



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2025 – 08:09 pm BST

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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

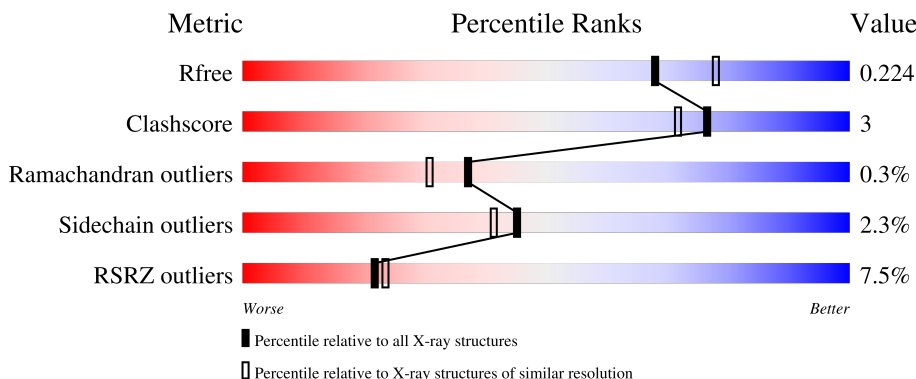
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (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	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	447	<div> <div>17%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	C	447	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	447	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>
1	E	447	<div> <div>11%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	447	<div><div></div><div>7%</div><div>87%</div><div>9%</div><div>• •</div></div>
1	G	447	<div><div></div><div>2%</div><div>85%</div><div>8%</div><div>• 5%</div></div>
1	H	447	<div><div></div><div>3%</div><div>89%</div><div>5%</div><div>5%</div></div>

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
C	?	-	SER	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	LYS	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	SER	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	ALA	deletion	UNP P30613
C	?	-	PHE	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	ALA	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	TRP	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	TYR	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613

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

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

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

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

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

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

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

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

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

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

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

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

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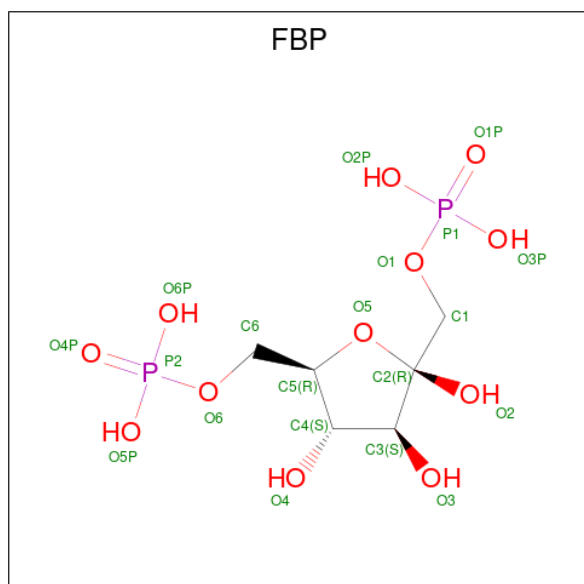
Chain	Residue	Modelled	Actual	Comment	Reference
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H	?	-	VAL	deletion	UNP P30613
H	?	-	TRP	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	TYR	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	ASN	deletion	UNP 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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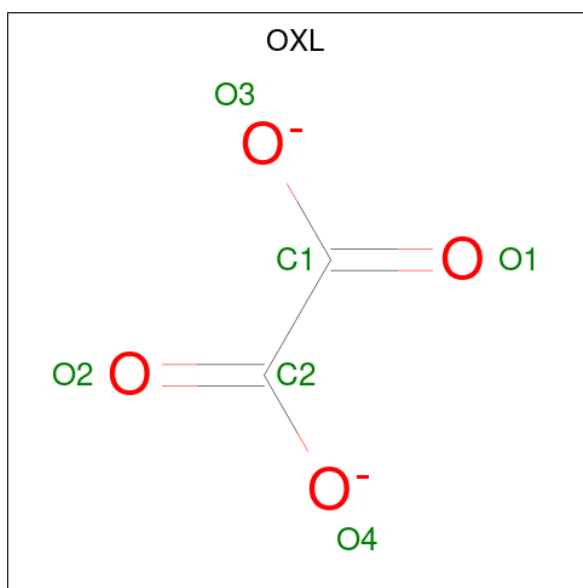
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLU	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	ARG	deletion	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).

