



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:38 AM UTC

PDB ID : 9R3H / pdb_00009r3h
Title : Structure of liver pyruvate kinase in complex with fluorescent probe 4b
Authors : Bogucka, A.; Nilsson, O.; Grotli, M.; Hyvonen, M.
Deposited on : 2025-05-05
Resolution : 2.10 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

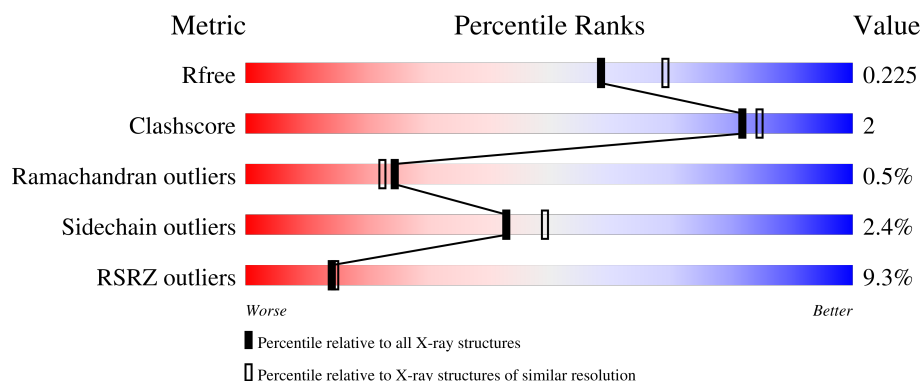
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	21% 85% 10% 5%
1	B	447	13% 89% 8% •
1	C	447	9% 87% 8% •
1	D	447	3% 87% 7% • 5%
1	E	447	13% 87% 7% • 5%

Continued on next page...

Continued from previous page...

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	602	-	X	-	-
3	OXL	B	602	-	X	-	-
3	OXL	C	602	-	X	-	-
3	OXL	D	602	-	X	-	-
3	OXL	E	602	-	X	-	-
3	OXL	G	603	-	X	-	-
3	OXL	H	602	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28940 atoms, of which 119 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
			3240	2036	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

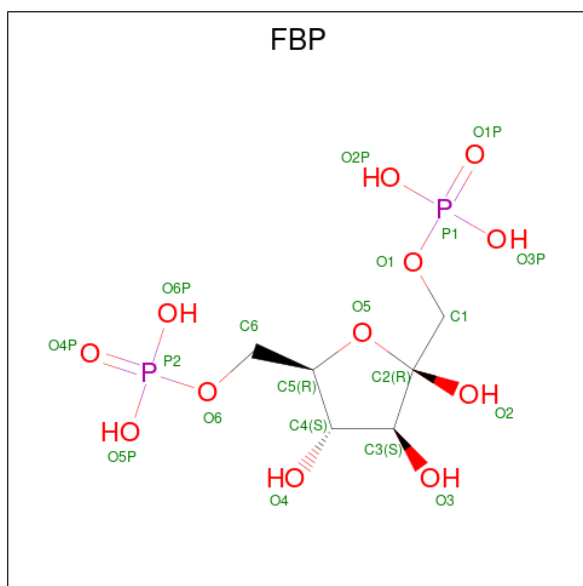
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	THR	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	TRP	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	TYR	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	ILE	deletion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

Continued on next page...

Continued from previous page...

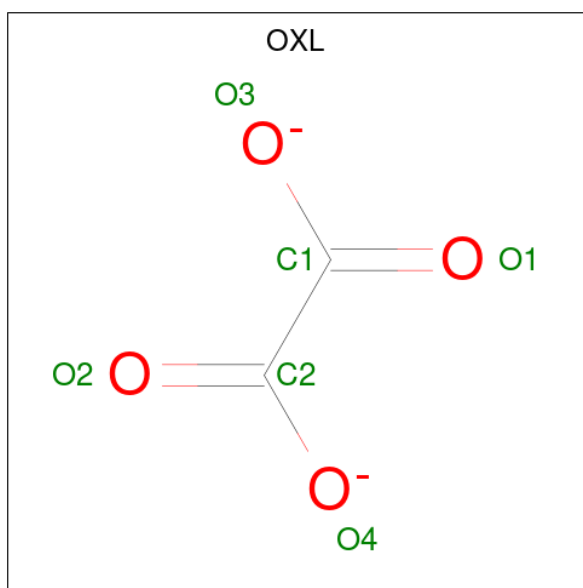
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLU	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	ARG	deletion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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	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		

Continued on next page...

Continued from previous page...

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).

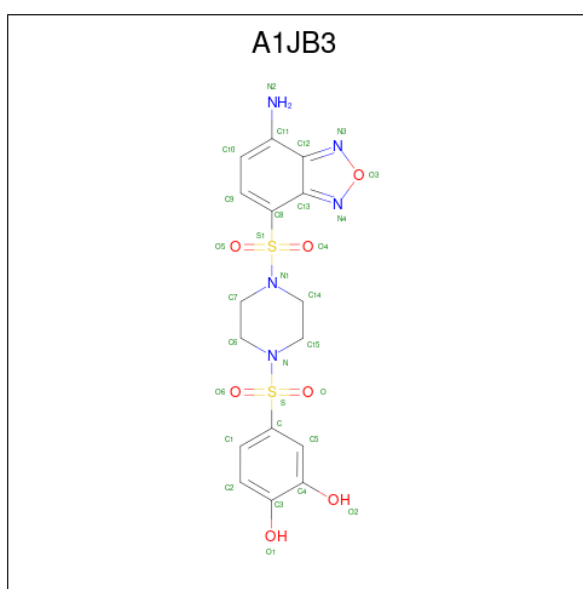
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	C	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		
5	E	1	Total	K	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is 4-[4-[(7-azanyl-2,1,3-benzoxadiazol-4-yl)sulfonyl]piperazin-1-yl]sulfonylbenzene-1,2-diol (CCD ID: A1JB3) (formula: C₁₆H₁₇N₅O₇S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	34	1
			94	32	34	10	14	4		
6	B	1	Total	C	H	N	O	S	17	0
			47	16	17	5	7	2		
6	F	1	Total	C	H	N	O	S	34	1
			94	32	34	10	14	4		
6	G	1	Total	C	H	N	O	S	34	1
			94	32	34	10	14	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	177	Total O 177 177	0	0

Continued on next page...

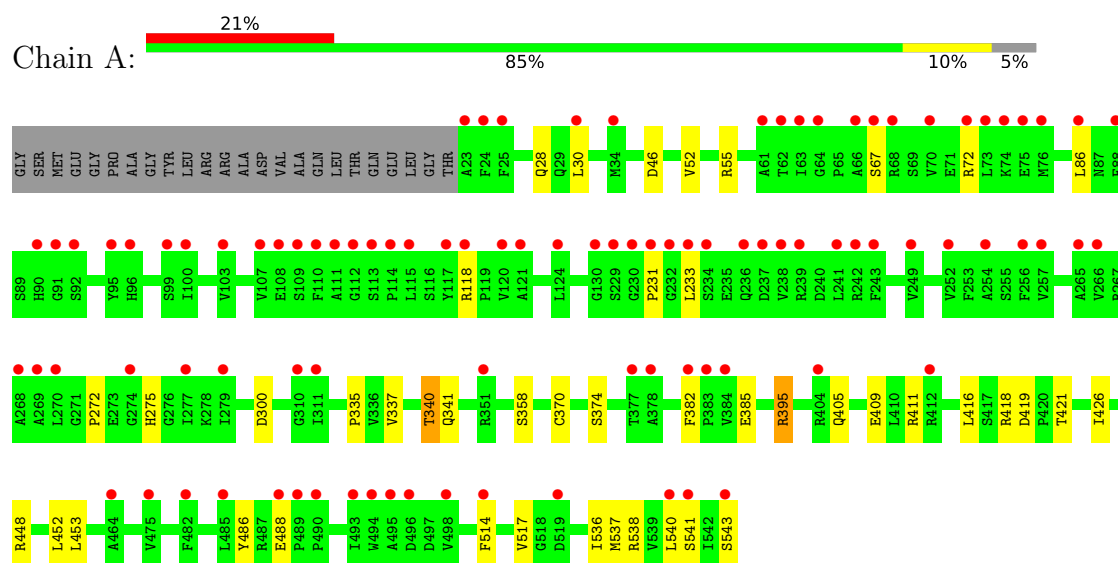
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	182	Total 182	O 182	0	0
7	C	270	Total 270	O 270	0	0
7	D	362	Total 362	O 362	0	0
7	E	221	Total 221	O 221	0	0
7	F	263	Total 263	O 263	0	0
7	G	388	Total 388	O 388	0	0
7	H	388	Total 388	O 388	0	0

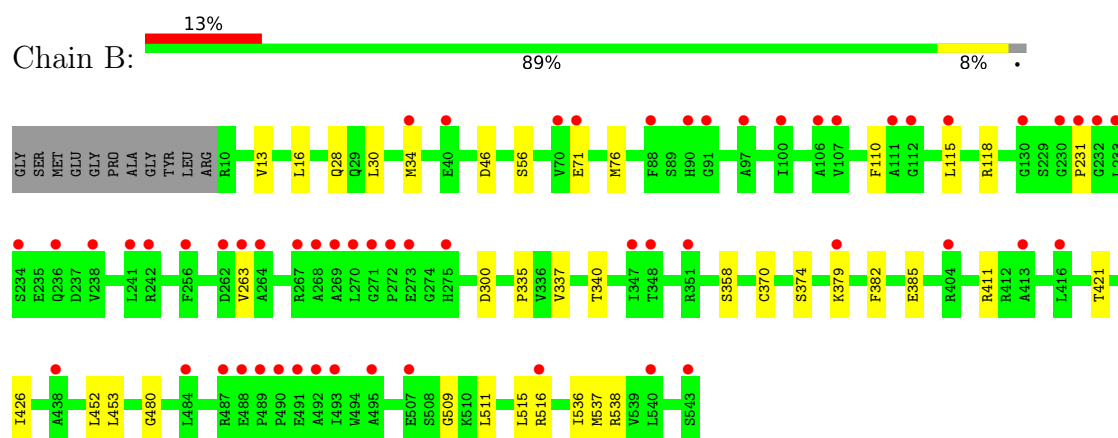
3 Residue-property plots

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.

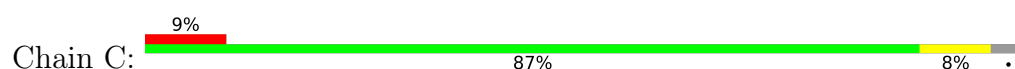
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

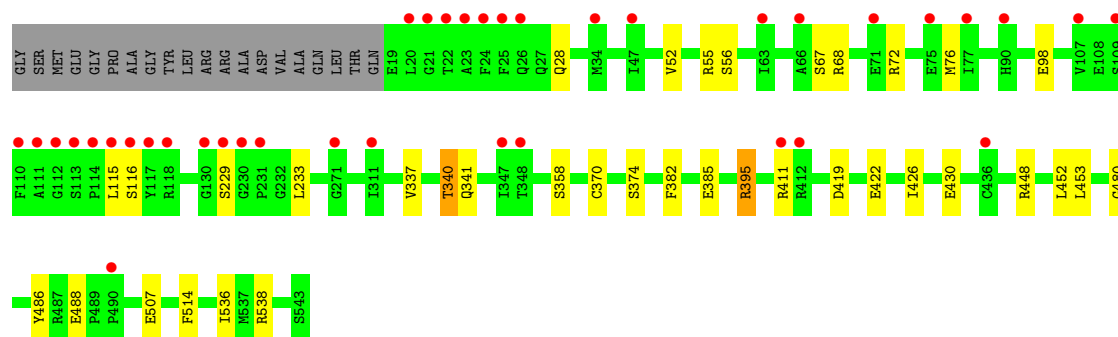


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

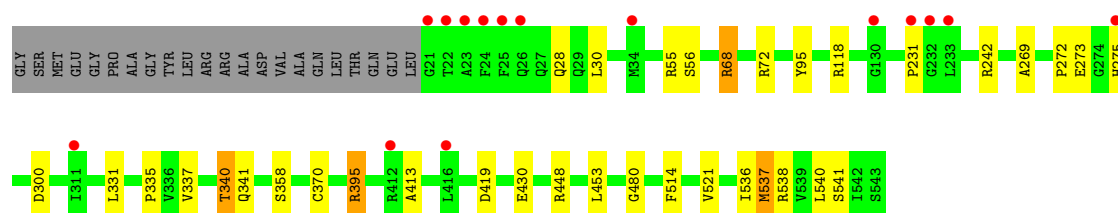
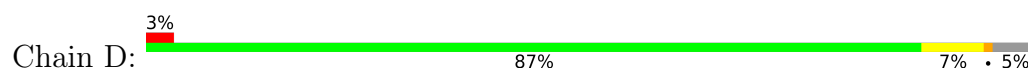


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

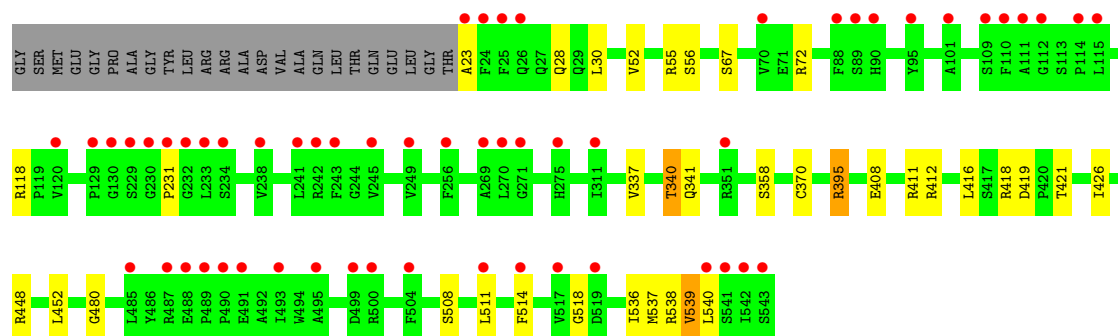
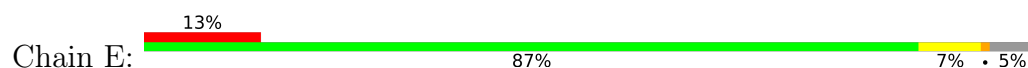




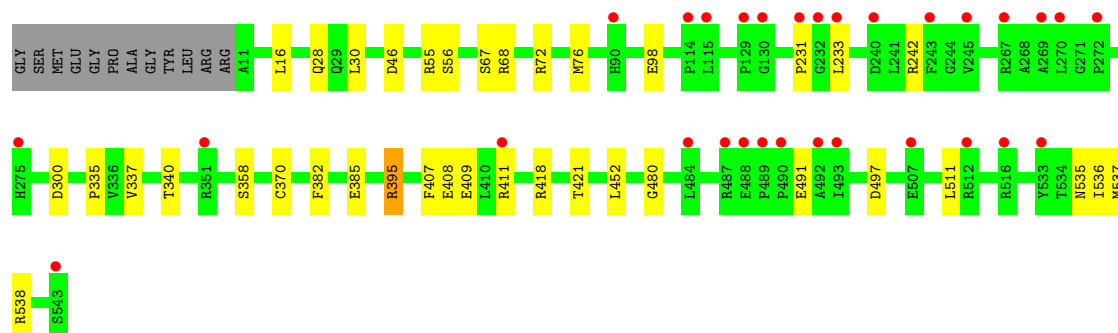
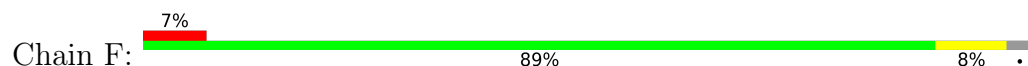
● Molecule 1: Isoform L-type of Pyruvate kinase PKLR



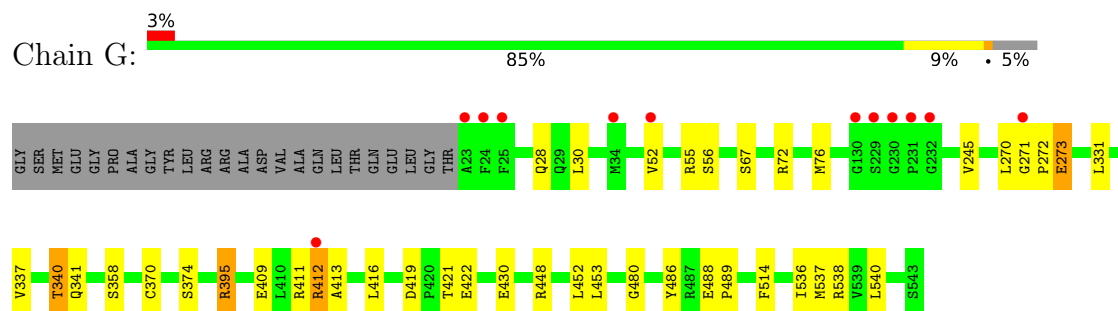
● Molecule 1: Isoform L-type of Pyruvate kinase PKLR



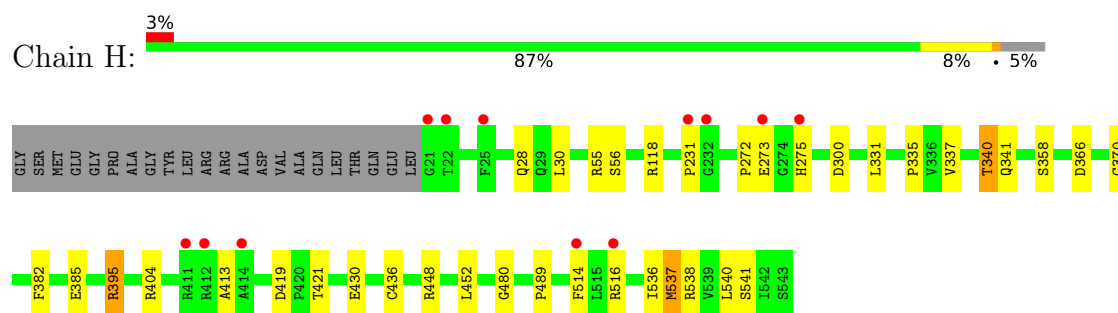
● Molecule 1: Isoform L-type of Pyruvate kinase PKLR



