



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:48 PM UTC

PDB ID : 9R3M / pdb_00009r3m
Title : Structure of liver pyruvate kinase in complex with fluorescent probe 8a
Authors : Bogucka, A.; Nilsson, O.; Grotli, M.; Hyvonen, M.
Deposited on : 2025-05-05
Resolution : 2.06 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

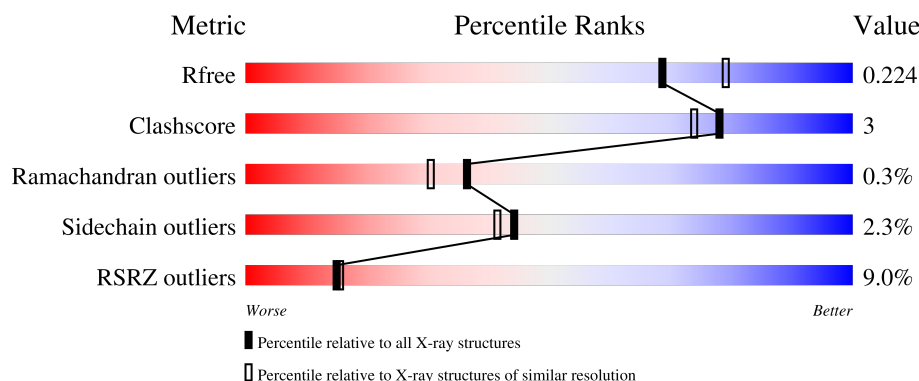
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	15% 86% 8% 5%
1	B	447	19% 89% 8% ..
1	C	447	5% 87% 8% .
1	D	447	2% 87% 7% 5%
1	E	447	14% 87% 7% 5%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	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	602	-	X	-	-
3	OXL	H	602	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28711 atoms, of which 100 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Isoform L-type of Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	6	0
			3243	2039	586	598	20			
1	B	436	Total	C	N	O	S	0	4	0
			3329	2090	604	615	20			
1	C	427	Total	C	N	O	S	0	4	0
			3257	2045	587	606	19			
1	D	425	Total	C	N	O	S	0	6	0
			3252	2042	590	601	19			
1	E	423	Total	C	N	O	S	0	5	0
			3231	2030	583	598	20			
1	F	435	Total	C	N	O	S	0	7	0
			3335	2097	600	618	20			
1	G	423	Total	C	N	O	S	0	6	0
			3241	2036	583	603	19			
1	H	425	Total	C	N	O	S	0	4	0
			3251	2040	594	598	19			

There are 832 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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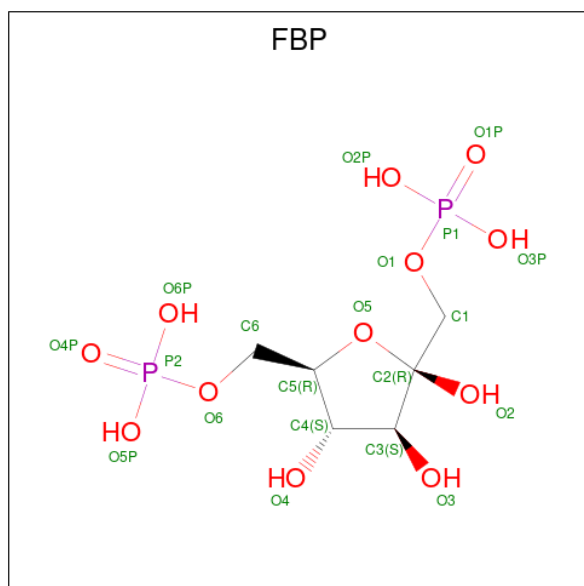
Chain	Residue	Modelled	Actual	Comment	Reference
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H	?	-	VAL	deletion	UNP P30613
H	?	-	TRP	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	TYR	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	ASN	deletion	UNP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

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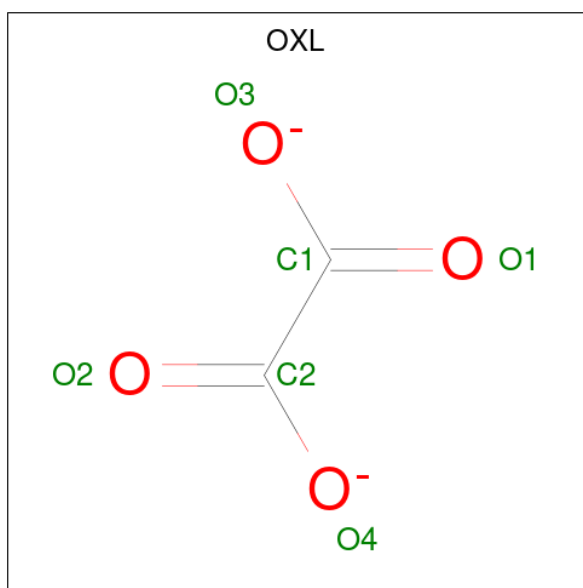
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLU	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	ARG	deletion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

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

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

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

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

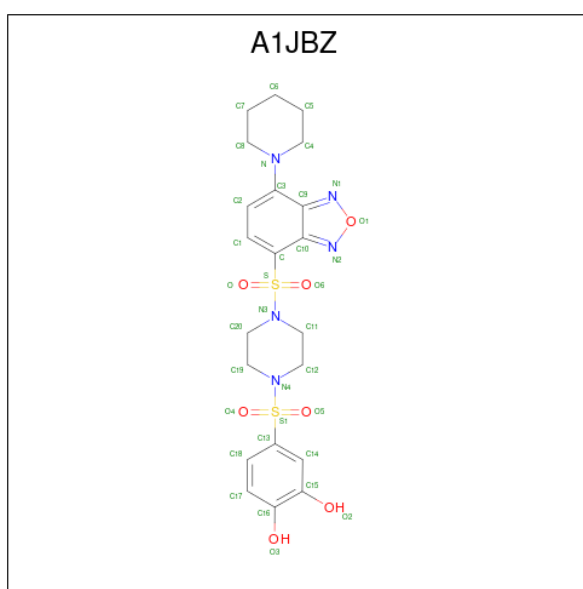
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	E	1	Total K 1 1	0	0

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

- Molecule 6 is 4-[4-[(7-piperidin-1-yl-2,1,3-benzoxadiazol-4-yl)sulfonyl]piperazin-1-yl]sulfonylbenzene-1,2-diol (CCD ID: A1JBZ) (formula: C₂₁H₂₅N₅O₇S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 60	C 21	H 25	N 5	O 7	S 2	25	0
6	D	1	Total 60	C 21	H 25	N 5	O 7	S 2	25	0
6	E	1	Total 60	C 21	H 25	N 5	O 7	S 2	25	0
6	F	1	Total 60	C 21	H 25	N 5	O 7	S 2	25	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	182	Total O 182 182	0	0

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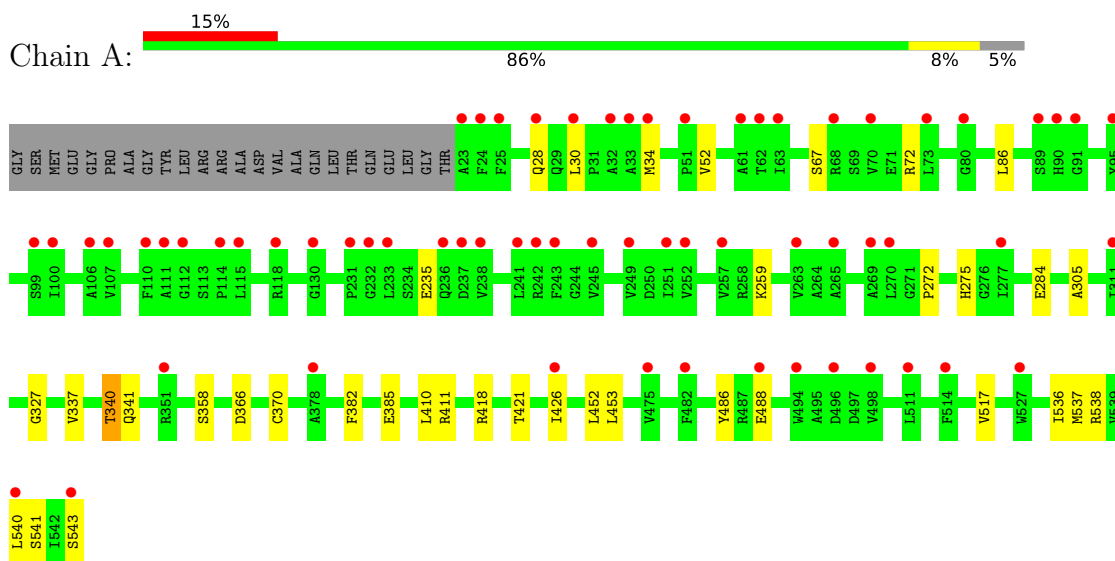
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	154	Total 154	O 154	0	0
7	C	299	Total 299	O 299	0	0
7	D	321	Total 321	O 321	0	0
7	E	181	Total 181	O 181	0	0
7	F	252	Total 252	O 252	0	0
7	G	322	Total 322	O 322	0	0
7	H	397	Total 397	O 397	0	0

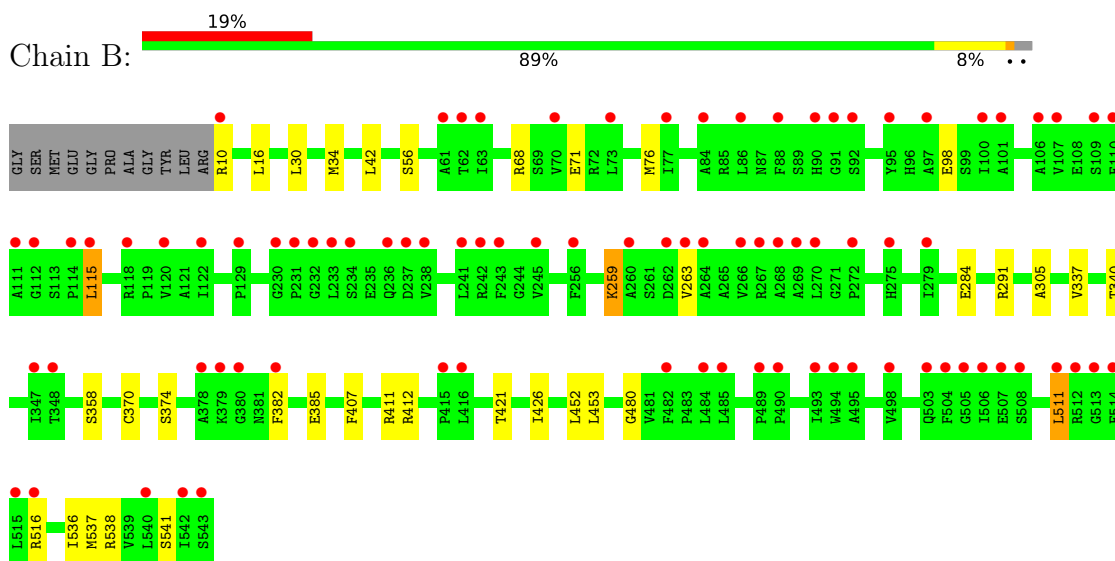
3 Residue-property plots [i](#)

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.

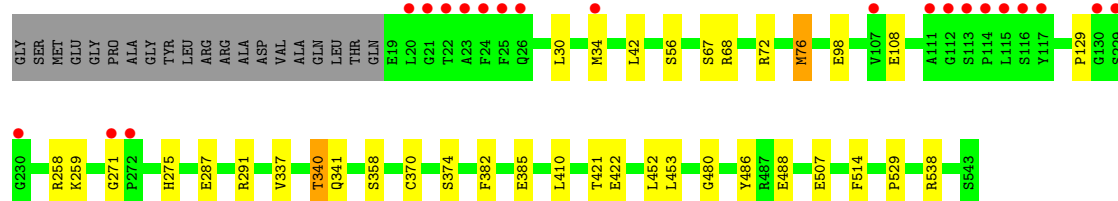
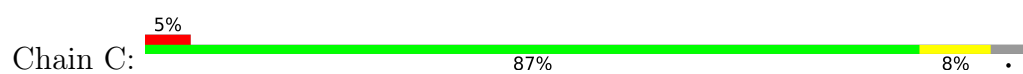
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



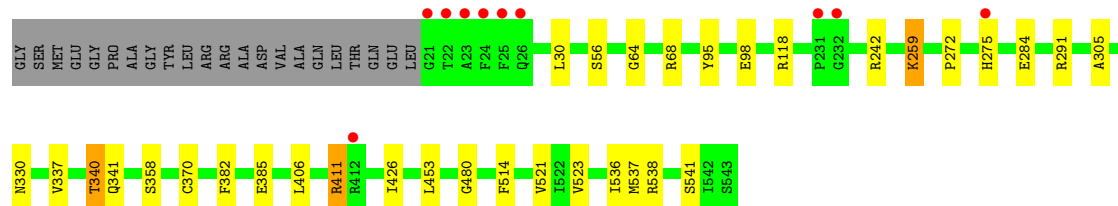
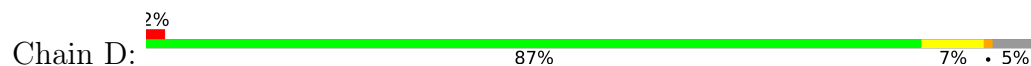
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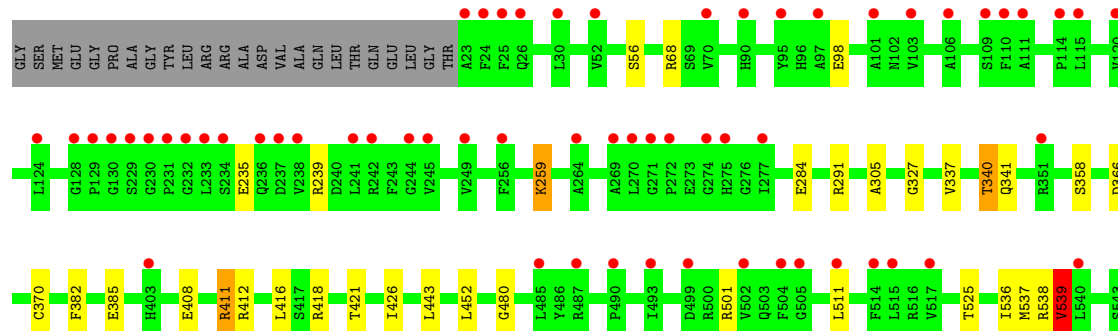
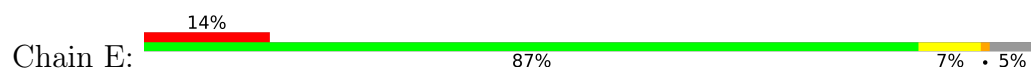
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



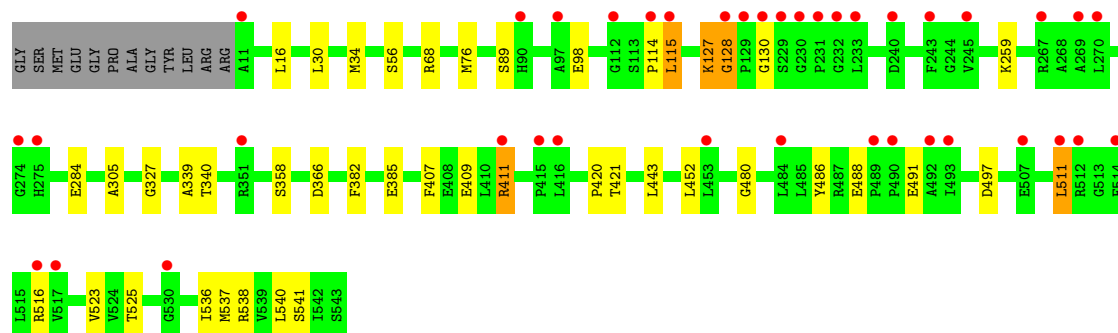
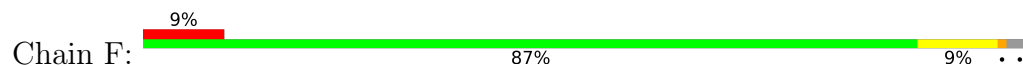
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