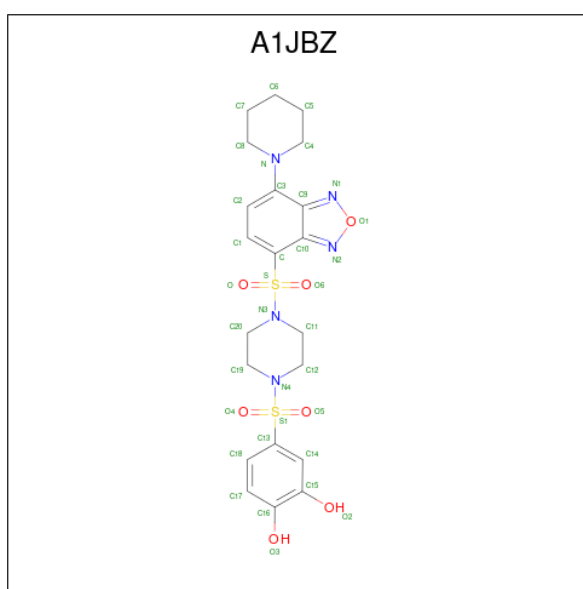
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	E	1	Total K 1 1	0	0

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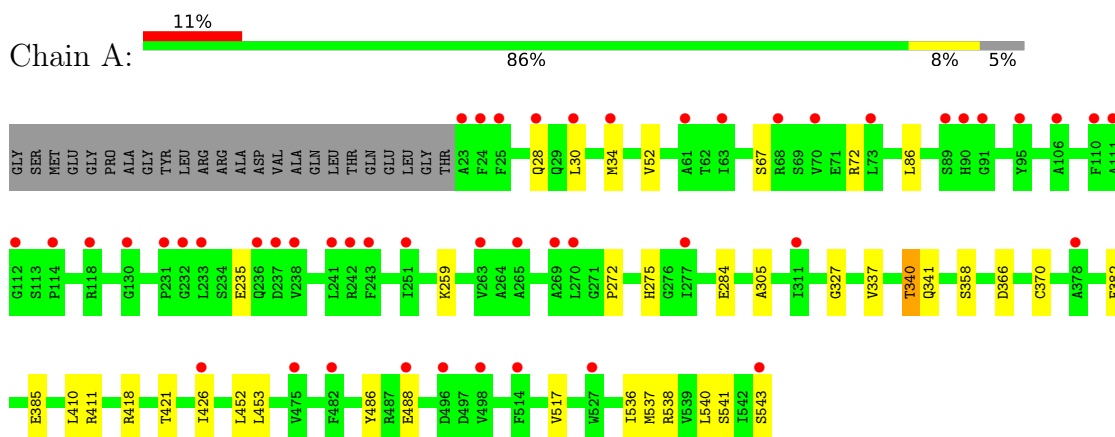
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	154	Total 154	O 154	0	0
7	C	299	Total 299	O 299	0	0
7	D	321	Total 321	O 321	0	0
7	E	181	Total 181	O 181	0	0
7	F	252	Total 252	O 252	0	0
7	G	322	Total 322	O 322	0	0
7	H	397	Total 397	O 397	0	0