- 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	208.52Å 112.55Å 189.31Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	189.28 – 2.10 189.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	81.4 (189.28-2.10) 81.4 (189.28-2.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.205 , 0.233 0.197 , 0.225	Depositor DCC
R_{free} test set	10119 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28940	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 53.58 % 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 4.1327e-05. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, K, FBP, MG, A1JB3

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	0.69	1/3312 (0.0%)	1.02	4/4477 (0.1%)
1	B	0.70	1/3396 (0.0%)	1.00	3/4592 (0.1%)
1	C	0.72	1/3324 (0.0%)	1.03	4/4495 (0.1%)
1	D	0.73	1/3326 (0.0%)	1.02	3/4497 (0.1%)
1	E	0.67	0/3301	1.01	3/4463 (0.1%)
1	F	0.71	0/3411	1.00	1/4613 (0.0%)
1	G	0.75	3/3314 (0.1%)	1.04	5/4481 (0.1%)
1	H	0.77	1/3316 (0.0%)	1.02	2/4483 (0.0%)
All	All	0.72	8/26700 (0.0%)	1.02	25/36101 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	SER	CA-C	7.17	1.56	1.52
1	G	489	PRO	CA-C	6.01	1.55	1.51
1	A	374	SER	CA-C	5.86	1.55	1.52
1	C	374	SER	CA-C	5.48	1.55	1.52
1	H	489	PRO	CA-C	5.33	1.54	1.51
1	G	374[A]	SER	CA-C	5.30	1.55	1.52
1	G	374[B]	SER	CA-C	5.30	1.55	1.52
1	D	537	MET	CA-C	5.16	1.58	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	514	PHE	CA-CB-CG	8.58	122.38	113.80
1	G	514	PHE	CA-CB-CG	8.24	122.04	113.80
1	D	514	PHE	CA-CB-CG	7.11	120.91	113.80
1	A	514	PHE	CA-CB-CG	6.94	120.74	113.80
1	E	514	PHE	CA-CB-CG	6.92	120.72	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	PHE	CA-CB-CG	6.41	120.21	113.80
1	E	23	ALA	CA-C-N	6.06	128.68	120.38
1	E	23	ALA	C-N-CA	6.06	128.68	120.38
1	C	507	GLU	CB-CG-CD	5.61	122.13	112.60
1	A	453	LEU	CA-C-N	5.48	127.63	120.28
1	A	453	LEU	C-N-CA	5.48	127.63	120.28
1	D	453	LEU	CA-C-N	5.32	127.40	120.28
1	D	453	LEU	C-N-CA	5.32	127.40	120.28
1	F	46	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	46	ASP	CA-CB-CG	5.28	117.88	112.60
1	G	270	LEU	CA-C-N	5.21	130.05	121.87
1	G	270	LEU	C-N-CA	5.21	130.05	121.87
1	C	453	LEU	CA-C-N	5.14	127.16	120.28
1	C	453	LEU	C-N-CA	5.14	127.16	120.28
1	A	46	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	453	LEU	CA-C-N	5.07	127.07	120.28
1	B	453	LEU	C-N-CA	5.07	127.07	120.28
1	G	453	LEU	CA-C-N	5.00	126.98	120.28
1	G	453	LEU	C-N-CA	5.00	126.98	120.28
1	H	366	ASP	CA-CB-CG	5.00	117.60	112.60

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	3240	0	3300	24	0
1	B	3329	0	3394	16	0
1	C	3257	0	3308	17	0
1	D	3252	0	3310	15	0
1	E	3231	0	3289	18	0
1	F	3335	0	3404	21	0
1	G	3241	0	3293	24	0
1	H	3251	0	3306	19	0
2	A	20	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	60	34	0	3	0
6	B	30	17	0	0	0
6	F	60	34	0	1	0
6	G	60	34	0	2	0
7	A	177	0	0	0	0
7	B	182	0	0	0	0
7	C	270	0	0	1	0
7	D	362	0	0	0	0
7	E	221	0	0	0	0
7	F	263	0	0	0	0
7	G	388	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	388	0	0	0	0
All	All	28821	119	26684	132	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 2.

All (132) 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:E:411:ARG:HG3	1:E:426:ILE:HD11	1.63	0.79
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.03	0.73
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.70	0.73
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.69	0.73
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.72	0.72
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.71	0.72
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.73	0.71
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.73	0.70
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.73	0.69
1:C:536:ILE:HG12	1:D:538:ARG:HG2	1.76	0.68
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.63	0.66
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.79	0.65
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.79	0.65
1:D:68:ARG:NH2	1:D:95:TYR:O	2.30	0.64
1:G:537:MET:HE3	1:H:537:MET:HG2	1.80	0.63
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.80	0.62
1:C:538:ARG:HD3	7:C:756:HOH:O	2.01	0.60
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.84	0.58
1:A:538:ARG:HG2	1:B:536:ILE:HG12	1.85	0.58
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.85	0.58
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.86	0.56
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.87	0.56
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.88	0.56
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.89	0.55
1:A:67:SER:HA	1:A:72:ARG:HG2	1.89	0.54
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.92	0.51
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.46	0.51
1:A:411:ARG:HG3	1:A:426:ILE:HD11	1.93	0.51
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.46	0.50
1:D:242[A]:ARG:HD2	1:D:269:ALA:O	2.12	0.50
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.12	0.50
1:A:416:LEU:HB3	1:B:16:LEU:HD22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.94	0.50
1:G:409:GLU:OE1	6:G:601[B]:A1JB3:O3	2.30	0.50
1:H:56:SER:HB2	1:H:480:GLY:CA	2.42	0.50
1:H:55:ARG:HB2	1:H:395:ARG:HG3	1.94	0.49
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.94	0.49
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.27	0.49
1:E:408:GLU:CD	1:F:411:ARG:HH21	2.21	0.48
1:B:13:VAL:HG11	1:B:34:MET:SD	2.53	0.48
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.95	0.48
1:E:418:ARG:HG3	1:F:16:LEU:HD11	1.96	0.48
1:H:419:ASP:OD2	1:H:448:ARG:NH2	2.48	0.47
1:H:331:LEU:CD1	1:H:413:ALA:HB1	2.45	0.47
1:A:55:ARG:HB2	1:A:395:ARG:HG3	1.96	0.47
1:G:56:SER:HB2	1:G:480:GLY:CA	2.44	0.46
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.44	0.46
1:C:340:THR:HG22	1:C:341:GLN:HG3	1.97	0.46
1:A:28:GLN:HB3	1:A:52:VAL:HG22	1.98	0.46
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.51	0.46
1:D:419:ASP:OD2	1:D:448:ARG:NH2	2.48	0.46
1:E:55:ARG:HB2	1:E:395:ARG:HG3	1.98	0.46
1:F:28:GLN:HG3	1:F:30:LEU:HG	1.98	0.46
1:A:409:GLU:OE1	6:A:605[B]:A1JB3:N3	2.49	0.46
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.98	0.46
1:F:409:GLU:OE1	6:F:605[B]:A1JB3:O3	2.33	0.46
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.51	0.45
1:G:409:GLU:OE1	6:G:601[B]:A1JB3:N3	2.49	0.45
1:D:55:ARG:HB2	1:D:395:ARG:HG3	1.99	0.45
1:A:419:ASP:OD2	1:A:448:ARG:NH2	2.50	0.45
1:E:539:VAL:HG13	1:F:535:ASN:HB2	1.98	0.45
1:G:430[A]:GLU:OE1	1:H:430:GLU:OE1	2.35	0.45
1:C:68:ARG:NH2	1:C:98:GLU:HB3	2.32	0.45
1:G:331:LEU:CD1	1:G:413:ALA:HB1	2.47	0.45
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.99	0.44
1:G:28:GLN:HB3	1:G:52:VAL:HG22	1.99	0.44
1:B:509:GLY:HA3	1:B:515:LEU:HD12	1.98	0.44
1:F:56:SER:HB2	1:F:480:GLY:CA	2.48	0.44
1:G:55:ARG:HB2	1:G:395:ARG:HG3	1.99	0.44
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.00	0.44
1:A:28:GLN:HG3	1:A:30:LEU:HG	2.00	0.44
1:D:56:SER:HB2	1:D:480:GLY:CA	2.46	0.44
1:F:491:GLU:HB2	1:F:497:ASP:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ARG:HB2	1:C:395:ARG:HG3	1.99	0.44
1:F:55:ARG:HB2	1:F:395:ARG:HG3	2.00	0.44
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.99	0.43
1:E:518:GLY:O	1:F:418:ARG:NH2	2.51	0.43
1:C:56:SER:HB2	1:C:480:GLY:CA	2.47	0.43
1:G:337:VAL:HG22	1:G:370:CYS:HB2	2.00	0.43
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.53	0.43
1:A:416:LEU:CB	1:B:16:LEU:HD22	2.48	0.43
1:D:300:ASP:O	1:D:335:PRO:HD2	2.19	0.43
1:A:272:PRO:HA	1:A:275:HIS:CD2	2.53	0.43
1:B:28:GLN:HG3	1:B:30:LEU:HG	1.99	0.43
1:B:56:SER:HB2	1:B:480:GLY:CA	2.48	0.43
1:B:337:VAL:HG22	1:B:370:CYS:HB2	2.00	0.43
1:C:28:GLN:HB3	1:C:52:VAL:HG22	2.00	0.43
1:A:421:THR:HG22	1:A:452:LEU:HD12	2.01	0.43
1:G:28:GLN:HG3	1:G:30:LEU:HG	2.01	0.43
1:G:416:LEU:HD13	1:H:436:CYS:SG	2.59	0.43
1:H:300:ASP:O	1:H:335:PRO:HD2	2.18	0.43
1:D:337:VAL:HG22	1:D:370:CYS:HB2	2.01	0.43
1:F:421:THR:HG22	1:F:452:LEU:HD12	2.01	0.43
1:A:405:GLN:HG2	6:A:605[B]:A1JB3:N4	2.34	0.42
1:G:419:ASP:OD2	1:G:448:ARG:NH2	2.51	0.42
1:E:56:SER:HB2	1:E:480:GLY:CA	2.48	0.42
1:E:67:SER:HA	1:E:72:ARG:HG2	2.01	0.42
1:G:412:ARG:NH2	1:H:404:ARG:HD3	2.34	0.42
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.55	0.42
1:F:382:PHE:HB3	1:F:385:GLU:HB2	2.01	0.42
1:F:407:PHE:CD2	1:F:411:ARG:NH1	2.76	0.42
1:A:337:VAL:HG22	1:A:370:CYS:HB2	2.00	0.42
1:A:300:ASP:O	1:A:335:PRO:HD2	2.20	0.42
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.99	0.42
1:A:517:VAL:HG13	1:A:543:SER:HB2	2.01	0.42
1:E:28:GLN:HB3	1:E:52:VAL:HG22	2.02	0.42
1:E:337:VAL:HG22	1:E:370:CYS:HB2	2.02	0.42
1:E:28:GLN:HG3	1:E:30:LEU:HG	2.01	0.41
1:A:382:PHE:HB3	1:A:385:GLU:HB2	2.02	0.41
1:F:67:SER:HA	1:F:72:ARG:HG2	2.02	0.41
1:C:382:PHE:HB3	1:C:385:GLU:HB2	2.03	0.41
1:G:430[B]:GLU:OE2	1:H:430:GLU:OE1	2.38	0.41
1:C:430[A]:GLU:OE1	1:D:430[A]:GLU:OE1	2.39	0.41
1:B:300:ASP:O	1:B:335:PRO:HD2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:421:THR:HG22	1:H:452:LEU:HD12	2.03	0.41
1:F:337:VAL:HG22	1:F:370:CYS:HB2	2.03	0.41
1:A:409:GLU:CD	6:A:605[B]:A1JB3:O3	2.64	0.41
1:B:421:THR:HG22	1:B:452:LEU:HD12	2.03	0.41
1:C:337:VAL:HG22	1:C:370:CYS:HB2	2.02	0.41
1:E:419:ASP:OD2	1:E:448:ARG:NH2	2.50	0.41
1:H:340:THR:HG22	1:H:341:GLN:HG3	2.03	0.41
1:D:28:GLN:HG3	1:D:30:LEU:HG	2.03	0.40
1:G:421:THR:HG22	1:G:452:LEU:HD12	2.03	0.40
1:H:382:PHE:HB3	1:H:385:GLU:HB2	2.03	0.40
1:E:416:LEU:HB3	1:F:16:LEU:HD22	2.02	0.40
1:B:110:PHE:CE1	1:B:118:ARG:NH1	2.90	0.40
1:C:419:ASP:OD2	1:C:448:ARG:NH2	2.54	0.40
1:C:67:SER:HA	1:C:72:ARG:HG2	2.03	0.40
1:G:67:SER:HA	1:G:72:ARG:HG2	2.03	0.40
1:D:331:LEU:CD1	1:D:413:ALA:HB1	2.52	0.40
1:F:300:ASP:O	1:F:335:PRO:HD2	2.21	0.40
1:H:28:GLN:HG3	1:H:30:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/447 (96%)	422 (99%)	3 (1%)	2 (0%)	24	22
1	B	438/447 (98%)	433 (99%)	3 (1%)	2 (0%)	24	22
1	C	429/447 (96%)	422 (98%)	5 (1%)	2 (0%)	24	22
1	D	429/447 (96%)	424 (99%)	3 (1%)	2 (0%)	24	22
1	E	426/447 (95%)	421 (99%)	3 (1%)	2 (0%)	24	22
1	F	440/447 (98%)	435 (99%)	3 (1%)	2 (0%)	24	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	427/447 (96%)	418 (98%)	7 (2%)	2 (0%)	24	22
1	H	427/447 (96%)	422 (99%)	3 (1%)	2 (0%)	24	22
All	All	3443/3576 (96%)	3397 (99%)	30 (1%)	16 (0%)	24	22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	271	GLY
1	A	231	PRO
1	A	340	THR
1	B	340	THR
1	C	229	SER
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR
1	E	231	PRO
1	F	231	PRO
1	H	231	PRO
1	D	231	PRO
1	B	231	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	340/352 (97%)	331 (97%)	9 (3%)	40	46
1	B	349/352 (99%)	338 (97%)	11 (3%)	34	38
1	C	342/352 (97%)	335 (98%)	7 (2%)	48	56
1	D	342/352 (97%)	332 (97%)	10 (3%)	37	42
1	E	340/352 (97%)	330 (97%)	10 (3%)	37	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	351/352 (100%)	341 (97%)	10 (3%)	38	43
1	G	341/352 (97%)	333 (98%)	8 (2%)	44	51
1	H	340/352 (97%)	332 (98%)	8 (2%)	43	49
All	All	2745/2816 (98%)	2672 (97%)	73 (3%)	43	45

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	118	ARG
1	A	233	LEU
1	A	358	SER
1	A	395	ARG
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	A	541	SER
1	B	71	GLU
1	B	76[A]	MET
1	B	76[B]	MET
1	B	115	LEU
1	B	263	VAL
1	B	358	SER
1	B	379	LYS
1	B	511	LEU
1	B	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	76[A]	MET
1	C	76[B]	MET
1	C	115	LEU
1	C	116	SER
1	C	233	LEU
1	C	358	SER
1	C	395	ARG
1	D	68	ARG
1	D	72	ARG
1	D	118	ARG
1	D	273	GLU
1	D	358	SER
1	D	395	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	521	VAL
1	D	537	MET
1	D	540	LEU
1	D	541	SER
1	E	118	ARG
1	E	358	SER
1	E	395	ARG
1	E	412	ARG
1	E	508	SER
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	E	540	LEU
1	F	76[A]	MET
1	F	76[B]	MET
1	F	233	LEU
1	F	242	ARG
1	F	358	SER
1	F	395	ARG
1	F	408	GLU
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	76[A]	MET
1	G	76[B]	MET
1	G	273	GLU
1	G	358	SER
1	G	395	ARG
1	G	411	ARG
1	G	412	ARG
1	G	540	LEU
1	H	118	ARG
1	H	273	GLU
1	H	358	SER
1	H	395	ARG
1	H	516	ARG
1	H	537	MET
1	H	540	LEU
1	H	541	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	B	90	HIS
1	B	390	GLN
1	B	405	GLN
1	C	90	HIS
1	C	275	HIS
1	C	390	GLN
1	D	90	HIS
1	D	390	GLN
1	D	405	GLN
1	E	90	HIS
1	E	390	GLN
1	F	90	HIS
1	F	236	GLN
1	F	390	GLN
1	F	405	GLN
1	G	26	GLN
1	G	90	HIS
1	G	275	HIS
1	G	390	GLN
1	H	90	HIS
1	H	390	GLN
1	H	405	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 16 are monoatomic - leaving 23 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
6	A1JB3	F	605[B]	-	33,33,33	0.91	3 (9%)	44,51,51	1.04	2 (4%)
2	FBP	G	602	-	18,20,20	0.47	0	21,32,32	0.82	0
3	OXL	G	603	4	5,5,5	2.30	2 (40%)	6,6,6	1.40	2 (33%)
3	OXL	F	602	4	5,5,5	2.01	2 (40%)	6,6,6	2.31	3 (50%)
2	FBP	H	601	-	18,20,20	0.67	0	21,32,32	0.66	1 (4%)
2	FBP	F	601	-	18,20,20	0.46	0	21,32,32	0.58	0
6	A1JB3	A	605[A]	-	33,33,33	1.02	4 (12%)	44,51,51	1.03	3 (6%)
3	OXL	D	602	4	5,5,5	2.40	2 (40%)	6,6,6	1.96	2 (33%)
2	FBP	B	601	-	18,20,20	0.39	0	21,32,32	0.66	0
3	OXL	E	602	4	5,5,5	2.07	2 (40%)	6,6,6	1.89	2 (33%)
6	A1JB3	G	601[A]	-	33,33,33	0.99	4 (12%)	44,51,51	0.87	1 (2%)
6	A1JB3	B	605	-	33,33,33	0.92	2 (6%)	44,51,51	0.87	1 (2%)
6	A1JB3	F	605[A]	-	33,33,33	1.12	4 (12%)	44,51,51	1.01	2 (4%)
2	FBP	E	601	-	18,20,20	0.55	0	21,32,32	0.58	0
2	FBP	D	601	-	18,20,20	0.58	0	21,32,32	0.78	1 (4%)
6	A1JB3	A	605[B]	-	33,33,33	0.96	3 (9%)	44,51,51	1.28	6 (13%)
3	OXL	A	602	4	5,5,5	2.21	2 (40%)	6,6,6	1.84	2 (33%)
2	FBP	A	601	-	18,20,20	0.57	0	21,32,32	0.60	0
3	OXL	B	602	4	5,5,5	2.23	2 (40%)	6,6,6	1.61	2 (33%)
3	OXL	C	602	4	5,5,5	2.06	2 (40%)	6,6,6	2.35	3 (50%)
2	FBP	C	601	-	18,20,20	0.55	0	21,32,32	0.60	0
3	OXL	H	602	4	5,5,5	1.87	2 (40%)	6,6,6	1.81	2 (33%)
6	A1JB3	G	601[B]	-	33,33,33	0.94	3 (9%)	44,51,51	0.76	1 (2%)

