	305	HIS	2.0
1	B	405	GLN	2.0
1	B	102	ASN	2.0
1	E	187	ASN	2.0
1	F	143	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	65	PRO	2.0
1	A	85	ARG	2.0
1	C	262	VAL	2.0
1	B	173	GLY	2.0
1	G	132	GLY	2.0
1	E	384	PHE	2.0
1	A	274	MET	2.0
1	E	76[A]	MET	2.0
1	A	321	ASP	2.0
1	A	422	LEU	2.0
1	B	83	ILE	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
5	K	E	504	1/1	0.54	0.24	142,142,142,142	0
5	K	B	504	1/1	0.78	0.11	108,108,108,108	0
3	OXL	A	502	6/6	0.80	0.18	124,124,124,125	0
6	A1JFT	C	501	33/33	0.83	0.20	84,87,91,91	19
6	A1JFT	E	505	33/33	0.83	0.18	68,78,84,84	19
6	A1JFT	F	505	33/33	0.84	0.20	82,87,88,88	19
5	K	A	504	1/1	0.85	0.09	125,125,125,125	0
3	OXL	E	502	6/6	0.86	0.13	86,86,86,86	0
2	FBP	A	501	20/20	0.86	0.14	77,78,79,79	0
6	A1JFT	B	505	33/33	0.86	0.17	65,74,79,79	19
2	FBP	B	501	20/20	0.88	0.12	72,76,80,80	0
5	K	G	504	1/1	0.89	0.10	80,80,80,80	0

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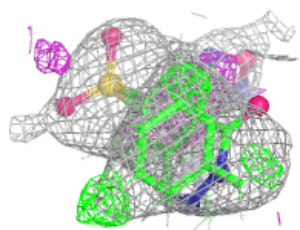
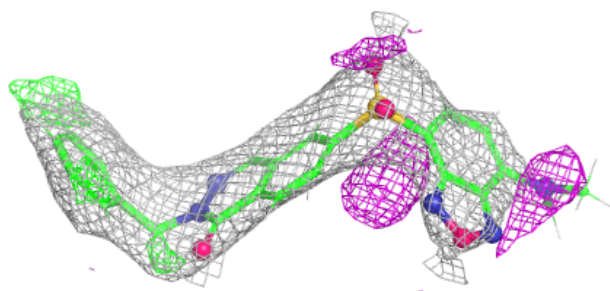
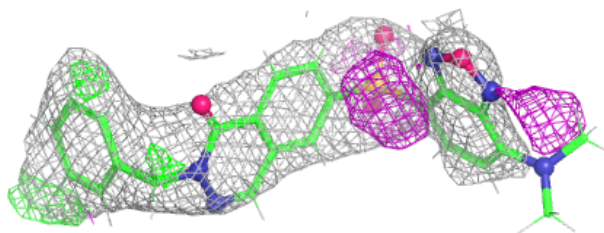
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OXL	C	503	6/6	0.91	0.09	66,66,66,67	0
2	FBP	F	501	20/20	0.91	0.10	57,63,66,66	0
5	K	F	504	1/1	0.91	0.09	105,105,105,105	0
2	FBP	E	501	20/20	0.91	0.10	67,69,72,72	0
3	OXL	G	502	6/6	0.92	0.09	54,55,55,56	0
3	OXL	B	502	6/6	0.92	0.09	63,63,64,64	0
3	OXL	F	502	6/6	0.93	0.12	84,84,85,85	0
3	OXL	H	502	6/6	0.94	0.10	48,49,51,51	0
5	K	C	505	1/1	0.94	0.10	75,75,75,75	0
3	OXL	D	502	6/6	0.94	0.09	58,58,58,58	0
4	MG	B	503	1/1	0.96	0.08	52,52,52,52	0
5	K	H	504	1/1	0.98	0.04	58,58,58,58	0
2	FBP	G	501	20/20	0.98	0.05	31,32,36,37	0
4	MG	E	503	1/1	0.98	0.03	46,46,46,46	0
2	FBP	H	501	20/20	0.98	0.05	25,27,30,31	0
4	MG	A	503	1/1	0.98	0.06	61,61,61,61	0
2	FBP	D	501	20/20	0.99	0.04	29,31,33,33	0
4	MG	C	504	1/1	0.99	0.07	45,45,45,45	0
4	MG	D	503	1/1	0.99	0.05	29,29,29,29	0
5	K	D	504	1/1	0.99	0.06	54,54,54,54	0
2	FBP	C	502	20/20	0.99	0.04	32,33,38,39	0
4	MG	F	503	1/1	0.99	0.06	36,36,36,36	0
4	MG	G	503	1/1	1.00	0.06	24,24,24,24	0
4	MG	H	503	1/1	1.00	0.05	22,22,22,22	0