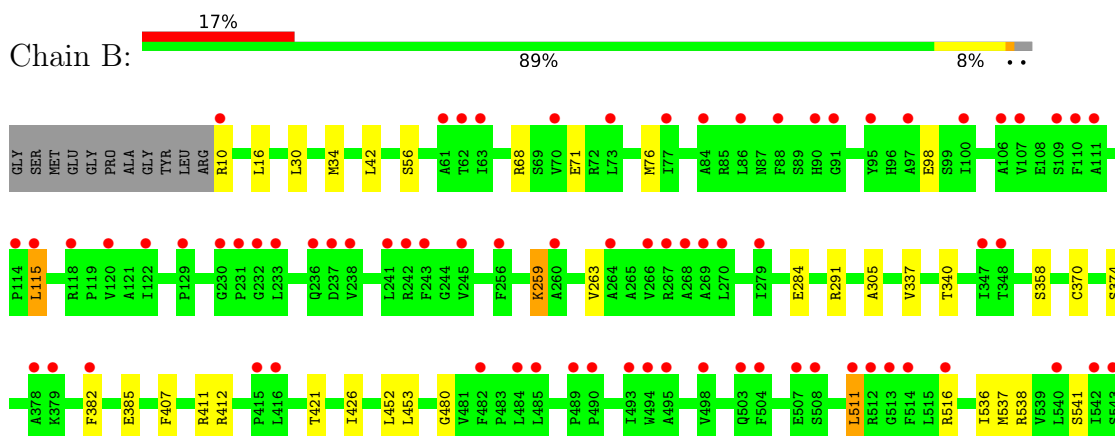
3 Residue-property plots [i](#)

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.

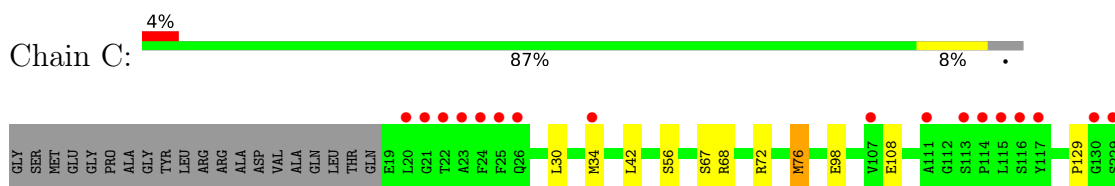
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



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

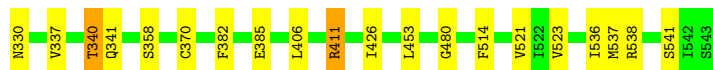
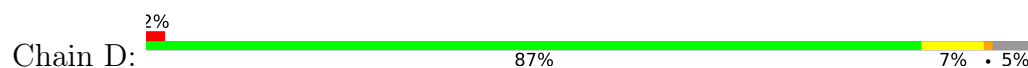


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

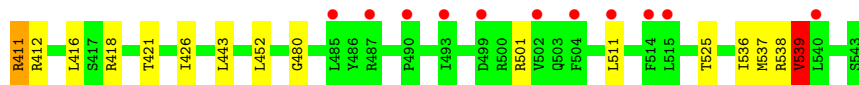
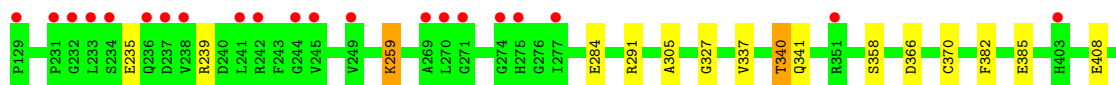
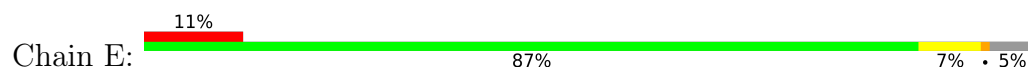




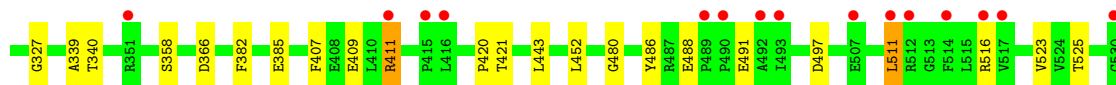
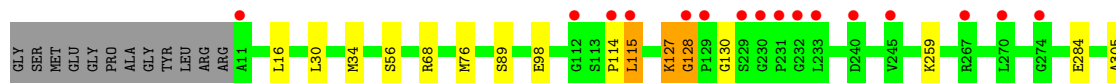
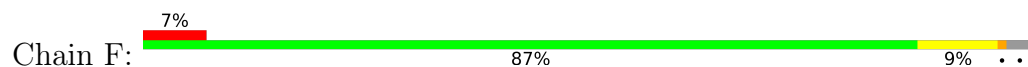
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