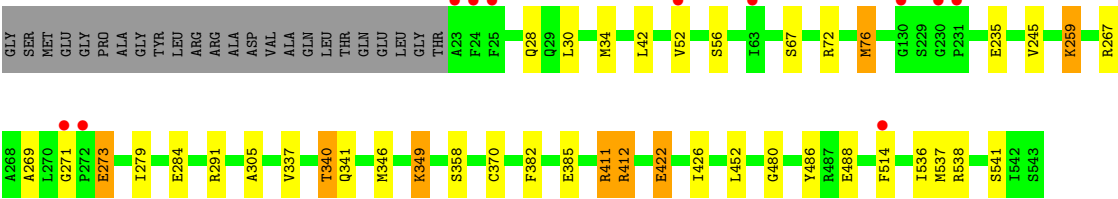
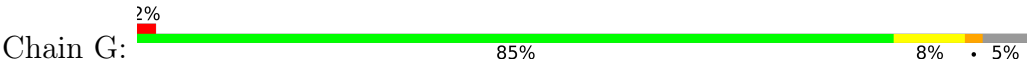
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



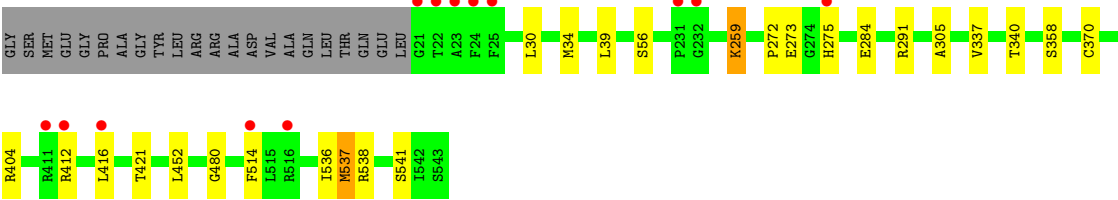
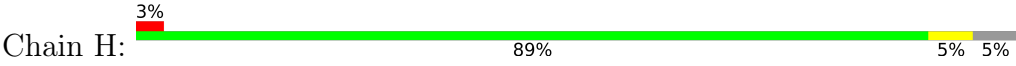
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



- 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	208.44Å 112.90Å 189.01Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	188.98 – 2.06 188.98 – 2.06	Depositor EDS
% Data completeness (in resolution range)	68.5 (188.98-2.06) 68.5 (188.98-2.06)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.07Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.199 , 0.235 0.190 , 0.224	Depositor DCC
R_{free} test set	9442 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.7	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	28711	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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 48.98 % 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 7.9614e-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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, OXL, MG, A1JBZ, FBP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.68	0/3316	1.01	4/4484 (0.1%)
1	B	0.70	1/3396 (0.0%)	1.00	2/4592 (0.0%)
1	C	0.73	1/3324 (0.0%)	1.03	6/4495 (0.1%)
1	D	0.75	0/3326	1.02	3/4497 (0.1%)
1	E	0.66	0/3301	1.01	3/4463 (0.1%)
1	F	0.71	0/3411	1.02	2/4613 (0.0%)
1	G	0.75	0/3314	1.01	1/4481 (0.0%)
1	H	0.77	0/3316	1.02	1/4483 (0.0%)
All	All	0.72	2/26704 (0.0%)	1.01	22/36108 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	SER	CA-C	8.46	1.56	1.52
1	C	374	SER	CA-C	5.04	1.54	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	PHE	CA-CB-CG	6.03	119.83	113.80
1	C	507	GLU	CB-CG-CD	6.02	122.84	112.60
1	H	514	PHE	CA-CB-CG	5.80	119.60	113.80
1	E	411	ARG	CA-C-N	5.68	128.17	120.44
1	E	411	ARG	C-N-CA	5.68	128.17	120.44
1	G	514	PHE	CA-CB-CG	5.66	119.46	113.80
1	D	514	PHE	CA-CB-CG	5.53	119.33	113.80
1	E	539	VAL	N-CA-CB	5.49	117.63	111.21
1	A	453	LEU	CA-C-N	5.24	127.30	120.28
1	A	453	LEU	C-N-CA	5.24	127.30	120.28
1	F	339	ALA	CA-C-N	5.22	131.52	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	339	ALA	C-N-CA	5.22	131.52	121.54
1	B	453	LEU	CA-C-N	5.20	127.25	120.28
1	B	453	LEU	C-N-CA	5.20	127.25	120.28
1	D	453	LEU	CA-C-N	5.18	127.22	120.28
1	D	453	LEU	C-N-CA	5.18	127.22	120.28
1	C	410	LEU	CA-C-N	5.10	127.07	120.44
1	C	410	LEU	C-N-CA	5.10	127.07	120.44
1	A	410	LEU	CA-C-N	5.06	127.01	120.44
1	A	410	LEU	C-N-CA	5.06	127.01	120.44
1	C	453	LEU	CA-C-N	5.00	126.98	120.28
1	C	453	LEU	C-N-CA	5.00	126.98	120.28

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	18	0
1	B	3329	0	3394	20	0
1	C	3257	0	3308	21	0
1	D	3252	0	3310	20	0
1	E	3231	0	3290	20	0
1	F	3335	0	3405	25	0
1	G	3241	0	3294	25	0
1	H	3251	0	3307	14	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	1	0
2	F	20	0	10	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	35	25	0	3	0
6	D	35	25	0	6	0
6	E	35	25	0	3	0
6	F	35	25	0	5	0
7	A	182	0	0	0	0
7	B	154	0	0	0	0
7	C	299	0	0	2	0
7	D	321	0	0	0	0
7	E	181	0	0	0	0
7	F	252	0	0	0	0
7	G	322	0	0	0	0
7	H	397	0	0	0	0
All	All	28611	100	26695	149	0

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

All (149) 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:A:272:PRO:HA	1:A:275:HIS:NE2	1.96	0.80
1:B:42:LEU:HD12	6:D:605:A1JBZ:C7	2.13	0.78
1:F:327:GLY:HA2	6:F:605:A1JBZ:C6	2.17	0.75
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.74	0.70
1:G:411:ARG:HG2	1:G:426:ILE:HD11	1.74	0.69
6:A:605:A1JBZ:C5	1:C:42:LEU:HD12	2.23	0.68
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.76	0.68
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.75	0.67
1:E:418:ARG:HD3	1:F:16:LEU:HD11	1.74	0.67
1:F:366:ASP:O	6:F:605:A1JBZ:C7	2.45	0.65
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.78	0.65
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.62	0.65
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.78	0.65
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.79	0.64
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.66	0.64
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.80	0.64
6:F:605:A1JBZ:C5	1:H:39:LEU:HD13	2.28	0.63
1:E:366:ASP:O	6:E:605:A1JBZ:C7	2.47	0.62
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.82	0.62
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.82	0.62
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.80	0.62
1:D:330:ASN:OD1	6:D:605:A1JBZ:C5	2.48	0.61
1:B:115:LEU:HD13	1:B:511:LEU:HB3	1.82	0.61
1:C:538:ARG:HD3	7:C:741:HOH:O	2.00	0.61
1:D:68:ARG:NH2	1:D:95:TYR:O	2.33	0.60
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.83	0.60
6:E:605:A1JBZ:C5	1:G:42:LEU:HD12	2.31	0.60
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.83	0.59
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.84	0.59
1:E:235:GLU:O	1:E:239:ARG:HD3	2.03	0.59
1:A:538:ARG:HG2	1:B:536:ILE:HG12	1.84	0.59
1:F:115:LEU:HD13	1:F:511:LEU:HD12	1.85	0.58
1:B:71:GLU:H	1:B:71:GLU:CD	2.11	0.58
1:B:42:LEU:CD1	6:D:605:A1JBZ:C7	2.80	0.57
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.86	0.57
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.88	0.56
1:E:443:LEU:HD13	1:E:525:THR:HG22	1.88	0.56
1:A:327:GLY:HA2	6:A:605:A1JBZ:C6	2.36	0.55
1:E:411:ARG:HG2	1:E:426:ILE:HD11	1.87	0.55
1:F:409:GLU:OE1	6:F:605:A1JBZ:O1	2.25	0.55
1:C:129:PRO:HG3	1:C:258:ARG:HH21	1.71	0.55
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASP:O	6:A:605:A1JBZ:C7	2.56	0.53
1:E:327:GLY:HA2	6:E:605:A1JBZ:C6	2.38	0.53
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.92	0.52
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.45	0.52
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.23	0.52
1:D:64:GLY:O	1:D:68:ARG:HG3	2.10	0.52
1:F:127:LYS:O	1:F:128:GLY:O	2.28	0.52
1:A:272:PRO:HA	1:A:275:HIS:CD2	2.46	0.51
1:B:407:PHE:CZ	1:B:411:ARG:HD2	2.45	0.51
1:A:411:ARG:HG3	1:A:426:ILE:HD11	1.93	0.51
1:A:67:SER:HA	1:A:72:ARG:HG2	1.93	0.50
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.93	0.50
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.47	0.50
1:C:67:SER:HB2	1:C:76[B]:MET:SD	2.52	0.49
1:H:56:SER:HB2	1:H:480:GLY:CA	2.43	0.49
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.93	0.49
1:D:411:ARG:HG2	1:D:426:ILE:HD11	1.94	0.49
1:F:491:GLU:HB2	1:F:497:ASP:HB2	1.95	0.49
1:E:501:ARG:NH1	2:E:601:FBP:O3P	2.38	0.48
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.48	0.48
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.94	0.48
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.47	0.48
1:F:30:LEU:O	1:F:34:MET:HG2	2.13	0.48
1:G:537:MET:HE3	1:H:537:MET:HG2	1.95	0.48
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.95	0.47
6:F:605:A1JBZ:N1	6:F:605:A1JBZ:C4	2.77	0.47
1:B:30:LEU:O	1:B:34:MET:HG2	2.14	0.47
1:F:89:SER:HA	1:F:127:LYS:HG3	1.96	0.47
1:C:30:LEU:O	1:C:34:MET:HG2	2.15	0.47
1:A:30:LEU:O	1:A:34:MET:HG2	2.15	0.47
1:H:30:LEU:O	1:H:34:MET:HG2	2.15	0.47
1:G:56:SER:HB2	1:G:480:GLY:CA	2.44	0.46
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.98	0.46
1:B:56:SER:HB2	1:B:480:GLY:CA	2.45	0.46
1:C:271:GLY:O	1:C:275:HIS:CE1	2.69	0.46
1:C:67:SER:HA	1:C:72:ARG:HG2	1.98	0.46
1:F:56:SER:HB2	1:F:480:GLY:CA	2.46	0.46
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.98	0.46
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.52	0.45
1:D:523:VAL:HB	1:D:538:ARG:HG2	1.99	0.45
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:LEU:O	1:G:34:MET:HG2	2.16	0.45
1:G:346:MET:HA	1:G:349:LYS:O	2.17	0.45
1:C:529:PRO:HG2	1:G:235:GLU:HG2	1.99	0.45
1:D:330:ASN:OD1	6:D:605:A1JBZ:C6	2.65	0.45
1:E:382:PHE:HB3	1:E:385:GLU:HB2	2.00	0.44
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.99	0.44
1:C:340:THR:HG22	1:C:341:GLN:HG3	2.00	0.44
1:F:443:LEU:HD22	1:F:525:THR:HG22	1.99	0.44
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.48	0.44
1:D:56:SER:HB2	1:D:480:GLY:CA	2.47	0.43
1:C:287:GLU:HG2	1:C:291:ARG:HD2	2.00	0.43
1:E:421:THR:HG22	1:E:452:LEU:HD12	2.00	0.43
1:B:71:GLU:CD	1:B:71:GLU:N	2.76	0.43
1:D:406:LEU:CD1	6:D:605:A1JBZ:C4	2.96	0.43
1:G:337:VAL:HG22	1:G:370:CYS:HB2	2.01	0.43
1:C:486:TYR:CE2	1:C:488:GLU:HB2	2.53	0.43
1:E:340:THR:HG22	1:E:341:GLN:HG3	2.00	0.43
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.99	0.43
1:G:259:LYS:HB3	1:G:291:ARG:HE	1.84	0.43
1:G:34:MET:HE1	1:H:416:LEU:HD11	2.01	0.43
1:B:407:PHE:CE2	1:B:411:ARG:HD2	2.53	0.43
1:C:56:SER:HB2	1:C:480:GLY:CA	2.48	0.43
1:F:486:TYR:CZ	1:F:488:GLU:HB2	2.54	0.43
1:G:269:ALA:C	1:G:271:GLY:H	2.26	0.43
1:E:68:ARG:NH2	1:E:98:GLU:HB3	2.34	0.42
1:D:337:VAL:HG22	1:D:370:CYS:HB2	2.01	0.42
1:F:421:THR:HG22	1:F:452:LEU:HD12	2.01	0.42
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.01	0.42
1:D:259:LYS:HB3	1:D:291:ARG:HE	1.84	0.42
1:E:284:GLU:HG2	1:E:305:ALA:HB3	2.01	0.42
1:F:114:PRO:HG2	1:F:115:LEU:HD23	2.01	0.42
1:A:284:GLU:HG2	1:A:305:ALA:HB3	2.01	0.42
1:B:68:ARG:NH2	1:B:98:GLU:HB3	2.35	0.42
1:E:259:LYS:HB3	1:E:291:ARG:HE	1.85	0.42
1:G:67:SER:HA	1:G:72:ARG:HG2	2.02	0.42
1:G:284:GLU:HG2	1:G:305:ALA:HB3	2.02	0.42
1:H:284:GLU:HG2	1:H:305:ALA:HB3	2.01	0.42
1:F:284:GLU:HG2	1:F:305:ALA:HB3	2.01	0.41
1:B:421:THR:HG22	1:B:452:LEU:HD12	2.02	0.41
1:C:108:GLU:HB3	7:C:886:HOH:O	2.20	0.41
1:C:337:VAL:HG22	1:C:370:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:VAL:HG22	1:E:370:CYS:HB2	2.01	0.41
1:G:382:PHE:HB3	1:G:385:GLU:HB2	2.02	0.41
1:D:382:PHE:HB3	1:D:385:GLU:HB2	2.02	0.41
1:H:421:THR:HG22	1:H:452:LEU:HD12	2.02	0.41
1:D:340:THR:HG22	1:D:341:GLN:HG3	2.02	0.41
1:H:259:LYS:HB3	1:H:291:ARG:HE	1.86	0.41
1:A:340:THR:HG22	1:A:341:GLN:HG3	2.02	0.41
1:F:89:SER:HA	1:F:127:LYS:HB2	2.02	0.41
1:C:68:ARG:NH2	1:C:98:GLU:HB3	2.35	0.41
1:C:421:THR:HG22	1:C:452:LEU:HD12	2.03	0.41
1:A:337:VAL:HG22	1:A:370:CYS:HB2	2.02	0.41
1:D:30:LEU:HD23	1:D:30:LEU:HA	1.97	0.41
1:D:406:LEU:HD13	6:D:605:A1JBZ:C4	2.51	0.41
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.36	0.41
1:G:245:VAL:HG11	1:G:273:GLU:HG2	2.01	0.41
1:G:267:ARG:HG2	1:G:279:ILE:HD12	2.03	0.41
1:A:28:GLN:HB3	1:A:52:VAL:HG22	2.03	0.40
1:B:259:LYS:HB3	1:B:291:ARG:HE	1.85	0.40
1:D:284:GLU:HG2	1:D:305:ALA:HB3	2.03	0.40
1:E:56:SER:HB2	1:E:480:GLY:CA	2.50	0.40
1:F:523:VAL:HG21	1:F:540[A]:LEU:HD12	2.03	0.40
1:B:284:GLU:HG2	1:B:305:ALA:HB3	2.04	0.40
1:E:416:LEU:HB3	1:F:16:LEU:HD22	2.03	0.40
1:G:28:GLN:HB3	1:G:52:VAL:HG22	2.03	0.40
1:G:67:SER:HB2	1:G:76[B]:MET:SD	2.62	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%)	423 (99%)	3 (1%)	1 (0%)	43 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	438/447 (98%)	434 (99%)	3 (1%)	1 (0%)	43	38
1	C	429/447 (96%)	423 (99%)	5 (1%)	1 (0%)	43	38
1	D	429/447 (96%)	425 (99%)	3 (1%)	1 (0%)	43	38
1	E	426/447 (95%)	421 (99%)	4 (1%)	1 (0%)	43	38
1	F	440/447 (98%)	435 (99%)	2 (0%)	3 (1%)	18	10
1	G	427/447 (96%)	420 (98%)	6 (1%)	1 (0%)	43	38
1	H	427/447 (96%)	424 (99%)	2 (0%)	1 (0%)	43	38
All	All	3443/3576 (96%)	3405 (99%)	28 (1%)	10 (0%)	36	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	128	GLY
1	F	130	GLY
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/352 (97%)	333 (98%)	8 (2%)	44	41
1	B	349/352 (99%)	336 (96%)	13 (4%)	30	24
1	C	342/352 (97%)	338 (99%)	4 (1%)	63	65
1	D	342/352 (97%)	333 (97%)	9 (3%)	40	37
1	E	340/352 (97%)	332 (98%)	8 (2%)	43	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	351/352 (100%)	339 (97%)	12 (3%)	32	27
1	G	341/352 (97%)	330 (97%)	11 (3%)	34	29
1	H	340/352 (97%)	334 (98%)	6 (2%)	51	51
All	All	2746/2816 (98%)	2675 (97%)	71 (3%)	44	37