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
6	A1JB3	F	605[B]	-	-	6/24/34/34	0/4/4/4
2	FBP	G	602	-	-	2/13/32/32	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	G	603	4	-	4/4/4/4	-
3	OXL	F	602	4	-	0/4/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
6	A1JB3	A	605[A]	-	-	3/24/34/34	0/4/4/4
3	OXL	D	602	4	-	4/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	E	602	4	-	4/4/4/4	-
6	A1JB3	G	601[A]	-	-	12/24/34/34	0/4/4/4
6	A1JB3	B	605	-	-	0/24/34/34	0/4/4/4
6	A1JB3	F	605[A]	-	-	9/24/34/34	0/4/4/4
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
6	A1JB3	A	605[B]	-	-	8/24/34/34	0/4/4/4
3	OXL	A	602	4	-	4/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	C	602	4	-	4/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	4/4/4/4	-
6	A1JB3	G	601[B]	-	-	12/24/34/34	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	603	OXL	O2-C2	4.48	1.33	1.22
3	B	602	OXL	O2-C2	4.04	1.32	1.22
3	A	602	OXL	O2-C2	3.87	1.32	1.22
3	D	602	OXL	O2-C2	3.81	1.32	1.22
3	C	602	OXL	O2-C2	3.66	1.31	1.22
3	F	602	OXL	O2-C2	3.60	1.31	1.22
6	F	605[A]	A1JB3	C12-N3	3.58	1.37	1.31
6	F	605[A]	A1JB3	C13-N4	3.43	1.36	1.31
6	G	601[A]	A1JB3	C13-N4	3.38	1.36	1.31
3	E	602	OXL	O4-C2	-3.28	1.21	1.30
3	D	602	OXL	O4-C2	-3.15	1.22	1.30
6	A	605[B]	A1JB3	C8-C13	-3.15	1.40	1.42
3	H	602	OXL	O2-C2	3.10	1.30	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605[A]	A1JB3	C13-N4	3.09	1.36	1.31
3	E	602	OXL	O2-C2	3.00	1.30	1.22
6	G	601[B]	A1JB3	C8-C13	-2.99	1.40	1.42
6	B	605	A1JB3	C8-C13	-2.90	1.40	1.42
3	B	602	OXL	O4-C2	-2.77	1.23	1.30
6	A	605[A]	A1JB3	C12-N3	2.72	1.35	1.31
6	G	601[B]	A1JB3	O3-N3	-2.71	1.33	1.39
3	H	602	OXL	O4-C2	-2.69	1.23	1.30
6	B	605	A1JB3	C13-N4	2.67	1.35	1.31
6	F	605[B]	A1JB3	O3-N3	-2.61	1.33	1.39
6	G	601[A]	A1JB3	O3-N3	-2.60	1.33	1.39
3	A	602	OXL	O4-C2	-2.56	1.23	1.30
6	G	601[A]	A1JB3	C12-N3	2.53	1.35	1.31
6	F	605[B]	A1JB3	C8-C13	-2.48	1.41	1.42
6	A	605[A]	A1JB3	C8-C13	-2.48	1.41	1.42
3	G	603	OXL	O4-C2	-2.44	1.23	1.30
6	A	605[B]	A1JB3	O3-N4	-2.42	1.33	1.39
6	A	605[B]	A1JB3	O3-N3	-2.42	1.33	1.39
6	A	605[A]	A1JB3	O3-N3	-2.39	1.33	1.39
3	C	602	OXL	O4-C2	-2.38	1.24	1.30
6	F	605[B]	A1JB3	C12-N3	2.35	1.35	1.31
6	G	601[B]	A1JB3	C12-N3	2.34	1.35	1.31
3	F	602	OXL	O4-C2	-2.28	1.24	1.30
6	F	605[A]	A1JB3	C8-C13	-2.21	1.41	1.42
6	F	605[A]	A1JB3	O3-N3	-2.20	1.34	1.39
6	G	601[A]	A1JB3	C8-C13	-2.12	1.41	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	601[A]	A1JB3	C8-C13-C12	-4.72	118.10	121.86
6	A	605[A]	A1JB3	C8-C13-C12	-4.61	118.18	121.86
6	F	605[B]	A1JB3	C8-C13-C12	-4.61	118.19	121.86
6	F	605[A]	A1JB3	C8-C13-C12	-4.39	118.36	121.86
3	C	602	OXL	O4-C2-C1	4.30	121.17	112.83
3	F	602	OXL	O4-C2-C1	4.13	120.84	112.83
6	A	605[B]	A1JB3	C8-C13-C12	-4.08	118.61	121.86
6	B	605	A1JB3	C8-C13-C12	-4.07	118.61	121.86
6	G	601[B]	A1JB3	C8-C13-C12	-3.95	118.71	121.86
3	H	602	OXL	O4-C2-C1	3.65	119.90	112.83
3	A	602	OXL	O4-C2-C1	3.51	119.64	112.83
3	E	602	OXL	O4-C2-C1	3.51	119.64	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	605[B]	A1JB3	C14-N1-C7	3.19	115.79	112.12
3	D	602	OXL	O4-C2-C1	3.18	119.00	112.83
6	A	605[B]	A1JB3	C15-N-C6	3.16	115.75	112.12
3	D	602	OXL	O3-C1-C2	2.99	118.64	112.83
3	F	602	OXL	O3-C1-C2	2.89	118.44	112.83
6	A	605[B]	A1JB3	C15-N-S	2.80	122.26	117.06
2	D	601	FBP	O6-P2-O4P	2.78	113.95	106.44
6	A	605[B]	A1JB3	C14-N1-S1	2.77	122.20	117.06
3	B	602	OXL	O4-C2-C1	2.66	117.98	112.83
3	C	602	OXL	O3-C1-C2	2.64	117.94	112.83
3	B	602	OXL	O3-C1-C2	2.61	117.90	112.83
3	C	602	OXL	O2-C2-C1	-2.61	115.19	120.63
6	F	605[B]	A1JB3	C14-N1-C7	2.43	114.91	112.12
3	E	602	OXL	O3-C1-C2	2.41	117.51	112.83
3	G	603	OXL	O4-C2-C1	2.39	117.46	112.83
3	F	602	OXL	O2-C2-C1	-2.36	115.72	120.63
2	H	601	FBP	O6-P2-O4P	2.33	112.74	106.44
6	F	605[A]	A1JB3	C14-N1-C7	2.33	114.79	112.12
6	A	605[A]	A1JB3	C14-N1-C7	2.31	114.77	112.12
6	A	605[A]	A1JB3	C15-N-C6	2.18	114.63	112.12
3	G	603	OXL	O3-C1-C2	2.18	117.06	112.83
3	A	602	OXL	O3-C1-C2	2.17	117.04	112.83
6	A	605[B]	A1JB3	C7-N1-S1	2.14	121.04	117.06
3	H	602	OXL	O2-C2-C1	-2.05	116.37	120.63

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	605[B]	A1JB3	C7-N1-S1-O4
6	A	605[B]	A1JB3	C7-N1-S1-O4
6	F	605[A]	A1JB3	C14-N1-S1-O5
6	F	605[B]	A1JB3	C7-N1-S1-O5
6	G	601[A]	A1JB3	C7-N1-S1-O4
6	G	601[A]	A1JB3	C15-N-S-O
6	G	601[B]	A1JB3	C14-N1-S1-O5
6	G	601[B]	A1JB3	C15-N-S-O
6	F	605[A]	A1JB3	C14-N1-S1-C8
6	G	601[A]	A1JB3	C15-N-S-C
6	G	601[B]	A1JB3	C15-N-S-C
6	G	601[B]	A1JB3	C7-N1-S1-O4
6	G	601[B]	A1JB3	C7-N1-S1-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	605[B]	A1JB3	C7-N1-S1-O5
6	A	605[B]	A1JB3	C6-N-S-O6
6	G	601[B]	A1JB3	C14-N1-S1-O4
6	F	605[B]	A1JB3	C7-N1-S1-C8
6	G	601[A]	A1JB3	C7-N1-S1-C8
6	F	605[A]	A1JB3	C14-N1-S1-O4
6	G	601[A]	A1JB3	C15-N-S-O6
6	G	601[B]	A1JB3	C15-N-S-O6
6	A	605[A]	A1JB3	C7-N1-S1-O4
6	A	605[B]	A1JB3	C6-N-S-O
6	G	601[A]	A1JB3	C7-N1-S1-O5
6	A	605[B]	A1JB3	C7-N1-S1-C8
6	G	601[B]	A1JB3	C7-N1-S1-C8
2	A	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	G	602	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	F	605[B]	A1JB3	C14-N1-S1-O5
6	G	601[B]	A1JB3	C14-N1-S1-C8
6	F	605[B]	A1JB3	C14-N1-S1-O4
6	A	605[A]	A1JB3	C7-N1-S1-C8
6	A	605[B]	A1JB3	C6-N-S-C
2	B	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
6	F	605[A]	A1JB3	C7-N1-S1-O4
6	F	605[A]	A1JB3	C7-N1-S1-O5
6	F	605[B]	A1JB3	C14-N1-S1-C8
6	G	601[A]	A1JB3	C14-N1-S1-O5
6	G	601[A]	A1JB3	C6-N-S-O6
6	G	601[B]	A1JB3	C6-N-S-O6
6	G	601[A]	A1JB3	C14-N1-S1-O4
6	G	601[A]	A1JB3	C6-N-S-O
2	A	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	G	602	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
6	G	601[B]	A1JB3	C6-N-S-O

Continued on next page...

Continued from previous page...

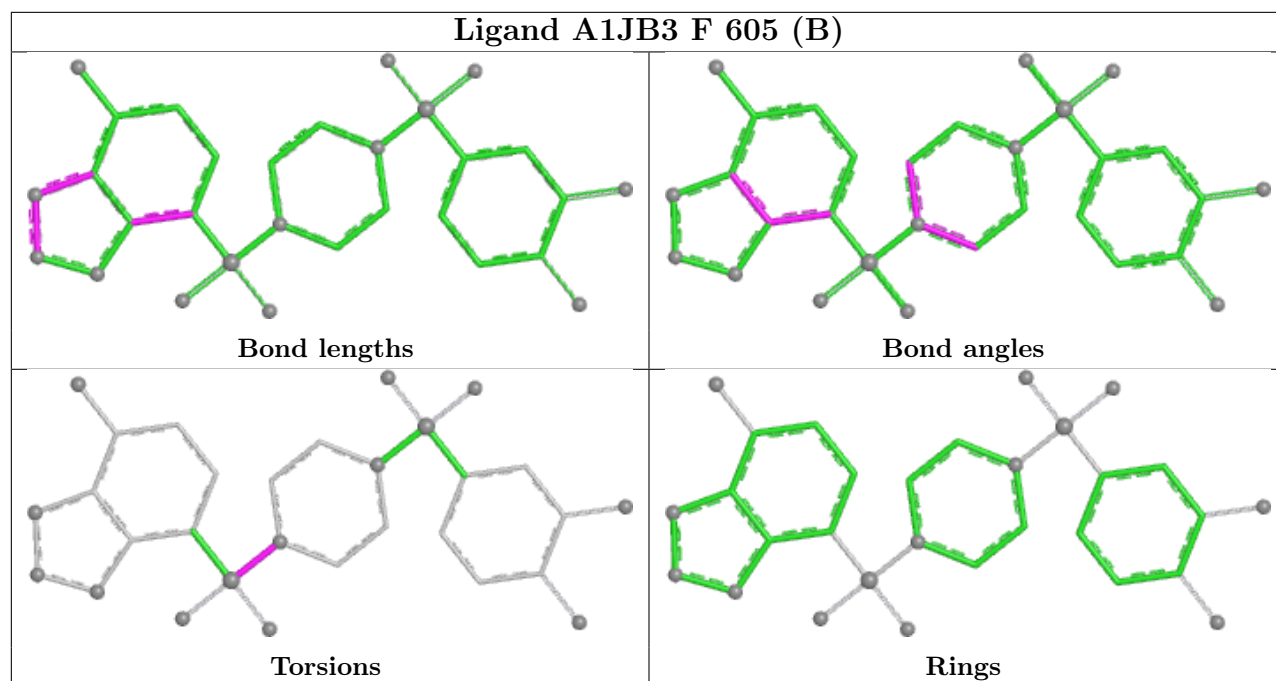
Mol	Chain	Res	Type	Atoms
2	B	601	FBP	O5-C5-C6-O6
6	F	605[A]	A1JB3	C7-N1-S1-C8
6	A	605[A]	A1JB3	C7-N1-S1-O5
6	G	601[A]	A1JB3	C6-N-S-C
3	A	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
6	G	601[B]	A1JB3	C6-N-S-C
3	D	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
6	G	601[A]	A1JB3	C14-N1-S1-C8
3	C	602	OXL	O3-C1-C2-O4
3	G	603	OXL	O3-C1-C2-O4
3	C	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O3-C1-C2-O4
3	G	603	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
6	F	605[A]	A1JB3	C15-N-S-O
3	C	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	G	603	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O2
3	G	603	OXL	O1-C1-C2-O4
6	A	605[B]	A1JB3	C15-N-S-O
6	F	605[A]	A1JB3	C6-N-S-O
6	A	605[B]	A1JB3	C15-N-S-O6
6	F	605[A]	A1JB3	C6-N-S-O6

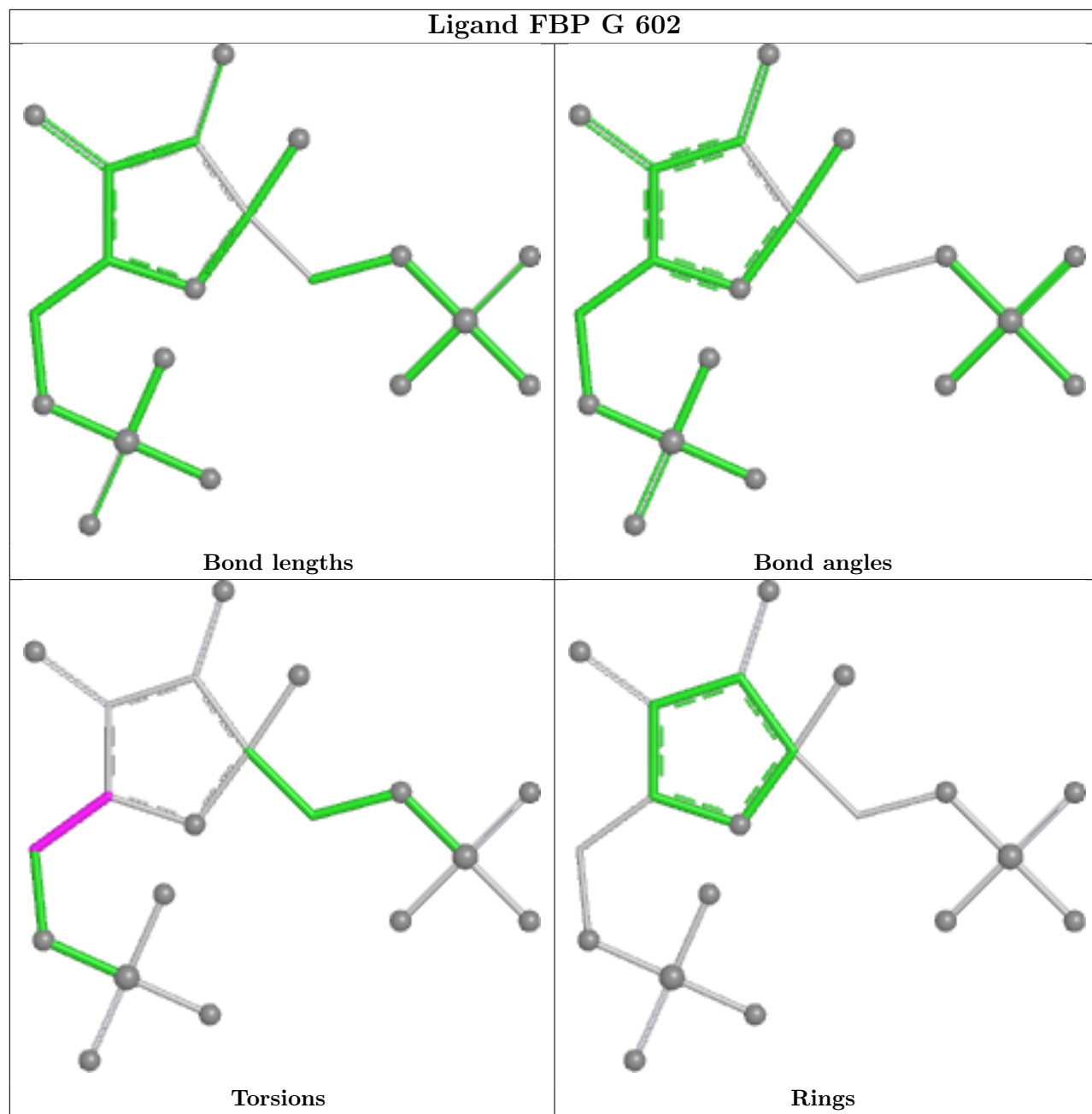
There are no ring outliers.

