



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 10:05 PM UTC

PDB ID : 9RFQ / pdb_00009rfq
Title : Structure of liver pyruvate kinase in complex with Liver pyruvate kinase in complex with fluorescent probe I
Authors : Bogucka, A.; Koteles, I.; Grotli, M.; Hyvonen, M.
Deposited on : 2025-06-04
Resolution : 2.38 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

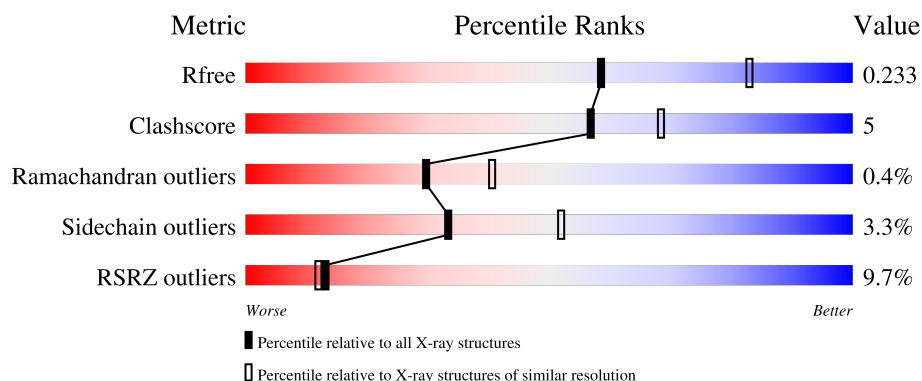
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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.



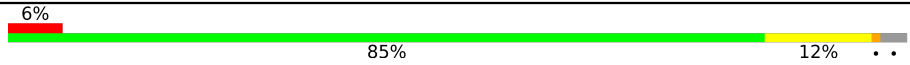

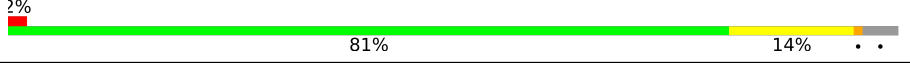
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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 ≥ 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>22%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	B	447	<div> <div>15%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>
1	C	447	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>
1	D	447	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	E	447	<div> <div>17%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	447	 6% 85% 12% . .
1	G	447	 2% 80% 13% . 6%
1	H	447	 2% 81% 14% . .

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	502	-	X	-	-
3	OXL	D	502	-	X	-	-
3	OXL	E	502	-	X	-	-
3	OXL	G	502	-	X	-	-
3	OXL	H	503	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27172 atoms, of which 64 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	424	Total	C	N	O	S	0	6	0
			3248	2040	589	600	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	422	Total	C	N	O	S	0	6	0
			3237	2034	582	602	19			
1	H	427	Total	C	N	O	S	0	4	0
			3268	2051	596	602	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
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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
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H	?	-	ASN	deletion	UNP P30613

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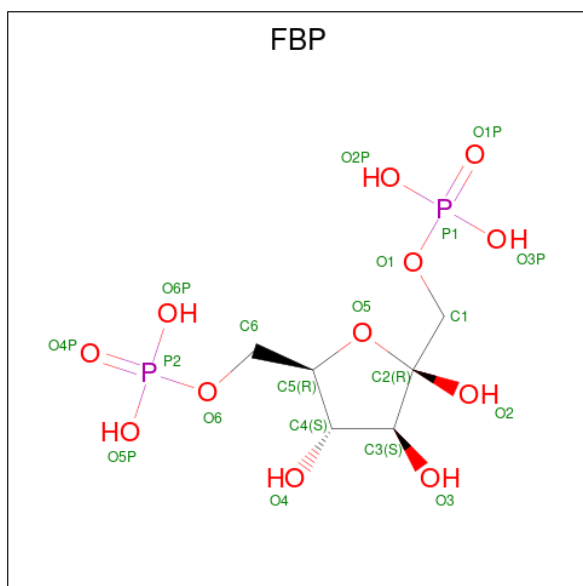
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H	?	-	TYR	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	PRO	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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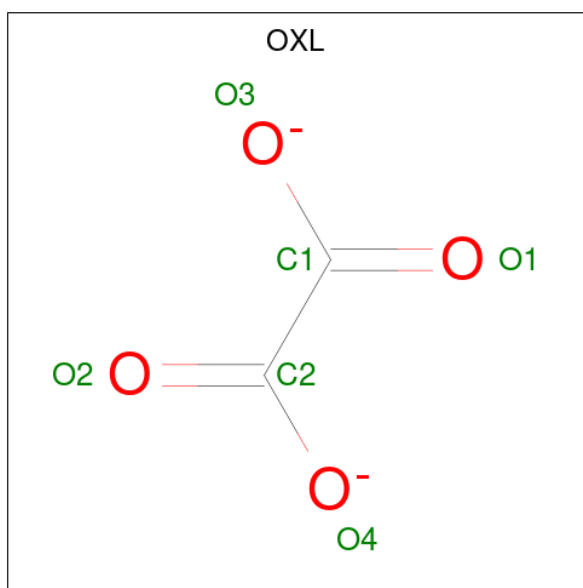
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLU	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	ARG	deletion	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	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
2	H	1	Total	C	O	P	0	0
			20	6	12	2		

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



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

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

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

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

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

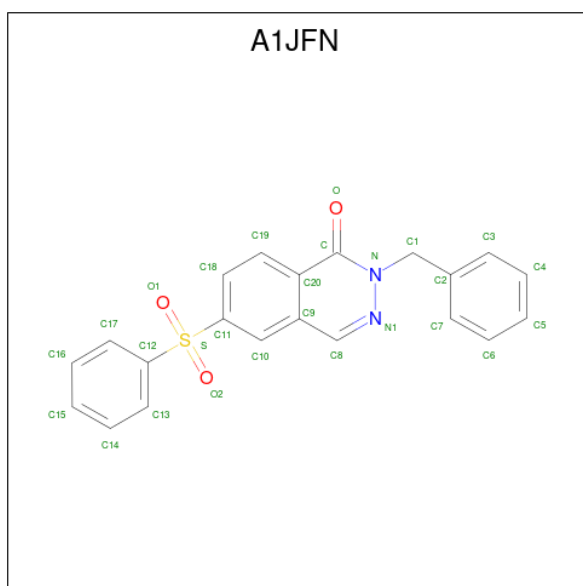
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	C	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		
5	E	1	Total	K	0	0
			1	1		

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

- Molecule 6 is 2-(phenylmethyl)-6-(phenylsulfonyl)phthalazin-1-one (CCD ID: A1JFN) (formula: C₂₁H₁₆N₂O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	S	16	0
			43	21	16	2	3	1		
6	C	1	Total	C	H	N	O	S	16	0
			43	21	16	2	3	1		
6	E	1	Total	C	H	N	O	S	16	0
			43	21	16	2	3	1		
6	H	1	Total	C	H	N	O	S	16	0
			43	21	16	2	3	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	45	Total O 45 45	0	0
7	B	49	Total O 49 49	0	0

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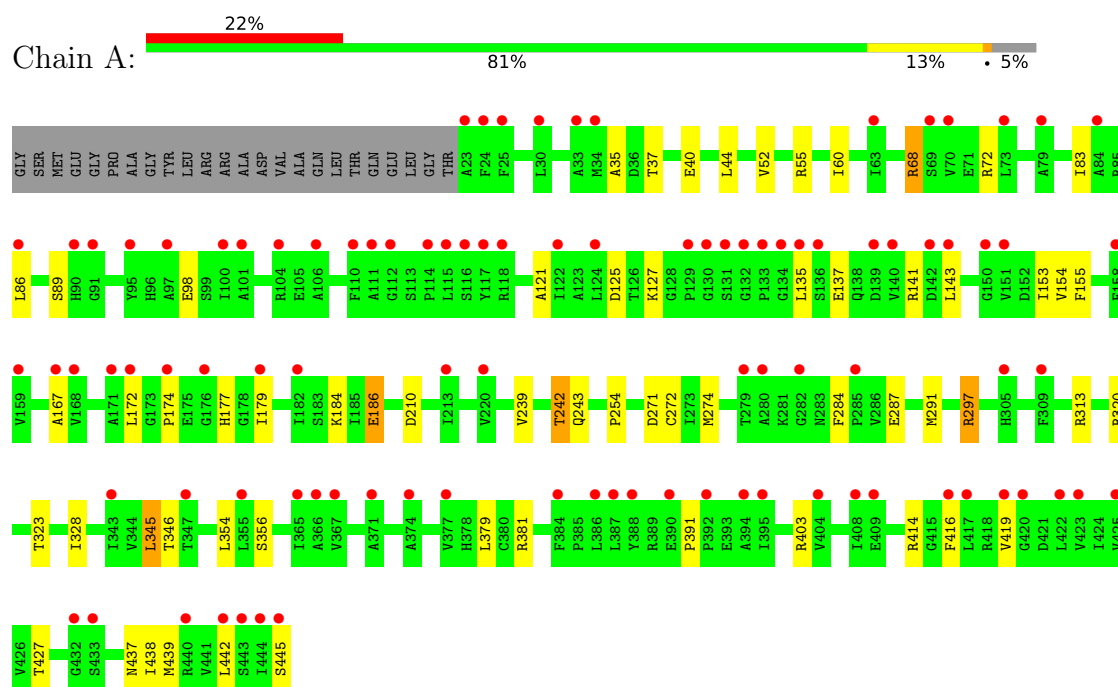
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	81	Total 81	O 81	0	0
7	D	99	Total 99	O 99	0	0
7	E	62	Total 62	O 62	0	0
7	F	79	Total 79	O 79	0	0
7	G	91	Total 91	O 91	0	0
7	H	122	Total 122	O 122	0	0

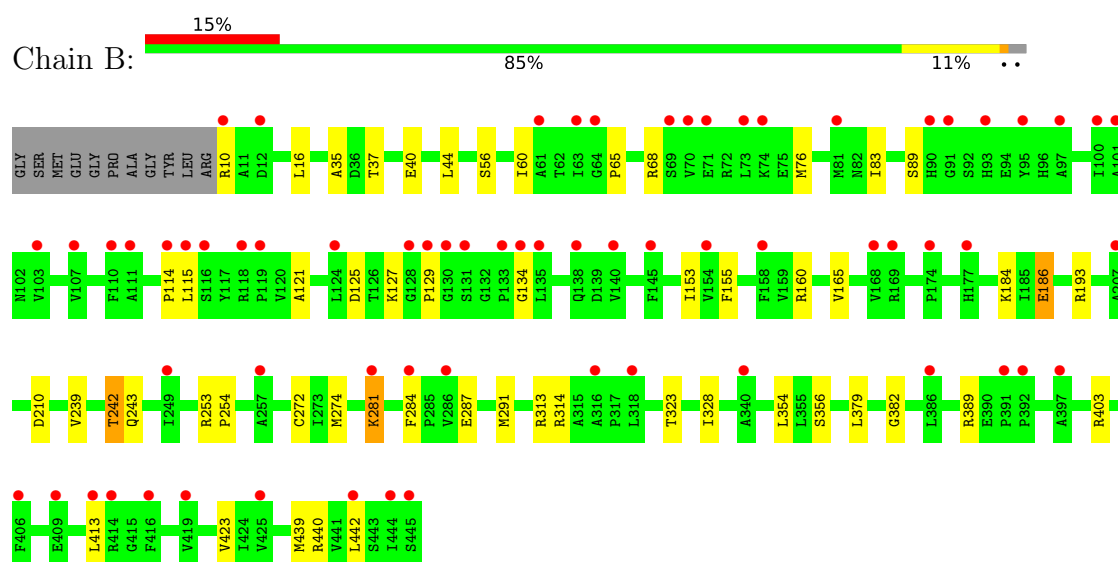
3 Residue-property plots [i](#)

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.

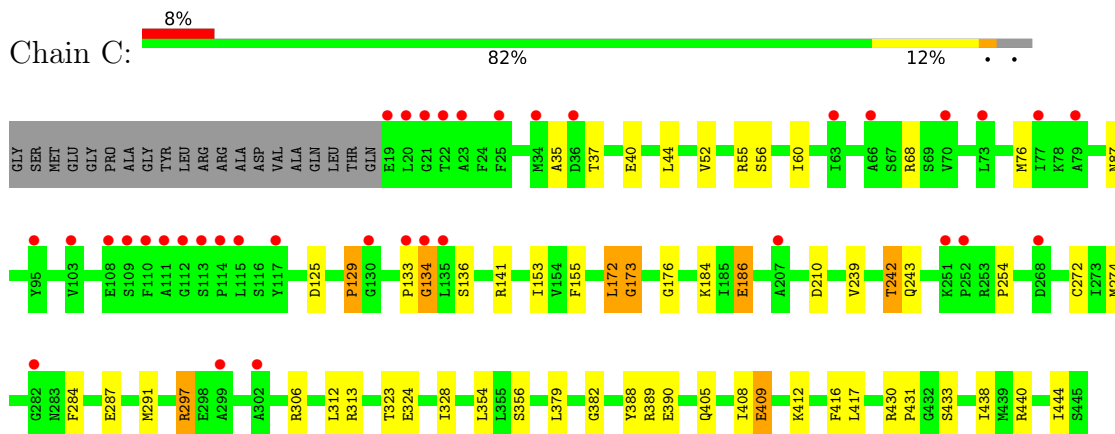
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



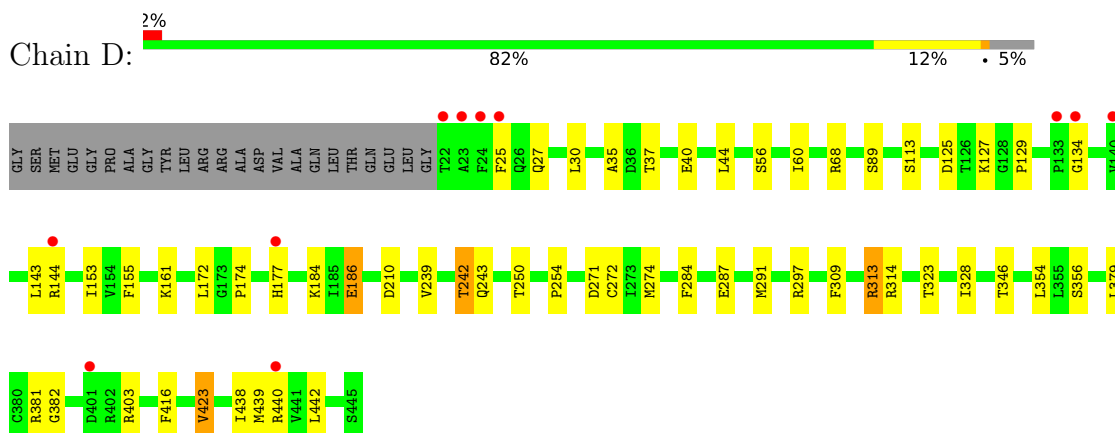
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



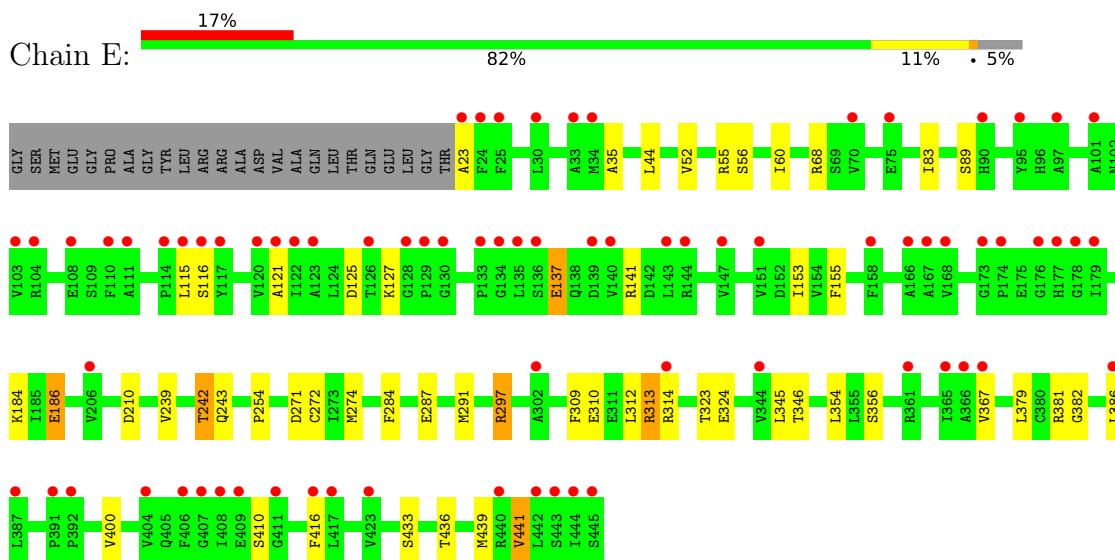
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR



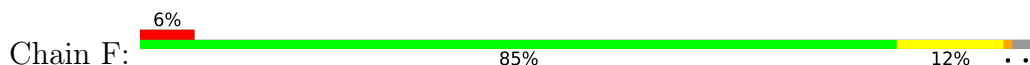
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