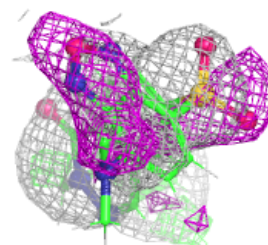
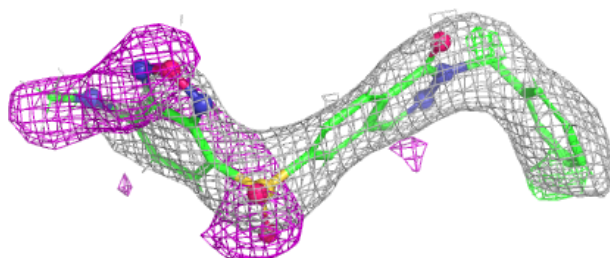
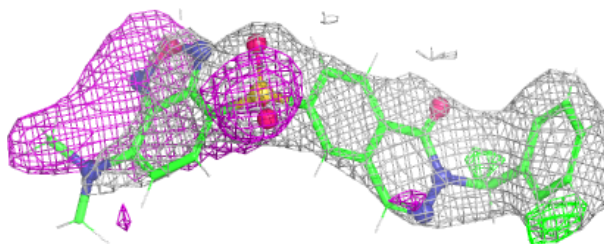
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1JFT C 501:**

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

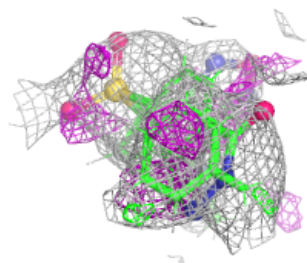
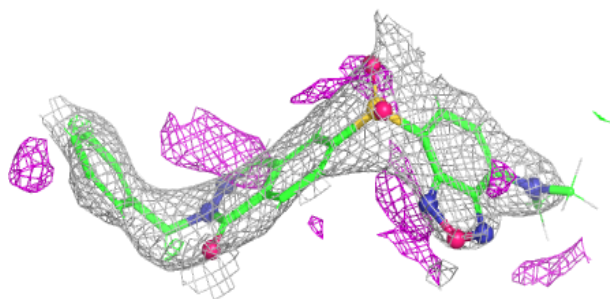
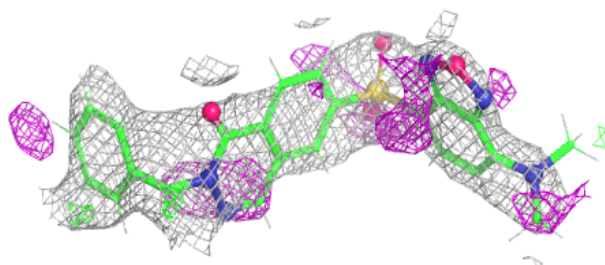
**Electron density around A1JFT E 505:**