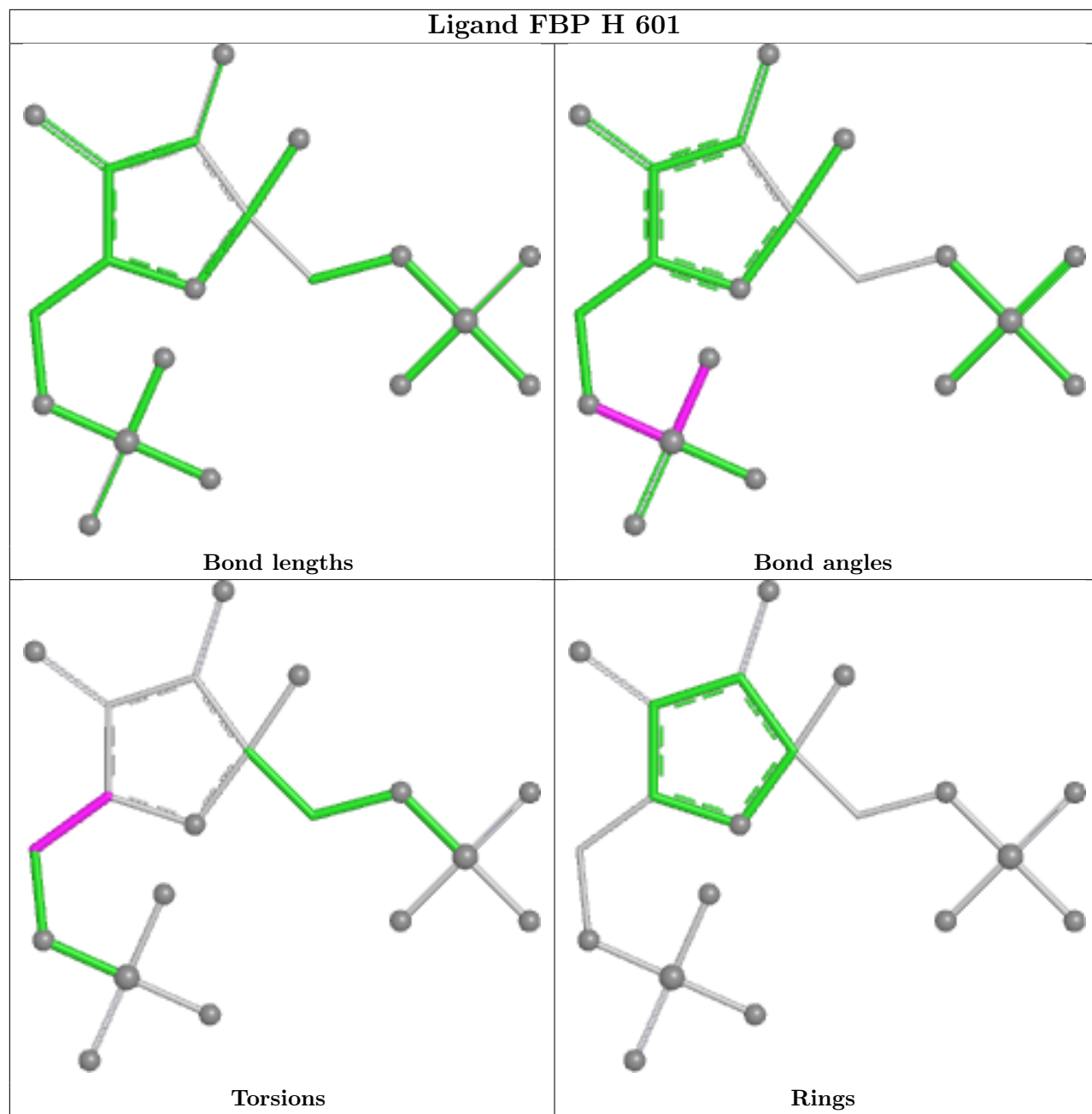
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	605[B]	A1JB3	1	0
6	A	605[B]	A1JB3	3	0
6	G	601[B]	A1JB3	2	0

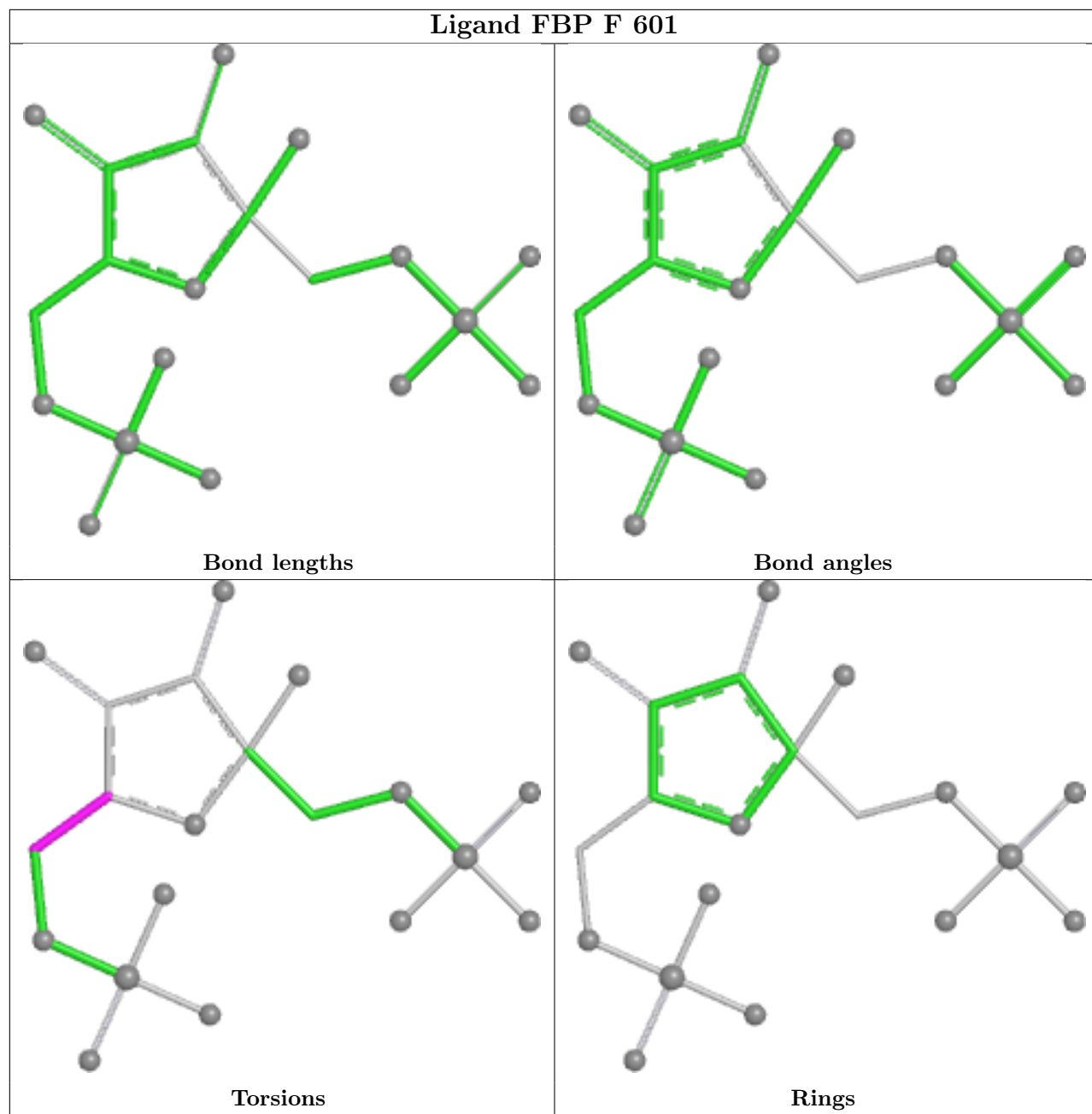
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