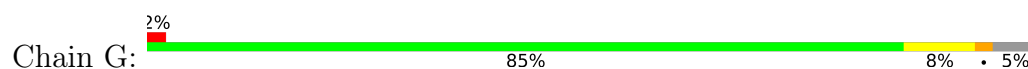
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

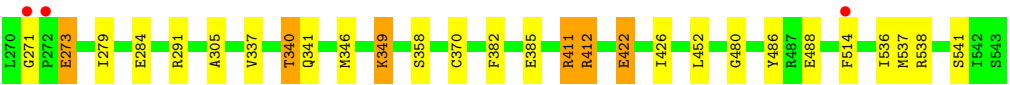


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

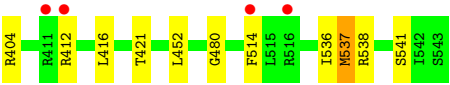
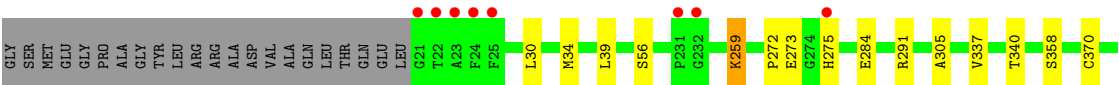
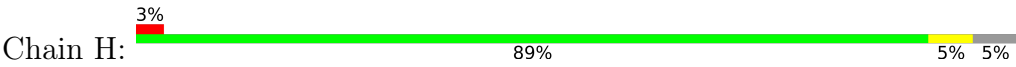


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR





● 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	208.44Å 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, A1JBZ, FBP, MG, OXL

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 [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%)	423 (99%)	3 (1%)	1 (0%)	44 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	438/447 (98%)	434 (99%)	3 (1%)	1 (0%)	44	38
1	C	429/447 (96%)	423 (99%)	5 (1%)	1 (0%)	44	38
1	D	429/447 (96%)	425 (99%)	3 (1%)	1 (0%)	44	38
1	E	426/447 (95%)	421 (99%)	4 (1%)	1 (0%)	44	38
1	F	440/447 (98%)	435 (99%)	2 (0%)	3 (1%)	19	10
1	G	427/447 (96%)	420 (98%)	6 (1%)	1 (0%)	44	38
1	H	427/447 (96%)	424 (99%)	2 (0%)	1 (0%)	44	38
All	All	3443/3576 (96%)	3405 (99%)	28 (1%)	10 (0%)	37	31