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

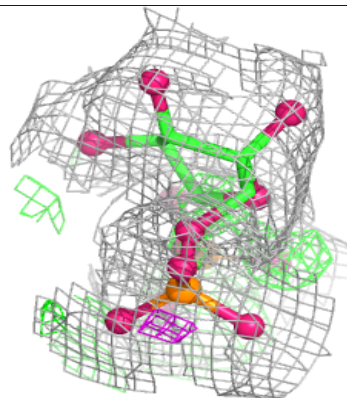
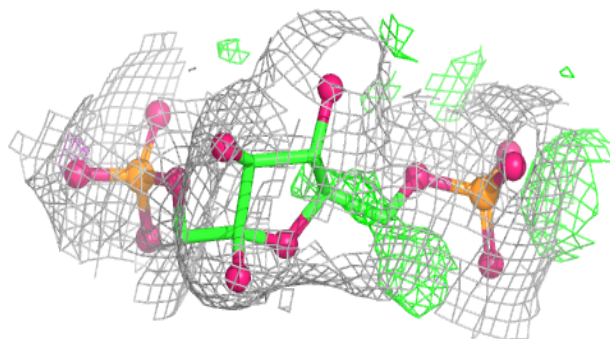
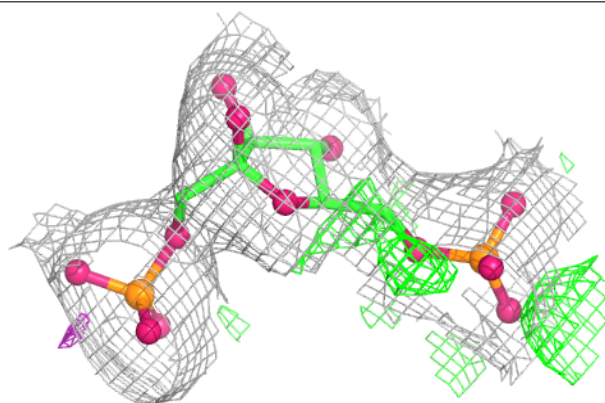


**Electron density around A1JFT F 505:**

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

**Electron density around FBP A 501:**

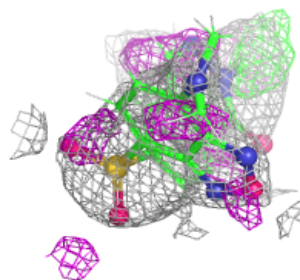
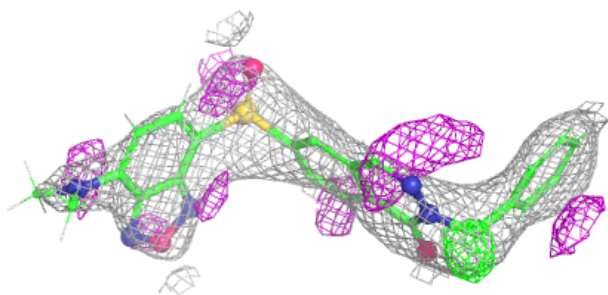
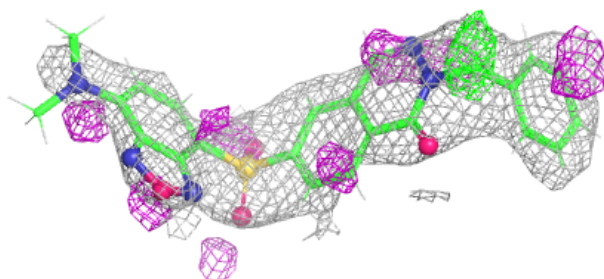
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around A1JFT B 505:**