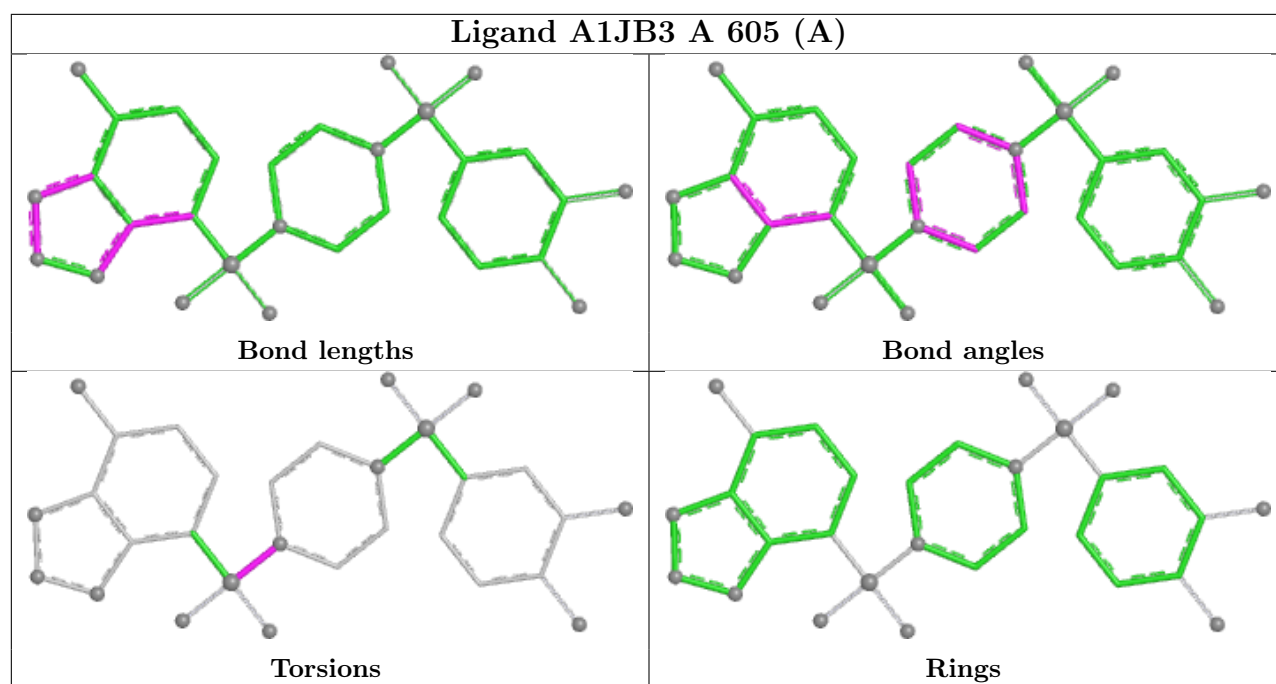




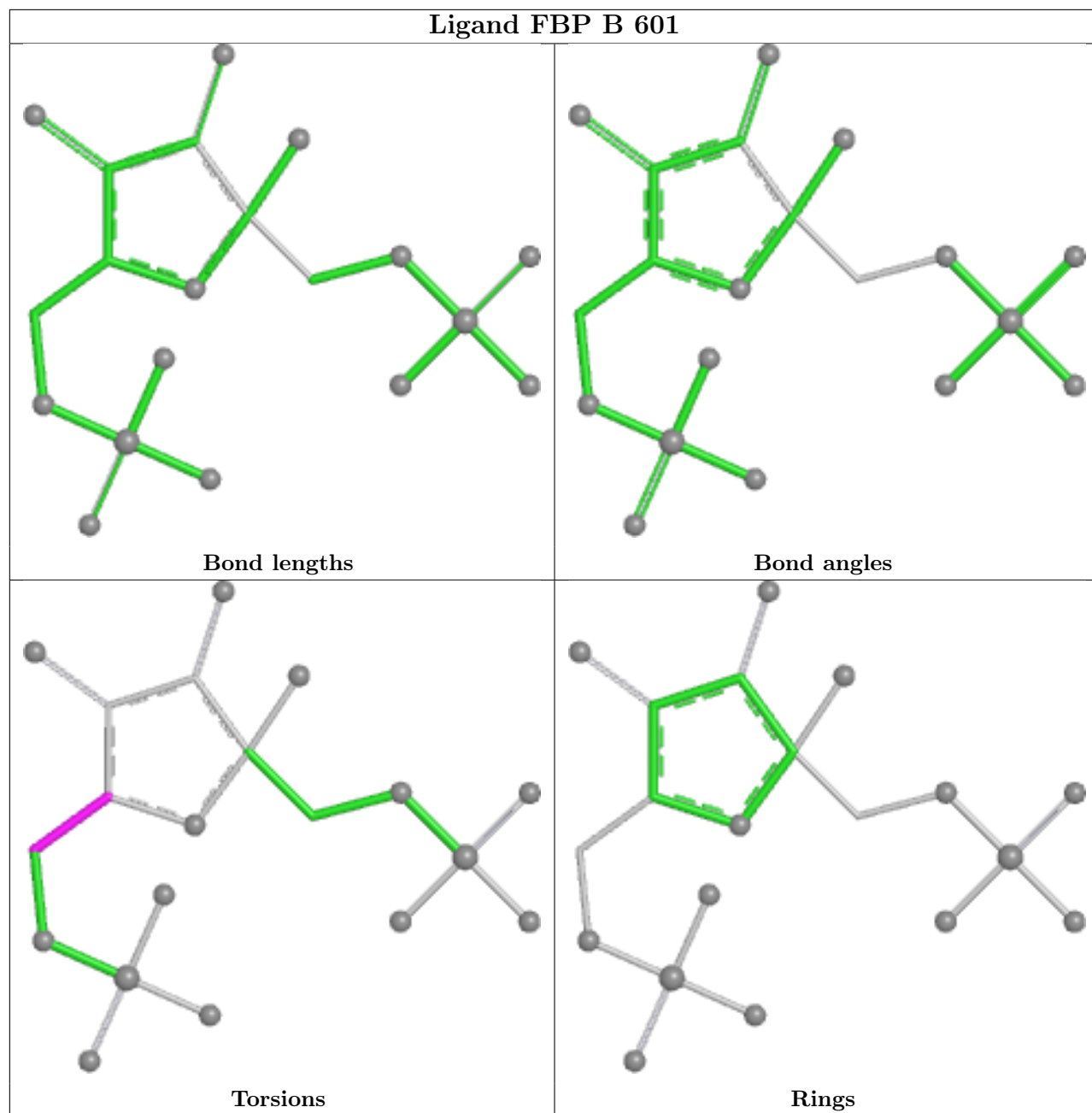


Ligand FBP F 601

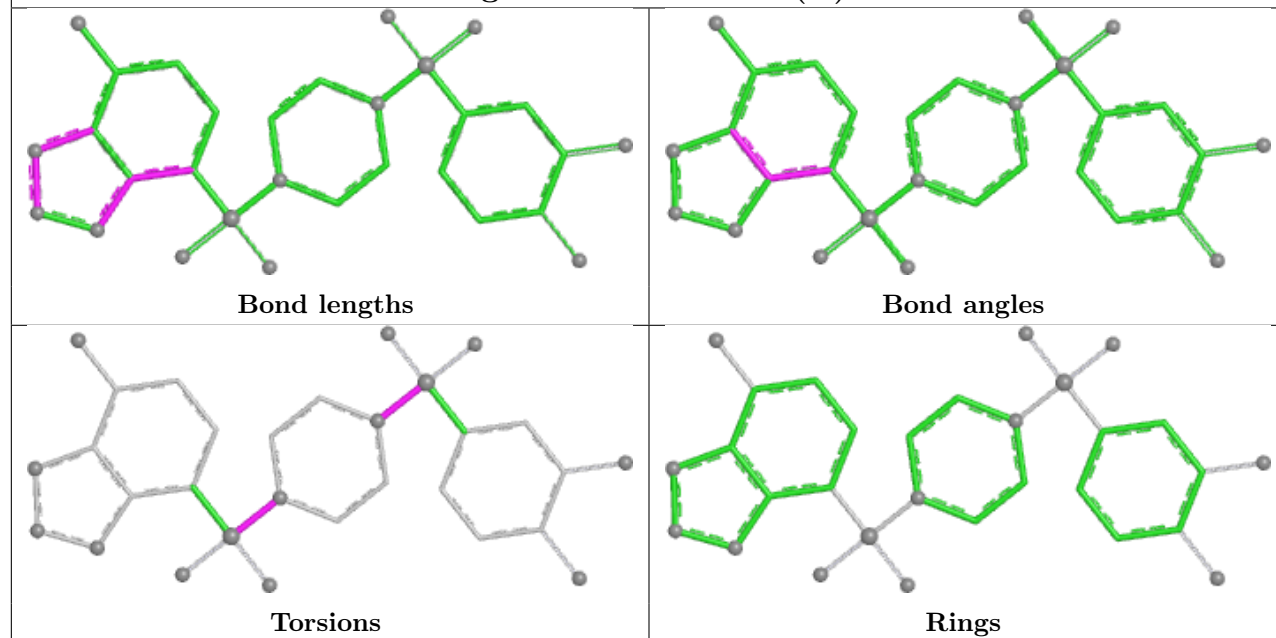




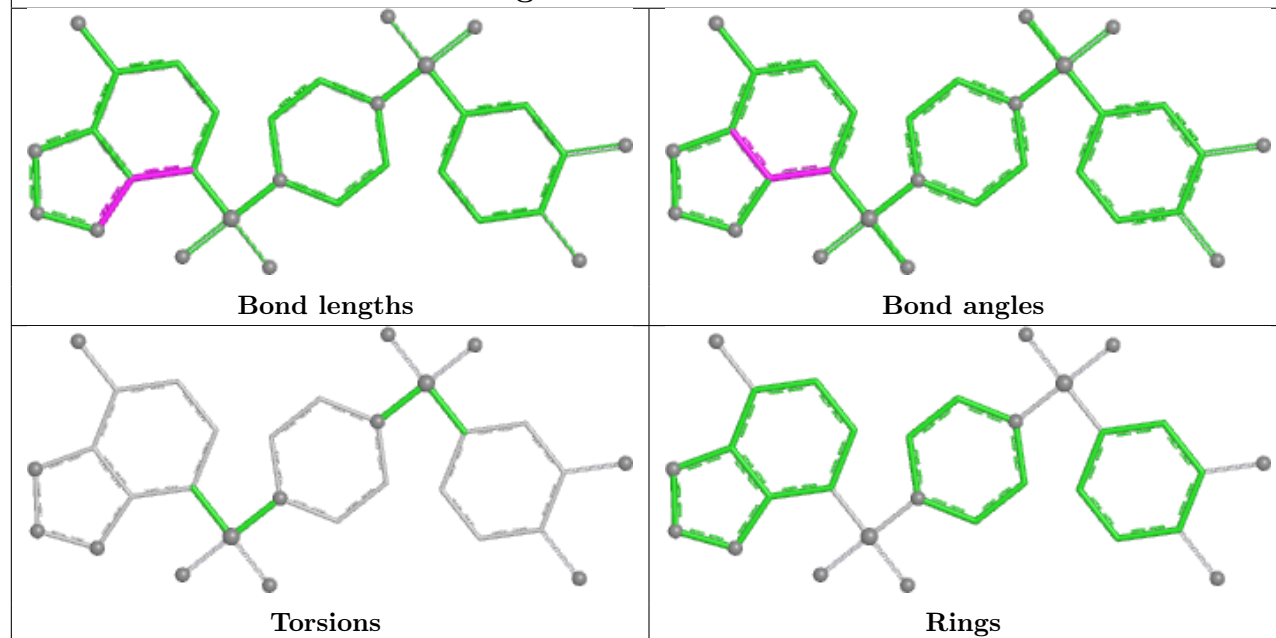
Ligand FBP B 601

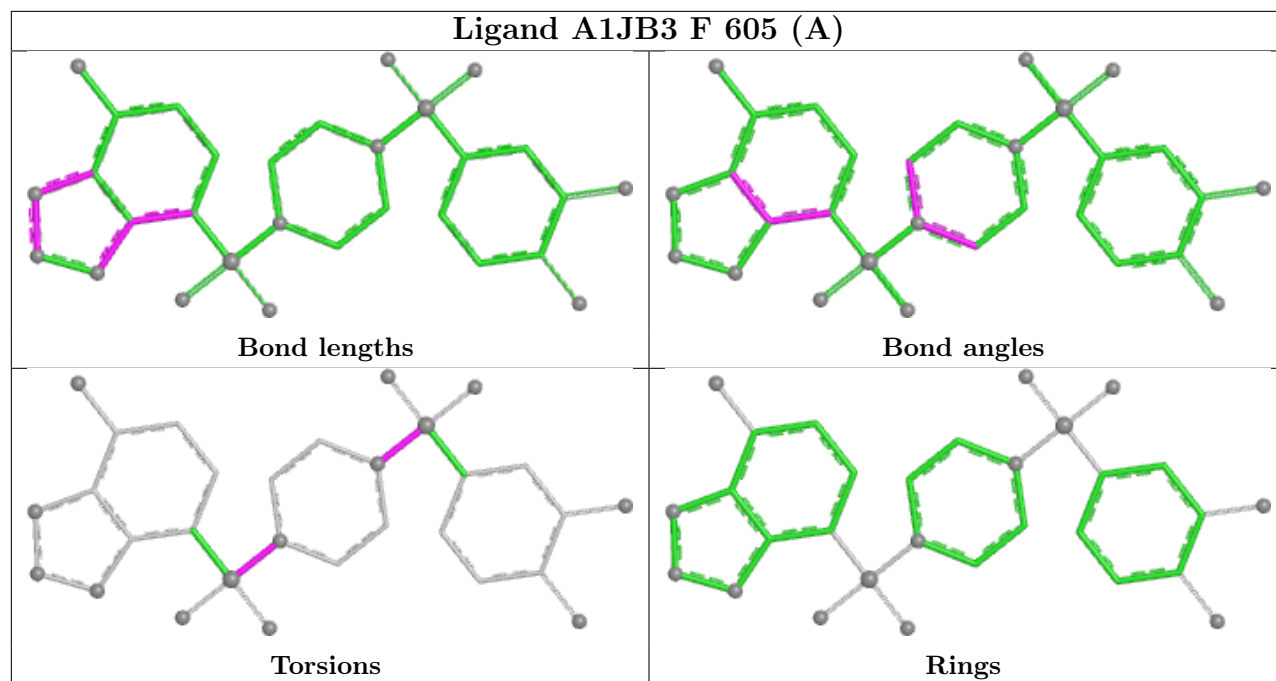


Ligand A1JB3 G 601 (A)