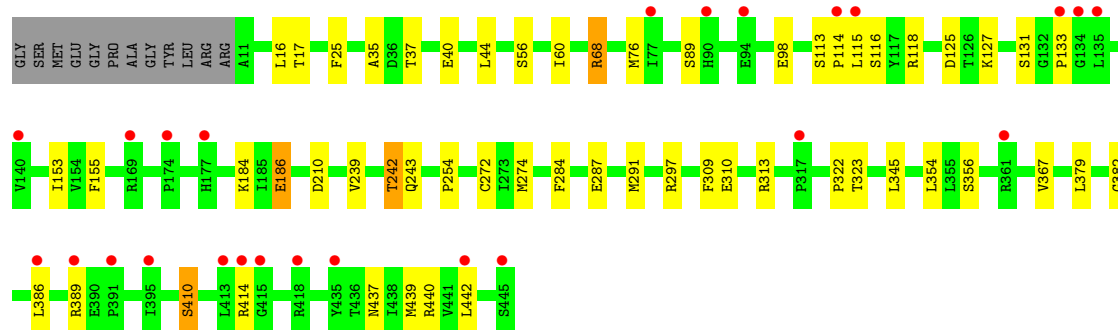


• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

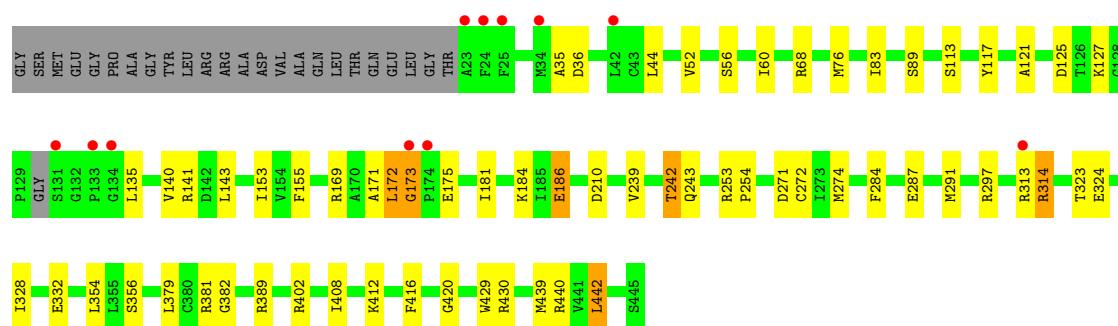
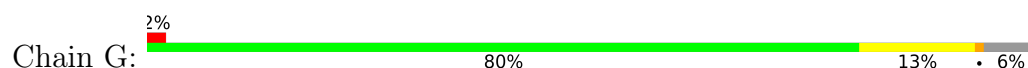


• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

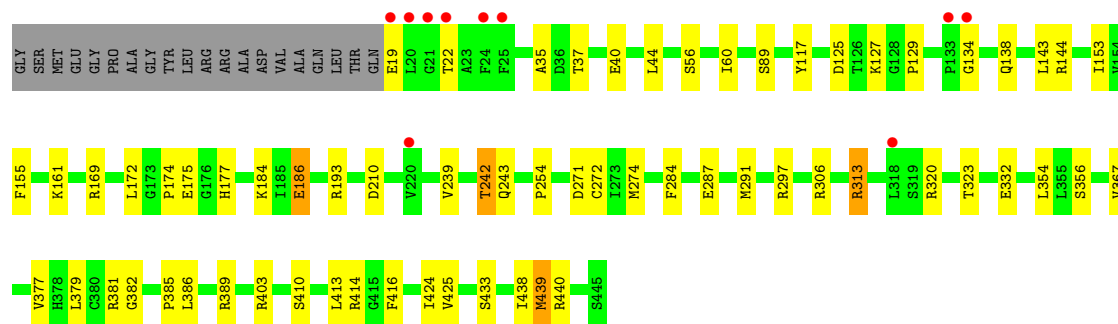
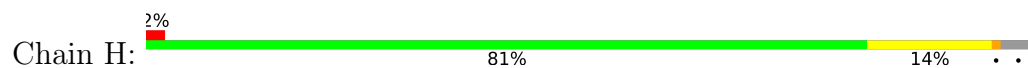




● Molecule 1: Isoform L-type of Pyruvate kinase PKLR



● 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, α , β , γ	207.36Å 112.74Å 187.80Å 90.00° 91.83° 90.00°	Depositor
Resolution (Å)	187.71 – 2.38 187.71 – 2.38	Depositor EDS
% Data completeness (in resolution range)	48.3 (187.71-2.38) 48.3 (187.71-2.38)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.209 , 0.242 0.204 , 0.233	Depositor DCC
R_{free} test set	4101 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27172	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 63.26 % 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 9.9381e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: A1JFN, FBP, MG, OXL, 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	0.68	0/3316	1.09	2/4484 (0.0%)
1	B	0.67	0/3396	1.06	0/4592
1	C	0.69	0/3324	1.09	6/4495 (0.1%)
1	D	0.69	0/3322	1.06	3/4492 (0.1%)
1	E	0.66	0/3301	1.09	6/4463 (0.1%)
1	F	0.69	0/3411	1.07	2/4613 (0.0%)
1	G	0.70	0/3309	1.05	3/4473 (0.1%)
1	H	0.72	0/3333	1.08	1/4506 (0.0%)
All	All	0.69	0/26712	1.08	23/36118 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	PRO	N-CA-C	7.71	120.10	110.70
1	C	416	PHE	CA-CB-CG	6.87	120.67	113.80
1	G	416	PHE	CA-CB-CG	6.27	120.07	113.80
1	E	23	ALA	CA-C-N	6.22	128.90	120.38
1	E	23	ALA	C-N-CA	6.22	128.90	120.38
1	A	416	PHE	CA-CB-CG	6.11	119.91	113.80
1	E	312	LEU	CA-C-N	6.10	128.37	120.44
1	E	312	LEU	C-N-CA	6.10	128.37	120.44
1	C	409	GLU	CB-CG-CD	5.93	122.68	112.60
1	F	116	SER	CA-C-N	5.65	131.12	122.93
1	F	116	SER	C-N-CA	5.65	131.12	122.93
1	D	416	PHE	CA-CB-CG	5.63	119.43	113.80
1	D	27	GLN	CA-C-N	5.63	130.12	122.07
1	D	27	GLN	C-N-CA	5.63	130.12	122.07
1	G	172	LEU	CA-C-N	5.62	130.69	121.87
1	G	172	LEU	C-N-CA	5.62	130.69	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	416	PHE	CA-CB-CG	5.61	119.41	113.80
1	E	416	PHE	CA-CB-CG	5.57	119.37	113.80
1	E	324	GLU	CB-CG-CD	5.27	121.56	112.60
1	C	172	LEU	CA-C-N	5.16	129.97	121.87
1	C	172	LEU	C-N-CA	5.16	129.97	121.87
1	C	312	LEU	CA-C-N	5.02	127.28	120.65
1	C	312	LEU	C-N-CA	5.02	127.28	120.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3243	0	3307	32	0
1	B	3329	0	3395	28	0
1	C	3257	0	3309	36	0
1	D	3248	0	3307	31	0
1	E	3231	0	3289	27	0
1	F	3335	0	3404	26	0
1	G	3237	0	3290	41	0
1	H	3268	0	3323	43	0
2	A	20	0	10	2	0
2	B	20	0	10	1	0
2	C	20	0	10	1	0
2	D	20	0	10	2	0
2	E	20	0	10	2	0
2	F	20	0	10	0	0
2	G	20	0	10	1	0
2	H	20	0	10	1	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	27	16	0	0	0
6	C	27	16	0	0	0
6	E	27	16	0	0	0
6	H	27	16	0	0	0
7	A	45	0	0	1	0
7	B	49	0	0	0	0
7	C	81	0	0	1	0
7	D	99	0	0	1	0
7	E	62	0	0	1	0
7	F	79	0	0	0	0
7	G	91	0	0	2	0
7	H	122	0	0	3	0
All	All	27108	64	26704	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (244) 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:313:ARG:HG3	1:C:328:ILE:HD11	1.51	0.90
7:G:615:HOH:O	1:H:313:ARG:HD3	1.72	0.87
1:A:174:PRO:HA	1:A:177:HIS:NE2	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:439:MET:HE3	1:H:439:MET:HG2	1.61	0.83
1:B:114:PRO:HB3	1:B:389:ARG:HE	1.43	0.81
1:F:114:PRO:HB3	1:F:389:ARG:HE	1.43	0.81
1:C:133:PRO:HG2	1:G:430:ARG:HH11	1.47	0.77
1:H:424:ILE:HG23	1:H:439:MET:HE3	1.69	0.73
1:C:324[A]:GLU:HG3	1:C:354:LEU:HD13	1.71	0.72
1:D:284:PHE:HB3	1:D:287:GLU:HB2	1.73	0.69
1:D:313:ARG:HB3	1:D:328:ILE:HD11	1.75	0.69
1:A:89:SER:HA	1:A:127:LYS:HG3	1.76	0.68
2:C:501:FBP:O3P	1:G:141:ARG:NH2	2.26	0.66
1:F:89:SER:HA	1:F:127:LYS:HG3	1.78	0.66
1:G:324[A]:GLU:HG3	1:G:354:LEU:HD13	1.76	0.66
1:B:89:SER:HA	1:B:127:LYS:HG3	1.79	0.65
1:D:89:SER:HA	1:D:127:LYS:HG3	1.77	0.65
1:A:403:ARG:NH1	2:A:501:FBP:O2P	2.30	0.65
1:G:89:SER:HA	1:G:127:LYS:HG3	1.80	0.63
1:G:56:SER:HB2	1:G:382:GLY:HA2	1.81	0.63
1:H:89:SER:HA	1:H:127:LYS:HG3	1.79	0.63
1:D:143:LEU:HD22	1:D:172:LEU:HD21	1.80	0.63
1:A:346:THR:HA	2:A:501:FBP:H61	1.81	0.63
1:E:89:SER:HA	1:E:127:LYS:HG3	1.78	0.63
1:A:414:ARG:HD3	7:A:617:HOH:O	1.99	0.62
1:F:440:ARG:HD2	1:F:442[A]:LEU:HD21	1.80	0.61
1:B:65:PRO:HG3	1:B:281:LYS:HE3	1.81	0.61
1:E:284:PHE:HB3	1:E:287:GLU:HB2	1.83	0.60
1:H:56:SER:HB2	1:H:382:GLY:HA2	1.82	0.60
1:B:114:PRO:CB	1:B:389:ARG:HE	2.13	0.60
1:F:309:PHE:CE2	1:F:313:ARG:NH1	2.64	0.60
1:B:284:PHE:HB3	1:B:287:GLU:HB2	1.84	0.60
1:B:313:ARG:HG2	1:B:328:ILE:HD11	1.82	0.60
1:B:56:SER:HB2	1:B:382:GLY:HA2	1.84	0.59
1:C:284:PHE:HB3	1:C:287:GLU:HB2	1.83	0.59
1:A:284:PHE:HB3	1:A:287:GLU:HB2	1.83	0.59
1:D:56:SER:HB2	1:D:382:GLY:HA2	1.84	0.59
1:E:56:SER:HB2	1:E:382:GLY:HA2	1.85	0.59
1:F:284:PHE:HB3	1:F:287:GLU:HB2	1.83	0.59
1:B:239:VAL:HG22	1:B:272:CYS:HB2	1.84	0.59
1:A:239:VAL:HG22	1:A:272:CYS:HB2	1.84	0.59
1:E:239:VAL:HG22	1:E:272:CYS:HB2	1.85	0.58
1:A:135:LEU:HD22	1:A:167:ALA:HB1	1.86	0.58
1:C:56:SER:HB2	1:C:382:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:PRO:HA	1:H:177[A]:HIS:CE1	2.38	0.58
1:H:239:VAL:HG22	1:H:272:CYS:HB2	1.86	0.58
1:D:239:VAL:HG22	1:D:272:CYS:HB2	1.86	0.58
1:C:239:VAL:HG22	1:C:272:CYS:HB2	1.86	0.57
1:G:239:VAL:HG22	1:G:272:CYS:HB2	1.86	0.57
1:D:423:VAL:HG12	1:D:442:LEU:HB3	1.85	0.57
1:F:239:VAL:HG22	1:F:272:CYS:HB2	1.85	0.57
1:A:320[A]:ARG:HG3	1:B:16:LEU:HD11	1.87	0.57
1:D:174:PRO:HA	1:D:177[A]:HIS:CE1	2.41	0.56
1:F:56:SER:HB2	1:F:382:GLY:HA2	1.87	0.56
1:G:284:PHE:HB3	1:G:287:GLU:HB2	1.86	0.56
1:G:313:ARG:HG3	1:G:328:ILE:HD11	1.87	0.56
1:B:440:ARG:HD2	1:B:442[A]:LEU:HD21	1.88	0.55
1:G:440:ARG:CG	1:H:438:ILE:HG12	2.37	0.55
1:C:153:ILE:HG12	1:C:379:LEU:HD11	1.89	0.55
1:A:68:ARG:HH22	1:A:98:GLU:HB3	1.73	0.54
1:H:143:LEU:HD22	1:H:172:LEU:HD21	1.89	0.54
1:B:65:PRO:CG	1:B:281:LYS:HE3	2.38	0.53
1:D:242:THR:HG22	1:D:243:GLN:HG3	1.90	0.53
1:G:242:THR:HG22	1:G:243:GLN:HG3	1.90	0.53
1:E:346:THR:HA	2:E:501:FBP:H61	1.90	0.53
1:C:405:GLN:O	1:C:409:GLU:HG2	2.09	0.53
1:C:242:THR:HG22	1:C:243:GLN:HG3	1.90	0.52
1:A:313:ARG:HG3	1:A:328:ILE:HD11	1.90	0.52
1:C:430:ARG:NH2	1:G:135:LEU:O	2.42	0.52
1:C:306:ARG:HD3	1:D:314:ARG:NH2	2.25	0.52
1:C:440:ARG:HG2	1:D:438:ILE:HG12	1.92	0.52
1:D:129:PRO:HB3	1:D:134:GLY:O	2.10	0.52
1:A:242:THR:HG22	1:A:243:GLN:HG3	1.92	0.51
1:E:242:THR:HG22	1:E:243:GLN:HG3	1.92	0.51
1:G:439:MET:CE	1:H:439:MET:HG2	2.38	0.51
1:G:35:ALA:HB2	1:G:44:LEU:HD12	1.92	0.51
1:H:403:ARG:NH1	2:H:502:FBP:O1P	2.39	0.51
1:A:35:ALA:HB2	1:A:44:LEU:HD12	1.92	0.51
1:D:35:ALA:HB1	1:D:40:GLU:HB3	1.92	0.51
1:E:309:PHE:O	1:E:313:ARG:HB2	2.10	0.51
1:A:35:ALA:HB1	1:A:40:GLU:HB3	1.93	0.51
1:H:284:PHE:HB3	1:H:287:GLU:HB2	1.92	0.50
1:C:35:ALA:HB2	1:C:44:LEU:HD12	1.94	0.50
1:A:153:ILE:HG12	1:A:379:LEU:HD11	1.94	0.50
1:F:35:ALA:HB2	1:F:44:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:ILE:HG12	1:F:379:LEU:HD11	1.94	0.50
1:H:144:ARG:HG2	7:H:692:HOH:O	2.12	0.50
1:H:35:ALA:HB2	1:H:44:LEU:HD12	1.93	0.50
1:F:17:THR:HA	1:F:25:PHE:CE2	2.46	0.50
1:G:117:TYR:CD2	1:G:389:ARG:NH2	2.80	0.50
1:G:153:ILE:HG12	1:G:379:LEU:HD11	1.93	0.50
1:E:137:GLU:O	1:E:141:ARG:HD3	2.12	0.50
1:D:35:ALA:HB2	1:D:44:LEU:HD12	1.93	0.49
1:B:35:ALA:HB2	1:B:44:LEU:HD12	1.93	0.49
1:B:129:PRO:HB3	1:B:134:GLY:O	2.12	0.49
1:E:153:ILE:HG12	1:E:379:LEU:HD11	1.95	0.49
1:C:60:ILE:HB	1:C:274:MET:HG3	1.95	0.49
1:A:137:GLU:O	1:A:141:ARG:HD3	2.12	0.49
1:H:60:ILE:HB	1:H:274:MET:HG3	1.94	0.49
1:E:60:ILE:HB	1:E:274:MET:HG3	1.94	0.49
1:H:129:PRO:HB3	1:H:134:GLY:O	2.12	0.49
1:F:60:ILE:HB	1:F:274:MET:HG3	1.94	0.48
1:H:35:ALA:HB1	1:H:40:GLU:HB3	1.95	0.48
1:B:242:THR:HG22	1:B:243:GLN:HG3	1.94	0.48
1:E:441:VAL:HG13	1:F:322:PRO:HB3	1.95	0.48
1:G:439:MET:HE3	1:H:439:MET:CG	2.38	0.48
1:G:56:SER:HB2	1:G:382:GLY:CA	2.43	0.48
1:E:35:ALA:HB2	1:E:44:LEU:HD12	1.94	0.48
1:G:314:ARG:NH2	1:H:306:ARG:HD3	2.28	0.48
1:F:35:ALA:HB1	1:F:40:GLU:HB3	1.95	0.48
1:C:56:SER:HB2	1:C:382:GLY:CA	2.44	0.48
1:H:56:SER:HB2	1:H:382:GLY:CA	2.43	0.48
1:A:60:ILE:HB	1:A:274:MET:HG3	1.95	0.48
1:C:438:ILE:HG12	1:D:440:ARG:CG	2.44	0.48
1:H:153:ILE:HG12	1:H:379:LEU:HD11	1.96	0.48
1:D:60:ILE:HB	1:D:274:MET:HG3	1.95	0.47
1:C:388:TYR:CE2	1:C:390:GLU:HB2	2.48	0.47
1:G:60:ILE:HB	1:G:274:MET:HG3	1.97	0.47
1:B:35:ALA:HB1	1:B:40:GLU:HB3	1.97	0.47
1:B:60:ILE:HB	1:B:274:MET:HG3	1.96	0.47
1:E:441:VAL:HG13	1:F:437:ASN:HB2	1.96	0.47
1:H:242:THR:HG22	1:H:243:GLN:HG3	1.97	0.47
1:A:143:LEU:HD22	1:A:172:LEU:HD21	1.97	0.47
1:C:388:TYR:CZ	1:C:390:GLU:HB2	2.50	0.47
1:F:113:SER:C	1:F:115:LEU:H	2.23	0.47
1:A:419:VAL:HG22	1:A:445:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:HG12	1:B:379:LEU:HD11	1.96	0.47
1:H:410:SER:O	1:H:414:ARG:HG3	2.14	0.47
1:A:154:VAL:HG23	1:A:179:ILE:HG21	1.97	0.47
1:D:153:ILE:HG12	1:D:379:LEU:HD11	1.97	0.47
1:G:143:LEU:HD22	1:G:172:LEU:HD21	1.97	0.46
1:E:254:PRO:HG3	1:E:291:MET:HG2	1.97	0.46
1:G:440:ARG:HG2	1:H:438:ILE:HG12	1.97	0.46
1:B:56:SER:HB2	1:B:382:GLY:CA	2.45	0.46
1:B:160:ARG:O	1:B:193:ARG:HD3	2.16	0.46
1:C:35:ALA:HB1	1:C:40:GLU:HB3	1.97	0.46
1:A:323:THR:HG22	1:A:354:LEU:HD12	1.97	0.46
1:C:323:THR:HG22	1:C:354:LEU:HD12	1.98	0.46
1:D:56:SER:HB2	1:D:382:GLY:CA	2.45	0.46
1:E:116:SER:O	7:E:601:HOH:O	2.21	0.46
1:C:125:ASP:HA	1:C:155:PHE:HB2	1.98	0.46
1:E:346:THR:OG1	2:E:501:FBP:O4P	2.28	0.46
1:F:242:THR:HG22	1:F:243:GLN:HG3	1.97	0.46
1:C:412:LYS:HG3	1:C:417:LEU:HB2	1.98	0.45
1:G:314:ARG:CZ	1:H:306:ARG:HD3	2.46	0.45
1:B:186:GLU:HB3	1:B:210:ASP:HB2	1.98	0.45
1:G:254:PRO:HG3	1:G:291:MET:HG2	1.99	0.45
1:G:440:ARG:HD2	1:G:442:LEU:HD21	1.97	0.45
1:C:186:GLU:HB3	1:C:210:ASP:HB2	1.99	0.45
1:E:56:SER:HB2	1:E:382:GLY:CA	2.45	0.45
1:E:345:LEU:HD22	1:E:400:VAL:HG13	1.98	0.45
1:F:37:THR:OG1	1:F:40:GLU:HB2	2.17	0.45
1:G:36:ASP:HB3	7:H:710:HOH:O	2.15	0.45
1:C:172:LEU:O	1:C:173:GLY:O	2.34	0.45
1:H:424:ILE:HG23	1:H:439:MET:CE	2.41	0.45
1:B:403:ARG:NH1	2:B:501:FBP:O3P	2.39	0.45
1:G:408:ILE:HG22	1:G:412:LYS:HD2	1.99	0.45
1:H:138:GLN:HG2	7:H:657:HOH:O	2.16	0.45
1:D:125:ASP:HA	1:D:155:PHE:HB2	1.99	0.45
1:F:56:SER:HB2	1:F:382:GLY:CA	2.47	0.45
1:A:37:THR:OG1	1:A:40:GLU:HB2	2.17	0.45
1:C:129:PRO:HB3	1:C:134:GLY:O	2.17	0.45
1:E:323:THR:HG22	1:E:354:LEU:HD12	1.99	0.45
1:G:171:ALA:C	1:G:173:GLY:H	2.25	0.45
1:A:186:GLU:HB3	1:A:210:ASP:HB2	1.99	0.45
1:F:186:GLU:HB3	1:F:210:ASP:HB2	1.99	0.45
1:F:125:ASP:HA	1:F:155:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:THR:OG1	1:H:40:GLU:HB2	2.17	0.44
1:F:410:SER:O	1:F:414:ARG:HB2	2.17	0.44
1:C:37:THR:OG1	1:C:40:GLU:HB2	2.18	0.44
1:H:425:VAL:HB	1:H:440[B]:ARG:CG	2.47	0.44
1:H:439:MET:O	1:H:439:MET:HG3	2.17	0.44
1:B:37:THR:OG1	1:B:40:GLU:HB2	2.18	0.44
1:D:323:THR:HG22	1:D:354:LEU:HD12	1.99	0.44
1:A:438:ILE:HG12	1:B:440:ARG:CG	2.47	0.44
1:C:129:PRO:HA	1:C:136:SER:HB3	1.99	0.44
1:D:186:GLU:HB3	1:D:210:ASP:HB2	1.98	0.44
1:E:155:PHE:HB3	1:E:184:LYS:HD2	2.00	0.44
1:F:323:THR:HG22	1:F:354:LEU:HD12	1.99	0.44
1:C:438:ILE:HG12	1:D:440:ARG:HG2	2.00	0.44
1:B:254:PRO:HG3	1:B:291:MET:HG2	1.99	0.44
1:G:186:GLU:HB3	1:G:210:ASP:HB2	1.99	0.44
1:A:125:ASP:HA	1:A:155:PHE:HB2	2.00	0.43
1:E:186:GLU:HB3	1:E:210:ASP:HB2	2.00	0.43
1:D:155:PHE:HB3	1:D:184:LYS:HD2	1.98	0.43
1:D:37:THR:OG1	1:D:40:GLU:HB2	2.18	0.43
1:G:125:ASP:HA	1:G:155:PHE:HB2	2.00	0.43
1:H:323:THR:HG22	1:H:354:LEU:HD12	1.99	0.43
1:H:367:VAL:HG22	1:H:386:LEU:HD12	2.01	0.43
1:C:210:ASP:OD2	3:C:502:OXL:O1	2.36	0.43
1:C:431:PRO:HB2	1:G:140:VAL:HG11	2.00	0.43
1:G:402:ARG:HD3	7:G:638:HOH:O	2.18	0.43
1:H:155:PHE:HB3	1:H:184:LYS:HD2	1.99	0.43
1:A:155:PHE:HB3	1:A:184:LYS:HD2	2.00	0.43
1:F:254:PRO:HG3	1:F:291:MET:HG2	1.99	0.43
1:C:408:ILE:HG23	1:C:444:ILE:HD12	2.01	0.43
1:H:169[B]:ARG:HD3	1:H:169[B]:ARG:HA	1.76	0.43
1:H:125:ASP:HA	1:H:155:PHE:HB2	2.00	0.43
1:G:420:GLY:O	1:H:320:ARG:NH2	2.51	0.42
1:H:117:TYR:CD2	1:H:389:ARG:NH2	2.87	0.42
1:H:254:PRO:HG3	1:H:291:MET:HG2	2.01	0.42
1:F:155:PHE:HB3	1:F:184:LYS:HD2	2.00	0.42
1:D:309:PHE:CE2	1:D:313:ARG:HD3	2.54	0.42
1:G:155:PHE:HB3	1:G:184:LYS:HD2	2.02	0.42
1:G:169:ARG:HG2	1:G:181:ILE:CD1	2.48	0.42
1:A:254:PRO:HG3	1:A:291:MET:HG2	2.00	0.42
1:H:377:VAL:CG2	1:H:385:PRO:HB3	2.50	0.42
1:C:55:ARG:HB2	1:C:297:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:PRO:HG3	1:C:291:MET:HG2	2.01	0.42
1:B:125:ASP:HA	1:B:155:PHE:HB2	2.01	0.42
1:B:323:THR:HG22	1:B:354:LEU:HD12	2.01	0.42
1:E:55:ARG:HB2	1:E:297:ARG:HG3	2.02	0.42
1:E:125:ASP:HA	1:E:155:PHE:HB2	2.00	0.42
1:D:403:ARG:NH1	2:D:501:FBP:O2P	2.40	0.42
1:G:332[A]:GLU:OE1	1:H:332:GLU:OE1	2.37	0.41
1:H:271:ASP:HA	1:H:381:ARG:HB2	2.02	0.41
1:B:155:PHE:HB3	1:B:184:LYS:HD2	2.02	0.41
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.36	0.41
1:A:271:ASP:HB3	1:A:379:LEU:O	2.21	0.41
1:C:155:PHE:HB3	1:C:184:LYS:HD2	2.01	0.41
1:G:429:TRP:CE2	1:G:430:ARG:HG2	2.56	0.41
1:A:345:LEU:HD22	1:A:427:THR:HG22	2.02	0.41
1:D:174:PRO:HD2	7:D:622:HOH:O	2.20	0.41
1:A:55:ARG:HB2	1:A:297:ARG:HG3	2.02	0.41
1:D:271:ASP:HA	1:D:381:ARG:HB2	2.01	0.41
1:G:323:THR:HG22	1:G:354:LEU:HD12	2.02	0.41
1:H:186:GLU:HB3	1:H:210:ASP:HB2	2.02	0.41
1:G:271:ASP:HB3	1:G:379:LEU:O	2.21	0.41
1:A:271:ASP:HA	1:A:381:ARG:HB2	2.02	0.41
1:D:25:PHE:HA	1:D:30:LEU:HD12	2.01	0.41
1:E:367:VAL:HG22	1:E:386:LEU:HD12	2.03	0.41
1:A:83:ILE:HG12	1:A:121:ALA:HB3	2.03	0.41
1:G:271:ASP:HA	1:G:381:ARG:HB2	2.01	0.41
1:D:254:PRO:HG3	1:D:291:MET:HG2	2.02	0.40
1:E:271:ASP:HA	1:E:381:ARG:HB2	2.02	0.40
1:E:83:ILE:HG12	1:E:121:ALA:HB3	2.03	0.40
1:G:83:ILE:HG12	1:G:121:ALA:HB3	2.03	0.40
1:H:161:LYS:HB3	1:H:193:ARG:HE	1.86	0.40
1:C:141:ARG:HH22	2:G:501:FBP:P1	2.44	0.40
1:F:367:VAL:HG22	1:F:386:LEU:HD12	2.02	0.40
1:B:83:ILE:HG12	1:B:121:ALA:HB3	2.03	0.40
1:C:87:ASN:HB3	7:C:669:HOH:O	2.20	0.40
1:D:346:THR:HA	2:D:501:FBP:H61	2.03	0.40
1:E:271:ASP:HB3	1:E:379:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/447 (96%)	416 (97%)	9 (2%)	2 (0%)	24	34
1	B	438/447 (98%)	428 (98%)	9 (2%)	1 (0%)	43	56
1	C	429/447 (96%)	418 (97%)	6 (1%)	5 (1%)	10	14
1	D	428/447 (96%)	424 (99%)	3 (1%)	1 (0%)	43	56
1	E	426/447 (95%)	421 (99%)	4 (1%)	1 (0%)	43	56
1	F	440/447 (98%)	431 (98%)	7 (2%)	2 (0%)	24	34
1	G	424/447 (95%)	416 (98%)	6 (1%)	2 (0%)	24	34
1	H	429/447 (96%)	423 (99%)	5 (1%)	1 (0%)	43	56
All	All	3441/3576 (96%)	3377 (98%)	49 (1%)	15 (0%)	30	40