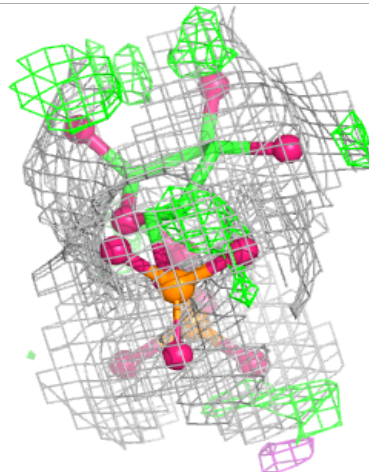
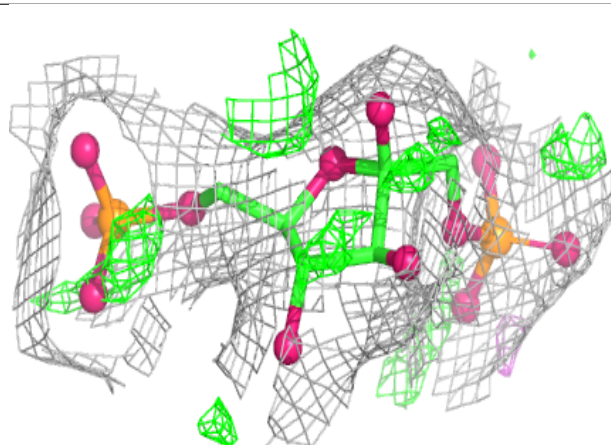
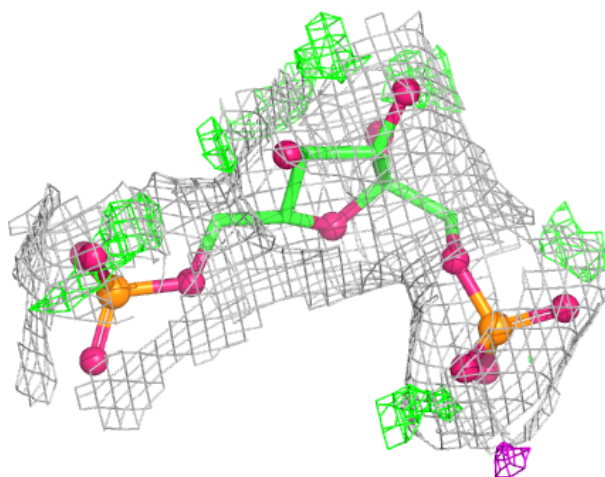
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





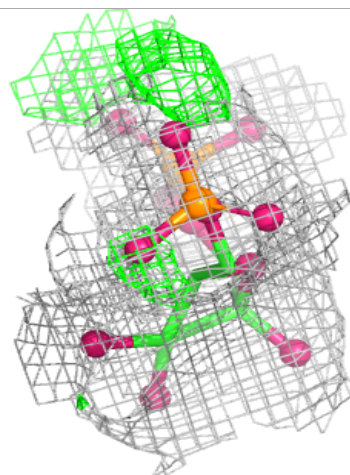
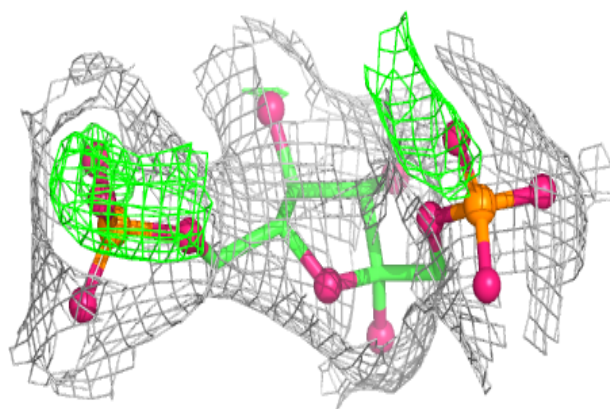
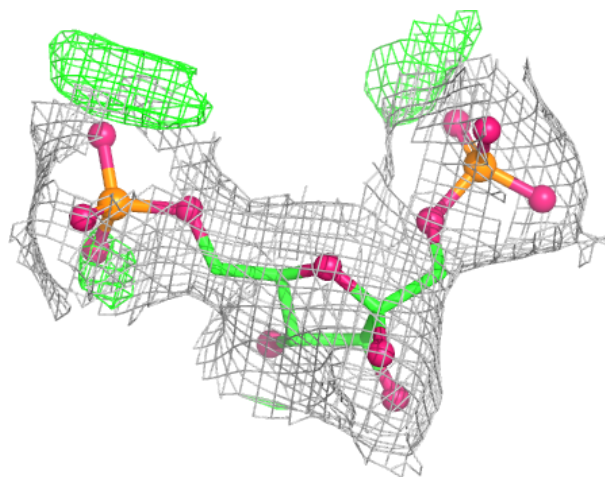
**Electron density around FBP B 501:**