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%)	45	41
1	B	349/352 (99%)	336 (96%)	13 (4%)	29	23
1	C	342/352 (97%)	338 (99%)	4 (1%)	67	68
1	D	342/352 (97%)	333 (97%)	9 (3%)	41	37
1	E	340/352 (97%)	332 (98%)	8 (2%)	44	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	351/352 (100%)	339 (97%)	12 (3%)	32	26
1	G	341/352 (97%)	330 (97%)	11 (3%)	34	28
1	H	340/352 (97%)	334 (98%)	6 (2%)	54	52
All	All	2746/2816 (98%)	2675 (97%)	71 (3%)	45	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	F	601	-	18,20,20	0.46	0	23,32,32	0.62	0
2	FBP	D	601	-	18,20,20	0.49	0	23,32,32	0.92	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	B	602	4	5,5,5	2.03	2 (40%)	6,6,6	0.80	0
6	A1JBZ	A	605	-	37,39,39	0.69	1 (2%)	50,59,59	0.68	0
2	FBP	C	601	-	18,20,20	0.52	0	23,32,32	0.62	0
3	OXL	F	602	4	5,5,5	1.80	2 (40%)	6,6,6	1.58	2 (33%)
3	OXL	E	602	4	5,5,5	1.83	2 (40%)	6,6,6	1.25	1 (16%)
3	OXL	C	602	4	5,5,5	1.73	1 (20%)	6,6,6	1.93	3 (50%)
6	A1JBZ	D	605	-	37,39,39	0.74	1 (2%)	50,59,59	0.67	0
3	OXL	A	602	4	5,5,5	1.80	2 (40%)	6,6,6	1.63	2 (33%)
6	A1JBZ	F	605	-	37,39,39	0.65	1 (2%)	50,59,59	0.77	1 (2%)
2	FBP	E	601	-	18,20,20	0.43	0	23,32,32	0.69	1 (4%)
2	FBP	B	601	-	18,20,20	0.42	0	23,32,32	0.85	1 (4%)
3	OXL	D	602	4	5,5,5	2.18	2 (40%)	6,6,6	1.77	2 (33%)
3	OXL	G	602	4	5,5,5	2.19	2 (40%)	6,6,6	0.65	0
2	FBP	A	601	-	18,20,20	0.48	0	23,32,32	0.69	0
2	FBP	H	601	-	18,20,20	0.70	0	23,32,32	0.73	1 (4%)
2	FBP	G	601	-	18,20,20	0.68	0	23,32,32	0.73	0
3	OXL	H	602	4	5,5,5	1.81	2 (40%)	6,6,6	1.32	1 (16%)
6	A1JBZ	E	605	-	37,39,39	0.68	1 (2%)	50,59,59	0.67	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
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	1/4/4/4	-
6	A1JBZ	A	605	-	-	13/28/46/46	0/5/5/5
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	OXL	F	602	4	-	0/4/4/4	-
3	OXL	E	602	4	-	0/4/4/4	-
3	OXL	C	602	4	-	0/4/4/4	-
6	A1JBZ	D	605	-	-	15/28/46/46	0/5/5/5
3	OXL	A	602	4	-	0/4/4/4	-
6	A1JBZ	F	605	-	-	17/28/46/46	0/5/5/5
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	4	-	0/4/4/4	-
3	OXL	G	602	4	-	0/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	1/4/4/4	-
6	A1JBZ	E	605	-	-	14/28/46/46	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	OXL	O2-C2	4.07	1.33	1.22
3	D	602	OXL	O2-C2	3.64	1.32	1.22
3	B	602	OXL	O2-C2	3.52	1.32	1.22
3	A	602	OXL	O2-C2	3.45	1.31	1.22
3	C	602	OXL	O2-C2	3.34	1.31	1.22
3	F	602	OXL	O2-C2	3.18	1.31	1.22
6	E	605	A1JBZ	C-C10	-3.15	1.40	1.42
6	D	605	A1JBZ	C-C10	-3.14	1.40	1.42
6	A	605	A1JBZ	C-C10	-3.12	1.40	1.42
3	H	602	OXL	O2-C2	3.09	1.30	1.22
6	F	605	A1JBZ	C-C10	-2.98	1.40	1.42
3	B	602	OXL	O4-C2	-2.81	1.22	1.30
3	E	602	OXL	O2-C2	2.81	1.30	1.22
3	E	602	OXL	O4-C2	-2.80	1.22	1.30
3	D	602	OXL	O4-C2	-2.67	1.22	1.30
3	G	602	OXL	O4-C2	-2.56	1.23	1.30
3	H	602	OXL	O4-C2	-2.33	1.23	1.30
3	F	602	OXL	O4-C2	-2.18	1.24	1.30
3	A	602	OXL	O4-C2	-2.07	1.24	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	OXL	O4-C2-C1	3.19	122.64	113.16
2	D	601	FBP	O6-P2-O4P	2.95	114.76	106.47
3	F	602	OXL	O4-C2-C1	2.93	121.85	113.16
3	A	602	OXL	O4-C2-C1	2.79	121.44	113.16
2	B	601	FBP	O6-P2-O4P	2.60	113.77	106.47
3	D	602	OXL	O4-C2-C1	2.60	120.88	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	605	A1JBZ	C10-C9-N1	-2.57	103.91	110.11
3	C	602	OXL	O2-C2-C1	-2.55	112.60	120.78
3	H	602	OXL	O4-C2-C1	2.53	120.69	113.16
2	H	601	FBP	O6-P2-O4P	2.40	113.19	106.47
3	D	602	OXL	O3-C1-C2	2.35	120.13	113.16
3	E	602	OXL	O4-C2-C1	2.34	120.12	113.16
6	E	605	A1JBZ	C10-C9-N1	-2.29	104.57	110.11
2	D	601	FBP	P1-O1-C1	2.29	124.59	118.30
3	F	602	OXL	O2-C2-C1	-2.25	113.54	120.78
2	E	601	FBP	P1-O1-C1	2.21	124.39	118.30
3	A	602	OXL	O2-C2-C1	-2.03	114.28	120.78
3	C	602	OXL	O3-C1-C2	2.02	119.15	113.16