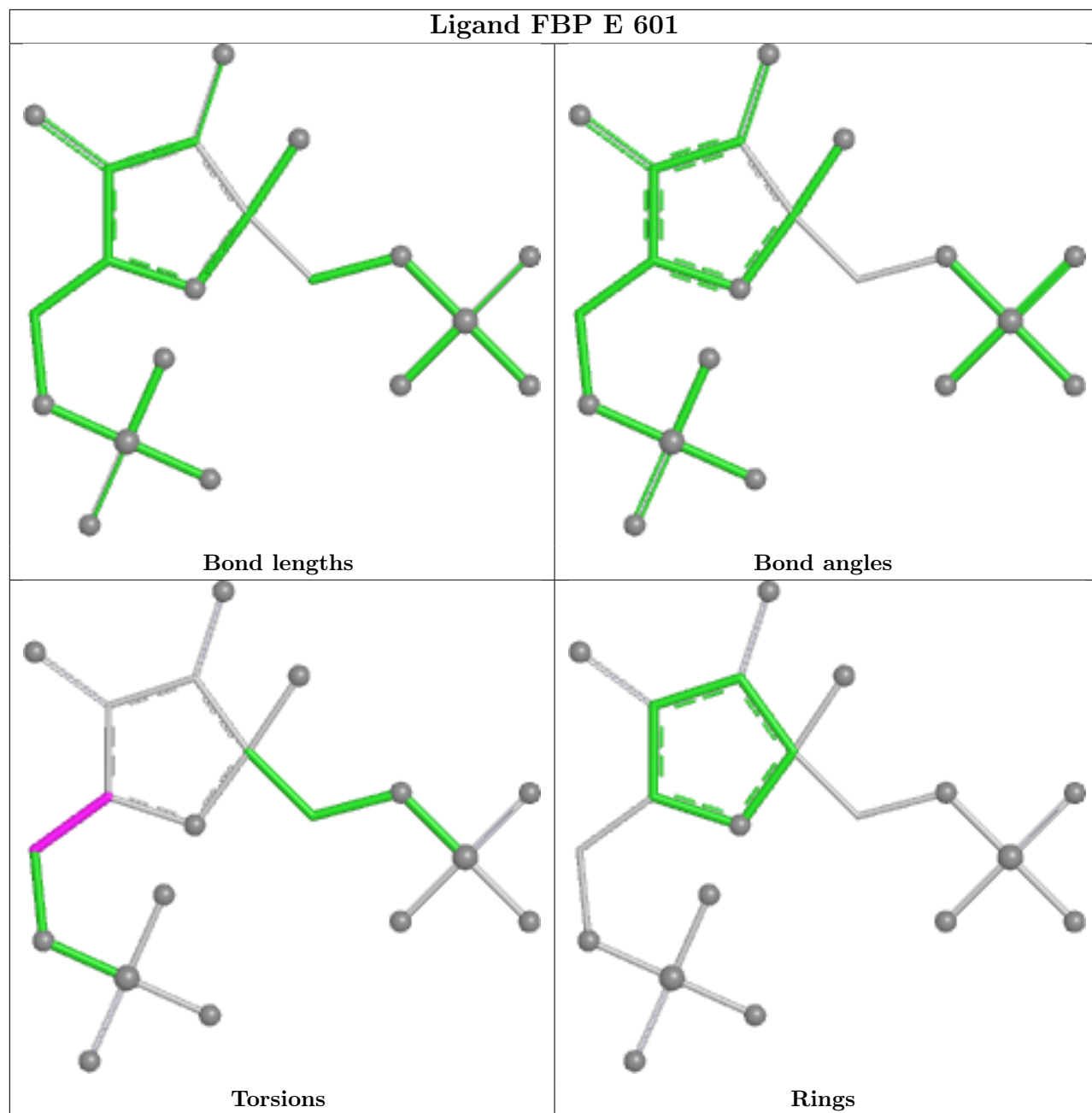


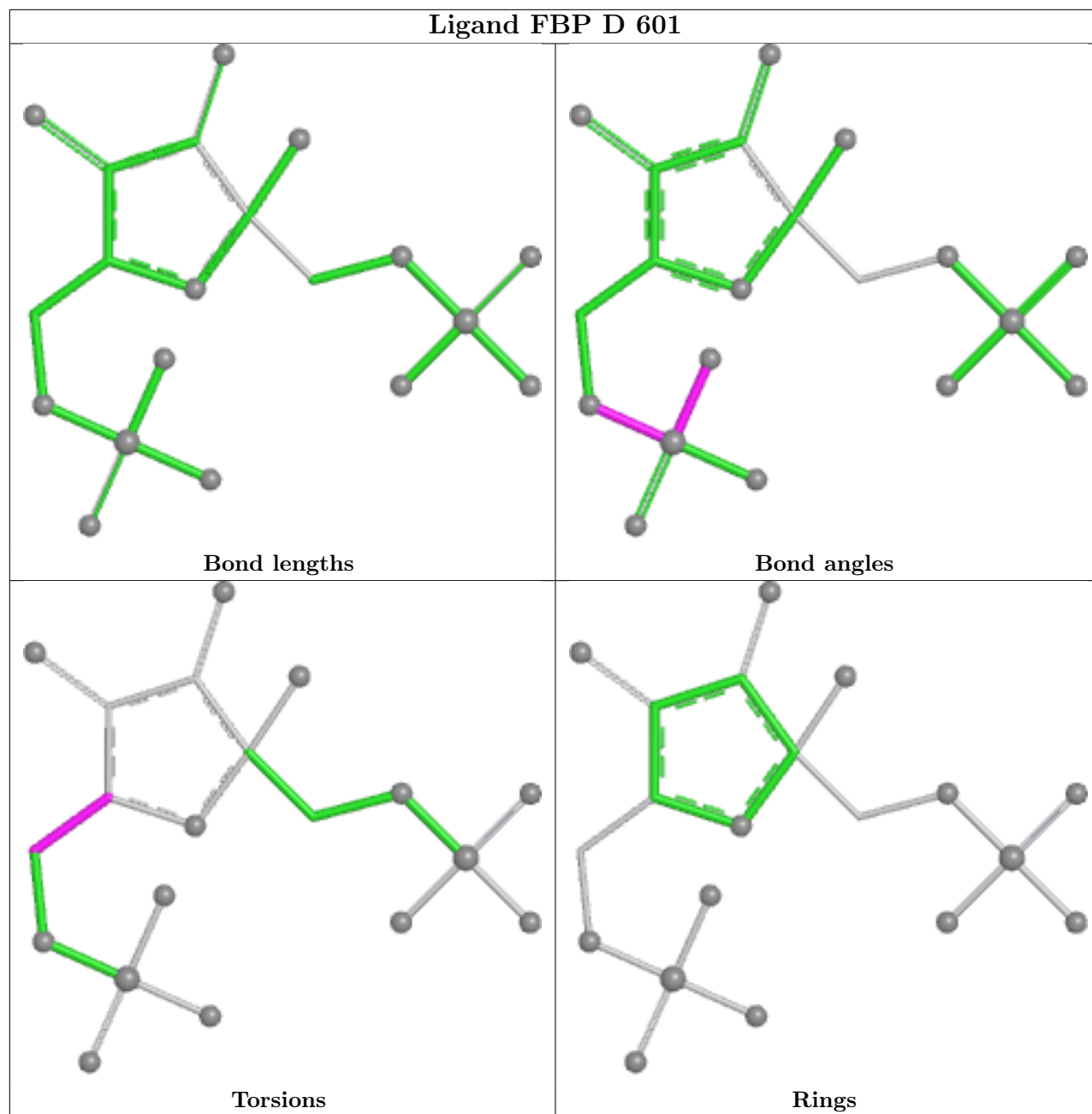
Ligand A1JB3 B 605

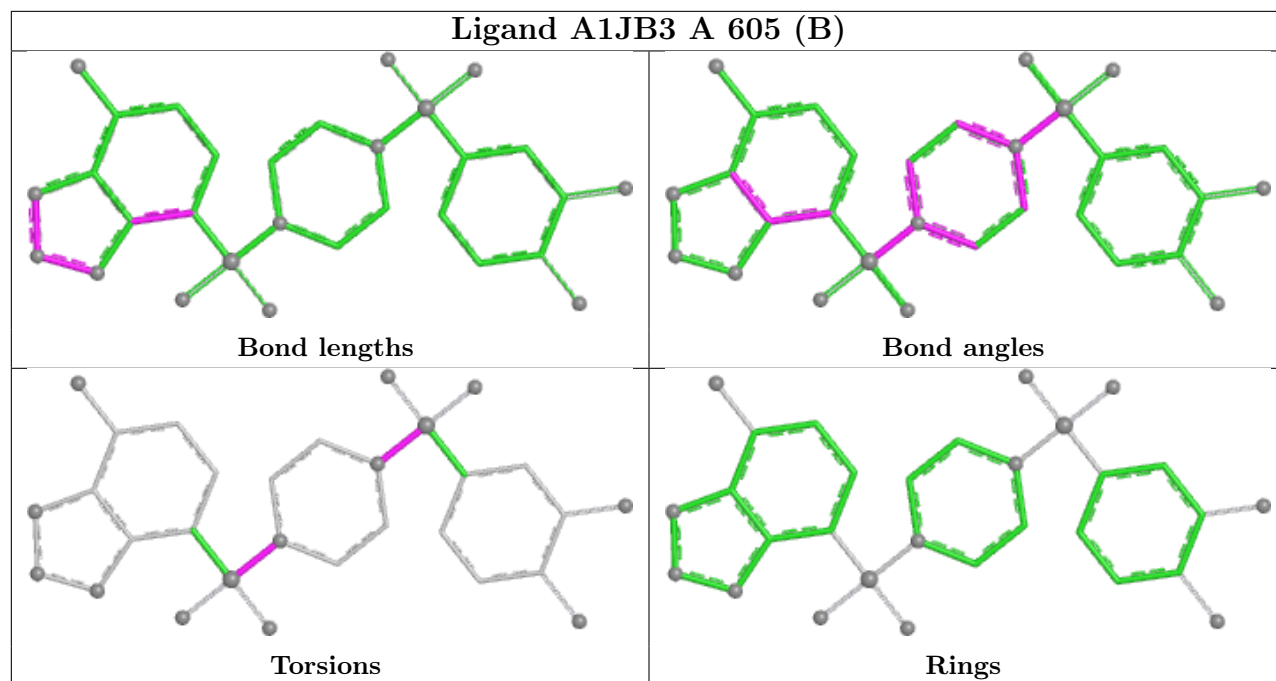




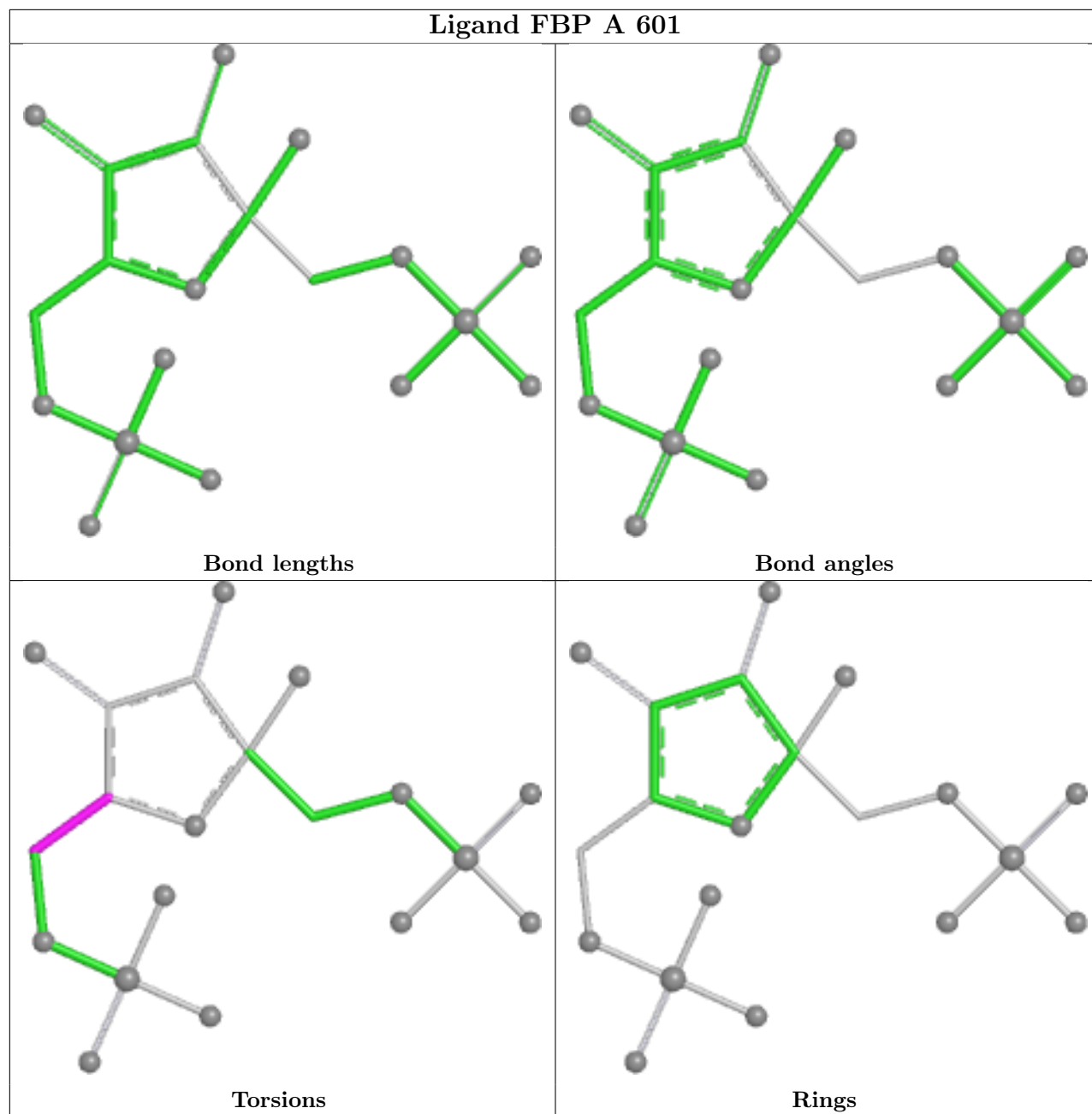
Ligand FBP E 601

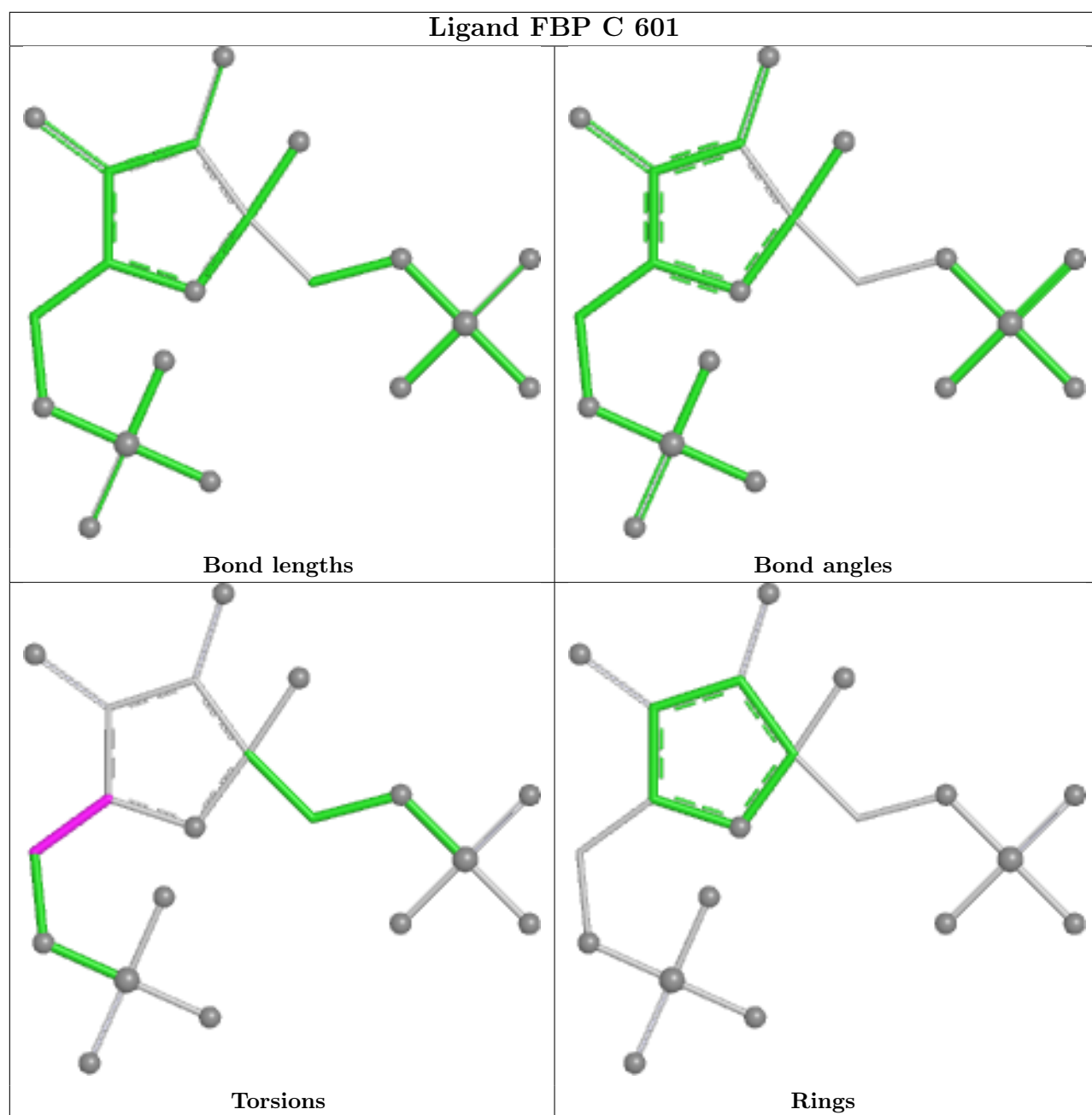


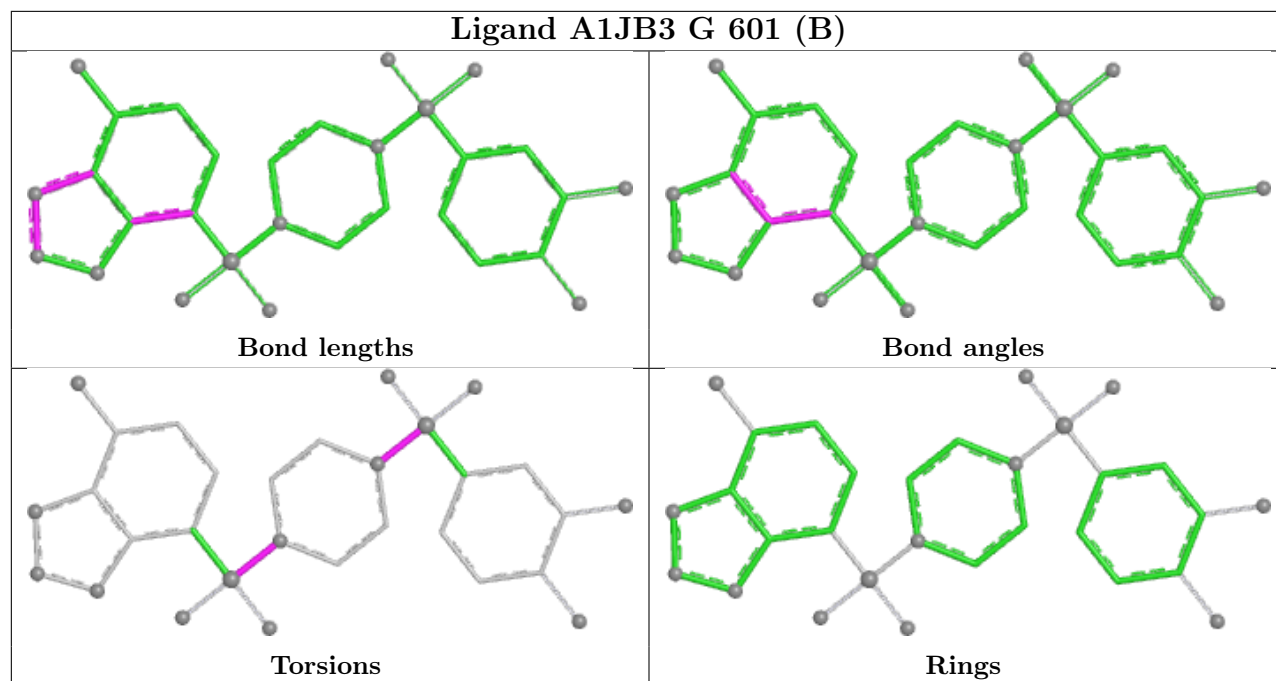




Ligand FBP A 601







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%)	1.23	96 (22%)	2 2	22, 47, 77, 96	6 (1%)
1	B	436/447 (97%)	0.86	57 (13%)	7 7	21, 43, 72, 94	4 (0%)
1	C	427/447 (95%)	0.41	38 (8%)	15 16	18, 33, 58, 86	4 (0%)
1	D	425/447 (95%)	-0.02	15 (3%)	47 49	14, 29, 52, 78	6 (1%)
1	E	423/447 (94%)	0.80	57 (13%)	7 7	19, 42, 70, 93	5 (1%)
1	F	435/447 (97%)	0.48	30 (6%)	23 24	20, 35, 64, 82	7 (1%)
1	G	423/447 (94%)	0.05	12 (2%)	55 57	17, 30, 46, 66	7 (1%)
1	H	425/447 (95%)	-0.16	12 (2%)	55 57	12, 26, 47, 65	4 (0%)
All	All	3417/3576 (95%)	0.46	317 (9%)	14 15	12, 35, 66, 96	43 (1%)

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	23	ALA	7.0
1	A	25	PHE	6.5
1	G	25	PHE	6.4
1	H	21	GLY	6.1
1	C	271	GLY	5.8
1	B	490	PRO	5.8
1	G	271	GLY	5.0
1	D	22	THR	4.8
1	A	238	VAL	4.8
1	A	543	SER	4.8
1	C	130	GLY	4.7
1	D	21	GLY	4.7
1	B	489	PRO	4.6
1	E	232	GLY	4.6
1	C	22	THR	4.5
1	A	232	GLY	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	490	PRO	4.4
1	A	70	VAL	4.4
1	E	231	PRO	4.4
1	H	411	ARG	4.3
1	C	21	GLY	4.3
1	G	229	SER	4.2
1	F	492	ALA	4.1
1	E	25	PHE	4.1
1	C	231	PRO	4.1
1	C	25	PHE	4.1
1	A	73	LEU	4.1
1	F	489	PRO	4.0
1	E	233	LEU	3.9
1	A	34	MET	3.9
1	B	507	GLU	3.9
1	A	270	LEU	3.8
1	C	34	MET	3.8
1	A	496	ASP	3.8
1	F	490	PRO	3.7
1	A	112	GLY	3.7
1	A	24	PHE	3.6
1	D	25	PHE	3.6
1	E	493	ILE	3.6
1	F	233	LEU	3.6
1	A	30	LEU	3.6
1	A	233	LEU	3.6
1	H	232	GLY	3.6
1	A	488[A]	GLU	3.6
1	B	543	SER	3.5
1	C	116	SER	3.5
1	A	90	HIS	3.5
1	H	231	PRO	3.4
1	C	111	ALA	3.4
1	E	514	PHE	3.4
1	E	238	VAL	3.4
1	E	541[A]	SER	3.4
1	G	412	ARG	3.4
1	G	130	GLY	3.4
1	B	270	LEU	3.4
1	F	507	GLU	3.3
1	A	118	ARG	3.3
1	A	114	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	231	PRO	3.3
1	B	416	LEU	3.2
1	C	115	LEU	3.2
1	F	232	GLY	3.2
1	G	52	VAL	3.2
1	B	269	ALA	3.2
1	B	267[A]	ARG	3.2
1	D	412	ARG	3.2
1	H	412	ARG	3.2
1	B	492	ALA	3.2
1	E	275	HIS	3.2
1	E	234	SER	3.2
1	E	129	PRO	3.2
1	E	90	HIS	3.1
1	A	230	GLY	3.1
1	H	514	PHE	3.1
1	E	114	PRO	3.1
1	A	241	LEU	3.1
1	E	229	SER	3.1
1	F	231	PRO	3.1
1	B	438	ALA	3.1
1	E	269	ALA	3.0
1	B	241	LEU	3.0
1	A	63	ILE	3.0
1	C	112	GLY	3.0
1	F	130	GLY	3.0
1	A	115	LEU	3.0
1	A	100	ILE	3.0
1	A	88	PHE	3.0
1	F	516	ARG	3.0
1	G	23	ALA	3.0
1	E	245	VAL	3.0
1	C	117	TYR	3.0
1	A	384	VAL	2.9
1	C	113	SER	2.9
1	F	484	LEU	2.9
1	E	351	ARG	2.9
1	A	66	ALA	2.9
1	E	130	GLY	2.9
1	E	499	ASP	2.9
1	A	311	ILE	2.9
1	C	26	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	26	GLN	2.9
1	D	24	PHE	2.9
1	B	230	GLY	2.9
1	B	233	LEU	2.8
1	A	249	VAL	2.8
1	B	231	PRO	2.8
1	A	111	ALA	2.8
1	B	268	ALA	2.8
1	E	511	LEU	2.8
1	A	75	GLU	2.8
1	F	512	ARG	2.8
1	D	275[A]	HIS	2.8
1	A	514	PHE	2.8
1	G	230	GLY	2.8
1	D	23	ALA	2.8
1	F	493	ILE	2.8
1	C	110	PHE	2.8
1	E	115	LEU	2.8
1	C	412	ARG	2.7
1	F	487	ARG	2.7
1	F	488	GLU	2.7
1	A	265	ALA	2.7
1	F	115	LEU	2.7
1	A	99	SER	2.7
1	C	109	SER	2.7
1	G	34	MET	2.7
1	B	379	LYS	2.7
1	A	269	ALA	2.7
1	B	487	ARG	2.7
1	C	20	LEU	2.7
1	A	236	GLN	2.7
1	A	107	VAL	2.7
1	B	488	GLU	2.7
1	B	493	ILE	2.7
1	A	124	LEU	2.7
1	B	238	VAL	2.7
1	D	233	LEU	2.6
1	F	114	PRO	2.6
1	A	237	ASP	2.6
1	A	91	GLY	2.6
1	B	236	GLN	2.6
1	A	23	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	62	THR	2.6
1	H	22	THR	2.6
1	B	484	LEU	2.6
1	F	270	LEU	2.6
1	A	64	GLY	2.6
1	A	351	ARG	2.6
1	F	267[A]	ARG	2.6
1	A	493	ILE	2.6
1	F	275	HIS	2.6
1	A	72	ARG	2.6
1	B	97	ALA	2.6
1	F	351	ARG	2.6
1	A	110	PHE	2.5
1	E	24	PHE	2.5
1	A	130	GLY	2.5
1	F	240	ASP	2.5
1	A	234	SER	2.5
1	D	26	GLN	2.5
1	C	75	GLU	2.5
1	B	256	PHE	2.5
1	H	25	PHE	2.5
1	B	130	GLY	2.5
1	A	254	ALA	2.5
1	C	229	SER	2.5
1	E	495	ALA	2.5
1	E	543	SER	2.5
1	E	230	GLY	2.5
1	C	311	ILE	2.5
1	A	95	TYR	2.5
1	C	23	ALA	2.5
1	G	231	PRO	2.5
1	E	241	LEU	2.5
1	E	270	LEU	2.5
1	E	500	ARG	2.5
1	C	230	GLY	2.5
1	A	257	VAL	2.4
1	A	279	ILE	2.5
1	E	101	ALA	2.4
1	A	485	LEU	2.4
1	H	516	ARG	2.4
1	A	243	PHE	2.4
1	A	494	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	86	LEU	2.4
1	B	232	GLY	2.4
1	E	271	GLY	2.4
1	E	88	PHE	2.4
1	E	491	GLU	2.4
1	A	266	VAL	2.4
1	B	107	VAL	2.4
1	E	249	VAL	2.4
1	C	118	ARG	2.4
1	E	487	ARG	2.4
1	E	489	PRO	2.4
1	A	96	HIS	2.4
1	A	61	ALA	2.4
1	A	268	ALA	2.4
1	A	540	LEU	2.4
1	A	482	PHE	2.4
1	A	495	ALA	2.3
1	B	264	ALA	2.3
1	E	540	LEU	2.3
1	A	274	GLY	2.3
1	B	271	GLY	2.3
1	B	34	MET	2.3
1	F	243	PHE	2.3
1	F	411	ARG	2.3
1	E	120	VAL	2.3
1	B	272	PRO	2.3
1	B	111	ALA	2.3
1	A	382	PHE	2.3
1	A	92	SER	2.3
1	F	543	SER	2.3
1	C	90	HIS	2.3
1	H	275[A]	HIS	2.3
1	E	70	VAL	2.3
1	H	273	GLU	2.3
1	A	68	ARG	2.3
1	D	130	GLY	2.3
1	B	71	GLU	2.3
1	B	491	GLU	2.3
1	A	277	ILE	2.3
1	B	347	ILE	2.3
1	B	351	ARG	2.3
1	G	232	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	256	PHE	2.2
1	C	24	PHE	2.2
1	F	245	VAL	2.2
1	F	272	PRO	2.2
1	B	242	ARG	2.2
1	A	310	GLY	2.2
1	A	378	ALA	2.2
1	C	66	ALA	2.2
1	A	109	SER	2.2
1	E	109	SER	2.2
1	E	256	PHE	2.2
1	G	24	PHE	2.2
1	B	348	THR	2.2
1	C	347	ILE	2.2
1	D	311	ILE	2.2
1	E	311	ILE	2.2
1	A	120	VAL	2.2
1	A	252	VAL	2.2
1	B	263	VAL	2.2
1	B	40	GLU	2.2
1	A	67	SER	2.2
1	E	89	SER	2.2
1	A	412	ARG	2.2
1	B	88	PHE	2.2
1	C	63	ILE	2.2
1	C	348	THR	2.2
1	A	76[A]	MET	2.2
1	A	103	VAL	2.2
1	C	107	VAL	2.2
1	E	517	VAL	2.2
1	A	121	ALA	2.2
1	A	490	PRO	2.1
1	D	231	PRO	2.1
1	B	91	GLY	2.1
1	E	112	GLY	2.1
1	B	106	ALA	2.1
1	B	495	ALA	2.1
1	A	242	ARG	2.1
1	A	229	SER	2.1
1	A	541	SER	2.1
1	E	519	ASP	2.1
1	A	377	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	100	ILE	2.1
1	E	110	PHE	2.1
1	E	243	PHE	2.1
1	E	504	PHE	2.1
1	E	542	ILE	2.1
1	B	70	VAL	2.1
1	E	242	ARG	2.1
1	B	413	ALA	2.1
1	H	414	ALA	2.1
1	A	117	TYR	2.1
1	E	95	TYR	2.1
1	A	489	PRO	2.1
1	C	490	PRO	2.1
1	F	90	HIS	2.1
1	A	239	ARG	2.1
1	C	77	ILE	2.1
1	A	464	ALA	2.1
1	A	383	PRO	2.1
1	B	90	HIS	2.1
1	B	516	ARG	2.1
1	F	129	PRO	2.1
1	A	74	LYS	2.1
1	A	475	VAL	2.1
1	A	498	VAL	2.1
1	C	71	GLU	2.0
1	E	488	GLU	2.0
1	F	269	ALA	2.1
1	D	34	MET	2.0
1	A	404	ARG	2.0
1	B	404	ARG	2.0
1	C	114	PRO	2.0
1	F	533	TYR	2.0
1	C	47	ILE	2.0
1	A	108	GLU	2.0
1	B	273	GLU	2.0
1	A	113	SER	2.0
1	B	234	SER	2.0
1	E	111	ALA	2.0
1	B	115	LEU	2.0
1	B	540[A]	LEU	2.0
1	D	416	LEU	2.0
1	E	485	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	519	ASP	2.0
1	B	262	ASP	2.0
1	C	411	ARG	2.0
1	C	436	CYS	2.0
1	B	275	HIS	2.0
1	B	112	GLY	2.0
1	D	232	GLY	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
3	OXL	A	602	6/6	0.84	0.14	80,80,81,81	0
3	OXL	B	602	6/6	0.87	0.14	58,59,60,60	0
3	OXL	E	602	6/6	0.89	0.12	58,58,59,59	0
3	OXL	C	602	6/6	0.91	0.12	53,53,53,53	0
5	K	A	604	1/1	0.91	0.12	74,74,74,74	0
6	A1JB3	G	601[A]	30/30	0.91	0.12	37,38,40,40	47
6	A1JB3	G	601[B]	30/30	0.91	0.12	35,39,41,41	47
6	A1JB3	B	605	30/30	0.92	0.12	36,38,41,44	17
3	OXL	G	603	6/6	0.92	0.11	42,43,44,44	0
5	K	E	604	1/1	0.92	0.17	70,70,70,70	0
6	A1JB3	A	605[B]	30/30	0.93	0.11	36,38,39,39	47
3	OXL	F	602	6/6	0.93	0.10	54,55,55,55	0
3	OXL	D	602	6/6	0.93	0.14	43,44,45,45	0
6	A1JB3	A	605[A]	30/30	0.93	0.11	36,40,42,42	47
6	A1JB3	F	605[A]	30/30	0.94	0.10	32,34,35,35	47
6	A1JB3	F	605[B]	30/30	0.94	0.10	34,35,36,36	47