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



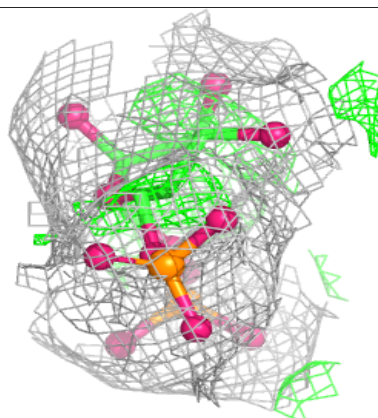
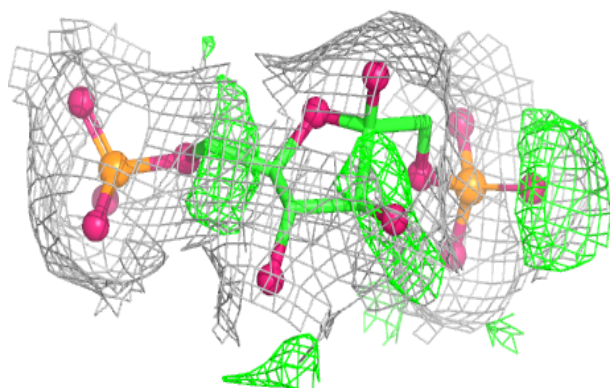
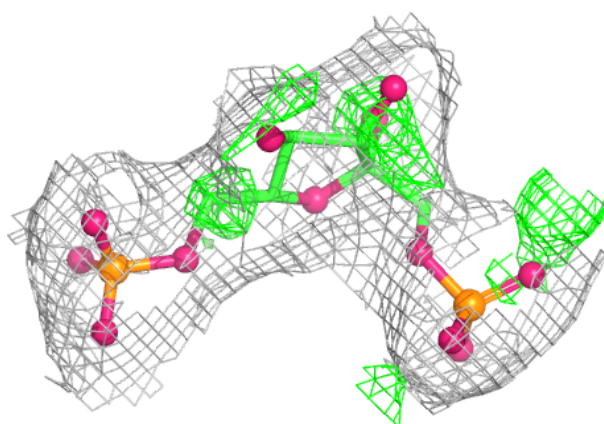
**Electron density around FBP F 501:**

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

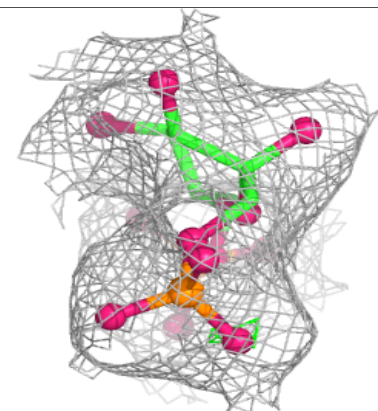
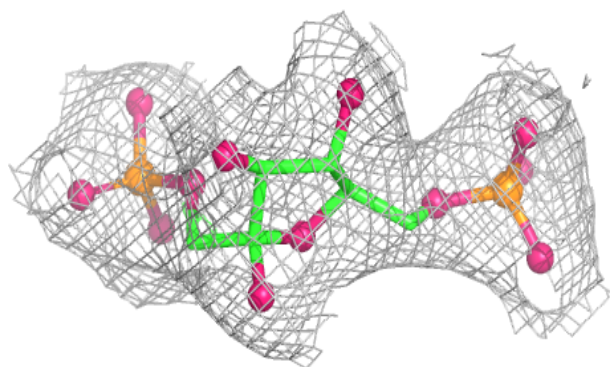
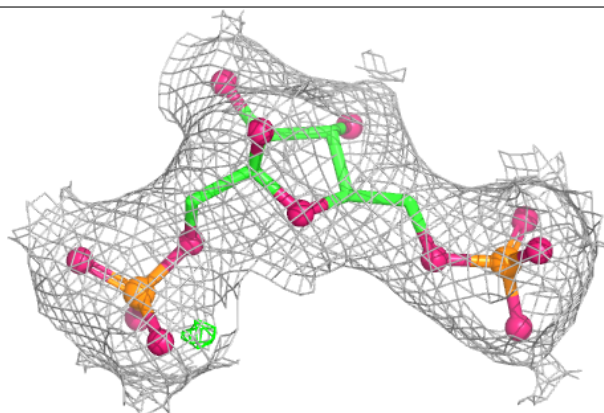