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
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	C10-C-S-O
6	E	605	A1JBZ	C10-C-S-O
6	F	605	A1JBZ	C2-C3-N-C4
6	F	605	A1JBZ	C9-C3-N-C4
6	A	605	A1JBZ	C19-N4-S1-O4
6	D	605	A1JBZ	C12-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	A	605	A1JBZ	C19-N4-S1-C13
6	D	605	A1JBZ	C20-N3-S-O
6	D	605	A1JBZ	C12-N4-S1-C13
6	E	605	A1JBZ	C11-N3-S-C
6	E	605	A1JBZ	C12-N4-S1-O4
6	E	605	A1JBZ	C12-N4-S1-O5
6	F	605	A1JBZ	C11-N3-S-O6
6	F	605	A1JBZ	C19-N4-S1-O5
6	F	605	A1JBZ	C12-N4-S1-O4

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Mol	Chain	Res	Type	Atoms
6	F	605	A1JBZ	C12-N4-S1-O5
6	A	605	A1JBZ	C11-N3-S-O
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	E	605	A1JBZ	C19-N4-S1-O5
6	A	605	A1JBZ	C11-N3-S-O6
6	A	605	A1JBZ	C20-N3-S-C
6	D	605	A1JBZ	C11-N3-S-C
6	D	605	A1JBZ	C12-N4-S1-O5
6	E	605	A1JBZ	C11-N3-S-O
6	E	605	A1JBZ	C19-N4-S1-O4
6	F	605	A1JBZ	C11-N3-S-C
6	F	605	A1JBZ	C19-N4-S1-C13
6	F	605	A1JBZ	C19-N4-S1-O4
6	F	605	A1JBZ	C12-N4-S1-C13
6	A	605	A1JBZ	C11-N3-S-C
6	D	605	A1JBZ	C20-N3-S-C
6	E	605	A1JBZ	C19-N4-S1-C13
6	E	605	A1JBZ	C12-N4-S1-C13
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
6	A	605	A1JBZ	C12-N4-S1-C13
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	E	605	A1JBZ	C20-N3-S-C
2	E	601	FBP	O5-C5-C6-O6
6	F	605	A1JBZ	C20-N3-S-O6
6	F	605	A1JBZ	C20-N3-S-O
6	D	605	A1JBZ	C2-C3-N-C4
6	D	605	A1JBZ	C9-C3-N-C4

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Mol	Chain	Res	Type	Atoms
6	F	605	A1JBZ	C2-C3-N-C8
6	F	605	A1JBZ	C9-C3-N-C8
6	D	605	A1JBZ	C19-N4-S1-C13
6	D	605	A1JBZ	C10-C-S-O6
6	F	605	A1JBZ	C10-C-S-O
2	G	601	FBP	O5-C5-C6-O6
6	F	605	A1JBZ	C20-N3-S-C
6	E	605	A1JBZ	C10-C-S-O6
3	H	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4