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	173	GLY
1	G	173	GLY
1	C	176	GLY
1	C	129	PRO
1	A	437	ASN
1	A	242	THR
1	B	242	THR
1	C	242	THR
1	D	242	THR
1	E	242	THR
1	F	242	THR
1	G	242	THR
1	H	242	THR
1	C	134	GLY
1	F	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%)	330 (97%)	11 (3%)	34	53
1	B	349/352 (99%)	334 (96%)	15 (4%)	26	41
1	C	342/352 (97%)	333 (97%)	9 (3%)	40	60
1	D	342/352 (97%)	330 (96%)	12 (4%)	32	50
1	E	340/352 (97%)	323 (95%)	17 (5%)	22	35
1	F	351/352 (100%)	337 (96%)	14 (4%)	28	44
1	G	341/352 (97%)	329 (96%)	12 (4%)	32	50
1	H	342/352 (97%)	332 (97%)	10 (3%)	37	57
All	All	2748/2816 (98%)	2648 (96%)	100 (4%)	33	49

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	68	ARG
1	A	72	ARG
1	A	86	LEU
1	A	186	GLU
1	A	297	ARG
1	A	345	LEU
1	A	356	SER
1	A	439[A]	MET
1	A	439[B]	MET
1	A	442	LEU
1	B	10	ARG
1	B	68	ARG
1	B	76[A]	MET
1	B	76[B]	MET
1	B	115	LEU
1	B	165	VAL
1	B	186	GLU
1	B	253	ARG

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Mol	Chain	Res	Type
1	B	281	LYS
1	B	314	ARG
1	B	356	SER
1	B	413	LEU
1	B	423	VAL
1	B	439[A]	MET
1	B	439[B]	MET
1	C	52	VAL
1	C	68	ARG
1	C	76[A]	MET
1	C	76[B]	MET
1	C	186	GLU
1	C	297	ARG
1	C	356	SER
1	C	389	ARG
1	C	433	SER
1	D	68	ARG
1	D	113	SER
1	D	144[A]	ARG
1	D	144[B]	ARG
1	D	161	LYS
1	D	186	GLU
1	D	250	THR
1	D	297	ARG
1	D	313	ARG
1	D	356	SER
1	D	423	VAL
1	D	439	MET
1	E	52	VAL
1	E	68	ARG
1	E	115	LEU
1	E	137	GLU
1	E	186	GLU
1	E	297	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	410	SER
1	E	433	SER
1	E	436	THR

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Mol	Chain	Res	Type
1	E	439[A]	MET
1	E	439[B]	MET
1	E	441	VAL
1	F	16	LEU
1	F	68	ARG
1	F	76[A]	MET
1	F	76[B]	MET
1	F	118	ARG
1	F	131	SER
1	F	186	GLU
1	F	297	ARG
1	F	310	GLU
1	F	345	LEU
1	F	356	SER
1	F	410	SER
1	F	439[A]	MET
1	F	439[B]	MET
1	G	52	VAL
1	G	68	ARG
1	G	76[A]	MET
1	G	76[B]	MET
1	G	113	SER
1	G	175	GLU
1	G	186	GLU
1	G	253	ARG
1	G	297	ARG
1	G	314	ARG
1	G	356	SER
1	G	442	LEU
1	H	19	GLU
1	H	22	THR
1	H	175	GLU
1	H	186	GLU
1	H	297	ARG
1	H	313	ARG
1	H	356	SER
1	H	413	LEU
1	H	433	SER
1	H	439	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	283	ASN
1	C	177	HIS
1	C	292	GLN
1	D	27	GLN
1	F	15	GLN
1	F	27	GLN
1	G	292	GLN
1	H	292	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FBP	F	501	-	18,20,20	0.34	0	21,32,32	0.67	1 (4%)
3	OXL	B	502	4	5,5,5	2.15	2 (40%)	6,6,6	1.81	2 (33%)
6	A1JFN	H	501	-	30,30,30	0.33	0	41,43,43	0.39	0
2	FBP	D	501	-	18,20,20	0.59	0	21,32,32	0.89	0
3	OXL	C	502	4	5,5,5	2.18	2 (40%)	6,6,6	1.48	1 (16%)
3	OXL	F	502	4	5,5,5	2.14	2 (40%)	6,6,6	1.93	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A1JFN	C	505	-	30,30,30	0.31	0	41,43,43	0.41	0
3	OXL	G	502	4	5,5,5	2.59	3 (60%)	6,6,6	1.61	2 (33%)
2	FBP	C	501	-	18,20,20	0.54	0	21,32,32	1.01	2 (9%)
2	FBP	H	502	-	18,20,20	0.81	1 (5%)	21,32,32	1.05	1 (4%)
3	OXL	E	502	4	5,5,5	2.20	2 (40%)	6,6,6	2.03	2 (33%)
3	OXL	A	502	4	5,5,5	2.05	2 (40%)	6,6,6	1.76	2 (33%)
6	A1JFN	B	505	-	30,30,30	0.30	0	41,43,43	0.45	0
2	FBP	B	501	-	18,20,20	0.51	0	21,32,32	0.70	0
2	FBP	G	501	-	18,20,20	0.51	0	21,32,32	0.70	0
2	FBP	A	501	-	18,20,20	0.35	0	21,32,32	0.64	0
3	OXL	H	503	4	5,5,5	1.93	2 (40%)	6,6,6	1.68	1 (16%)
6	A1JFN	E	505	-	30,30,30	0.26	0	41,43,43	0.46	0
3	OXL	D	502	4	5,5,5	2.03	2 (40%)	6,6,6	2.26	3 (50%)
2	FBP	E	501	-	18,20,20	0.52	0	21,32,32	0.77	1 (4%)