Continued on next page...

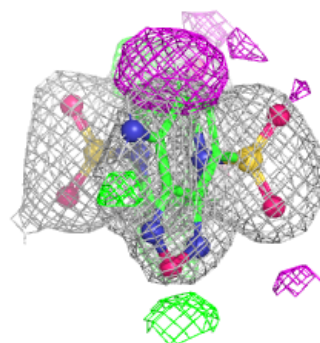
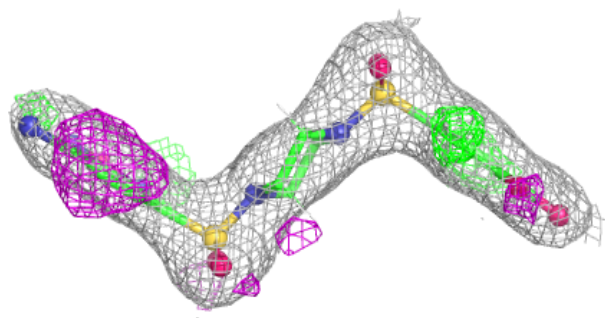
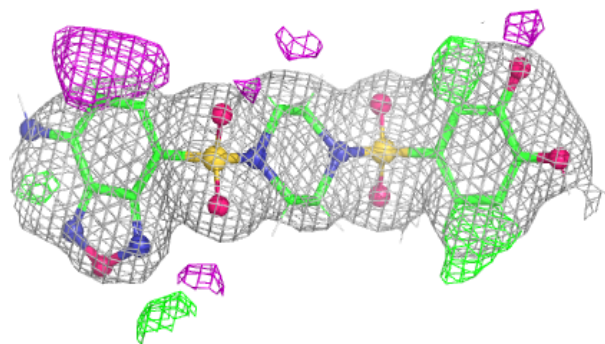
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	K	B	604	1/1	0.95	0.07	72,72,72,72	0
2	FBP	A	601	20/20	0.95	0.08	40,40,42,43	0
5	K	F	604	1/1	0.95	0.07	67,67,67,67	0
3	OXL	H	602	6/6	0.95	0.10	42,42,42,43	0
2	FBP	B	601	20/20	0.95	0.08	37,38,41,41	0
4	MG	A	603	1/1	0.96	0.09	48,48,48,48	0
2	FBP	E	601	20/20	0.96	0.07	34,36,37,38	0
2	FBP	F	601	20/20	0.96	0.07	31,37,39,40	0
4	MG	E	603	1/1	0.97	0.07	31,31,31,31	0
5	K	C	604	1/1	0.98	0.10	56,56,56,56	0
2	FBP	C	601	20/20	0.98	0.04	21,24,27,27	0
2	FBP	D	601	20/20	0.98	0.04	22,23,25,25	0
5	K	G	605	1/1	0.98	0.07	46,46,46,46	0
5	K	H	604	1/1	0.98	0.05	42,42,42,42	0
2	FBP	H	601	20/20	0.98	0.04	18,21,23,23	0
4	MG	B	603	1/1	0.99	0.07	39,39,39,39	0
4	MG	D	603	1/1	0.99	0.06	21,21,21,21	0
2	FBP	G	602	20/20	0.99	0.04	19,22,23,24	0
5	K	D	604	1/1	0.99	0.10	40,40,40,40	0
4	MG	F	603	1/1	0.99	0.02	27,27,27,27	0
4	MG	C	603	1/1	1.00	0.09	29,29,29,29	0
4	MG	G	604	1/1	1.00	0.06	17,17,17,17	0
4	MG	H	603	1/1	1.00	0.06	18,18,18,18	0

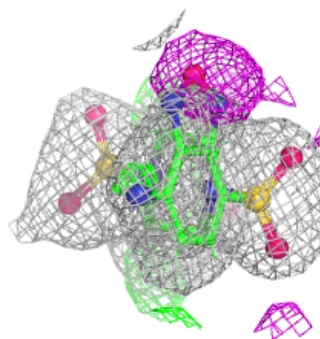
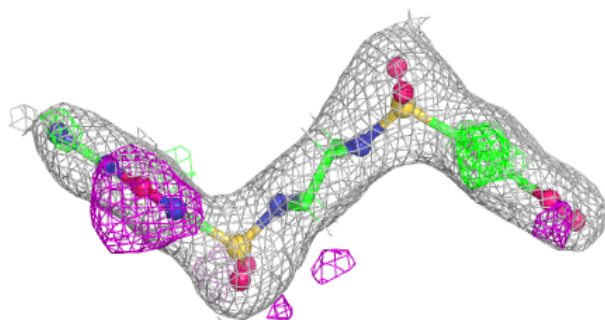
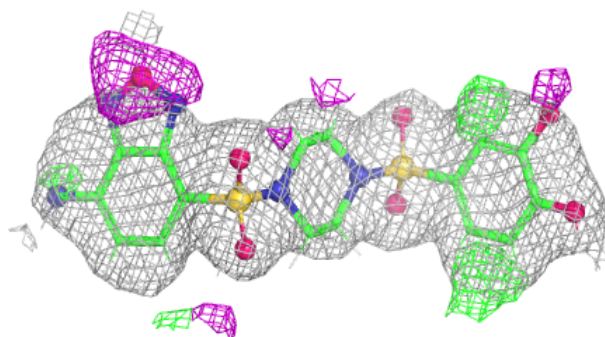
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1JB3 G 601 (A):

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

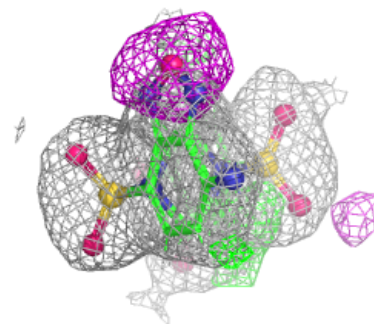
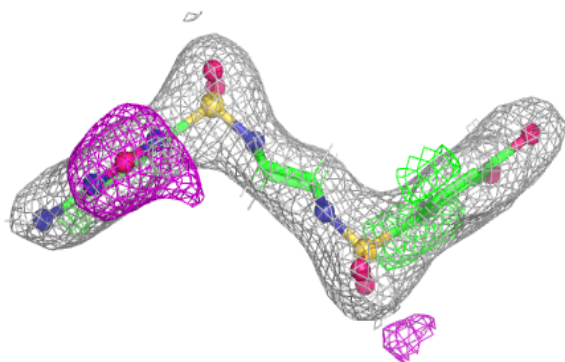
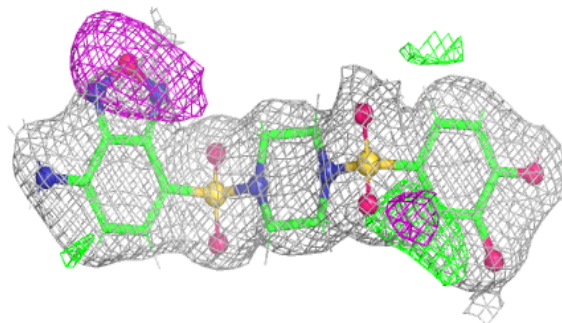
**Electron density around A1JB3 G 601 (B):**

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

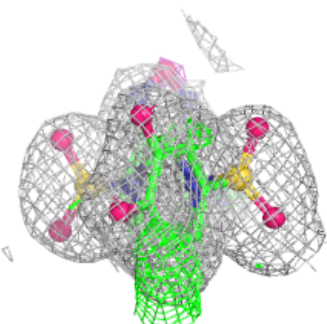
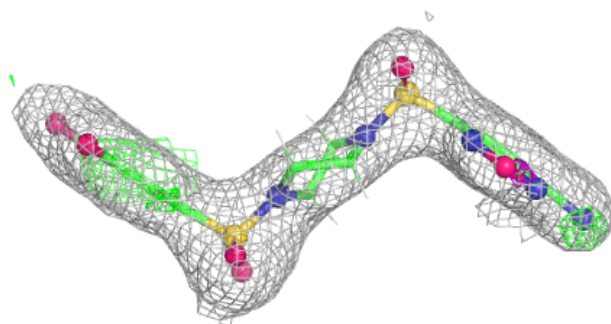
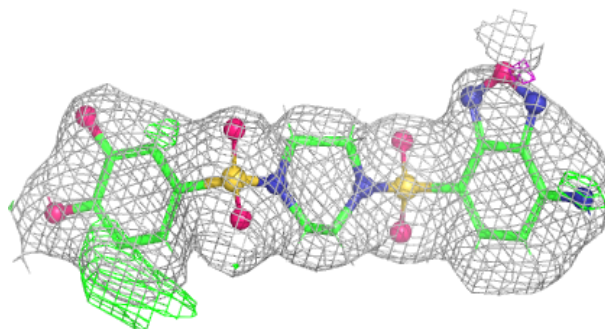


Electron density around A1JB3 B 605:

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

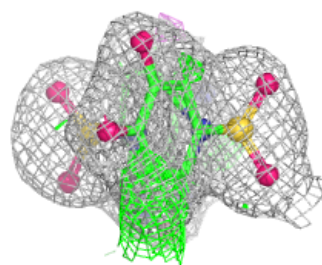
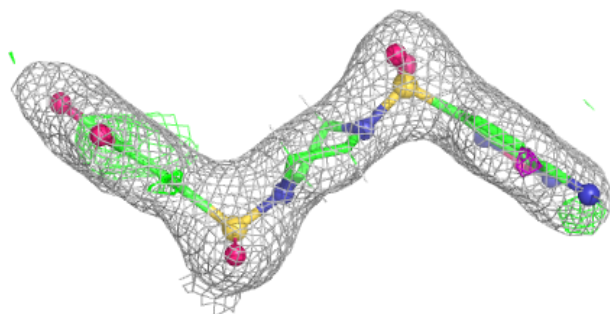
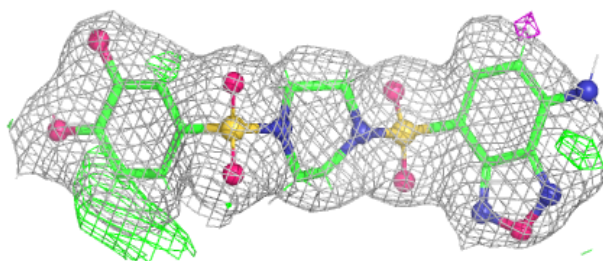
**Electron density around A1JB3 A 605 (B):**

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

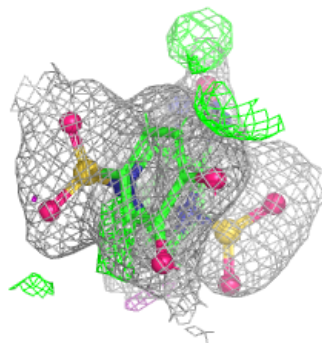
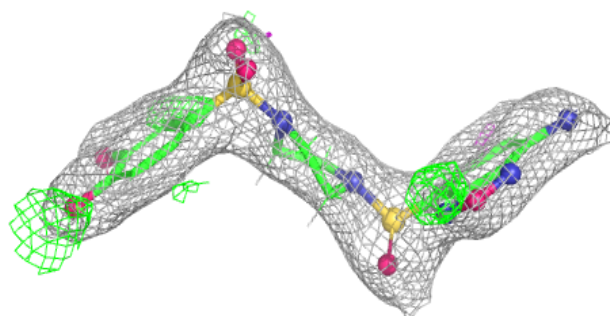
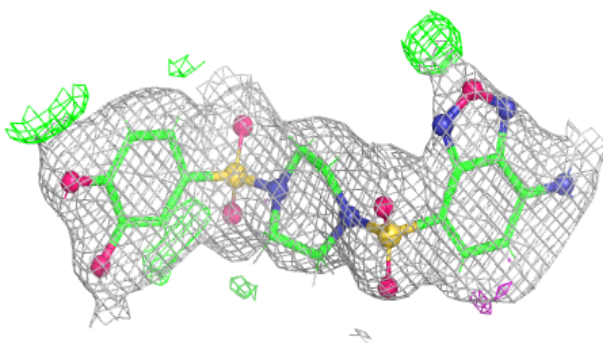


Electron density around A1JB3 A 605 (A):

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

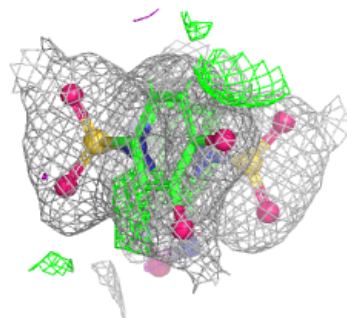
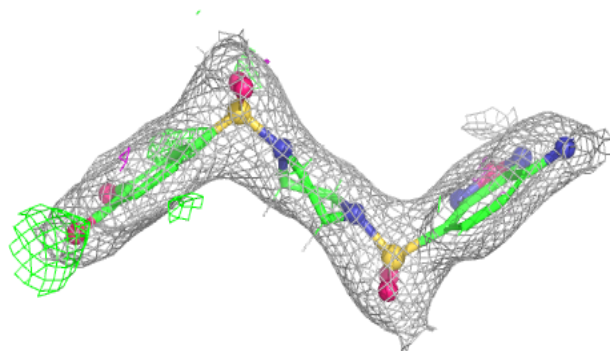
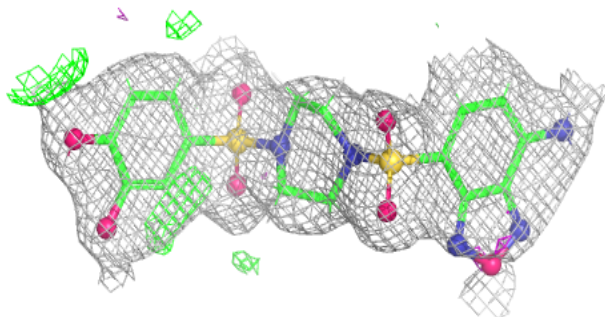
**Electron density around A1JB3 F 605 (A):**