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	235	GLU
1	A	259	LYS
1	A	358	SER
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	A	541	SER
1	B	10	ARG
1	B	76[A]	MET
1	B	76[B]	MET
1	B	115	LEU
1	B	259	LYS
1	B	263	VAL
1	B	358	SER
1	B	412	ARG
1	B	511	LEU
1	B	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	B	541	SER
1	C	76[A]	MET
1	C	76[B]	MET
1	C	259	LYS
1	C	358	SER
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	259	LYS
1	D	358	SER
1	D	411	ARG
1	D	521	VAL
1	D	537	MET

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Mol	Chain	Res	Type
1	D	541	SER
1	E	259	LYS
1	E	358	SER
1	E	408	GLU
1	E	412	ARG
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	76[A]	MET
1	F	76[B]	MET
1	F	115	LEU
1	F	127	LYS
1	F	259	LYS
1	F	358	SER
1	F	411	ARG
1	F	511	LEU
1	F	516	ARG
1	F	537[A]	MET
1	F	537[B]	MET
1	F	541	SER
1	G	76[A]	MET
1	G	76[B]	MET
1	G	259	LYS
1	G	273	GLU
1	G	349	LYS
1	G	358	SER
1	G	411	ARG
1	G	412	ARG
1	G	422[A]	GLU
1	G	422[B]	GLU
1	G	541	SER
1	H	259	LYS
1	H	273	GLU
1	H	358	SER
1	H	412	ARG
1	H	537	MET
1	H	541	SER

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

Mol	Chain	Res	Type
1	A	27	GLN
1	B	27	GLN
1	B	405	GLN
1	C	26	GLN
1	C	275	HIS
1	D	27	GLN
1	D	405	GLN
1	E	27	GLN
1	F	27	GLN
1	F	405	GLN
1	G	26	GLN
1	G	275	HIS
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 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	G	601	-	18,20,20	0.69	0	21,32,32	0.73	0
3	OXL	B	602	4	5,5,5	2.21	2 (40%)	6,6,6	1.30	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	D	602	4	5,5,5	2.36	2 (40%)	6,6,6	2.76	4 (66%)
3	OXL	C	602	4	5,5,5	1.87	2 (40%)	6,6,6	3.01	3 (50%)
3	OXL	H	602	4	5,5,5	1.95	2 (40%)	6,6,6	2.06	2 (33%)
6	A1JBZ	F	605	-	39,39,39	1.14	4 (10%)	52,59,59	1.27	3 (5%)
2	FBP	F	601	-	18,20,20	0.47	0	21,32,32	0.58	0
2	FBP	H	601	-	18,20,20	0.72	0	21,32,32	0.68	1 (4%)
6	A1JBZ	A	605	-	39,39,39	0.97	4 (10%)	52,59,59	1.15	3 (5%)
2	FBP	E	601	-	18,20,20	0.43	0	21,32,32	0.53	0
2	FBP	D	601	-	18,20,20	0.51	0	21,32,32	0.85	1 (4%)
6	A1JBZ	E	605	-	39,39,39	1.07	4 (10%)	52,59,59	1.14	5 (9%)
3	OXL	G	602	4	5,5,5	2.42	2 (40%)	6,6,6	1.05	0
2	FBP	A	601	-	18,20,20	0.49	0	21,32,32	0.59	0
3	OXL	A	602	4	5,5,5	1.94	2 (40%)	6,6,6	2.56	3 (50%)
3	OXL	F	602	4	5,5,5	2.04	2 (40%)	6,6,6	2.47	2 (33%)
2	FBP	C	601	-	18,20,20	0.53	0	21,32,32	0.52	0
2	FBP	B	601	-	18,20,20	0.42	0	21,32,32	0.80	1 (4%)
6	A1JBZ	D	605	-	39,39,39	0.98	2 (5%)	52,59,59	1.04	3 (5%)
3	OXL	E	602	4	5,5,5	1.98	2 (40%)	6,6,6	1.98	2 (33%)

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	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	D	602	4	-	4/4/4/4	-
3	OXL	C	602	4	-	4/4/4/4	-
3	OXL	H	602	4	-	4/4/4/4	-
6	A1JBZ	F	605	-	-	16/28/46/46	0/5/5/5
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
6	A1JBZ	A	605	-	-	12/28/46/46	0/5/5/5
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	A1JBZ	E	605	-	-	12/28/46/46	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	G	602	4	-	4/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	4	-	4/4/4/4	-
3	OXL	F	602	4	-	0/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
6	A1JBZ	D	605	-	-	13/28/46/46	0/5/5/5
3	OXL	E	602	4	-	4/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	OXL	O2-C2	4.41	1.33	1.22
3	D	602	OXL	O2-C2	3.94	1.32	1.22
3	B	602	OXL	O2-C2	3.82	1.32	1.22
6	D	605	A1JBZ	O1-N1	-3.76	1.30	1.39
3	A	602	OXL	O2-C2	3.74	1.31	1.22
6	F	605	A1JBZ	O1-N1	-3.73	1.30	1.39
6	F	605	A1JBZ	C9-N1	3.62	1.37	1.31
3	C	602	OXL	O2-C2	3.62	1.31	1.22
3	F	602	OXL	O2-C2	3.45	1.31	1.22
6	E	605	A1JBZ	O1-N1	-3.42	1.31	1.39
3	H	602	OXL	O2-C2	3.35	1.30	1.22
6	E	605	A1JBZ	C-C10	-3.19	1.40	1.42
6	D	605	A1JBZ	C-C10	-3.18	1.40	1.42
6	A	605	A1JBZ	C-C10	-3.16	1.40	1.42
6	A	605	A1JBZ	O1-N1	-3.08	1.32	1.39
3	E	602	OXL	O2-C2	3.06	1.30	1.22
6	F	605	A1JBZ	C-C10	-3.01	1.40	1.42
3	B	602	OXL	O4-C2	-3.01	1.22	1.30
3	E	602	OXL	O4-C2	-3.00	1.22	1.30
6	E	605	A1JBZ	C9-N1	2.99	1.36	1.31
3	D	602	OXL	O4-C2	-2.86	1.22	1.30
3	G	602	OXL	O4-C2	-2.74	1.23	1.30
6	E	605	A1JBZ	O1-N2	-2.60	1.33	1.39
3	H	602	OXL	O4-C2	-2.49	1.23	1.30
6	F	605	A1JBZ	O1-N2	-2.45	1.33	1.39
3	F	602	OXL	O4-C2	-2.33	1.24	1.30
3	A	602	OXL	O4-C2	-2.21	1.24	1.30
6	A	605	A1JBZ	O1-N2	-2.18	1.34	1.39
6	A	605	A1JBZ	C9-N1	2.17	1.34	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	OXL	O4-C2	-2.01	1.25	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	605	A1JBZ	C-C10-C9	-6.06	117.03	121.86
6	A	605	A1JBZ	C-C10-C9	-5.41	117.54	121.86
6	E	605	A1JBZ	C-C10-C9	-5.27	117.66	121.86
3	C	602	OXL	O4-C2-C1	5.06	122.64	112.83
6	D	605	A1JBZ	C-C10-C9	-4.67	118.14	121.86
3	F	602	OXL	O4-C2-C1	4.65	121.85	112.83
6	F	605	A1JBZ	C1-C2-C3	4.53	120.80	116.82
3	A	602	OXL	O4-C2-C1	4.44	121.44	112.83
3	D	602	OXL	O4-C2-C1	4.15	120.88	112.83
3	H	602	OXL	O4-C2-C1	4.05	120.69	112.83
3	C	602	OXL	O2-C2-C1	-3.85	112.60	120.63
3	D	602	OXL	O3-C1-C2	3.76	120.13	112.83
3	E	602	OXL	O4-C2-C1	3.76	120.12	112.83
6	E	605	A1JBZ	C1-C2-C3	3.60	119.98	116.82
3	F	602	OXL	O2-C2-C1	-3.40	113.54	120.63
6	D	605	A1JBZ	C1-C2-C3	3.40	119.80	116.82
6	A	605	A1JBZ	C1-C2-C3	3.39	119.80	116.82
3	C	602	OXL	O3-C1-C2	3.26	119.15	112.83
2	D	601	FBP	O6-P2-O4P	3.08	114.76	106.44
3	A	602	OXL	O2-C2-C1	-3.05	114.28	120.63
3	A	602	OXL	O3-C1-C2	2.92	118.50	112.83
6	F	605	A1JBZ	O1-N1-C9	2.89	109.10	105.65
3	D	602	OXL	O1-C1-C2	-2.75	114.91	120.63
2	B	601	FBP	O6-P2-O4P	2.71	113.77	106.44
3	D	602	OXL	O2-C2-C1	-2.56	115.30	120.63
3	H	602	OXL	O2-C2-C1	-2.54	115.34	120.63
2	H	601	FBP	O6-P2-O4P	2.50	113.19	106.44
6	D	605	A1JBZ	C9-C3-N	-2.47	116.20	120.54
6	A	605	A1JBZ	C9-C3-N	-2.45	116.25	120.54
6	E	605	A1JBZ	O1-N1-C9	2.37	108.48	105.65
3	B	602	OXL	O4-C2-C1	2.26	117.21	112.83
3	E	602	OXL	O3-C1-C2	2.23	117.15	112.83
6	E	605	A1JBZ	C9-C3-N	-2.07	116.91	120.54
6	E	605	A1JBZ	C8-N-C3	2.06	121.09	116.19
3	B	602	OXL	O3-C1-C2	2.00	116.71	112.83

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	605	A1JBZ	C19-N4-S1-O4
6	E	605	A1JBZ	C11-N3-S-O6
6	A	605	A1JBZ	C20-N3-S-O6
6	A	605	A1JBZ	C20-N3-S-O
6	D	605	A1JBZ	C20-N3-S-O
6	D	605	A1JBZ	C12-N4-S1-O4
6	E	605	A1JBZ	C12-N4-S1-O4
6	E	605	A1JBZ	C12-N4-S1-O5
6	F	605	A1JBZ	C19-N4-S1-O5
6	F	605	A1JBZ	C12-N4-S1-O4
6	F	605	A1JBZ	C12-N4-S1-O5
6	A	605	A1JBZ	C19-N4-S1-C13
6	E	605	A1JBZ	C11-N3-S-C
6	A	605	A1JBZ	C19-N4-S1-O5
6	D	605	A1JBZ	C11-N3-S-O6
6	D	605	A1JBZ	C20-N3-S-O6
6	D	605	A1JBZ	C11-N3-S-O
6	A	605	A1JBZ	C11-N3-S-O
6	E	605	A1JBZ	C19-N4-S1-O5
6	F	605	A1JBZ	C11-N3-S-O6
6	F	605	A1JBZ	C19-N4-S1-O4
6	A	605	A1JBZ	C20-N3-S-C
6	D	605	A1JBZ	C12-N4-S1-C13
6	F	605	A1JBZ	C12-N4-S1-C13
6	E	605	A1JBZ	C11-N3-S-O
6	A	605	A1JBZ	C11-N3-S-O6
6	D	605	A1JBZ	C12-N4-S1-O5
6	E	605	A1JBZ	C19-N4-S1-O4
6	D	605	A1JBZ	C11-N3-S-C
6	D	605	A1JBZ	C20-N3-S-C
6	E	605	A1JBZ	C12-N4-S1-C13
6	F	605	A1JBZ	C11-N3-S-C
6	F	605	A1JBZ	C19-N4-S1-C13
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	A	605	A1JBZ	C11-N3-S-C
6	E	605	A1JBZ	C19-N4-S1-C13

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Mol	Chain	Res	Type	Atoms
6	F	605	A1JBZ	C2-C3-N-C4
6	F	605	A1JBZ	C9-C3-N-C4
6	A	605	A1JBZ	C12-N4-S1-O5
6	A	605	A1JBZ	C12-N4-S1-O4
6	E	605	A1JBZ	C20-N3-S-O6
6	E	605	A1JBZ	C20-N3-S-O
2	G	601	FBP	C4-C5-C6-O6
6	D	605	A1JBZ	C19-N4-S1-O5
6	D	605	A1JBZ	C19-N4-S1-O4
6	F	605	A1JBZ	C11-N3-S-O
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
6	A	605	A1JBZ	C12-N4-S1-C13
6	E	605	A1JBZ	C20-N3-S-C
2	E	601	FBP	O5-C5-C6-O6
6	F	605	A1JBZ	C20-N3-S-O
6	F	605	A1JBZ	C2-C3-N-C8
6	F	605	A1JBZ	C20-N3-S-O6
6	D	605	A1JBZ	C19-N4-S1-C13
3	H	602	OXL	O3-C1-C2-O4
6	D	605	A1JBZ	C2-C3-N-C4
3	B	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	A	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
6	F	605	A1JBZ	C20-N3-S-C
2	G	601	FBP	O5-C5-C6-O6
6	F	605	A1JBZ	C9-C3-N-C8
3	B	602	OXL	O1-C1-C2-O4