**Electron density around FBP E 501:**

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

**Electron density around FBP G 501:**

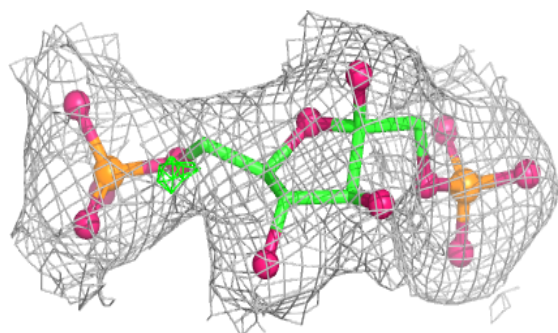
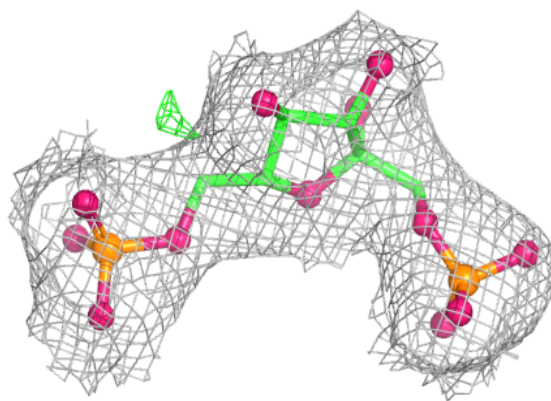
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



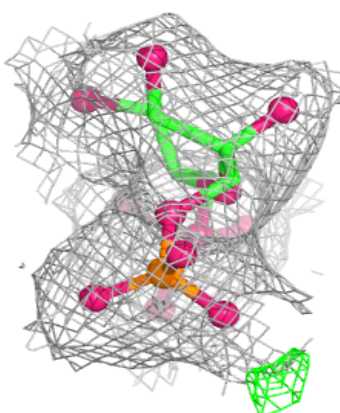
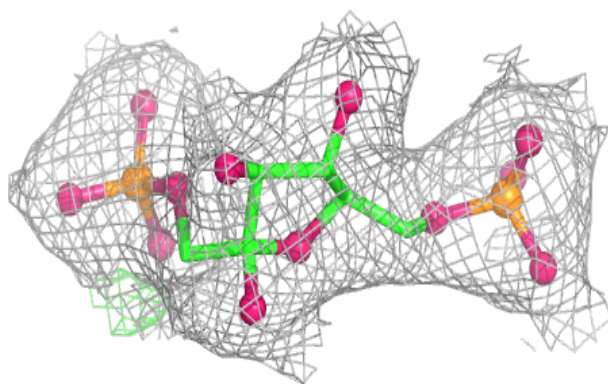
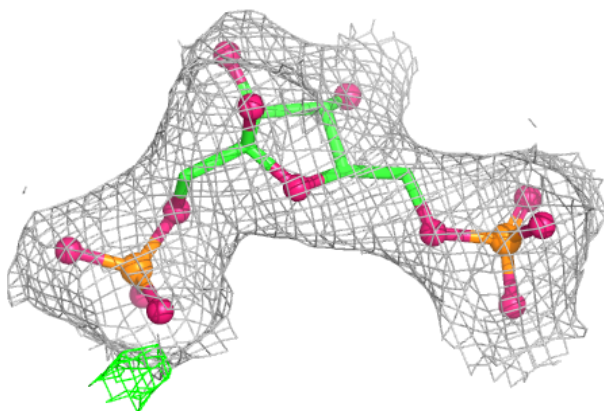