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	F	501	-	-	4/13/32/32	0/1/1/1
3	OXL	B	502	4	-	4/4/4/4	-
6	A1JFN	H	501	-	-	0/16/16/16	0/4/4/4
2	FBP	D	501	-	-	3/13/32/32	0/1/1/1
3	OXL	C	502	4	-	4/4/4/4	-
3	OXL	F	502	4	-	0/4/4/4	-
6	A1JFN	C	505	-	-	0/16/16/16	0/4/4/4
3	OXL	G	502	4	-	4/4/4/4	-
2	FBP	C	501	-	-	2/13/32/32	0/1/1/1
2	FBP	H	502	-	-	2/13/32/32	0/1/1/1
3	OXL	E	502	4	-	4/4/4/4	-
3	OXL	A	502	4	-	4/4/4/4	-
6	A1JFN	B	505	-	-	0/16/16/16	0/4/4/4
2	FBP	B	501	-	-	5/13/32/32	0/1/1/1
2	FBP	G	501	-	-	7/13/32/32	0/1/1/1
2	FBP	A	501	-	-	5/13/32/32	0/1/1/1
3	OXL	H	503	4	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1JFN	E	505	-	-	0/16/16/16	0/4/4/4
3	OXL	D	502	4	-	4/4/4/4	-
2	FBP	E	501	-	-	7/13/32/32	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	502	OXL	O2-C2	4.35	1.33	1.22
3	F	502	OXL	O2-C2	4.03	1.32	1.22
3	B	502	OXL	O2-C2	3.88	1.32	1.22
3	C	502	OXL	O2-C2	3.65	1.31	1.22
3	E	502	OXL	O2-C2	3.62	1.31	1.22
3	A	502	OXL	O2-C2	3.60	1.31	1.22
3	D	502	OXL	O2-C2	3.34	1.30	1.22
3	H	503	OXL	O2-C2	3.20	1.30	1.22
3	D	502	OXL	O4-C2	-2.92	1.22	1.30
3	E	502	OXL	O4-C2	-2.92	1.22	1.30
3	H	503	OXL	O4-C2	-2.81	1.22	1.30
3	C	502	OXL	O4-C2	-2.76	1.23	1.30
3	G	502	OXL	C2-C1	2.73	1.59	1.54
3	A	502	OXL	O4-C2	-2.71	1.23	1.30
3	G	502	OXL	O4-C2	-2.59	1.23	1.30
3	B	502	OXL	O4-C2	-2.55	1.23	1.30
3	F	502	OXL	O4-C2	-2.39	1.24	1.30
2	H	502	FBP	P1-O1	-2.39	1.52	1.60

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	OXL	O4-C2-C1	3.90	120.39	112.83
3	F	502	OXL	O4-C2-C1	3.63	119.86	112.83
3	E	502	OXL	O4-C2-C1	3.48	119.58	112.83
3	H	503	OXL	O4-C2-C1	3.47	119.56	112.83
3	A	502	OXL	O4-C2-C1	3.39	119.42	112.83
3	B	502	OXL	O4-C2-C1	3.36	119.36	112.83
2	H	502	FBP	O6-P2-O4P	3.32	115.42	106.44
3	C	502	OXL	O4-C2-C1	3.14	118.91	112.83
3	D	502	OXL	O3-C1-C2	2.98	118.62	112.83
3	E	502	OXL	O3-C1-C2	2.90	118.46	112.83
3	G	502	OXL	O3-C1-C2	2.72	118.10	112.83
3	G	502	OXL	O4-C2-C1	2.59	117.86	112.83
3	B	502	OXL	O3-C1-C2	2.30	117.29	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FBP	O1-P1-O1P	2.26	112.55	106.44
2	C	501	FBP	O6-P2-O4P	2.17	112.32	106.44
3	F	502	OXL	O3-C1-C2	2.12	116.94	112.83
3	F	502	OXL	O2-C2-C1	-2.10	116.25	120.63
2	E	501	FBP	O6-P2-O4P	2.10	112.12	106.44
3	D	502	OXL	O2-C2-C1	-2.08	116.30	120.63
2	F	501	FBP	O1-P1-O1P	2.03	111.94	106.44
3	A	502	OXL	O3-C1-C2	2.00	116.72	112.83

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FBP	C6-O6-P2-O4P
2	A	501	FBP	C6-O6-P2-O5P
2	A	501	FBP	C6-O6-P2-O6P
2	B	501	FBP	C1-O1-P1-O2P
2	B	501	FBP	C1-O1-P1-O3P
2	D	501	FBP	O5-C5-C6-O6
2	E	501	FBP	C6-O6-P2-O4P
2	E	501	FBP	C6-O6-P2-O5P
2	E	501	FBP	C6-O6-P2-O6P
2	F	501	FBP	C4-C5-C6-O6
2	G	501	FBP	C1-O1-P1-O1P
2	G	501	FBP	C1-O1-P1-O2P
2	G	501	FBP	C1-O1-P1-O3P
2	G	501	FBP	O1-C1-C2-O2
2	G	501	FBP	O1-C1-C2-O5
2	G	501	FBP	C6-O6-P2-O5P
2	G	501	FBP	C6-O6-P2-O6P
2	B	501	FBP	C4-C5-C6-O6
2	C	501	FBP	C4-C5-C6-O6
2	D	501	FBP	C4-C5-C6-O6
2	H	502	FBP	C4-C5-C6-O6
2	F	501	FBP	O5-C5-C6-O6
2	H	502	FBP	O5-C5-C6-O6
2	C	501	FBP	O5-C5-C6-O6
2	B	501	FBP	C1-O1-P1-O1P
2	E	501	FBP	C1-O1-P1-O1P
3	H	503	OXL	O3-C1-C2-O4
3	E	502	OXL	O3-C1-C2-O4
3	A	502	OXL	O3-C1-C2-O4

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Mol	Chain	Res	Type	Atoms
3	B	502	OXL	O3-C1-C2-O4
3	C	502	OXL	O3-C1-C2-O4
3	D	502	OXL	O3-C1-C2-O4
3	G	502	OXL	O3-C1-C2-O4
2	E	501	FBP	O5-C5-C6-O6
3	C	502	OXL	O1-C1-C2-O2
3	D	502	OXL	O1-C1-C2-O2
3	E	502	OXL	O1-C1-C2-O2
3	A	502	OXL	O1-C1-C2-O2
3	B	502	OXL	O1-C1-C2-O2
3	G	502	OXL	O1-C1-C2-O2
3	H	503	OXL	O1-C1-C2-O2
2	D	501	FBP	C6-O6-P2-O4P
2	F	501	FBP	C1-O1-P1-O1P
2	B	501	FBP	O5-C5-C6-O6
2	E	501	FBP	C4-C5-C6-O6
2	A	501	FBP	O5-C5-C6-O6
3	A	502	OXL	O1-C1-C2-O4
3	A	502	OXL	O3-C1-C2-O2
3	B	502	OXL	O3-C1-C2-O2
3	C	502	OXL	O1-C1-C2-O4
3	C	502	OXL	O3-C1-C2-O2
3	D	502	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	B	502	OXL	O1-C1-C2-O4
2	E	501	FBP	C1-O1-P1-O2P
2	F	501	FBP	C1-O1-P1-O2P
3	H	503	OXL	O1-C1-C2-O4
3	H	503	OXL	O3-C1-C2-O2
2	A	501	FBP	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FBP	2	0
3	C	502	OXL	1	0
2	C	501	FBP	1	0

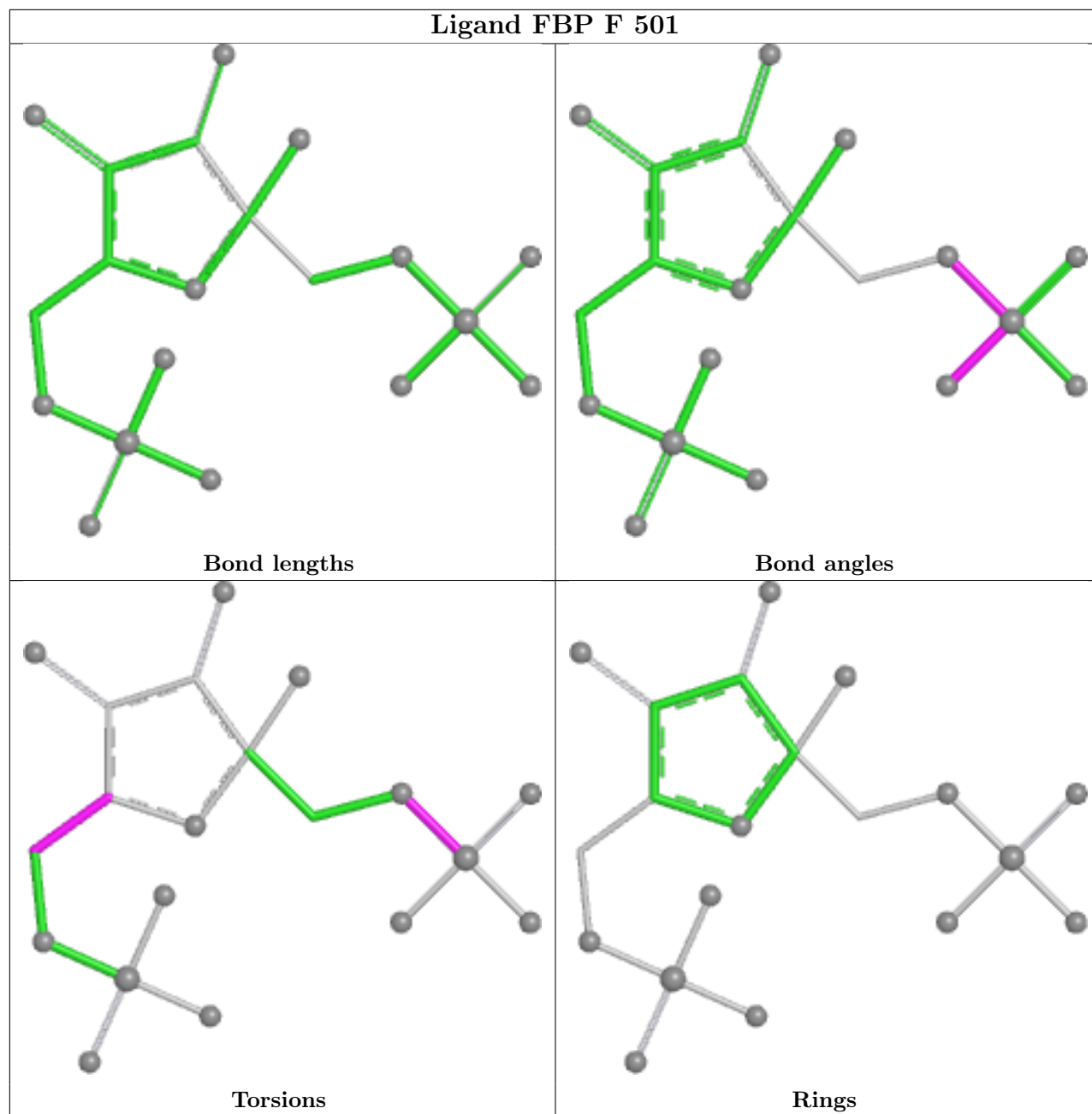
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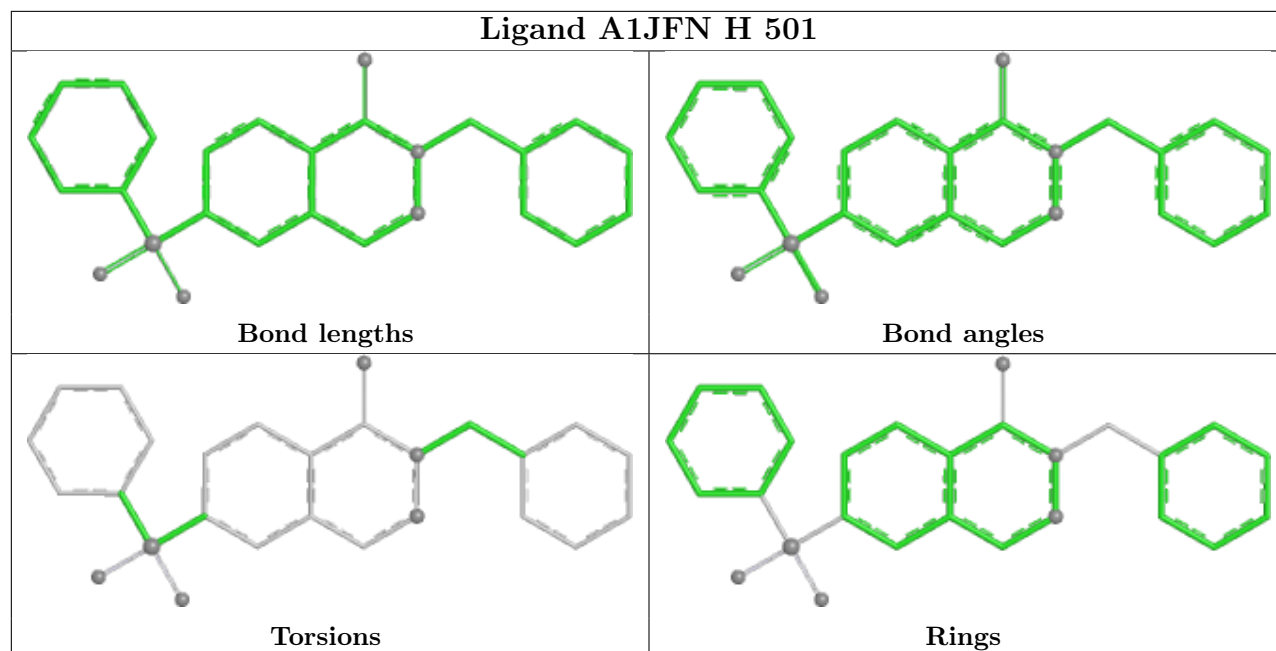
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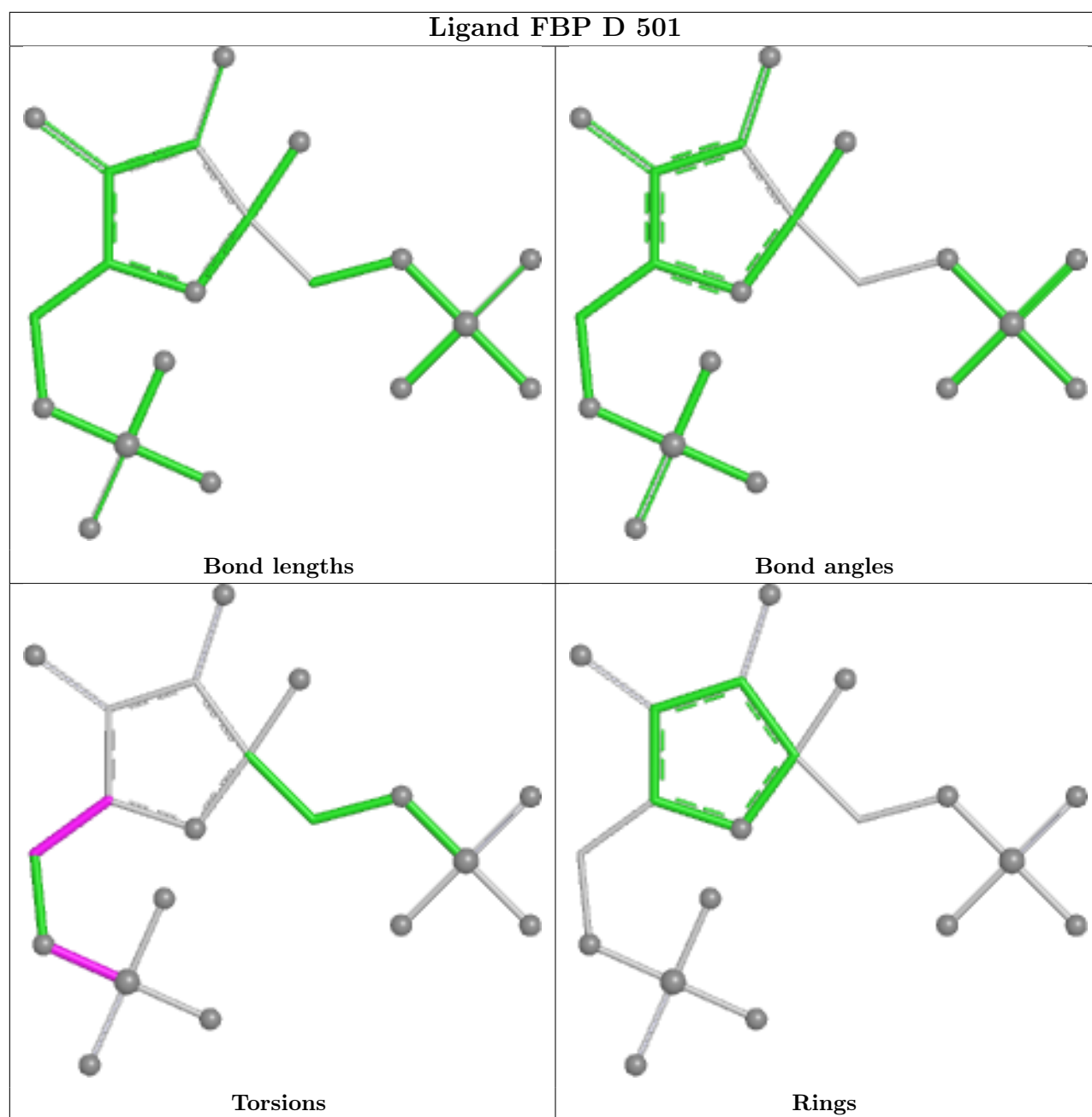
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	502	FBP	1	0
2	B	501	FBP	1	0
2	G	501	FBP	1	0
2	A	501	FBP	2	0
2	E	501	FBP	2	0