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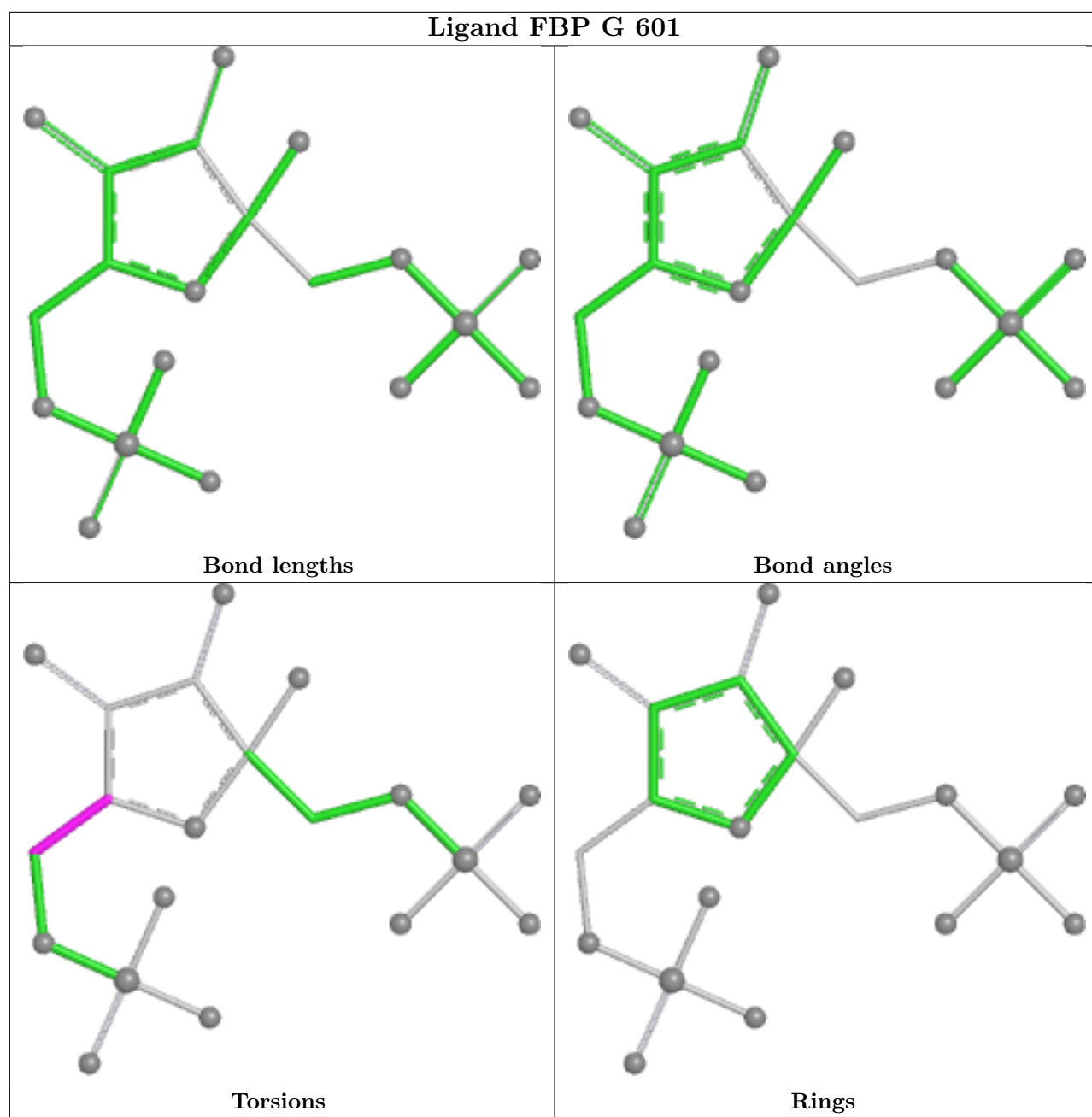
Mol	Chain	Res	Type	Atoms
3	B	602	OXL	O3-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O2

There are no ring outliers.

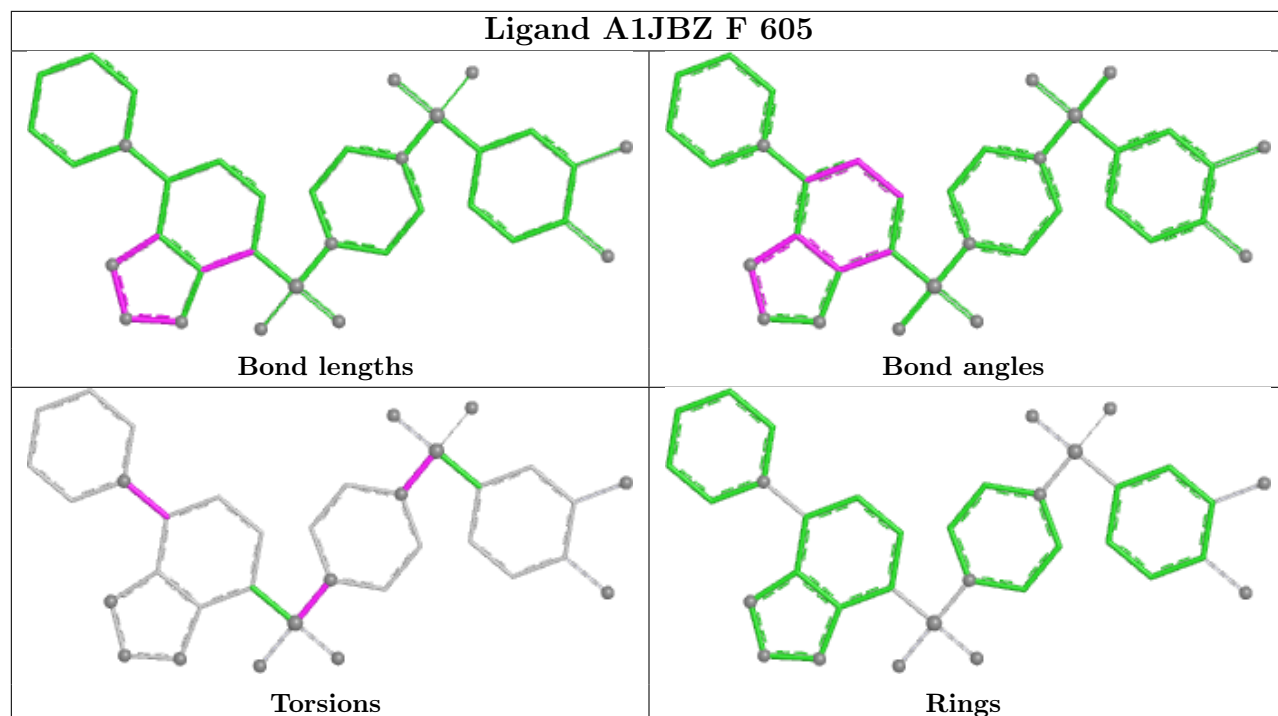
5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	605	A1JBZ	5	0
6	A	605	A1JBZ	3	0
2	E	601	FBP	1	0
6	E	605	A1JBZ	3	0
6	D	605	A1JBZ	6	0

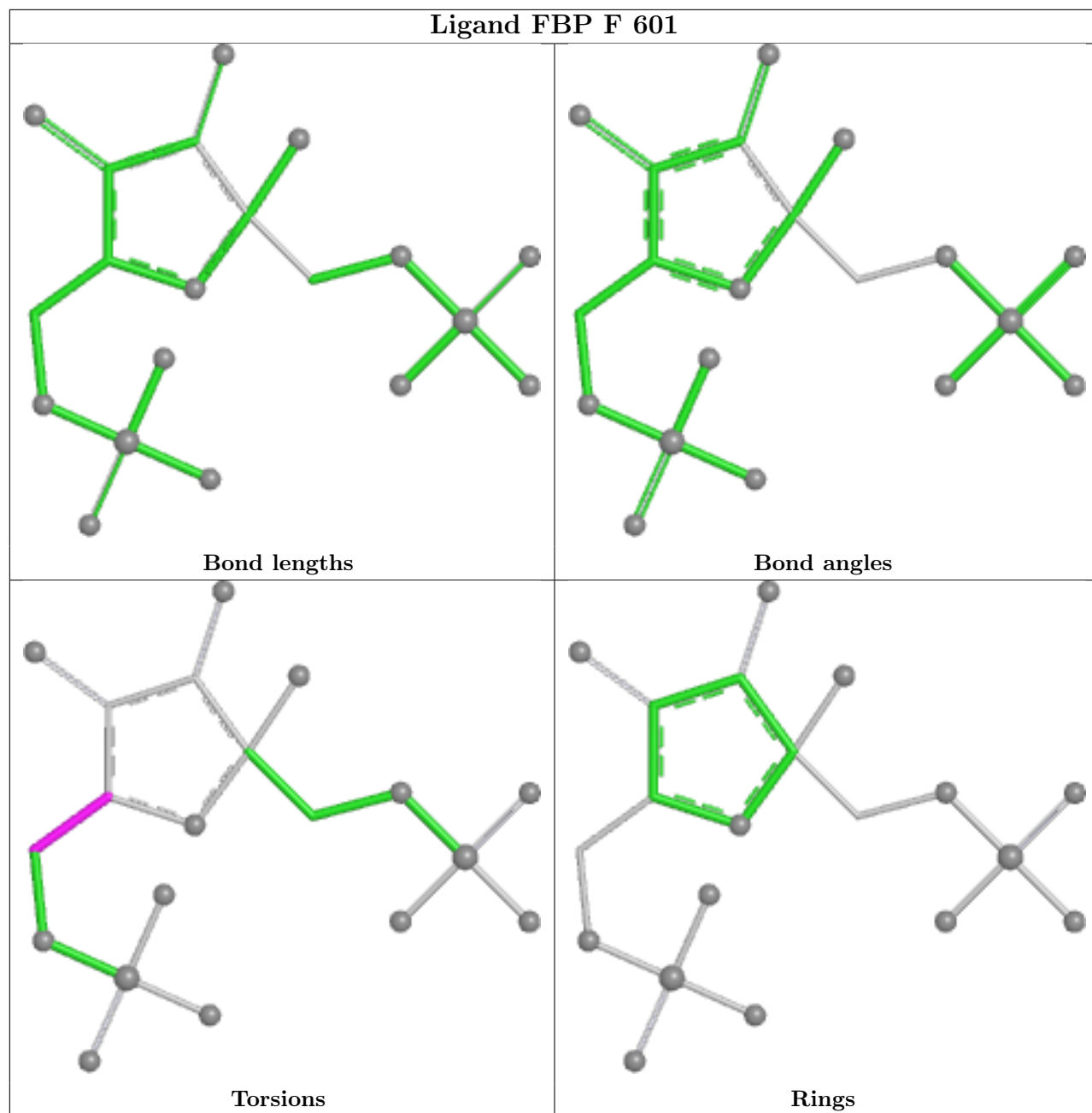
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