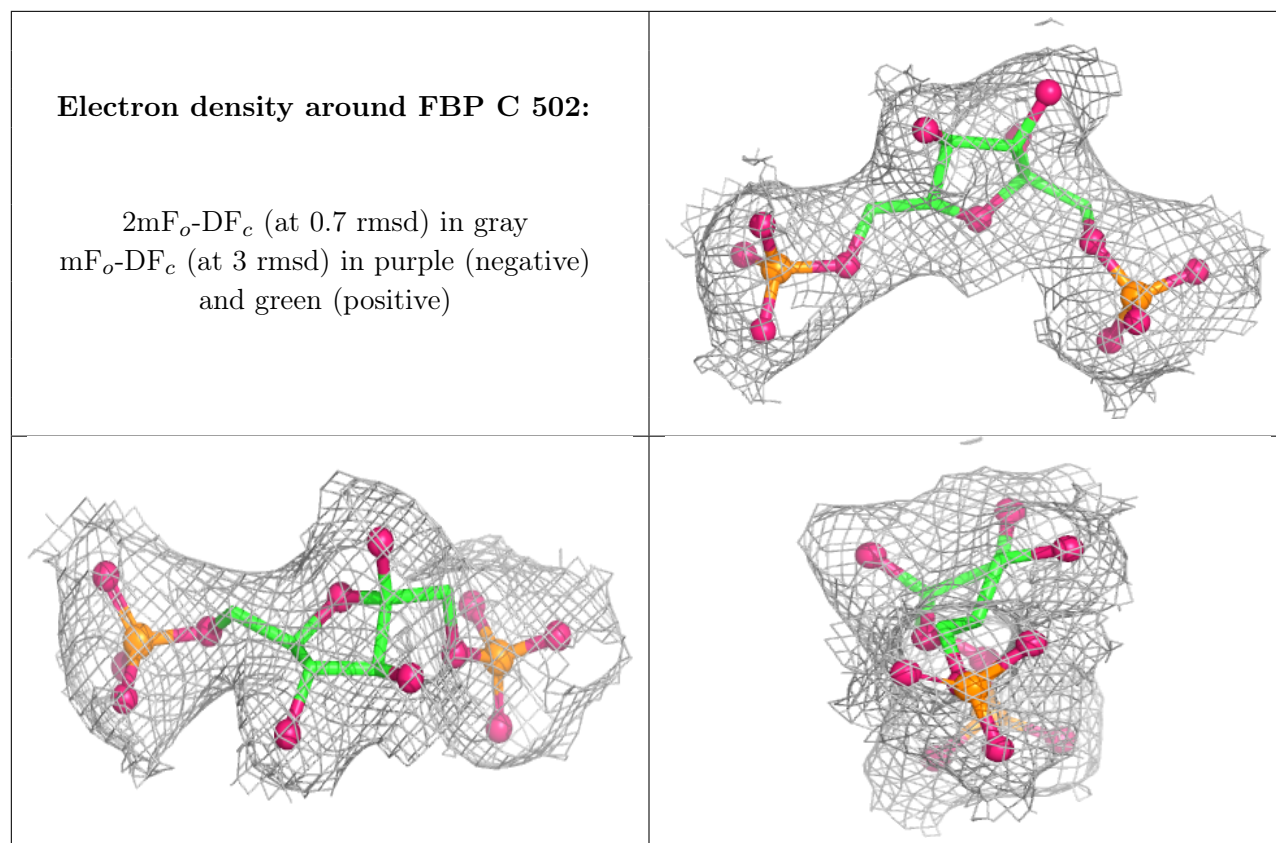
**Electron density around FBP H 501:**

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

**Electron density around FBP D 501:**

$2mF_o-DF_c$  (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.