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

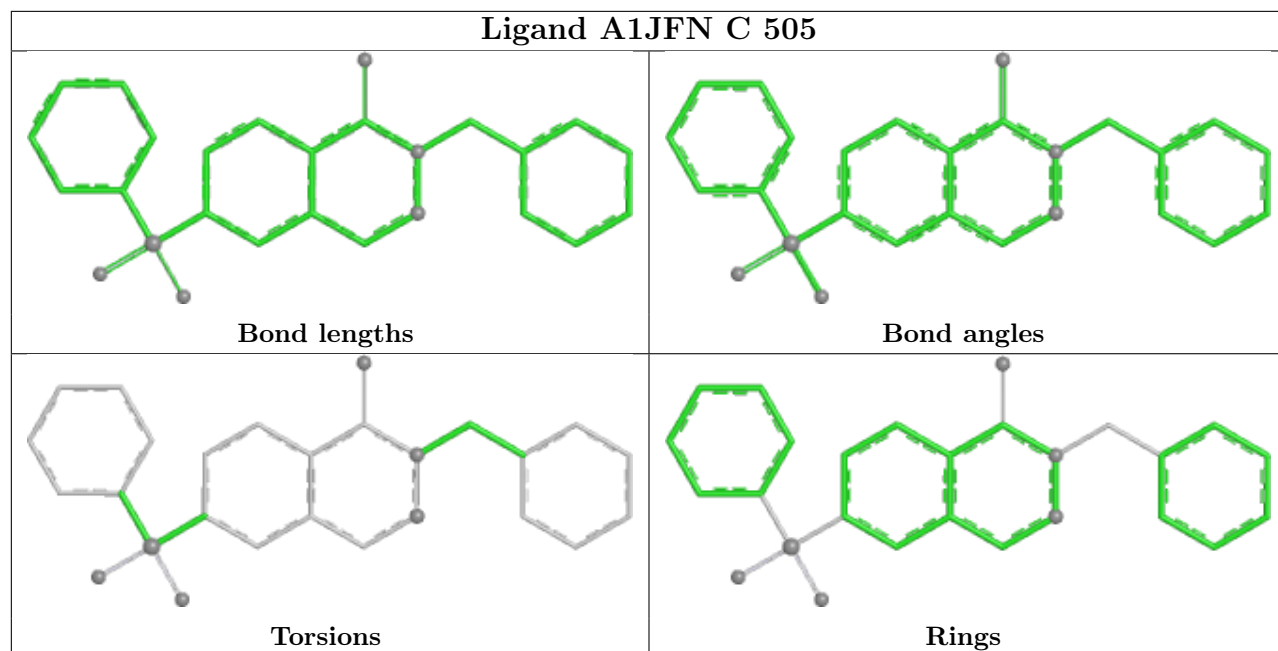
Ligand FBP F 501

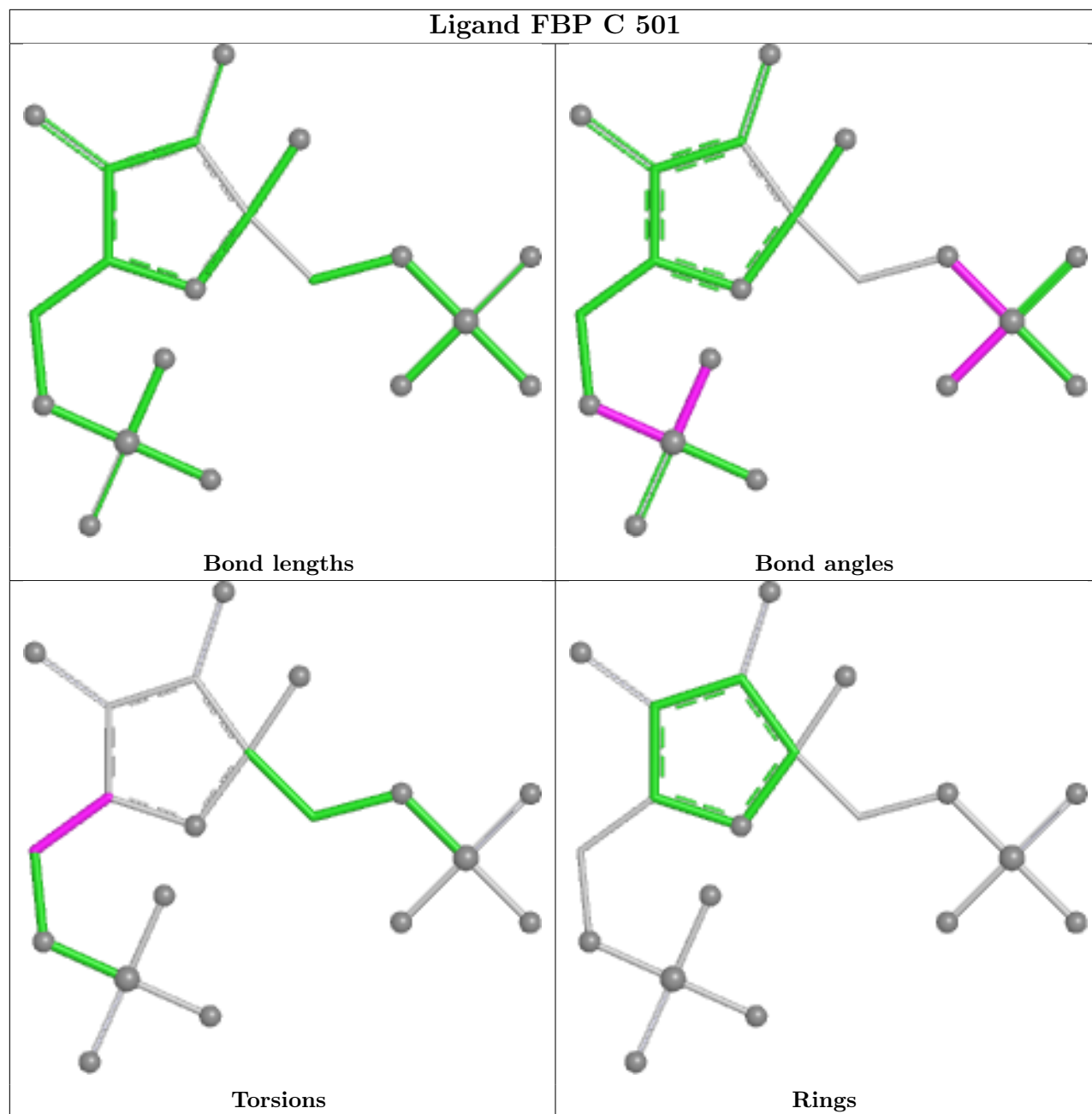


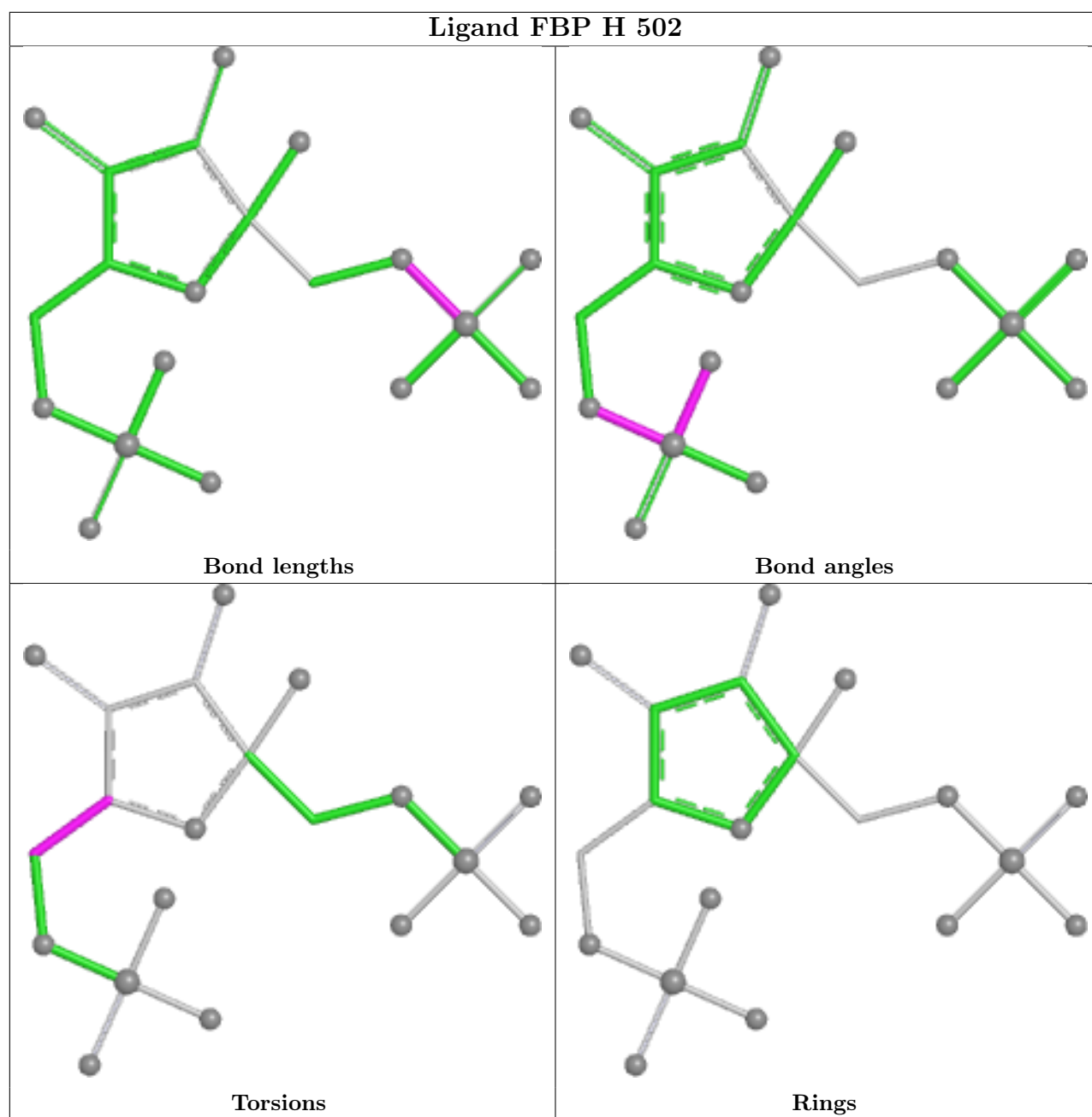


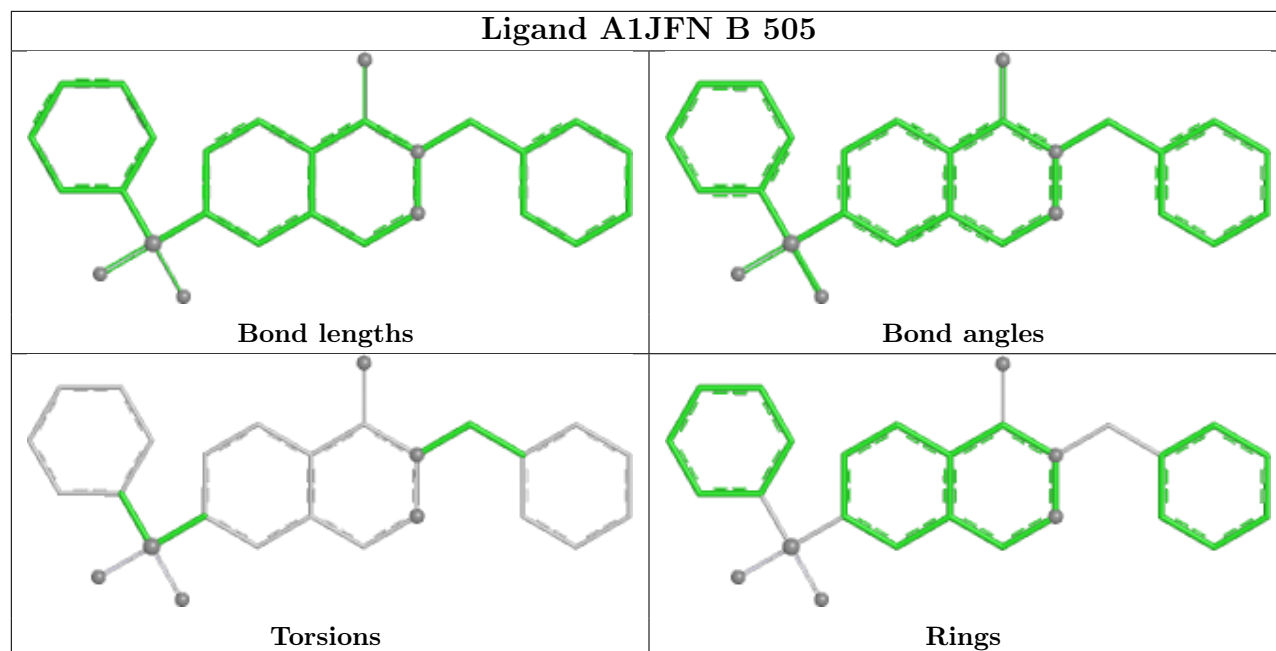


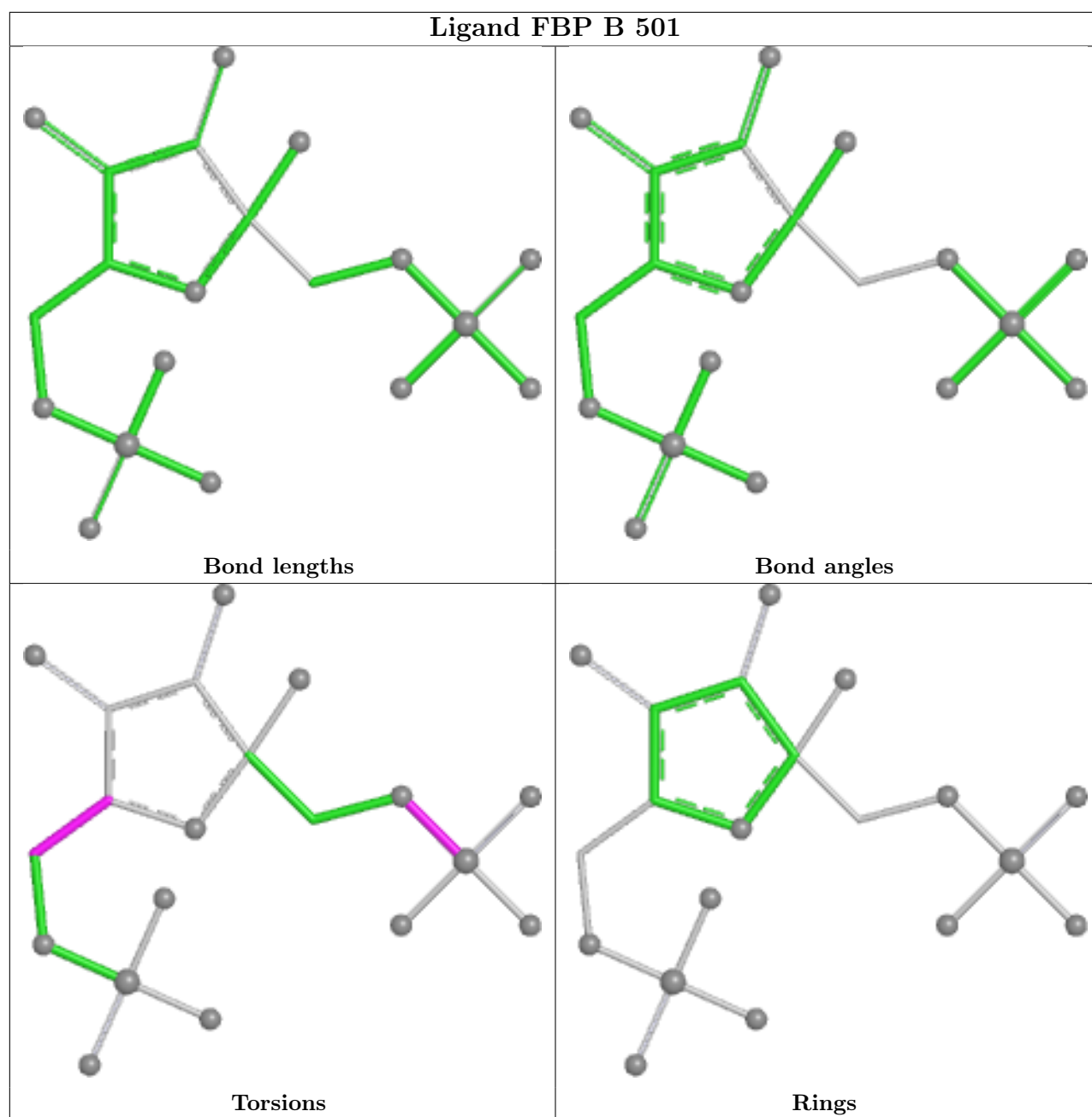
Ligand A1JFN C 505

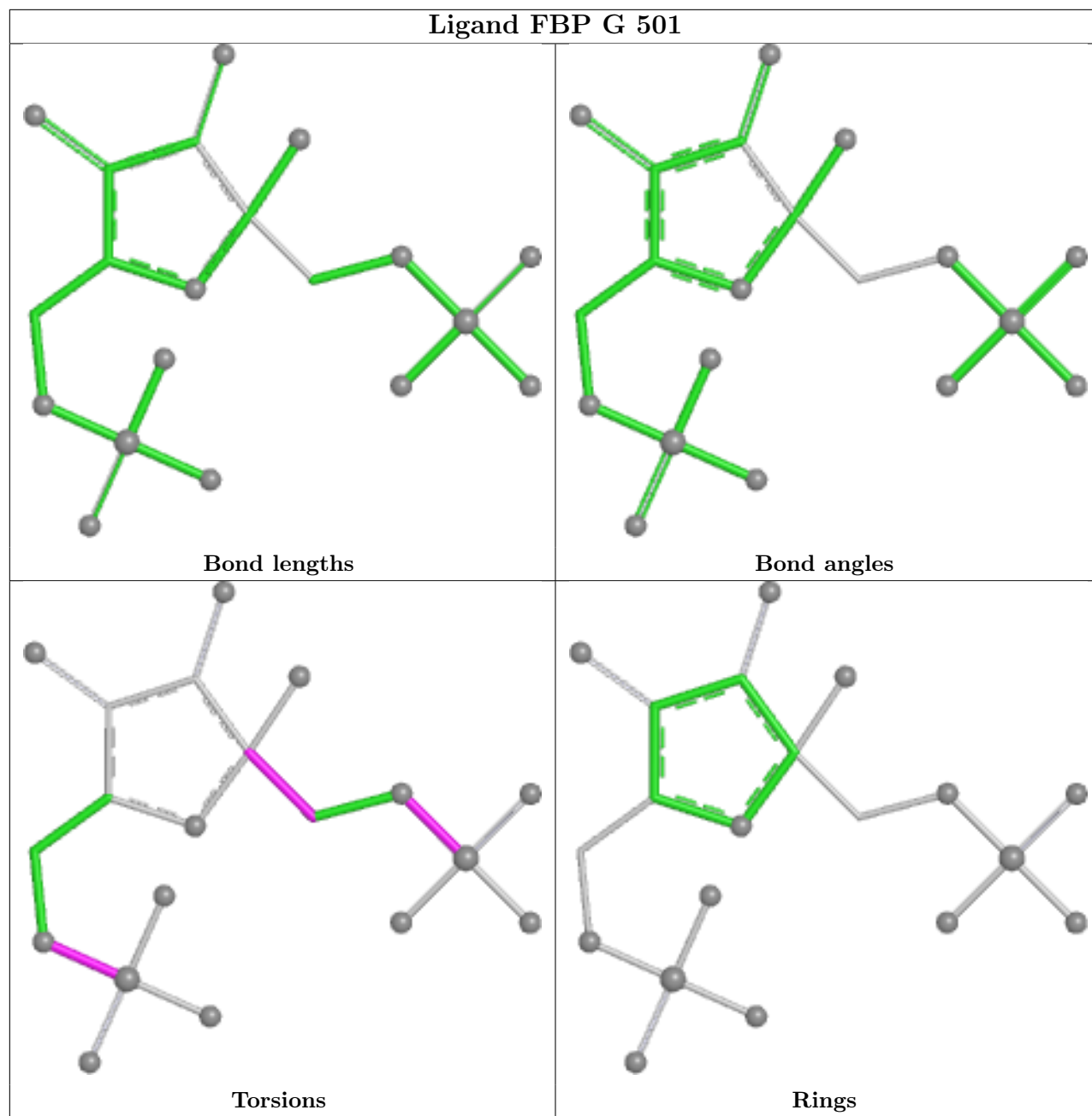


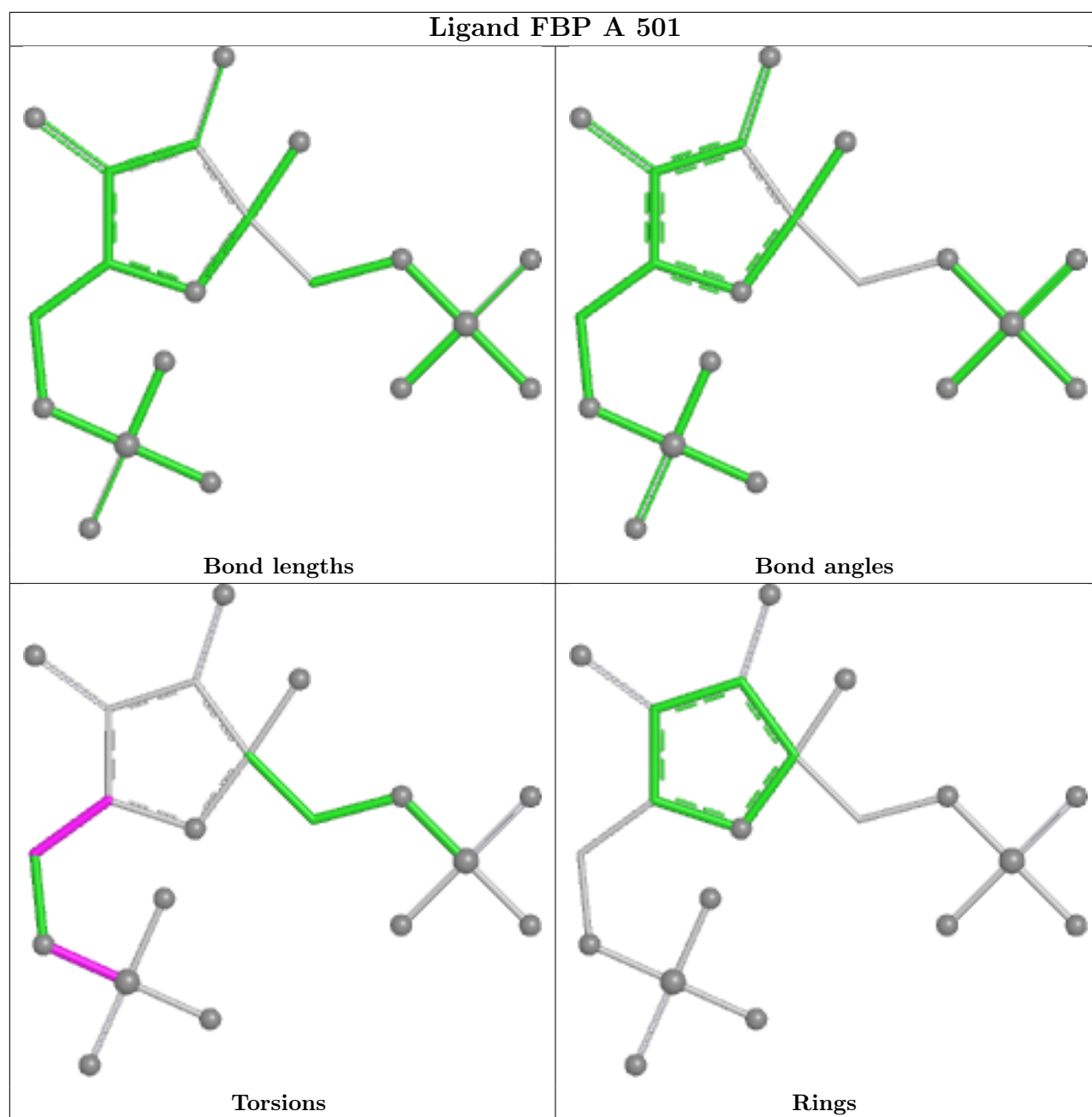


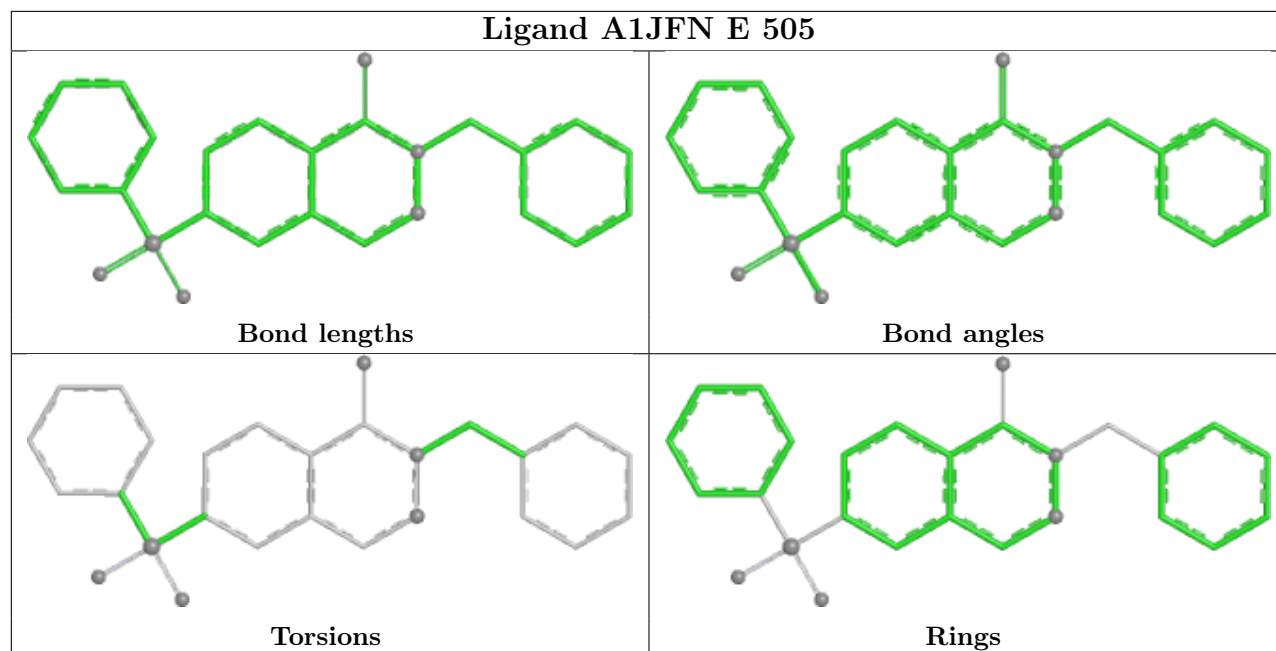


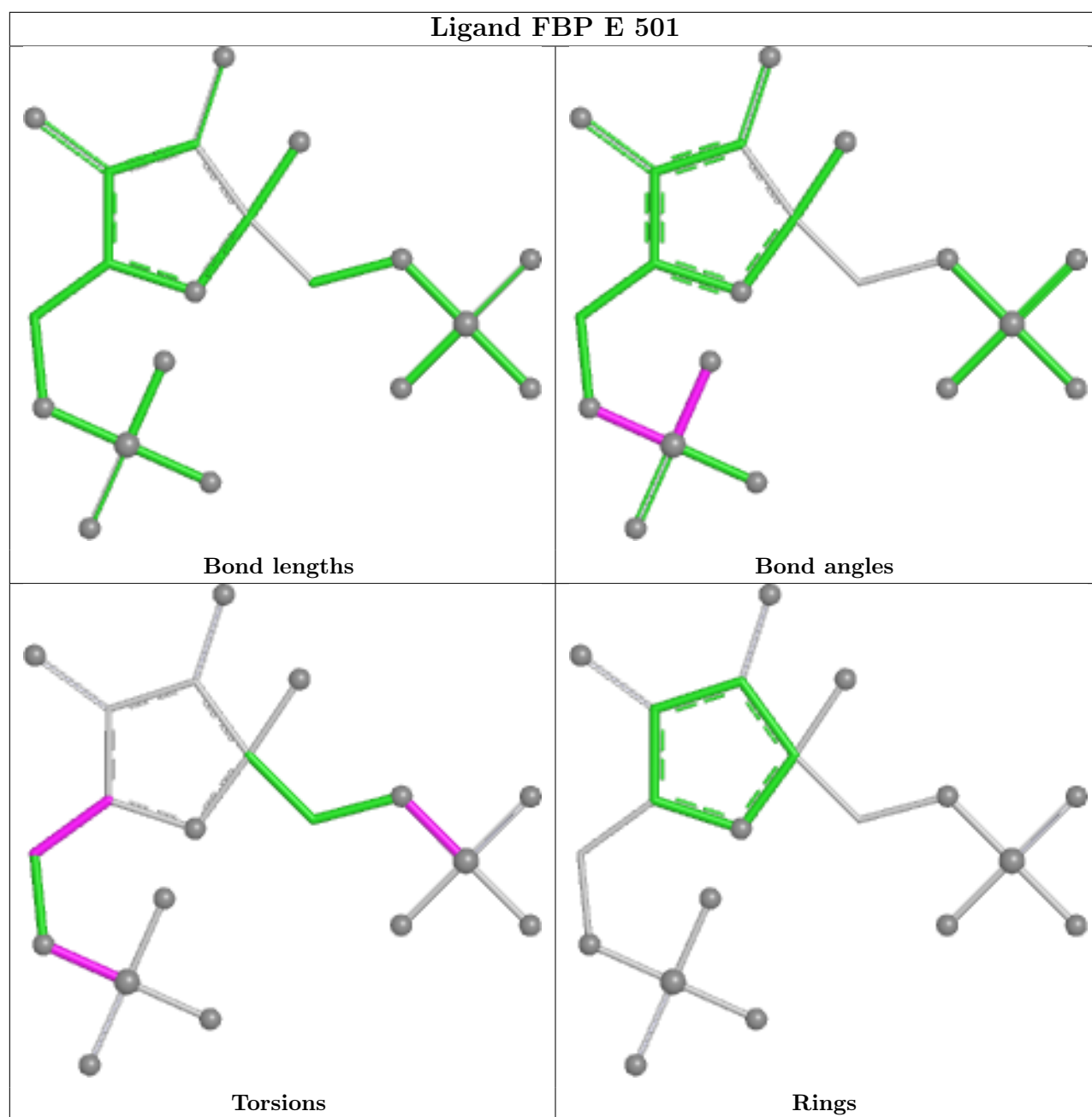












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	423/447 (94%)	1.38	97 (22%)	2 1	32, 65, 98, 120	6 (1%)
1	B	436/447 (97%)	0.98	67 (15%)	5 4	30, 55, 87, 99	4 (0%)
1	C	427/447 (95%)	0.59	36 (8%)	17 15	23, 51, 78, 105	4 (0%)
1	D	424/447 (94%)	0.13	11 (2%)	57 56	16, 36, 61, 100	6 (1%)
1	E	423/447 (94%)	1.02	75 (17%)	4 3	27, 55, 89, 108	5 (1%)
1	F	435/447 (97%)	0.55	25 (5%)	29 28	27, 46, 76, 95	7 (1%)
1	G	422/447 (94%)	0.23	11 (2%)	57 56	20, 42, 60, 85	7 (1%)
1	H	427/447 (95%)	-0.05	10 (2%)	61 60	14, 33, 58, 91	4 (0%)
All	All	3417/3576 (95%)	0.60	332 (9%)	13 12	14, 48, 85, 120	43 (1%)