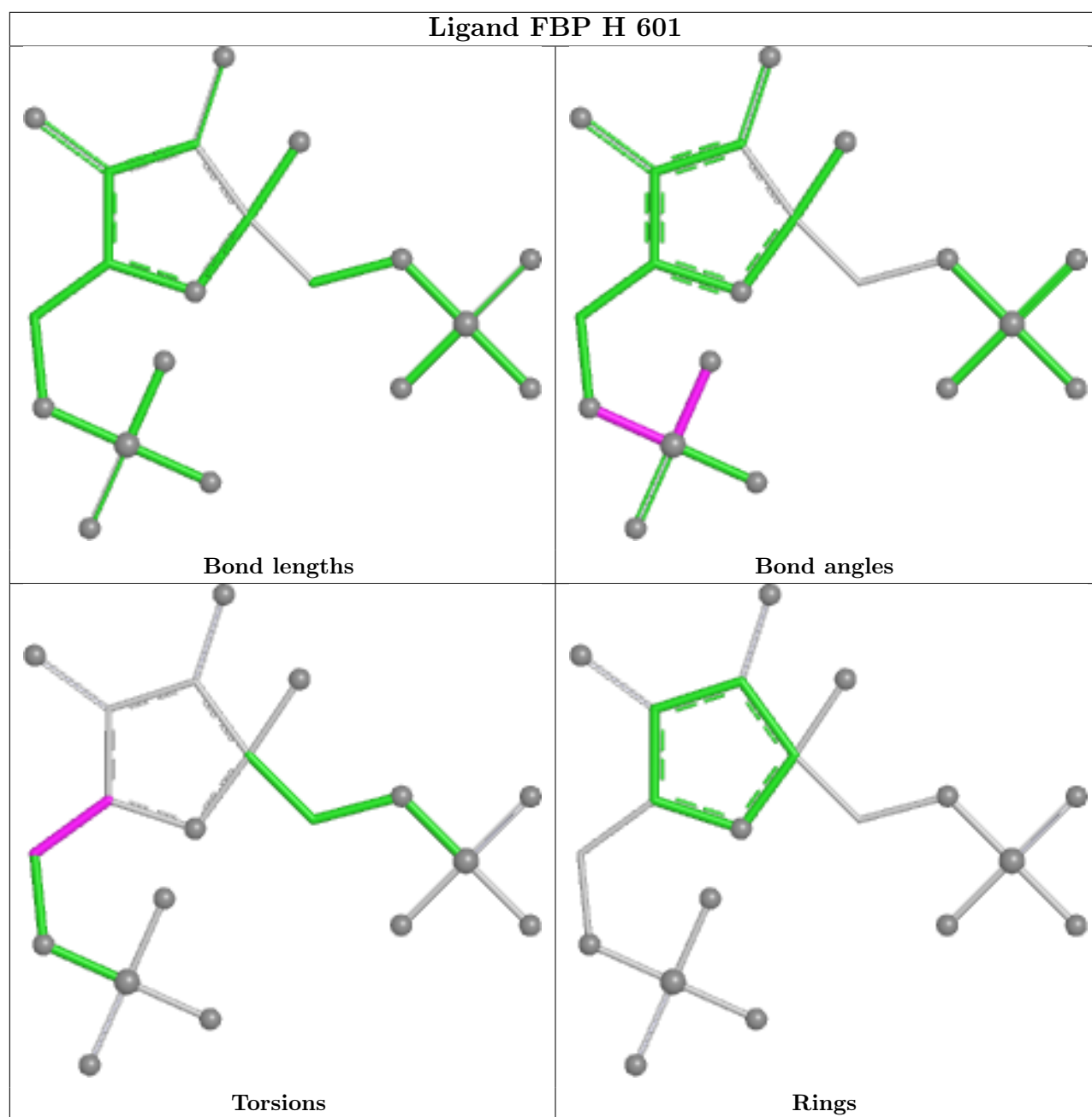


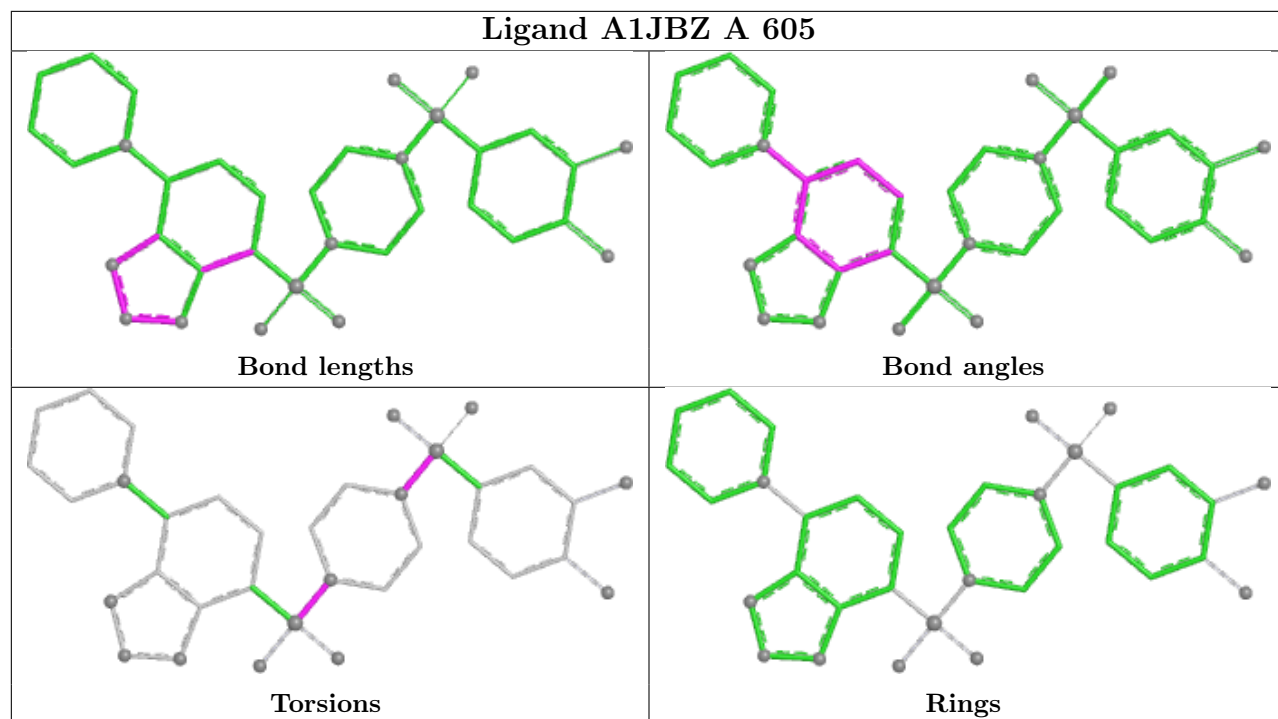
Ligand A1JBZ F 605



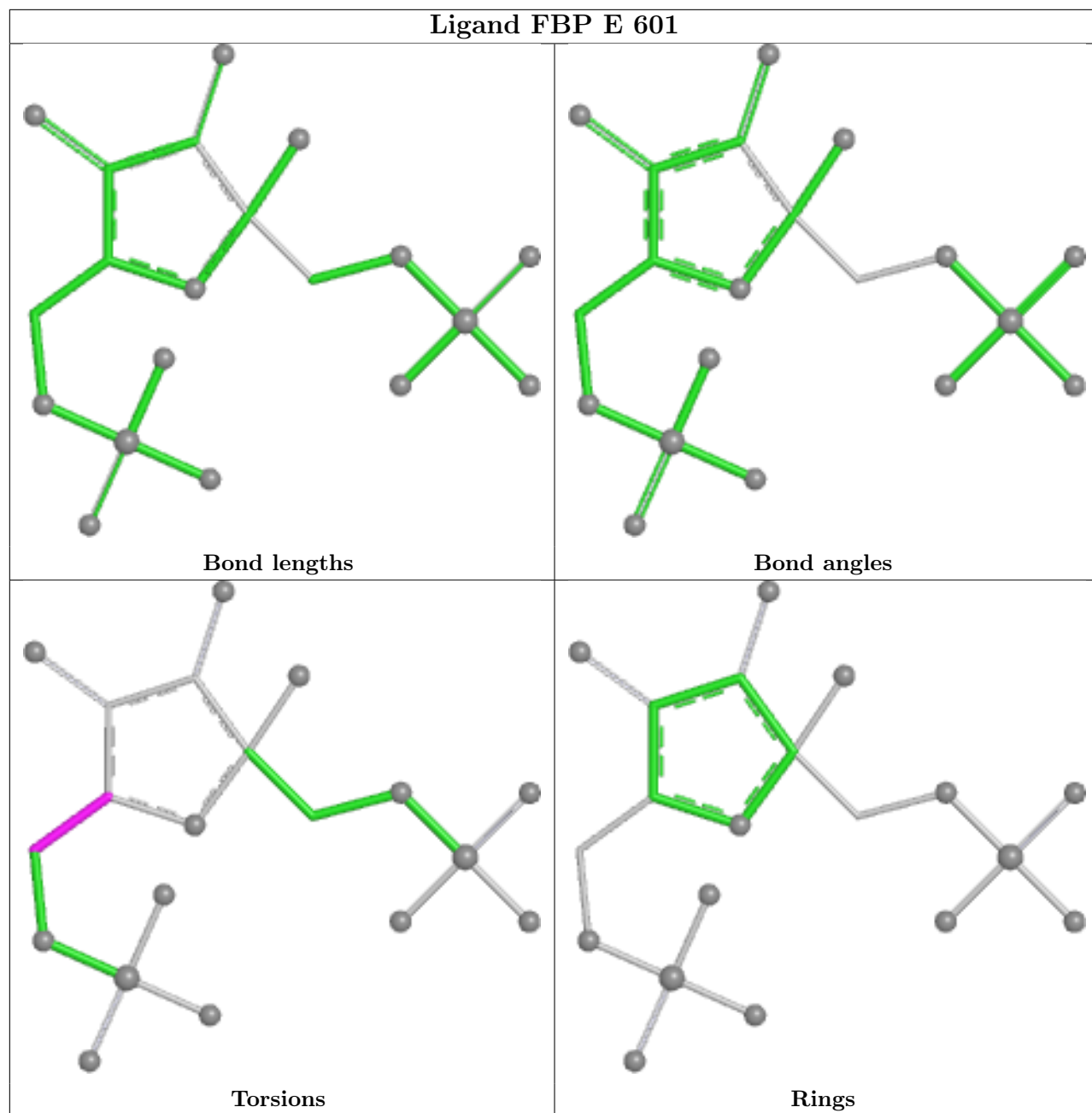
Ligand FBP F 601

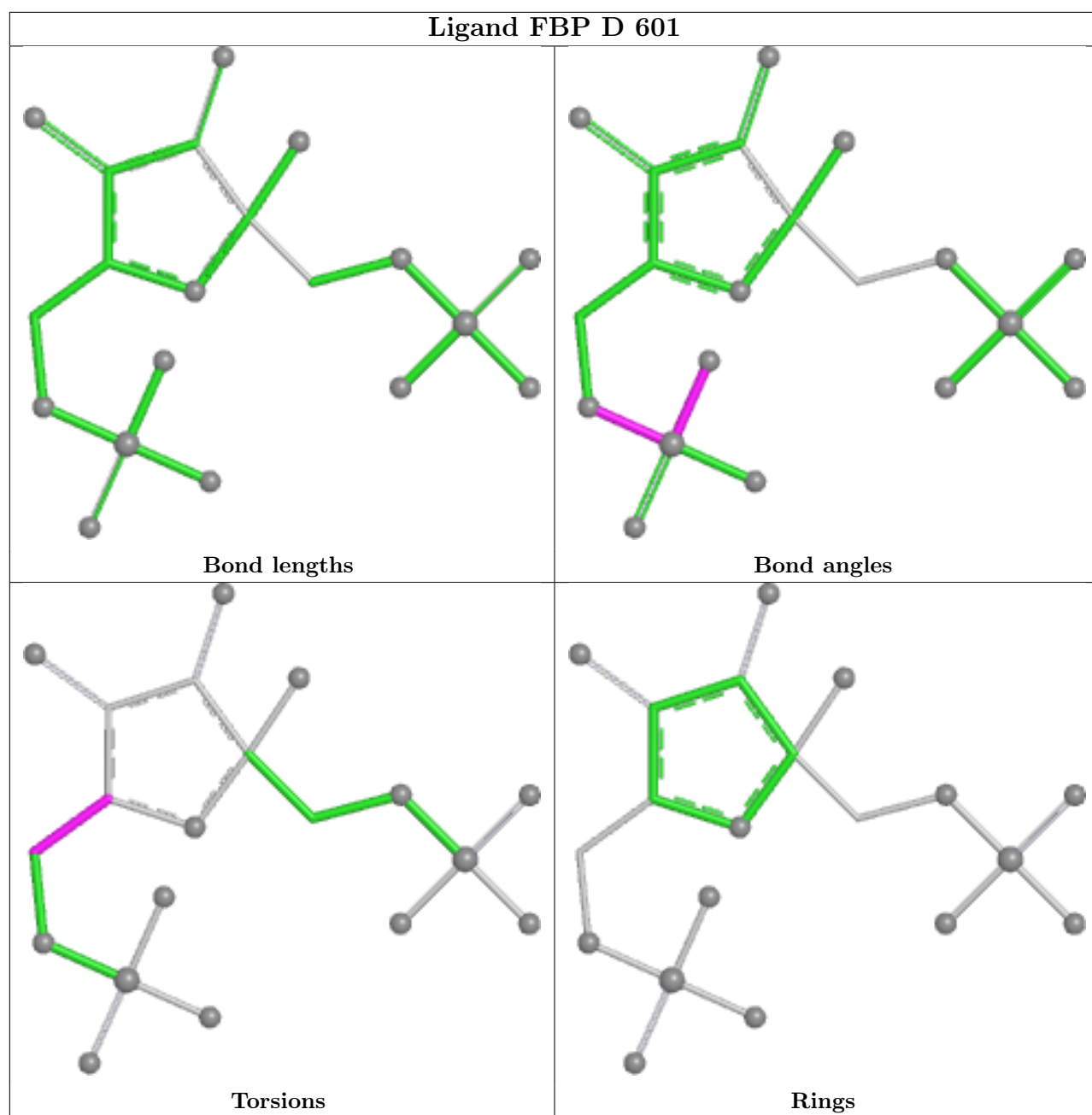




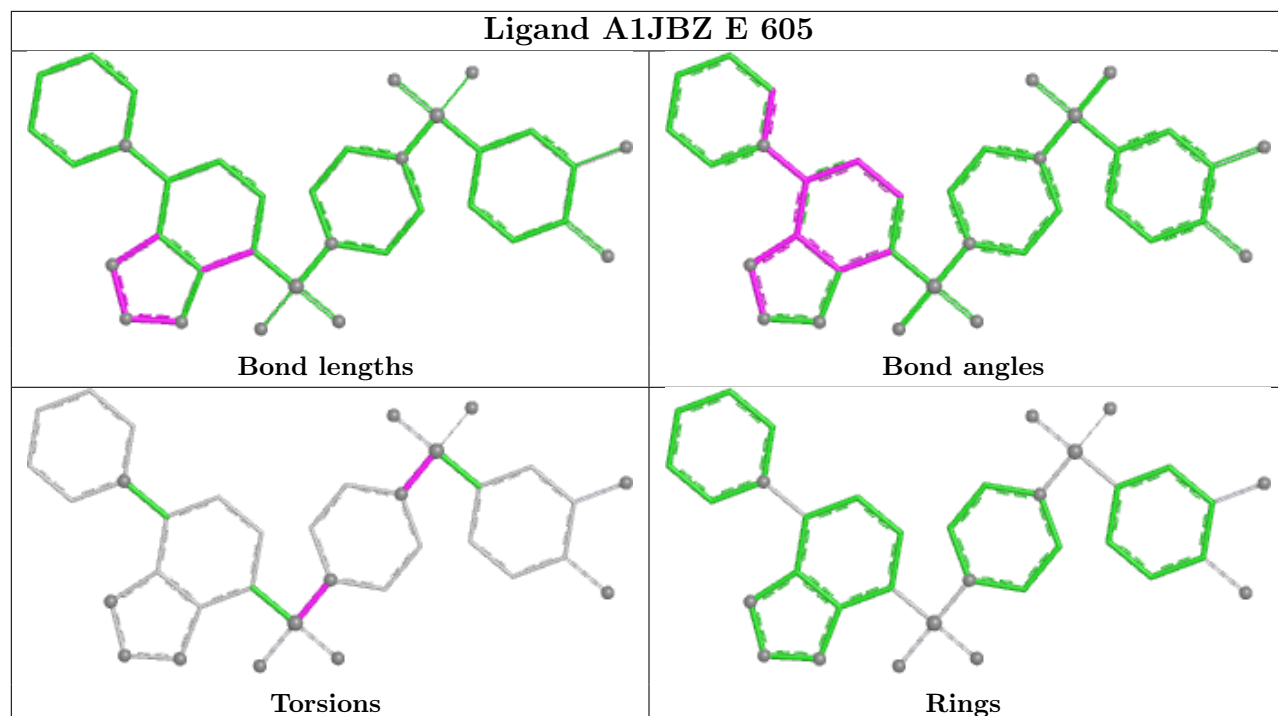


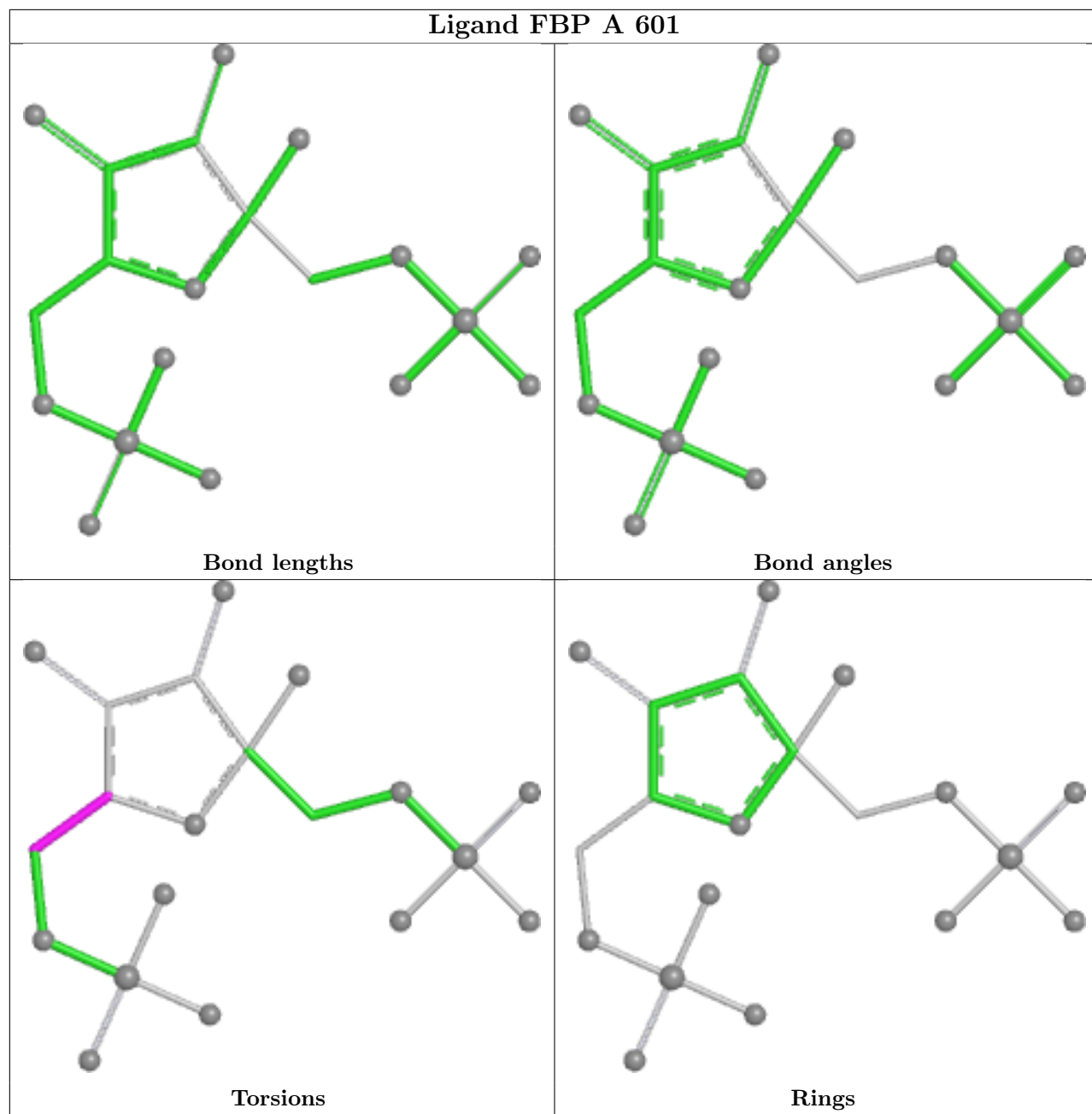
Ligand FBP E 601

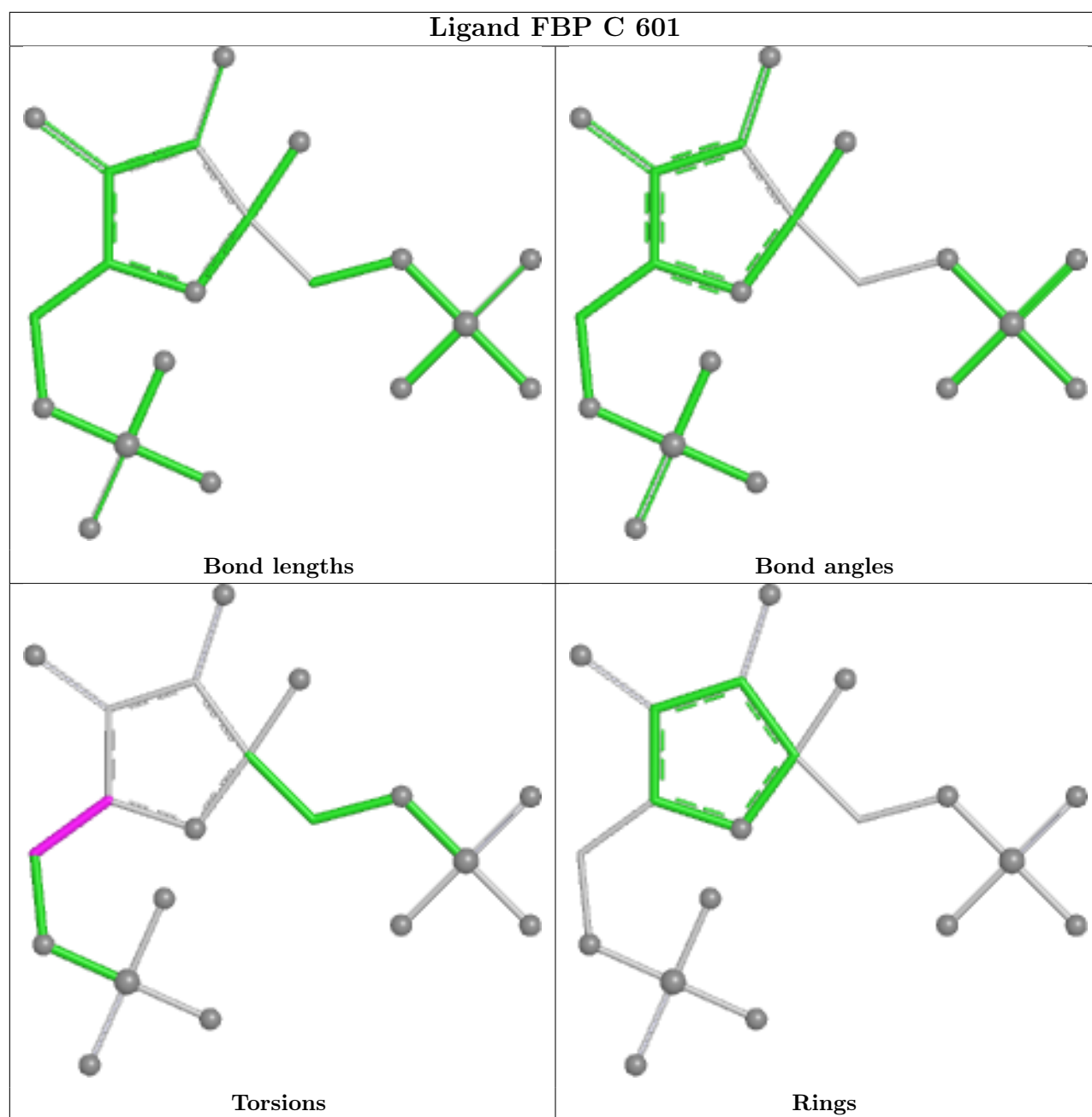


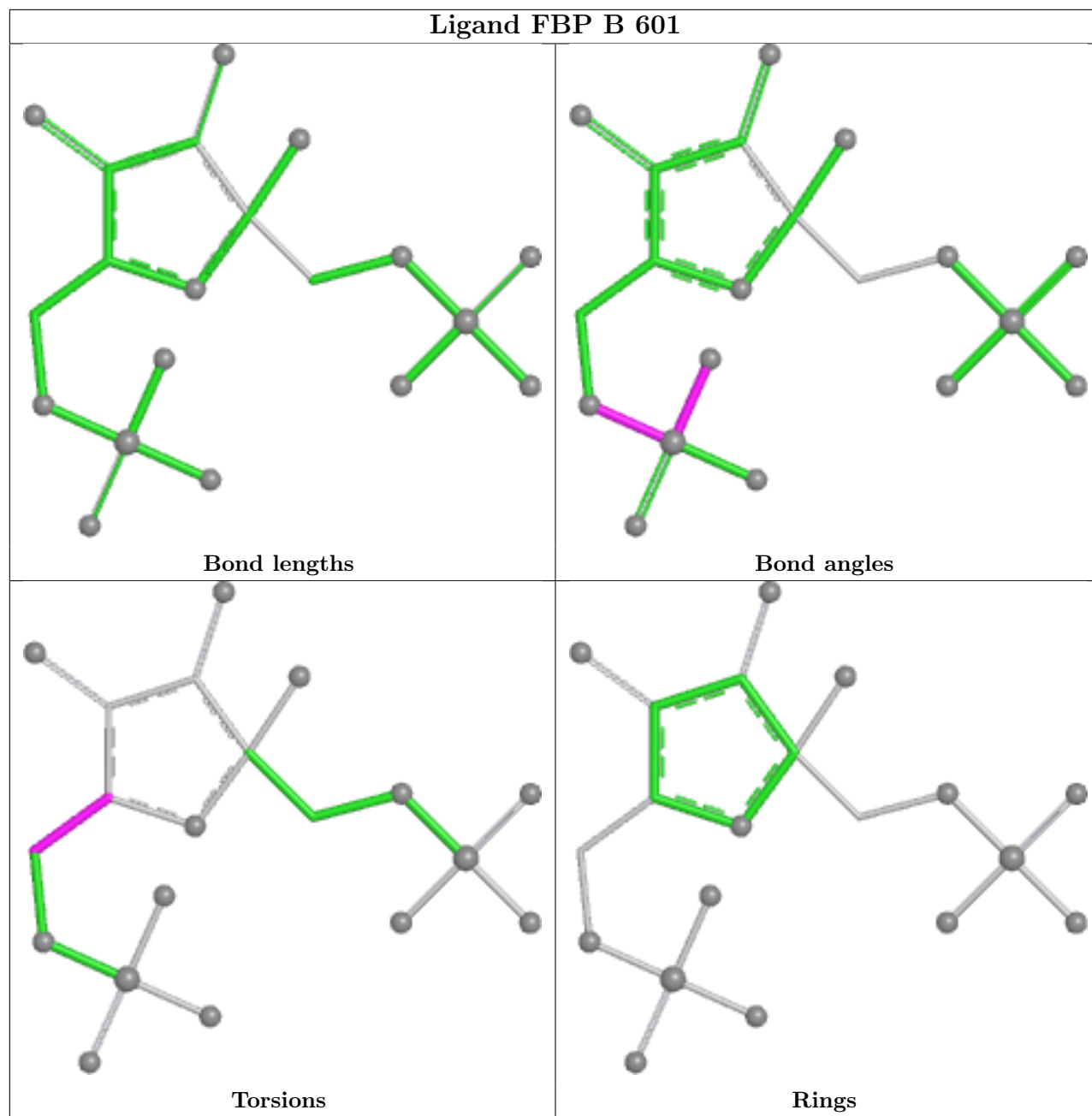


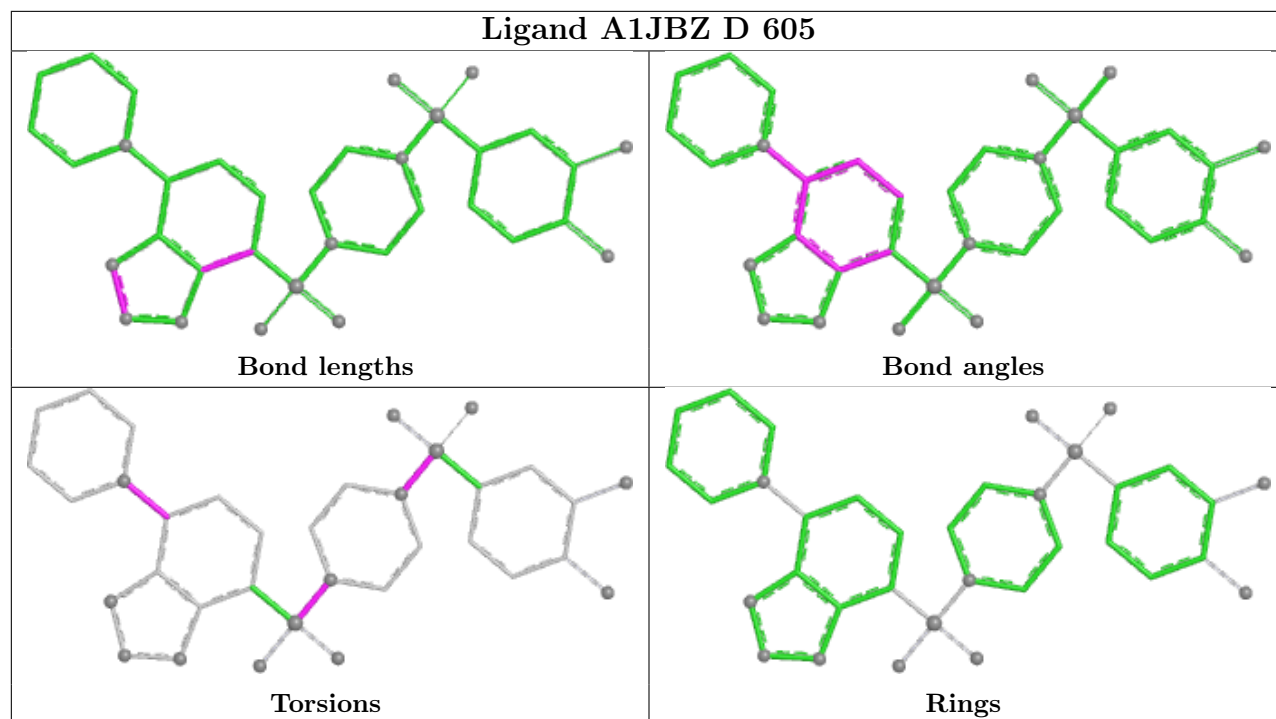
Ligand A1JBZ E 605











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	1.04	65 (15%)	5 5	24, 47, 77, 95	6 (1%)
1	B	436/447 (97%)	1.14	86 (19%)	3 3	22, 46, 78, 94	4 (0%)
1	C	427/447 (95%)	0.23	21 (4%)	35 35	18, 34, 61, 104	4 (0%)
1	D	425/447 (95%)	-0.06	10 (2%)	59 61	14, 28, 54, 101	6 (1%)
1	E	423/447 (94%)	0.91	61 (14%)	6 6	22, 46, 77, 94	5 (1%)
1	F	435/447 (97%)	0.53	39 (8%)	15 15	21, 37, 68, 87	7 (1%)
1	G	423/447 (94%)	0.02	11 (2%)	57 59	18, 30, 50, 71	7 (1%)
1	H	425/447 (95%)	-0.21	13 (3%)	51 52	13, 25, 48, 85	4 (0%)
All	All	3417/3576 (95%)	0.45	306 (8%)	15 15	13, 37, 70, 104	43 (1%)