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

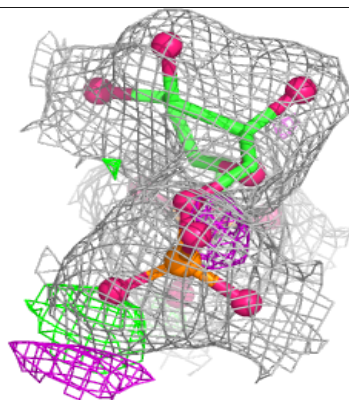
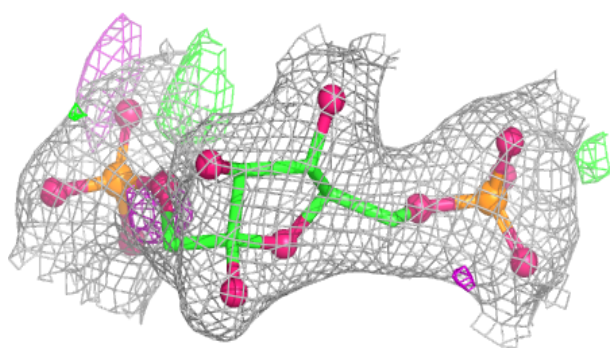
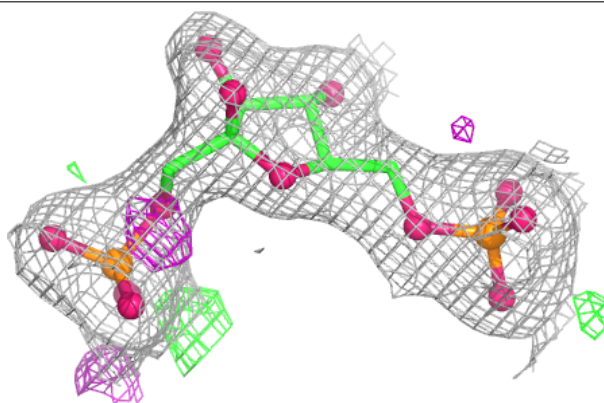


Electron density around A1JB3 F 605 (B):

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

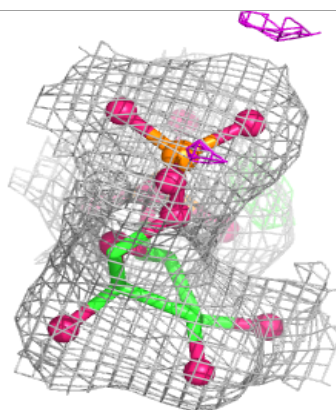
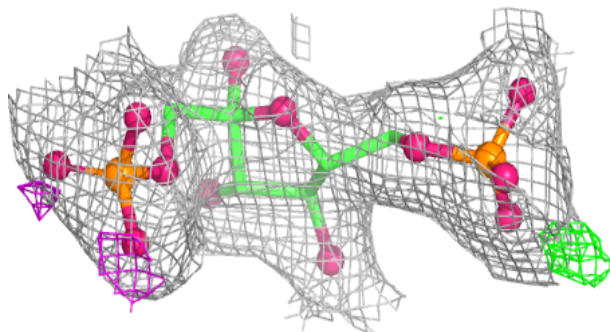
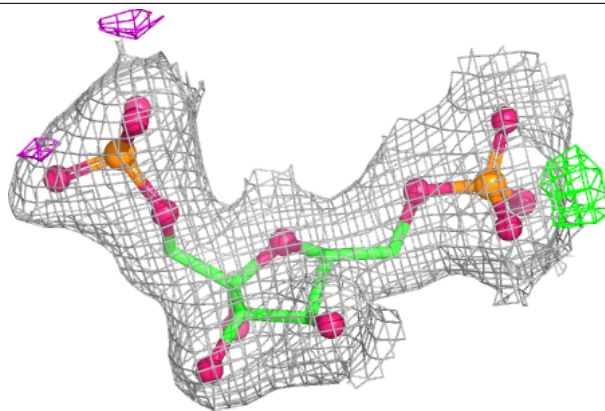
**Electron density around FBP A 601:**

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

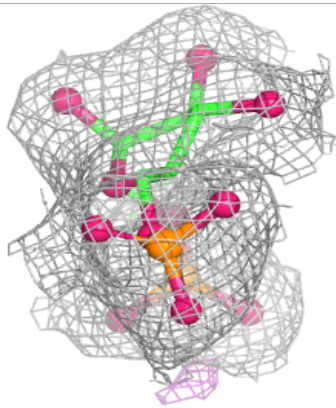
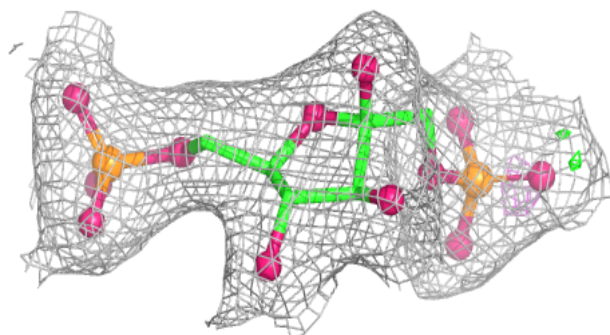
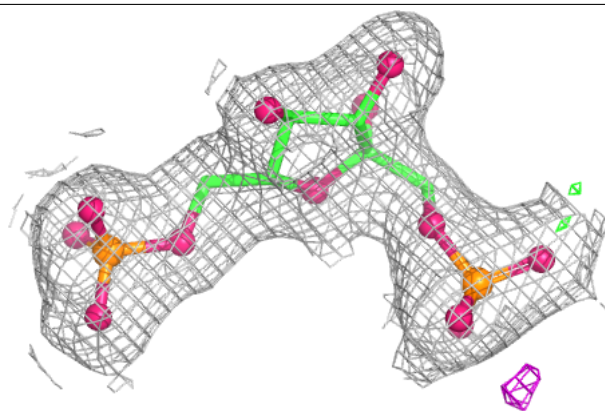


Electron density around FBP B 601:

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

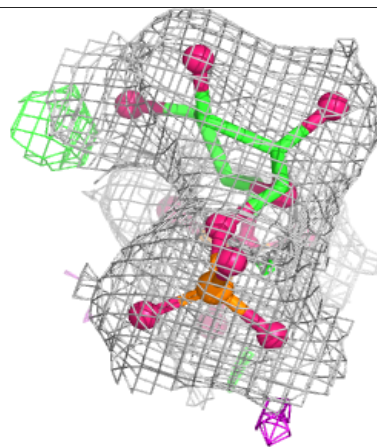
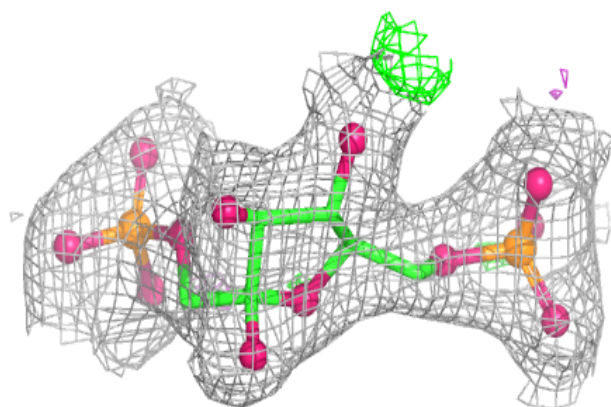
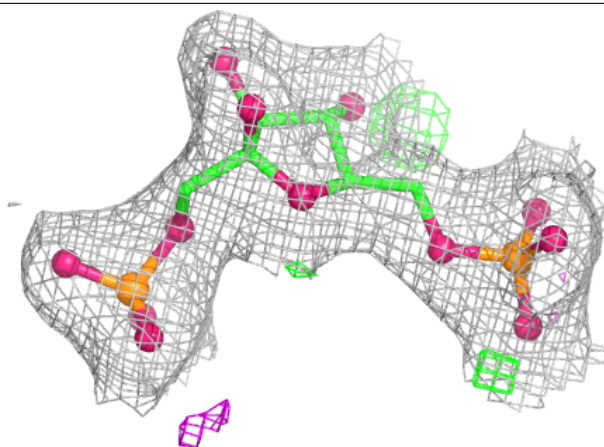
**Electron density around FBP E 601:**

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

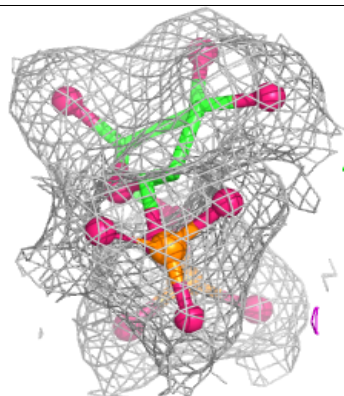
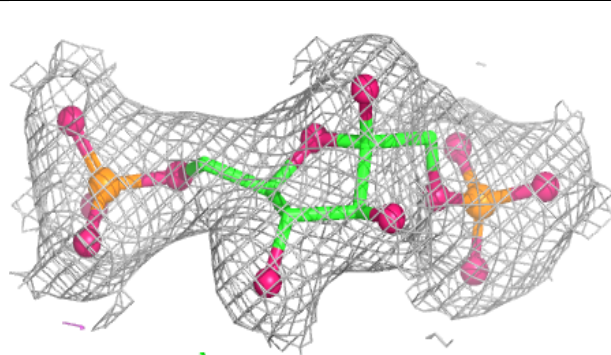
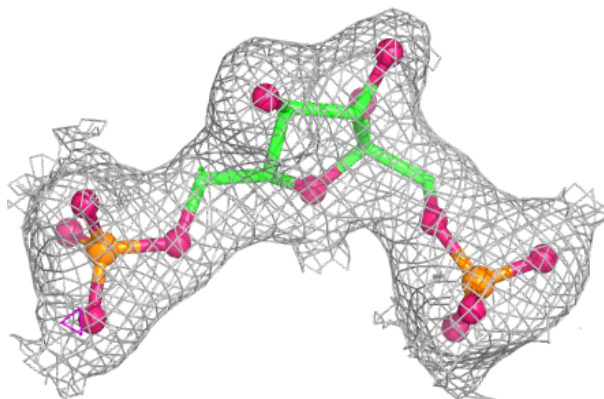


Electron density around FBP F 601:

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

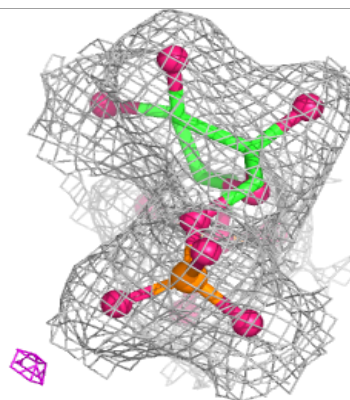
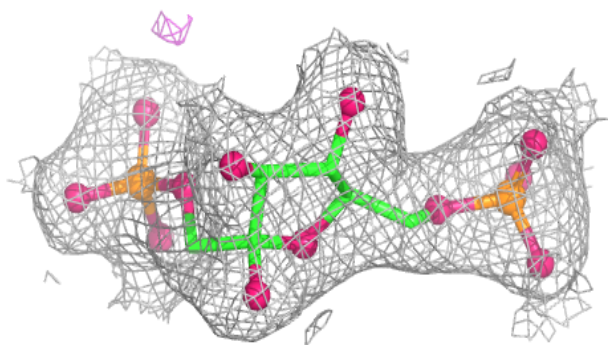
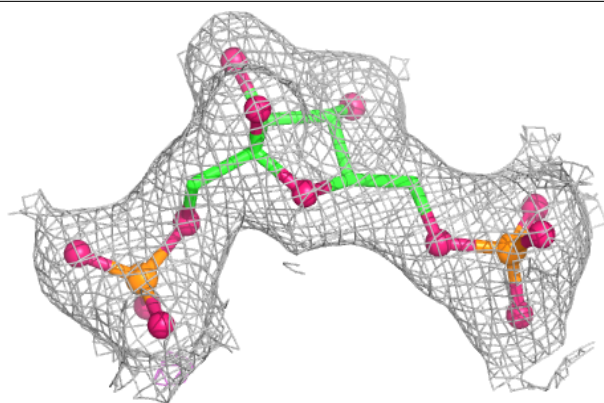
**Electron density around FBP C 601:**

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

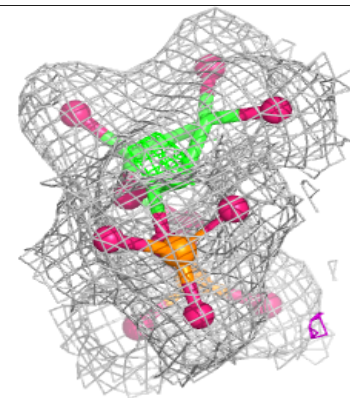
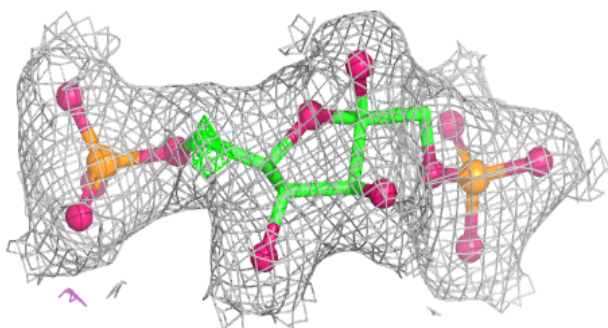
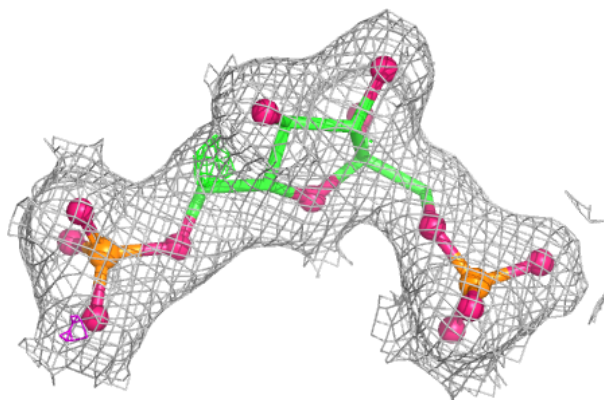


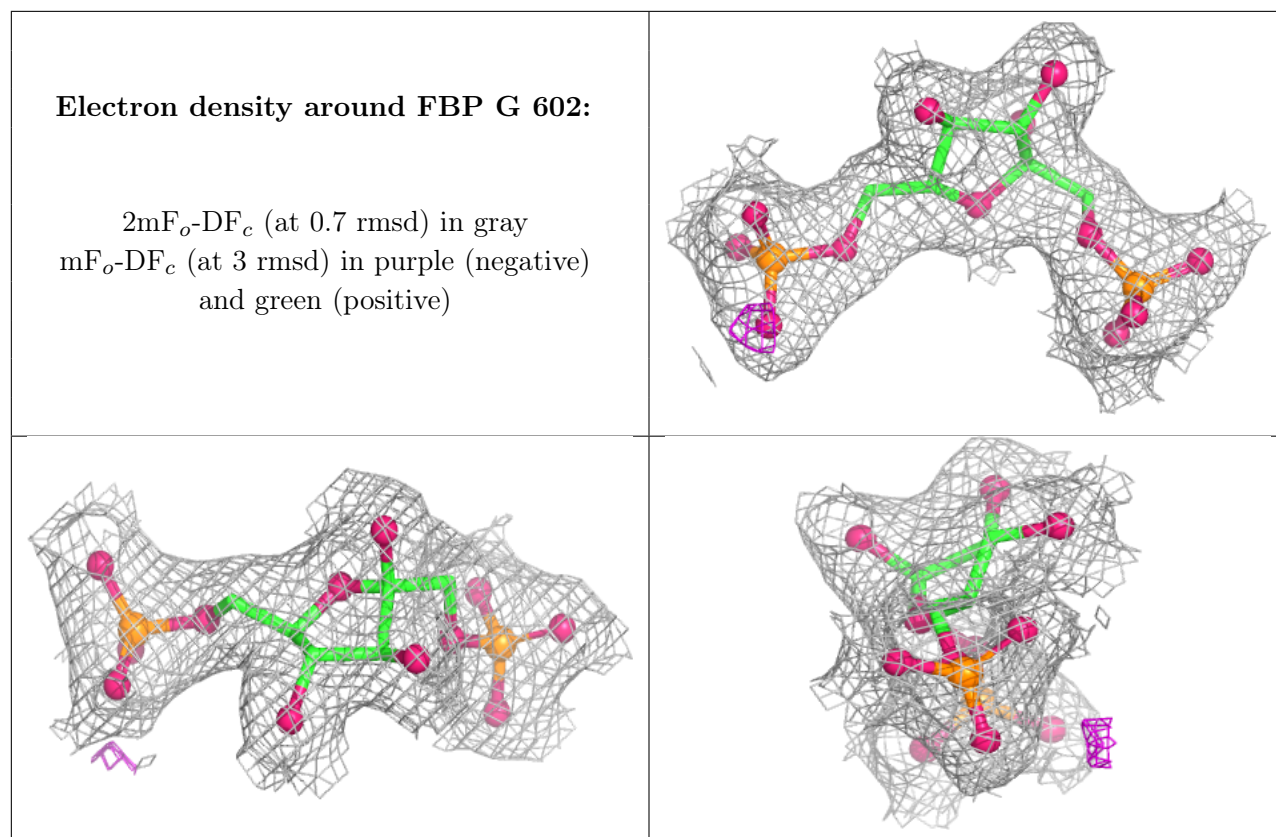
Electron density around FBP D 601:

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

**Electron density around FBP H 601:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.