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	SER	9.9
1	A	384	PHE	7.0
1	A	365	ILE	6.4
1	E	23	ALA	6.1
1	D	25	PHE	5.9
1	D	24	PHE	5.7
1	B	445	SER	5.6
1	A	25	PHE	5.5
1	A	408	ILE	5.4
1	A	115	LEU	5.2
1	A	404	VAL	5.2
1	C	133	PRO	5.2
1	A	343	ILE	5.1
1	A	140	VAL	5.1
1	E	442	LEU	5.0
1	E	111	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	404	VAL	4.8
1	A	366	ALA	4.7
1	E	133	PRO	4.6
1	F	135	LEU	4.5
1	A	63	ILE	4.5
1	C	115	LEU	4.4
1	E	135	LEU	4.3
1	A	133	PRO	4.3
1	D	22	THR	4.3
1	B	419	VAL	4.3
1	E	366	ALA	4.2
1	A	143	LEU	4.2
1	B	133	PRO	4.2
1	A	442	LEU	4.2
1	A	132	GLY	4.2
1	E	444	ILE	4.2
1	H	24	PHE	4.2
1	H	25	PHE	4.1
1	E	365	ILE	4.1
1	A	392	PRO	4.1
1	F	418	ARG	4.1
1	F	133	PRO	4.1
1	G	23	ALA	4.0
1	A	130	GLY	4.0
1	E	130	GLY	4.0
1	E	416	PHE	4.0
1	B	114	PRO	3.9
1	E	25	PHE	3.8
1	B	115	LEU	3.8
1	B	413	LEU	3.8
1	A	23	ALA	3.8
1	C	302	ALA	3.8
1	B	70	VAL	3.8
1	A	417	LEU	3.7
1	E	443[A]	SER	3.7
1	A	416	PHE	3.6
1	A	419	VAL	3.6
1	A	95	TYR	3.6
1	G	25	PHE	3.6
1	B	61	ALA	3.6
1	G	24	PHE	3.6
1	A	34	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	134	GLY	3.6
1	A	386	LEU	3.6
1	B	169[A]	ARG	3.5
1	A	444	ILE	3.5
1	E	140	VAL	3.5
1	B	135	LEU	3.5
1	B	391	PRO	3.5
1	E	151	VAL	3.4
1	E	407	GLY	3.4
1	A	33	ALA	3.4
1	C	34	MET	3.4
1	C	114	PRO	3.4
1	E	344	VAL	3.4
1	C	111	ALA	3.4
1	A	135	LEU	3.3
1	A	213	ILE	3.3
1	B	95	TYR	3.3
1	E	101	ALA	3.3
1	G	133	PRO	3.3
1	D	177[A]	HIS	3.3
1	A	390[A]	GLU	3.3
1	A	111	ALA	3.3
1	E	103	VAL	3.3
1	F	114	PRO	3.3
1	A	367	VAL	3.2
1	C	207	ALA	3.2
1	A	134	GLY	3.2
1	E	129	PRO	3.2
1	B	444	ILE	3.2
1	E	179	ILE	3.2
1	A	101	ALA	3.2
1	E	445	SER	3.2
1	A	124	LEU	3.2
1	E	24	PHE	3.1
1	G	173	GLY	3.1
1	H	21	GLY	3.1
1	D	140	VAL	3.1
1	C	109	SER	3.1
1	E	386	LEU	3.1
1	F	317	PRO	3.1
1	A	279	THR	3.1
1	A	24	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	134	GLY	3.1
1	A	423	VAL	3.1
1	A	114	PRO	3.1
1	A	122	ILE	3.1
1	D	134	GLY	3.1
1	G	34	MET	3.1
1	A	443	SER	3.0
1	F	361	ARG	3.0
1	E	114	PRO	3.0
1	A	387	LEU	3.0
1	B	107	VAL	3.0
1	E	136	SER	3.0
1	C	25	PHE	3.0
1	A	100	ILE	3.0
1	E	367	VAL	3.0
1	A	377	VAL	2.9
1	H	22	THR	2.9
1	E	417	LEU	2.9
1	A	171	ALA	2.9
1	F	115	LEU	2.9
1	C	103	VAL	2.9
1	E	147	VAL	2.9
1	A	172	LEU	2.8
1	E	30	LEU	2.8
1	B	316	ALA	2.8
1	H	134	GLY	2.8
1	E	120	VAL	2.8
1	C	112	GLY	2.8
1	A	129	PRO	2.8
1	A	118	ARG	2.8
1	A	73	LEU	2.8
1	B	397	ALA	2.8
1	E	97	ALA	2.8
1	A	70	VAL	2.8
1	C	77	ILE	2.7
1	A	158	PHE	2.7
1	E	115	LEU	2.7
1	C	23	ALA	2.7
1	A	90	HIS	2.7
1	B	145	PHE	2.7
1	C	22	THR	2.7
1	E	122	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	174	PRO	2.7
1	F	391	PRO	2.7
1	F	414	ARG	2.7
1	A	182	ILE	2.7
1	A	420	GLY	2.7
1	E	408	ILE	2.7
1	E	314	ARG	2.7
1	B	174	PRO	2.6
1	E	392	PRO	2.6
1	E	143	LEU	2.6
1	F	177	HIS	2.6
1	E	75	GLU	2.6
1	A	110	PHE	2.6
1	B	140	VAL	2.6
1	C	70	VAL	2.6
1	F	90	HIS	2.6
1	A	167	ALA	2.6
1	B	130	GLY	2.6
1	A	116	SER	2.6
1	E	387	LEU	2.5
1	H	318	LEU	2.5
1	B	10	ARG	2.5
1	D	144[A]	ARG	2.5
1	G	313	ARG	2.5
1	B	101	ALA	2.5
1	E	121	ALA	2.5
1	A	151	VAL	2.5
1	B	97	ALA	2.5
1	H	133	PRO	2.5
1	A	136	SER	2.5
1	D	401	ASP	2.5
1	A	309	PHE	2.5
1	B	414	ARG	2.5
1	B	425	VAL	2.5
1	G	131	SER	2.5
1	E	90	HIS	2.5
1	F	415	GLY	2.5
1	A	409	GLU	2.4
1	B	118	ARG	2.4
1	B	158	PHE	2.4
1	E	406	PHE	2.4
1	C	20	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	117	TYR	2.4
1	E	34	MET	2.4
1	B	138	GLN	2.4
1	B	257	ALA	2.4
1	B	340	ALA	2.4
1	A	282	GLY	2.4
1	E	104	ARG	2.4
1	F	169[A]	ARG	2.4
1	F	445	SER	2.4
1	A	395	ILE	2.4
1	A	425	VAL	2.4
1	E	70	VAL	2.4
1	E	423	VAL	2.4
1	B	129	PRO	2.4
1	E	33	ALA	2.4
1	F	174	PRO	2.4
1	E	128	GLY	2.4
1	E	173	GLY	2.4
1	E	126	THR	2.4
1	A	433	SER	2.4
1	C	63	ILE	2.4
1	C	110	PHE	2.4
1	E	95	TYR	2.4
1	E	108	GLU	2.4
1	A	371	ALA	2.4
1	C	130	GLY	2.4
1	E	168	VAL	2.4
1	E	409	GLU	2.4
1	B	131	SER	2.3
1	A	440	ARG	2.3
1	F	442[A]	LEU	2.3
1	B	71	GLU	2.3
1	G	134	GLY	2.3
1	B	111	ALA	2.3
1	B	116	SER	2.3
1	A	104	ARG	2.3
1	E	440	ARG	2.3
1	B	168	VAL	2.3
1	E	177	HIS	2.3
1	A	30	LEU	2.3
1	H	20	LEU	2.3
1	B	281	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	392	PRO	2.3
1	A	112	GLY	2.3
1	A	176	GLY	2.3
1	A	432	GLY	2.3
1	E	134	GLY	2.3
1	C	299	ALA	2.3
1	B	90	HIS	2.3
1	B	110	PHE	2.3
1	E	158	PHE	2.3
1	B	73	LEU	2.3
1	B	442[A]	LEU	2.3
1	E	139	ASP	2.3
1	B	91	GLY	2.3
1	E	166	ALA	2.3
1	E	302	ALA	2.3
1	B	177	HIS	2.3
1	C	108	GLU	2.3
1	F	395	ILE	2.3
1	B	416	PHE	2.2
1	C	73	LEU	2.2
1	C	268	ASP	2.2
1	C	134	GLY	2.2
1	E	411	GLY	2.2
1	C	66	ALA	2.2
1	B	69	SER	2.2
1	B	63	ILE	2.2
1	F	386	LEU	2.2
1	A	142	ASP	2.2
1	B	119	PRO	2.2
1	B	64	GLY	2.2
1	C	21	GLY	2.2
1	E	176	GLY	2.2
1	A	79	ALA	2.2
1	A	84	ALA	2.2
1	B	74	LYS	2.2
1	B	207	ALA	2.2
1	E	167	ALA	2.2
1	B	100	ILE	2.2
1	B	318	LEU	2.2
1	F	413	LEU	2.2
1	E	110	PHE	2.2
1	A	150	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	305	HIS	2.2
1	B	93	HIS	2.2
1	A	347	THR	2.2
1	A	394	ALA	2.2
1	B	386	LEU	2.2
1	D	440	ARG	2.2
1	A	139	ASP	2.2
1	A	168	VAL	2.2
1	B	284	PHE	2.2
1	C	36	ASP	2.2
1	A	91	GLY	2.2
1	A	69	SER	2.2
1	A	131	SER	2.2
1	A	117	TYR	2.1
1	C	95	TYR	2.1
1	G	42	LEU	2.1
1	B	12	ASP	2.1
1	B	406	PHE	2.1
1	B	409	GLU	2.1
1	C	252	PRO	2.1
1	D	23	ALA	2.1
1	E	116	SER	2.1
1	F	435	TYR	2.1
1	B	124	LEU	2.1
1	C	135	LEU	2.1
1	C	251	LYS	2.1
1	B	103	VAL	2.1
1	B	286	VAL	2.1
1	D	133	PRO	2.1
1	E	206	VAL	2.1
1	H	220	VAL	2.1
1	C	282	GLY	2.1
1	E	178	GLY	2.1
1	A	106	ALA	2.1
1	E	123	ALA	2.1
1	B	81	MET	2.1
1	H	19	GLU	2.1
1	E	117	TYR	2.1
1	A	159	VAL	2.1
1	A	220	VAL	2.1
1	E	361	ARG	2.1
1	C	19	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	249	ILE	2.1
1	A	174	PRO	2.1
1	G	174	PRO	2.1
1	B	128	GLY	2.1
1	C	113	SER	2.0
1	A	374	ALA	2.0
1	C	79	ALA	2.0
1	F	94	GLU	2.0
1	A	355	LEU	2.0
1	A	422	LEU	2.0
1	A	285	PRO	2.0
1	A	388	TYR	2.0
1	B	154	VAL	2.0
1	E	144	ARG	2.0
1	F	140	VAL	2.0
1	F	389	ARG	2.0
1	A	97	ALA	2.0
1	A	280	ALA	2.0
1	A	86	LEU	2.0
1	A	179	ILE	2.0
1	E	391	PRO	2.0
1	F	77	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	K	E	504	1/1	0.78	0.13	95,95,95,95	0

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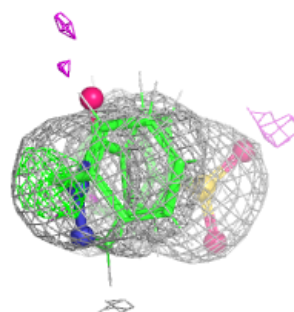
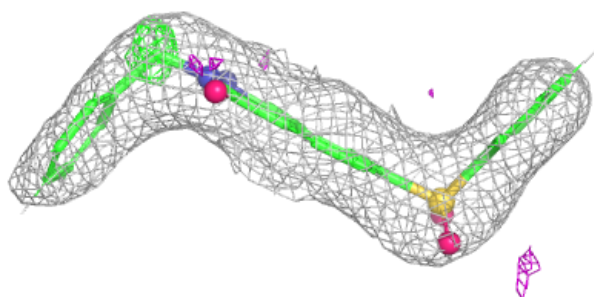
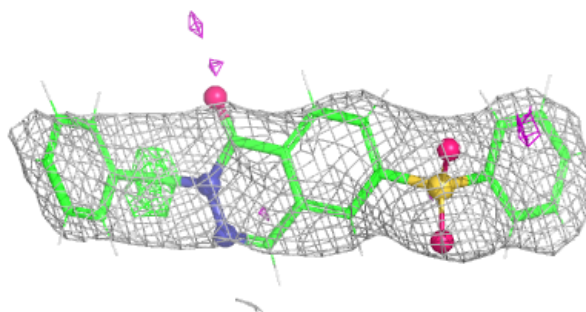
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	K	C	504	1/1	0.83	0.11	97,97,97,97	0
5	K	A	504	1/1	0.85	0.10	105,105,105,105	0
3	OXL	A	502	6/6	0.89	0.15	100,100,100,100	0
3	OXL	G	502	6/6	0.90	0.11	61,61,62,62	0
3	OXL	C	502	6/6	0.90	0.13	69,69,69,69	0
6	A1JFN	C	505	27/27	0.90	0.13	58,59,61,61	16
6	A1JFN	B	505	27/27	0.91	0.12	51,53,54,55	16
6	A1JFN	H	501	27/27	0.91	0.11	41,45,46,47	16
6	A1JFN	E	505	27/27	0.92	0.10	43,49,50,52	16
3	OXL	B	502	6/6	0.92	0.11	71,71,72,72	0
3	OXL	H	503	6/6	0.93	0.10	39,40,41,41	0
2	FBP	B	501	20/20	0.93	0.09	56,57,60,60	0
2	FBP	E	501	20/20	0.93	0.09	52,54,56,56	0
2	FBP	A	501	20/20	0.93	0.09	62,65,66,66	0
3	OXL	F	502	6/6	0.94	0.10	67,68,68,69	0
2	FBP	F	501	20/20	0.94	0.07	45,48,54,54	0
3	OXL	E	502	6/6	0.94	0.09	69,70,70,70	0
5	K	G	504	1/1	0.94	0.06	65,65,65,65	0
4	MG	C	503	1/1	0.95	0.15	37,37,37,37	0
5	K	D	504	1/1	0.95	0.06	49,49,49,49	0
5	K	F	504	1/1	0.96	0.05	80,80,80,80	0
3	OXL	D	502	6/6	0.96	0.09	58,58,58,59	0
4	MG	F	503	1/1	0.96	0.10	22,22,22,22	0
5	K	H	505	1/1	0.97	0.04	57,57,57,57	0
4	MG	B	503	1/1	0.97	0.09	39,39,39,39	0
4	MG	A	503	1/1	0.97	0.09	44,44,44,44	0
5	K	B	504	1/1	0.97	0.06	70,70,70,70	0
4	MG	D	503	1/1	0.97	0.13	32,32,32,32	0
2	FBP	C	501	20/20	0.98	0.05	28,29,32,33	0
4	MG	G	503	1/1	0.98	0.10	17,17,17,17	0
4	MG	H	504	1/1	0.98	0.12	21,21,21,21	0
2	FBP	D	501	20/20	0.98	0.05	28,29,31,31	0
2	FBP	G	501	20/20	0.98	0.05	34,37,38,38	0
4	MG	E	503	1/1	0.99	0.08	43,43,43,43	0
2	FBP	H	502	20/20	0.99	0.04	22,23,25,25	0

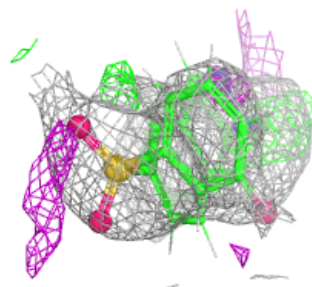
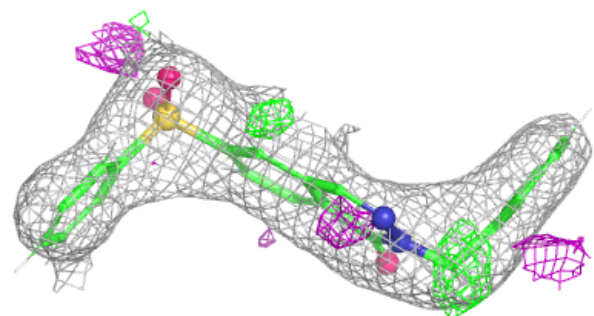
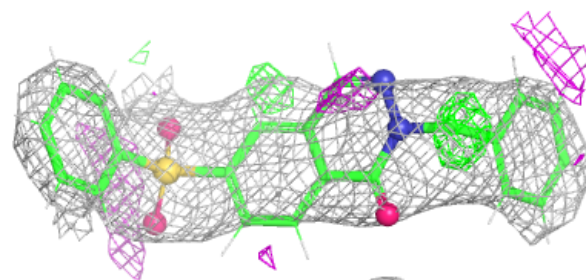
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1JFN C 505:

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

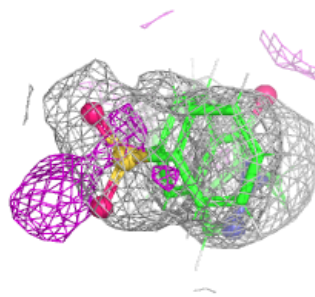
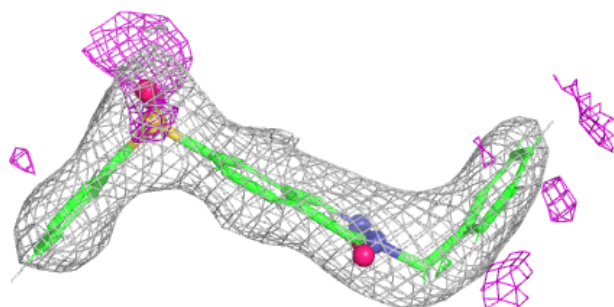
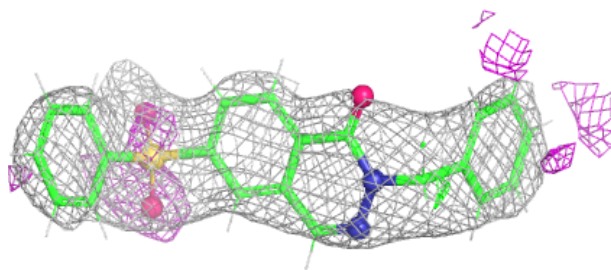
**Electron density around A1JFN B 505:**

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

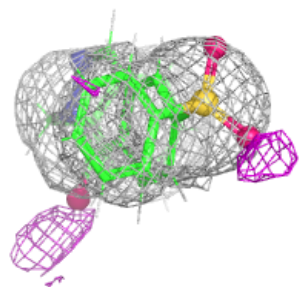
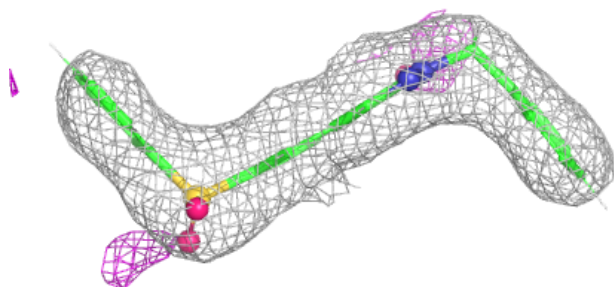
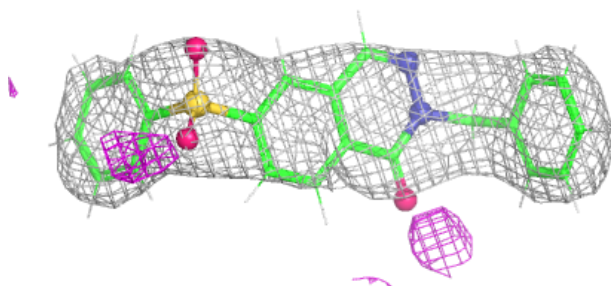


Electron density around A1JFN H 501:

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

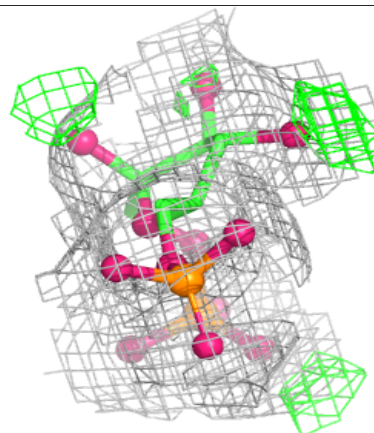
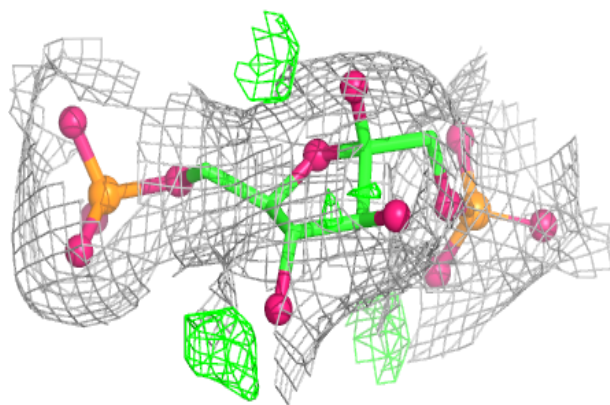
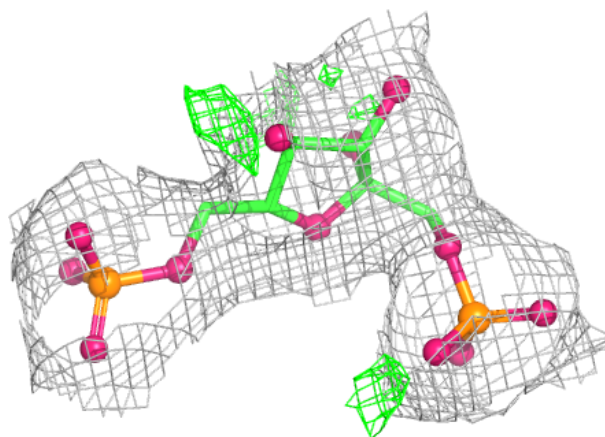
**Electron density around A1JFN E 505:**

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



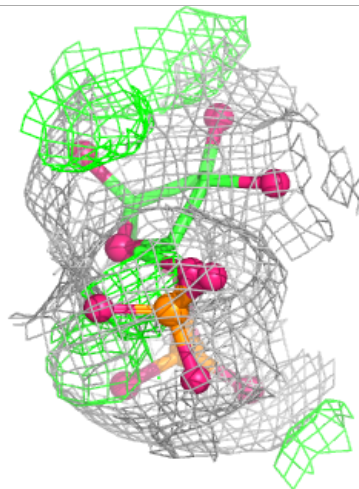
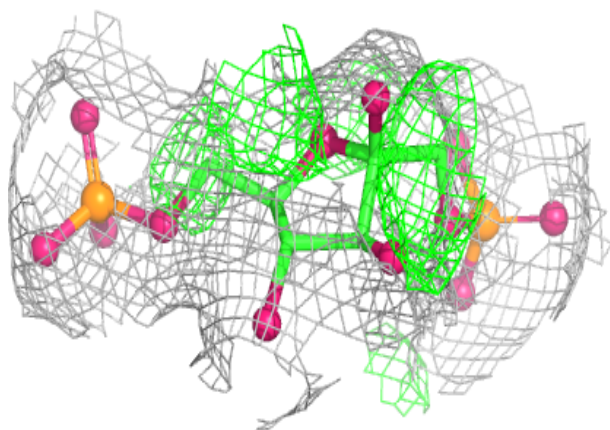
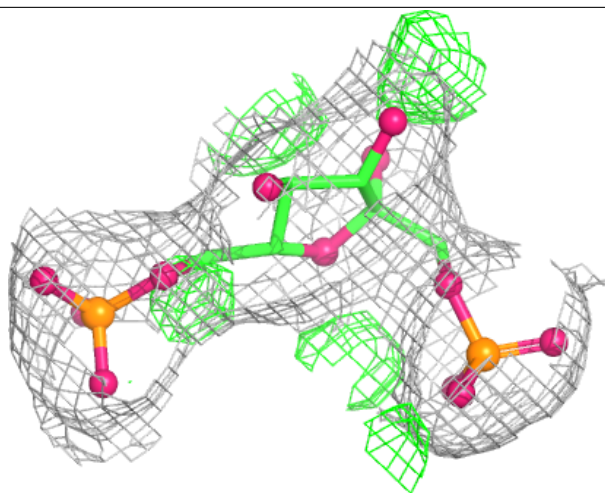
Electron density around FBP B 501:

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



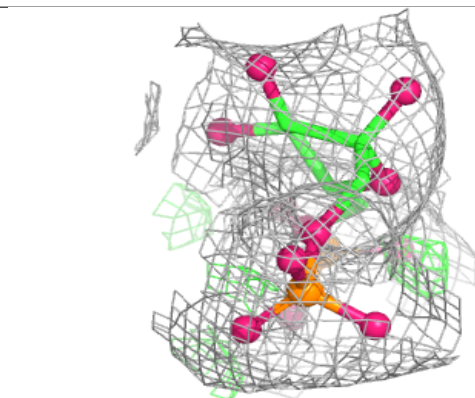
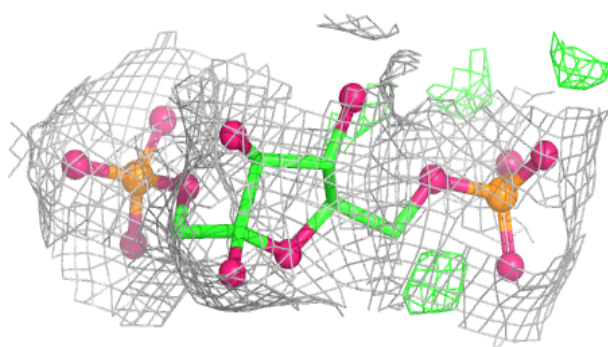
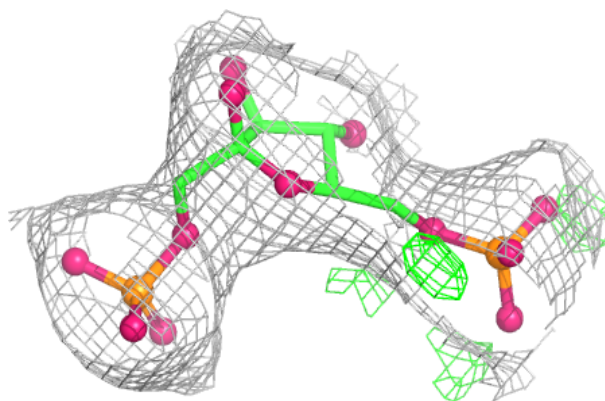
Electron density around FBP E 501:

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

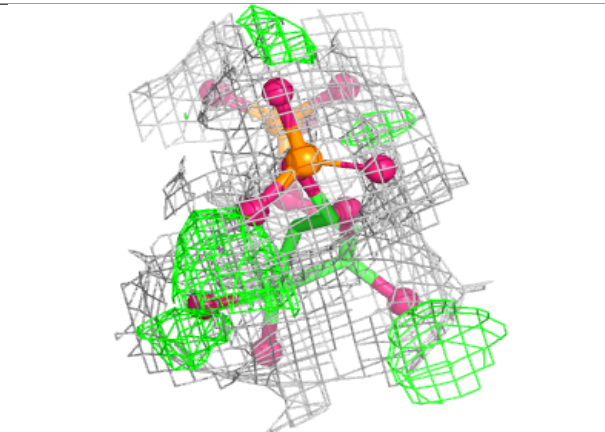
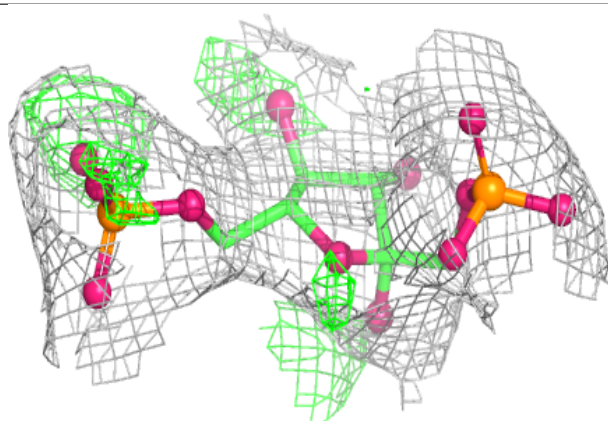
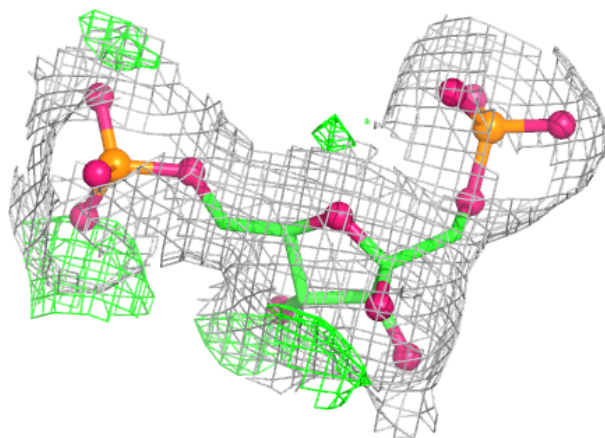


Electron density around FBP A 501:

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

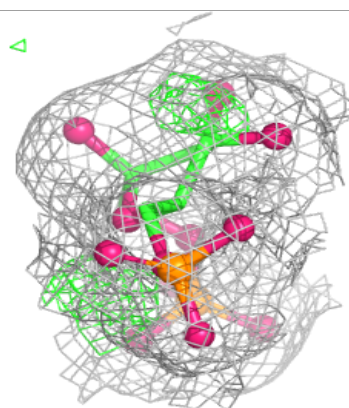
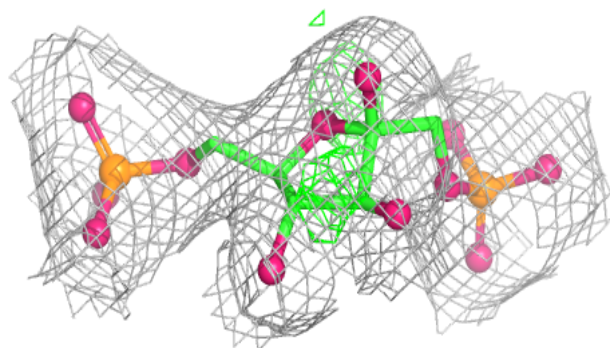
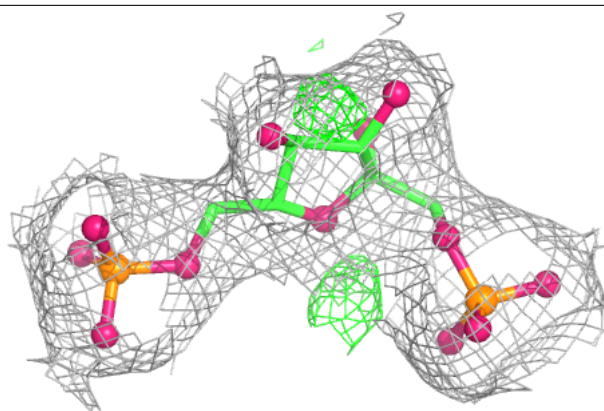
**Electron density around FBP F 501:**

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

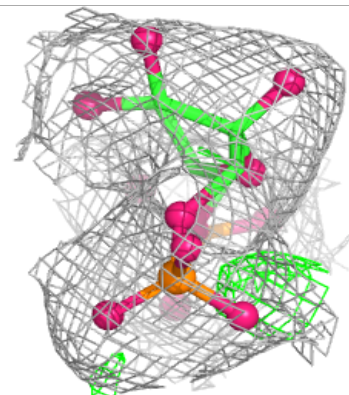
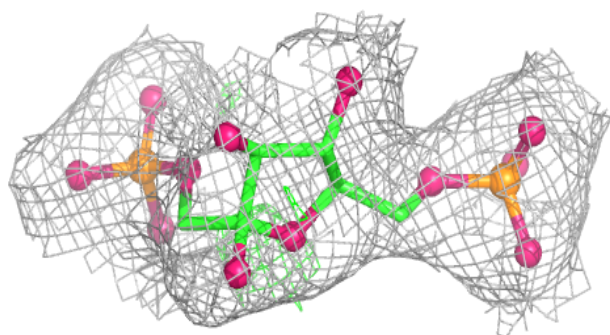
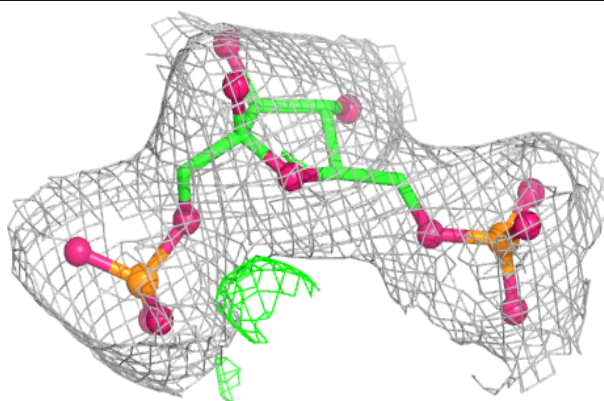


Electron density around FBP C 501:

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

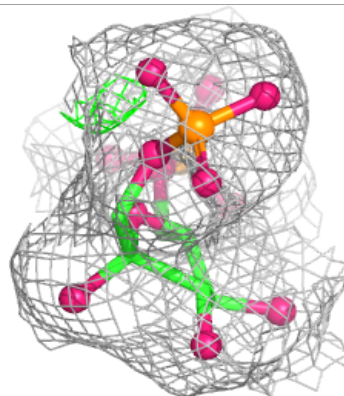
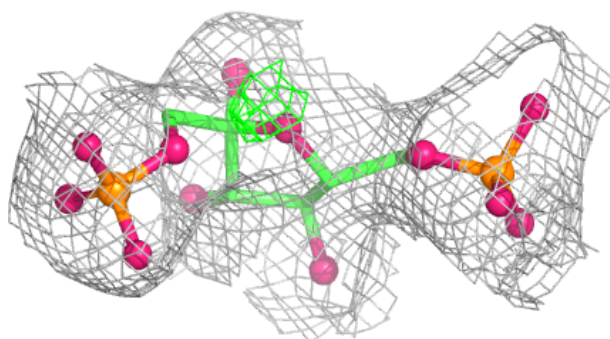
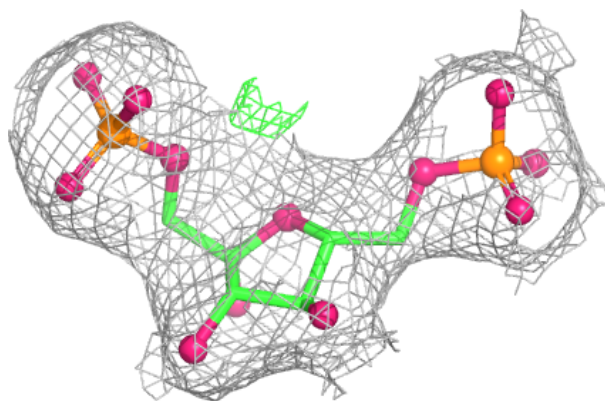
**Electron density around FBP D 501:**

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

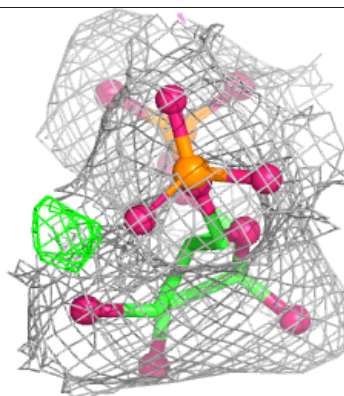
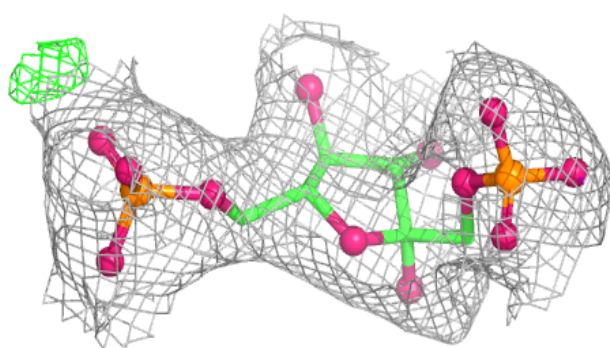
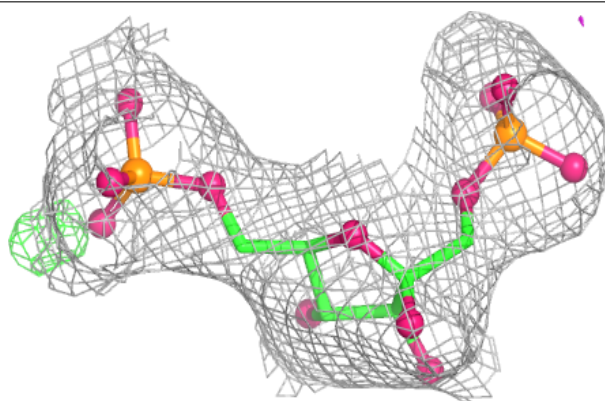


Electron density around FBP G 501:

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

**Electron density around FBP H 502:**

$2mF_o-DF_c$ (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.