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	6.8
1	E	23	ALA	6.1
1	H	21	GLY	5.7
1	A	25	PHE	5.6
1	B	511	LEU	5.5
1	D	25	PHE	5.1
1	G	25	PHE	4.9
1	E	25	PHE	4.9
1	F	115	LEU	4.8
1	F	511	LEU	4.7
1	D	22	THR	4.6
1	B	507	GLU	4.6
1	A	231	PRO	4.4
1	C	25	PHE	4.4
1	B	114	PRO	4.2
1	D	21	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	271	GLY	4.1
1	A	238	VAL	4.1
1	D	23	ALA	4.1
1	C	271	GLY	4.0
1	E	490	PRO	4.0
1	E	514	PHE	3.9
1	A	63	ILE	3.9
1	B	267[A]	ARG	3.9
1	F	516	ARG	3.7
1	H	232	GLY	3.7
1	A	23	ALA	3.7
1	B	490	PRO	3.7
1	C	117	TYR	3.7
1	A	543	SER	3.6
1	C	22	THR	3.6
1	F	114	PRO	3.5
1	F	230	GLY	3.5
1	C	111	ALA	3.5
1	C	229	SER	3.5
1	C	21	GLY	3.5
1	B	493	ILE	3.4
1	H	231	PRO	3.4
1	B	269	ALA	3.4
1	B	543	SER	3.4
1	A	70	VAL	3.4
1	B	348	THR	3.4
1	B	61	ALA	3.4
1	E	232	GLY	3.4
1	B	241	LEU	3.4
1	C	20	LEU	3.4
1	F	512	ARG	3.3
1	E	249	VAL	3.3
1	A	95	TYR	3.3
1	E	233	LEU	3.3
1	B	513	GLY	3.3
1	B	238	VAL	3.3
1	B	485	LEU	3.3
1	D	24	PHE	3.3
1	C	230	GLY	3.2
1	A	233	LEU	3.2
1	B	484	LEU	3.2
1	C	26	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	482	PHE	3.2
1	A	514	PHE	3.2
1	E	493	ILE	3.1
1	F	493	ILE	3.1
1	A	24	PHE	3.1
1	B	88	PHE	3.1
1	C	130	GLY	3.1
1	H	22	THR	3.1
1	F	231	PRO	3.1
1	F	233	LEU	3.1
1	F	490	PRO	3.1
1	B	111	ALA	3.1
1	B	268	ALA	3.1
1	B	122	ILE	3.1
1	A	114	PRO	3.1
1	G	23	ALA	3.1
1	A	68	ARG	3.0
1	E	114	PRO	3.0
1	E	129	PRO	3.0
1	C	115	LEU	3.0
1	B	91	GLY	3.0
1	B	512	ARG	3.0
1	E	231	PRO	3.0
1	B	495	ALA	3.0
1	E	70	VAL	3.0
1	F	267[A]	ARG	3.0
1	E	271	GLY	3.0
1	G	24	PHE	3.0
1	A	61	ALA	3.0
1	A	73	LEU	3.0
1	E	270	LEU	3.0
1	B	70	VAL	2.9
1	B	107	VAL	2.9
1	F	112	GLY	2.9
1	E	234	SER	2.9
1	A	241	LEU	2.9
1	E	502	VAL	2.9
1	A	232	GLY	2.9
1	G	52	VAL	2.9
1	B	100	ILE	2.9
1	B	379	LYS	2.9
1	B	382	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	25	PHE	2.9
1	B	230	GLY	2.9
1	B	540[A]	LEU	2.8
1	E	238	VAL	2.8
1	B	489	PRO	2.8
1	A	28	GLN	2.8
1	A	270	LEU	2.8
1	B	416	LEU	2.8
1	E	504	PHE	2.8
1	E	115	LEU	2.8
1	C	23	ALA	2.8
1	A	30	LEU	2.8
1	B	270	LEU	2.8
1	E	511	LEU	2.8
1	F	415	PRO	2.8
1	B	118	ARG	2.7
1	D	275[A]	HIS	2.7
1	C	24	PHE	2.7
1	B	97	ALA	2.7
1	A	488[A]	GLU	2.7
1	B	508	SER	2.7
1	B	84	ALA	2.7
1	B	106	ALA	2.7
1	F	416	LEU	2.7
1	G	272	PRO	2.7
1	E	274	GLY	2.7
1	F	128	GLY	2.7
1	E	269	ALA	2.7
1	F	270	LEU	2.7
1	D	231	PRO	2.7
1	A	496	ASP	2.7
1	F	411	ARG	2.7
1	H	411	ARG	2.7
1	C	114	PRO	2.6
1	E	275	HIS	2.6
1	E	101	ALA	2.6
1	E	24	PHE	2.6
1	F	240	ASP	2.6
1	A	475	VAL	2.6
1	G	63	ILE	2.6
1	B	231	PRO	2.6
1	D	232	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	232	GLY	2.6
1	B	73	LEU	2.6
1	H	514	PHE	2.5
1	A	236	GLN	2.5
1	E	95	TYR	2.5
1	A	34	MET	2.5
1	E	241	LEU	2.5
1	E	485	LEU	2.5
1	F	507	GLU	2.5
1	A	110	PHE	2.5
1	A	527	TRP	2.5
1	B	243	PHE	2.5
1	B	120	VAL	2.5
1	B	245	VAL	2.5
1	B	542	ILE	2.5
1	F	489	PRO	2.5
1	E	30	LEU	2.5
1	B	256	PHE	2.5
1	C	34	MET	2.5
1	B	90	HIS	2.5
1	B	232	GLY	2.5
1	B	498	VAL	2.5
1	E	237	ASP	2.5
1	A	269	ALA	2.5
1	C	272	PRO	2.5
1	A	118	ARG	2.5
1	B	10	ARG	2.5
1	E	487	ARG	2.5
1	F	351	ARG	2.5
1	A	130	GLY	2.5
1	A	263	VAL	2.4
1	E	236	GLN	2.4
1	E	109	SER	2.4
1	E	540	LEU	2.4
1	A	90	HIS	2.4
1	A	112	GLY	2.4
1	E	26	GLN	2.4
1	F	517	VAL	2.4
1	A	378	ALA	2.4
1	F	11	ALA	2.4
1	B	95	TYR	2.4
1	E	106	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	111	ALA	2.4
1	E	515	LEU	2.4
1	D	26	GLN	2.4
1	B	504	PHE	2.4
1	E	242	ARG	2.4
1	E	97	ALA	2.3
1	G	230	GLY	2.3
1	A	277	ILE	2.3
1	B	77	ILE	2.3
1	B	62	THR	2.3
1	B	494	TRP	2.3
1	E	124	LEU	2.3
1	E	244	GLY	2.3
1	B	514	PHE	2.3
1	G	514	PHE	2.3
1	A	498	VAL	2.3
1	B	129	PRO	2.3
1	F	129	PRO	2.3
1	B	260	ALA	2.3
1	B	264	ALA	2.3
1	F	492	ALA	2.3
1	H	23	ALA	2.3
1	B	237	ASP	2.3
1	C	116	SER	2.3
1	F	229	SER	2.3
1	B	63	ILE	2.3
1	C	107	VAL	2.3
1	G	231	PRO	2.3
1	B	516	ARG	2.3
1	B	233	LEU	2.3
1	A	426	ILE	2.2
1	B	347	ILE	2.2
1	A	106	ALA	2.2
1	F	530	GLY	2.2
1	B	86	LEU	2.2
1	B	503	GLN	2.2
1	A	242	ARG	2.2
1	B	110	PHE	2.2
1	B	482	PHE	2.2
1	F	514	PHE	2.2
1	H	24	PHE	2.2
1	H	412	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	251	ILE	2.2
1	B	279	ILE	2.2
1	E	103	VAL	2.2
1	F	245	VAL	2.2
1	E	128	GLY	2.2
1	F	274	GLY	2.2
1	A	111	ALA	2.2
1	E	90	HIS	2.2
1	H	275[A]	HIS	2.2
1	A	243	PHE	2.2
1	A	311	ILE	2.2
1	E	110	PHE	2.2
1	E	277	ILE	2.2
1	B	266	VAL	2.2
1	E	245	VAL	2.2
1	A	91	GLY	2.2
1	A	265	ALA	2.2
1	B	236	GLN	2.2
1	B	378	ALA	2.2
1	A	89	SER	2.2
1	B	109	SER	2.2
1	E	351	ARG	2.2
1	B	415	PRO	2.1
1	E	499	ASP	2.2
1	F	130	GLY	2.1
1	A	33	ALA	2.1
1	A	115	LEU	2.1
1	A	540	LEU	2.1
1	C	113	SER	2.1
1	A	252	VAL	2.1
1	B	263	VAL	2.1
1	B	505	GLY	2.1
1	C	112	GLY	2.1
1	E	130	GLY	2.1
1	E	403	HIS	2.1
1	H	516	ARG	2.1
1	B	101	ALA	2.1
1	E	264	ALA	2.1
1	A	99	SER	2.1
1	A	237	ASP	2.1
1	A	100	ILE	2.1
1	B	242	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	506	ILE	2.1
1	G	130	GLY	2.1
1	A	249	VAL	2.1
1	F	484	LEU	2.1
1	B	262	ASP	2.1
1	A	62	THR	2.1
1	A	351	ARG	2.1
1	B	275	HIS	2.1
1	E	272	PRO	2.1
1	A	80	GLY	2.1
1	B	380	GLY	2.1
1	E	230	GLY	2.1
1	E	52	VAL	2.1
1	E	256	PHE	2.1
1	E	517	VAL	2.1
1	F	243	PHE	2.1
1	A	494	TRP	2.1
1	B	234	SER	2.1
1	E	229	SER	2.1
1	F	97	ALA	2.1
1	F	269	ALA	2.1
1	A	511	LEU	2.0
1	B	515	LEU	2.0
1	F	453	LEU	2.0
1	H	416	LEU	2.0
1	F	90	HIS	2.0
1	F	275	HIS	2.0
1	A	51	PRO	2.0
1	A	107	VAL	2.0
1	A	245	VAL	2.0
1	A	257	VAL	2.0
1	E	120	VAL	2.0
1	B	92	SER	2.0
1	A	32	ALA	2.0
1	D	412	ARG	2.0
1	B	272	PRO	2.0
1	B	112	GLY	2.0
1	E	505	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	A1JBZ	F	605	35/35	0.88	0.16	62,68,73,73	25
6	A1JBZ	E	605	35/35	0.89	0.15	59,65,69,69	25
5	K	A	604	1/1	0.90	0.10	90,90,90,90	0
5	K	E	604	1/1	0.90	0.17	90,90,90,90	0
3	OXL	A	602	6/6	0.90	0.11	51,51,52,52	0
3	OXL	E	602	6/6	0.90	0.11	54,54,54,55	0
6	A1JBZ	A	605	35/35	0.91	0.14	50,57,62,62	25
6	A1JBZ	D	605	35/35	0.91	0.14	58,60,63,63	25
3	OXL	B	602	6/6	0.92	0.12	46,47,48,48	0
2	FBP	B	601	20/20	0.93	0.10	47,49,54,54	0
3	OXL	H	602	6/6	0.93	0.10	33,34,34,34	0
5	K	C	604	1/1	0.94	0.16	58,58,58,58	0
3	OXL	D	602	6/6	0.94	0.08	30,32,33,34	0
3	OXL	G	602	6/6	0.94	0.11	38,39,39,39	0
2	FBP	E	601	20/20	0.95	0.08	41,43,44,44	0
5	K	F	604	1/1	0.95	0.09	76,76,76,76	0
3	OXL	C	602	6/6	0.95	0.09	42,43,43,43	0
2	FBP	F	601	20/20	0.95	0.07	35,39,44,44	0
5	K	B	604	1/1	0.95	0.10	81,81,81,81	0
2	FBP	A	601	20/20	0.95	0.07	37,39,41,41	0
3	OXL	F	602	6/6	0.96	0.10	45,46,47,48	0
5	K	G	604	1/1	0.97	0.07	54,54,54,54	0
2	FBP	C	601	20/20	0.98	0.04	21,22,26,27	0
5	K	H	604	1/1	0.98	0.05	44,44,44,44	0
2	FBP	D	601	20/20	0.98	0.04	22,25,26,27	0
5	K	D	604	1/1	0.98	0.07	43,43,43,43	0
4	MG	E	603	1/1	0.98	0.12	21,21,21,21	0
2	FBP	H	601	20/20	0.98	0.05	19,21,22,23	0
4	MG	A	603	1/1	0.99	0.10	24,24,24,24	0
4	MG	B	603	1/1	0.99	0.12	22,22,22,22	0
2	FBP	G	601	20/20	0.99	0.04	20,21,23,23	0
4	MG	F	603	1/1	1.00	0.09	13,13,13,13	0

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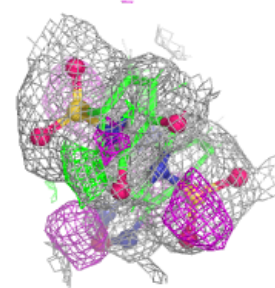
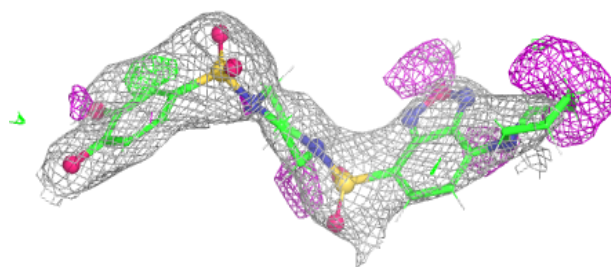
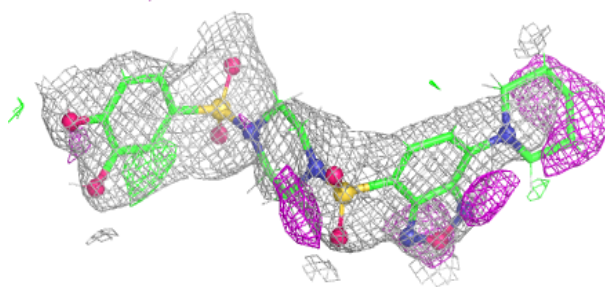
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	G	603	1/1	1.00	0.09	6,6,6,6	0
4	MG	H	603	1/1	1.00	0.09	4,4,4,4	0
4	MG	D	603	1/1	1.00	0.09	5,5,5,5	0
4	MG	C	603	1/1	1.00	0.11	15,15,15,15	0

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.

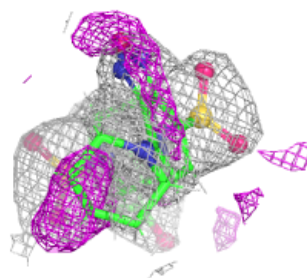
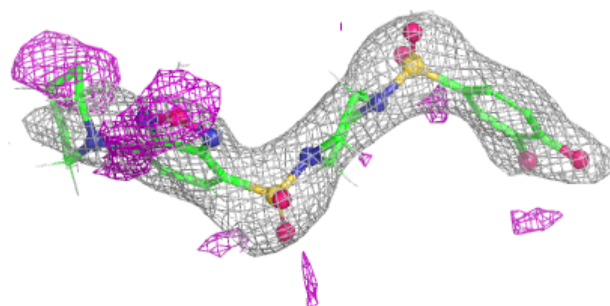
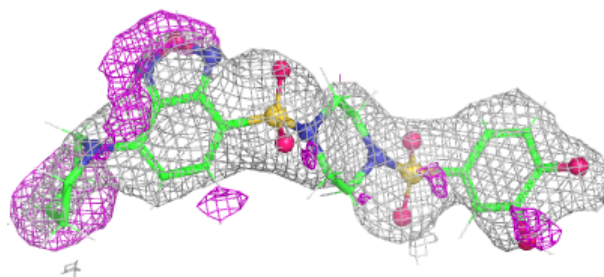
Electron density around A1JBZ F 605:

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

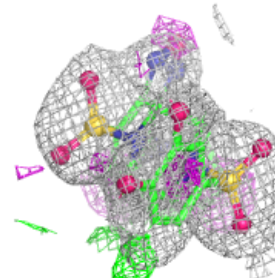
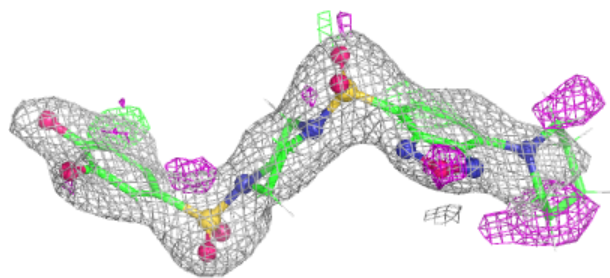
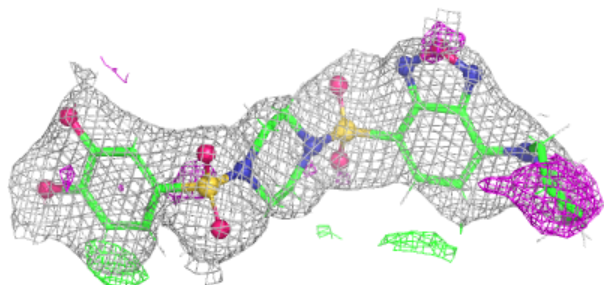


Electron density around A1JBZ E 605:

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

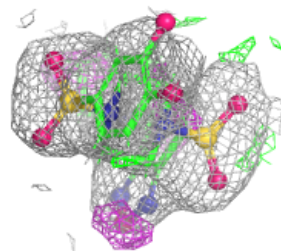
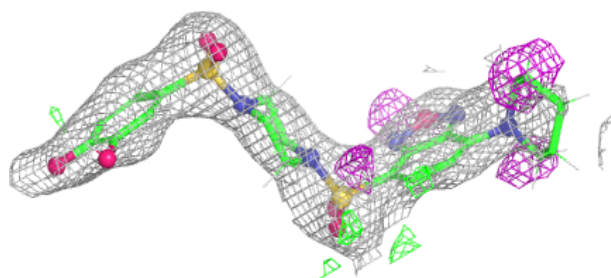
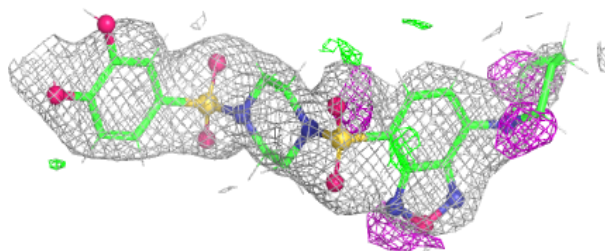
**Electron density around A1JBZ A 605:**

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

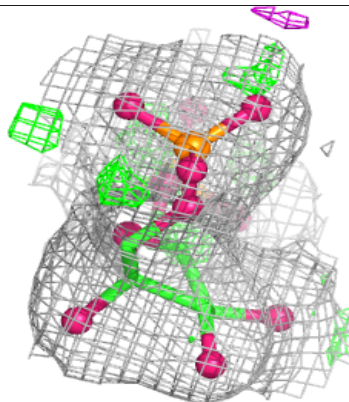
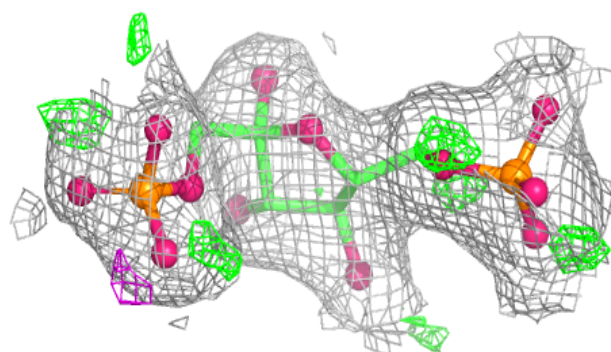
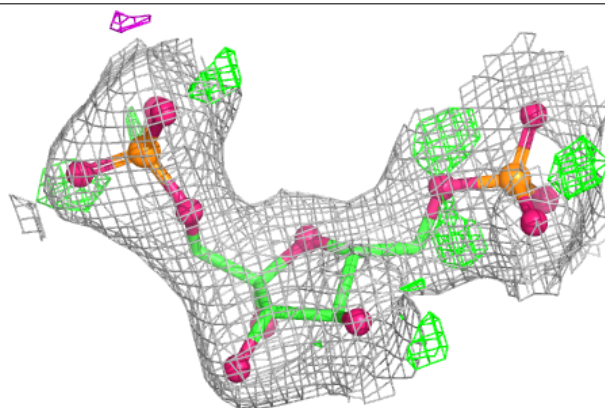


Electron density around A1JBZ D 605:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

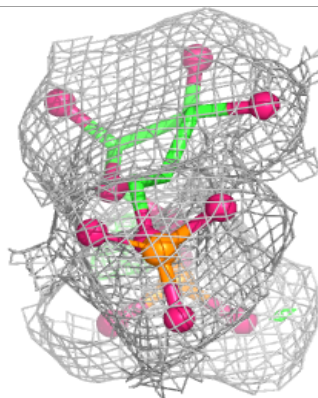
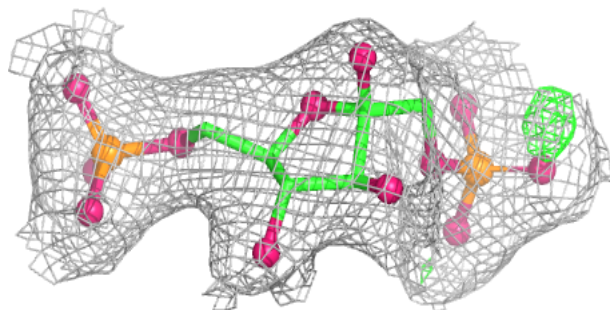
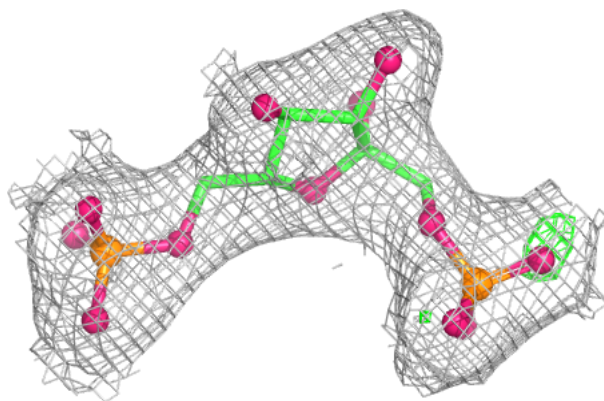
**Electron density around FBP B 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

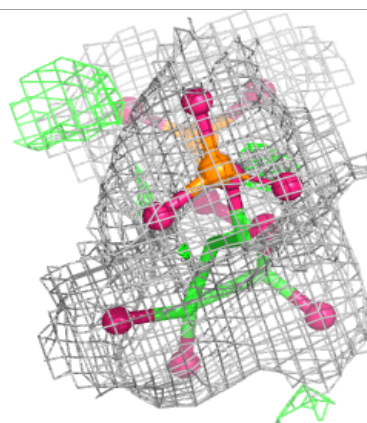
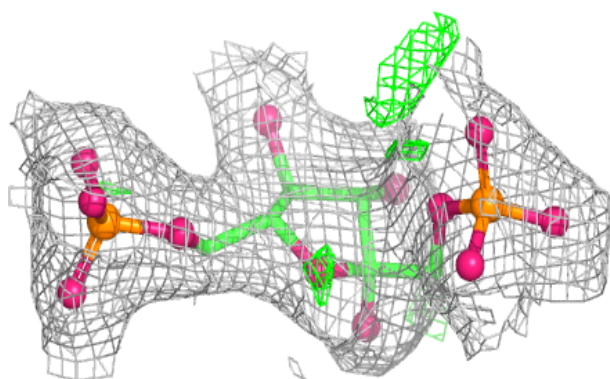
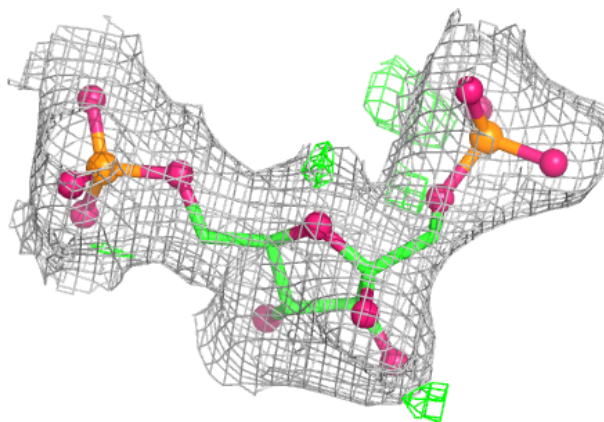


Electron density around FBP E 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

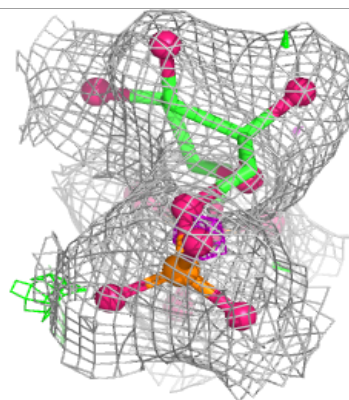
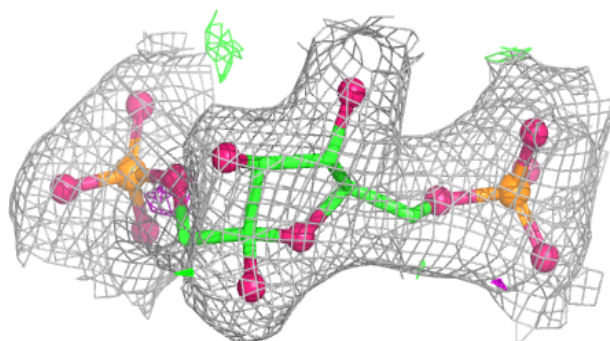
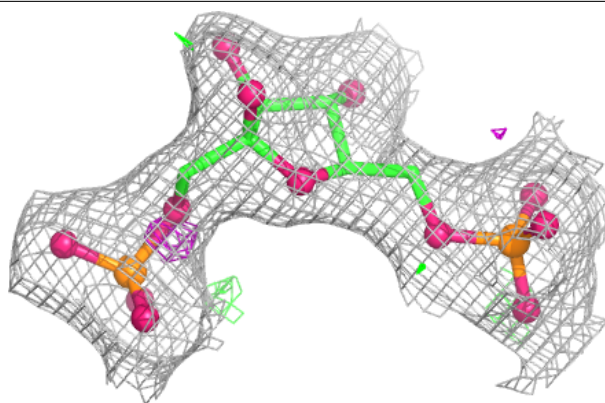
**Electron density around FBP F 601:**

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

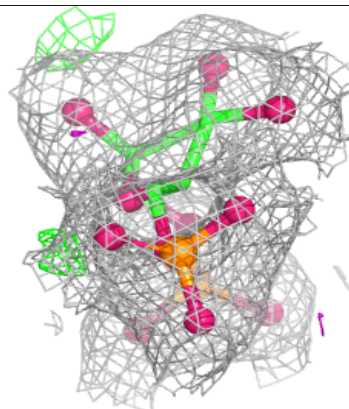
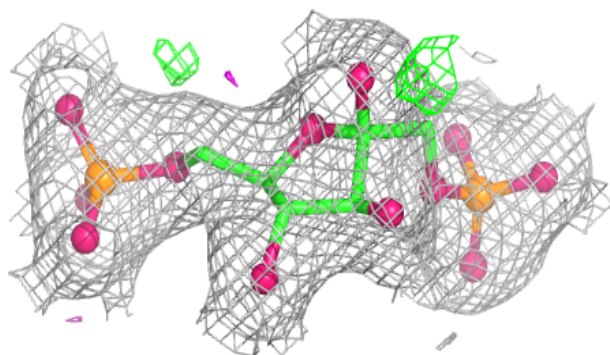
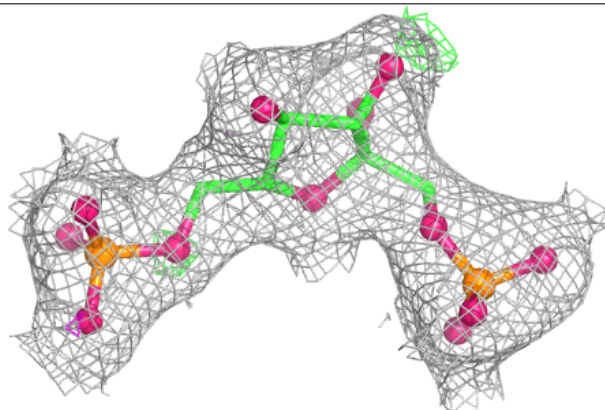


Electron density around FBP A 601:

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

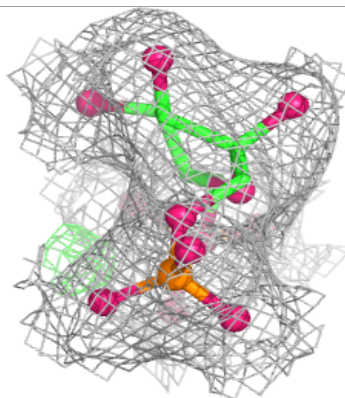
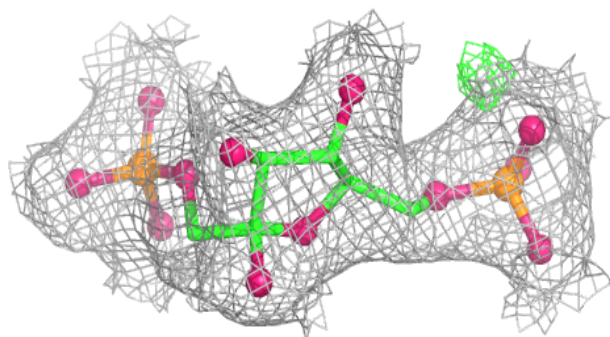
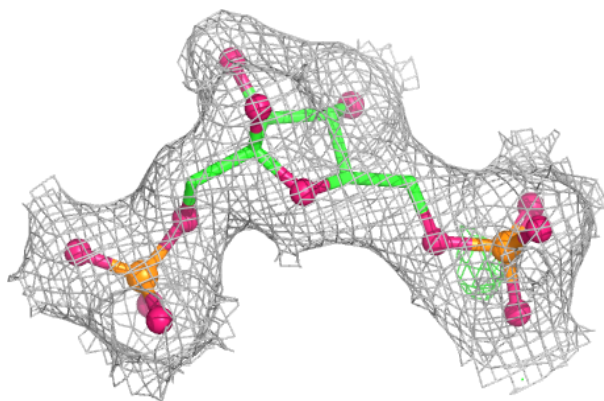
**Electron density around FBP C 601:**

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

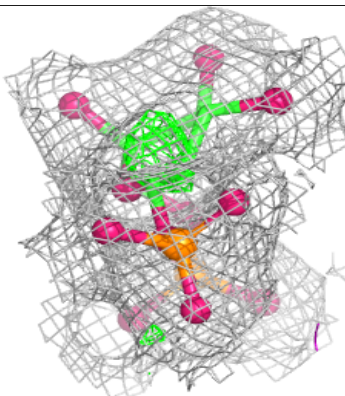
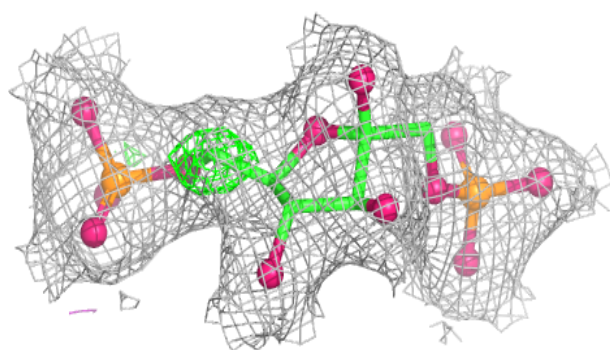
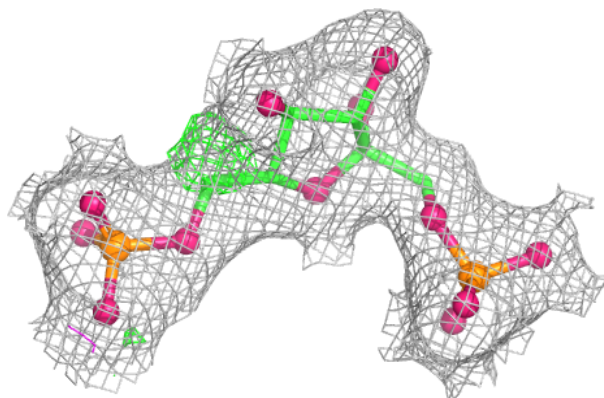


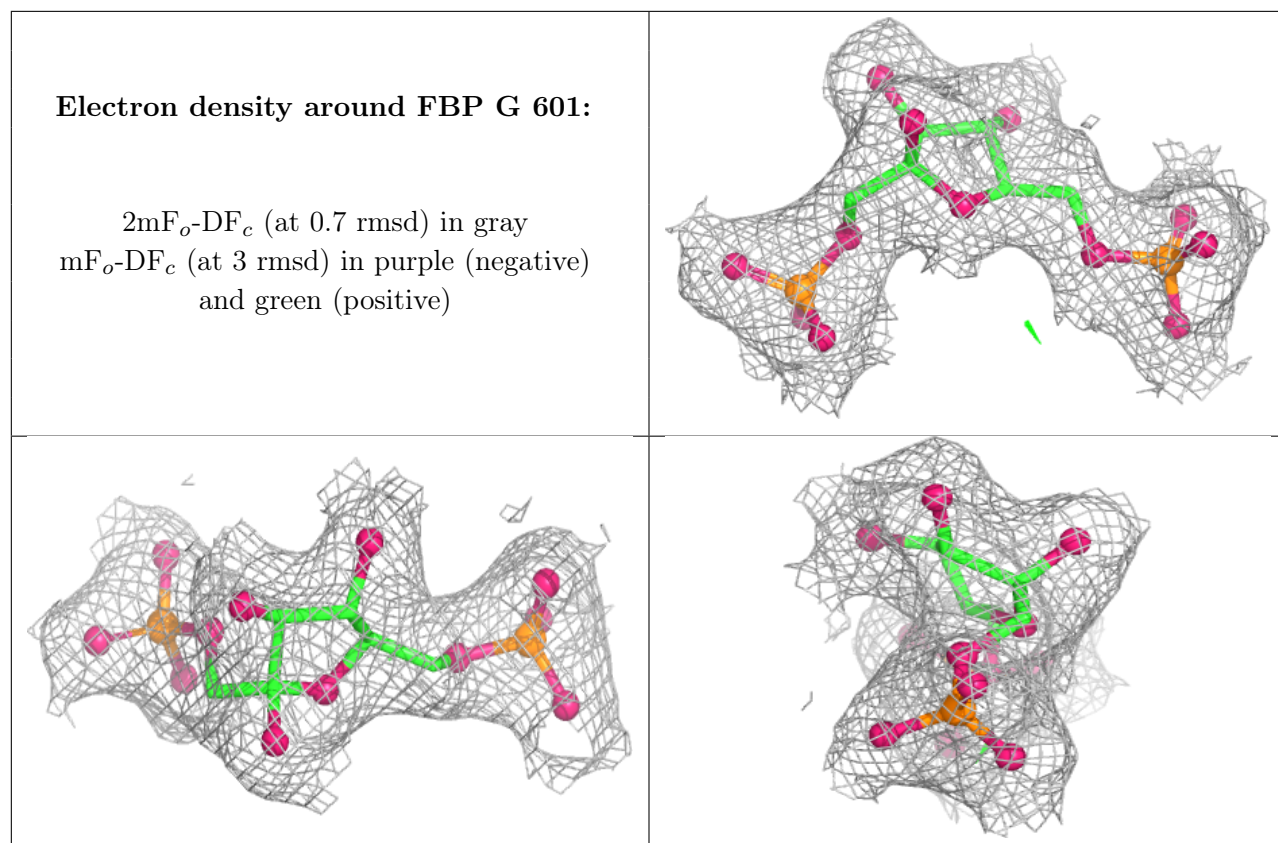
Electron density around FBP D 601:

$2mF_o-DF_c$ (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.