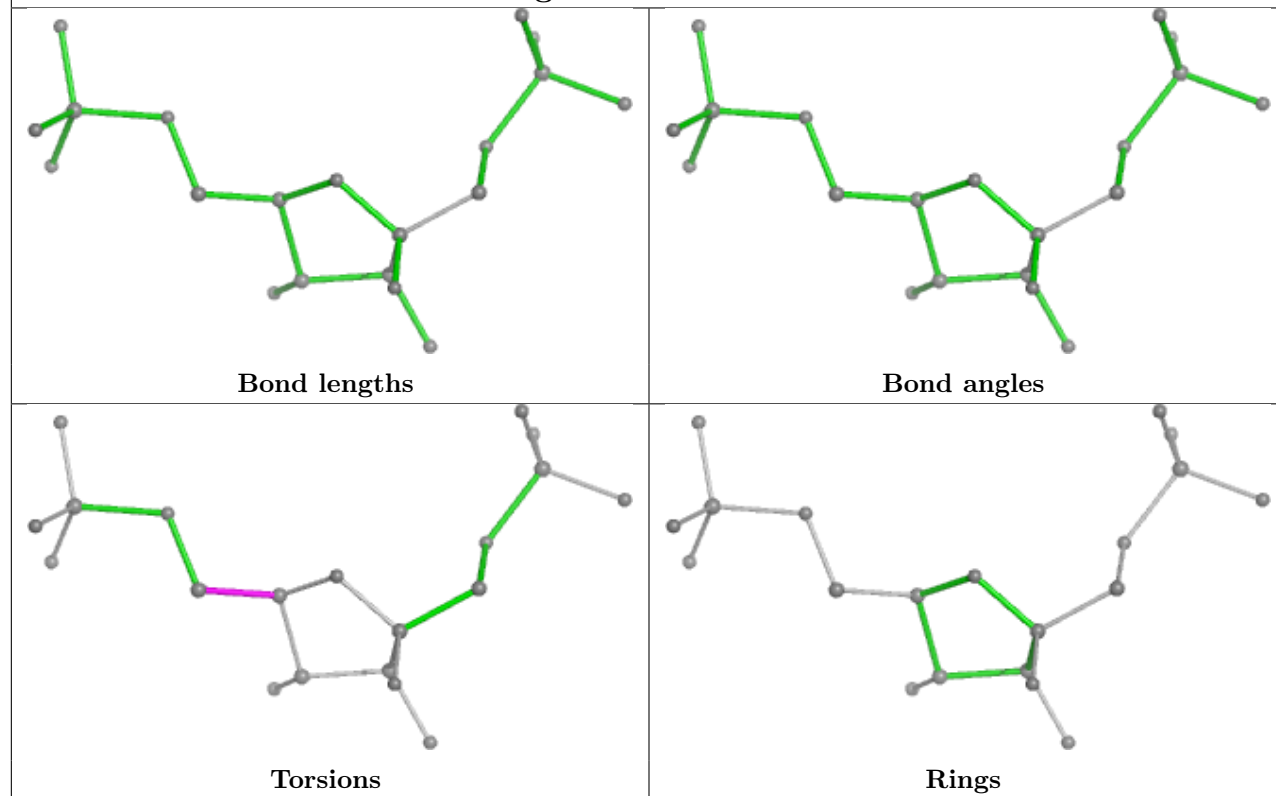
There are no ring outliers.

5 monomers are involved in 18 short contacts:

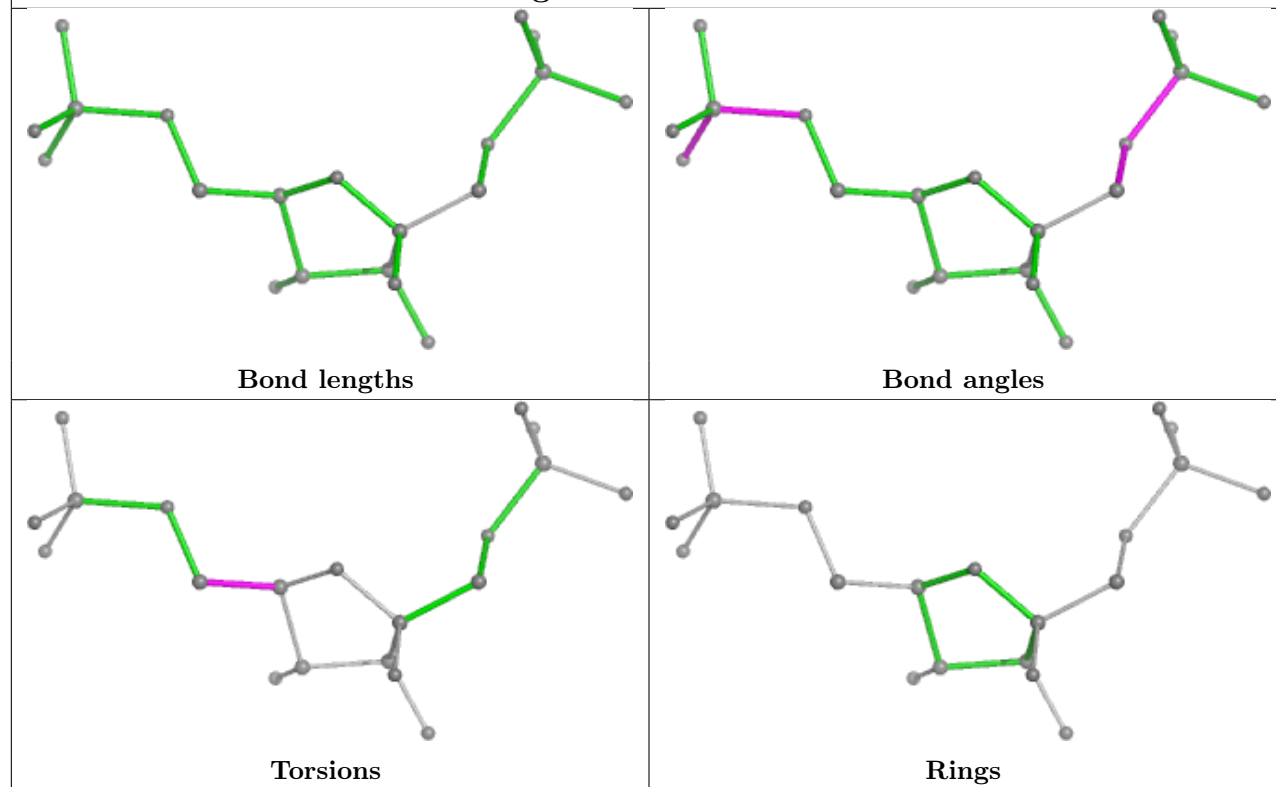
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	605	A1JBZ	3	0
6	D	605	A1JBZ	6	0
6	F	605	A1JBZ	5	0
2	E	601	FBP	1	0
6	E	605	A1JBZ	3	0

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.

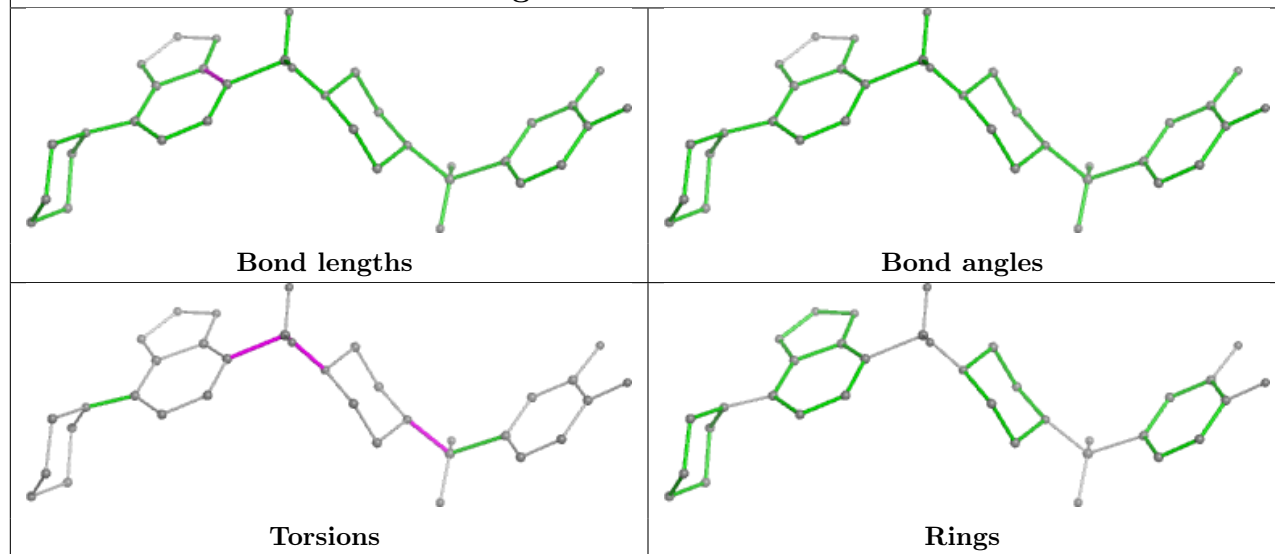
Ligand FBP F 601



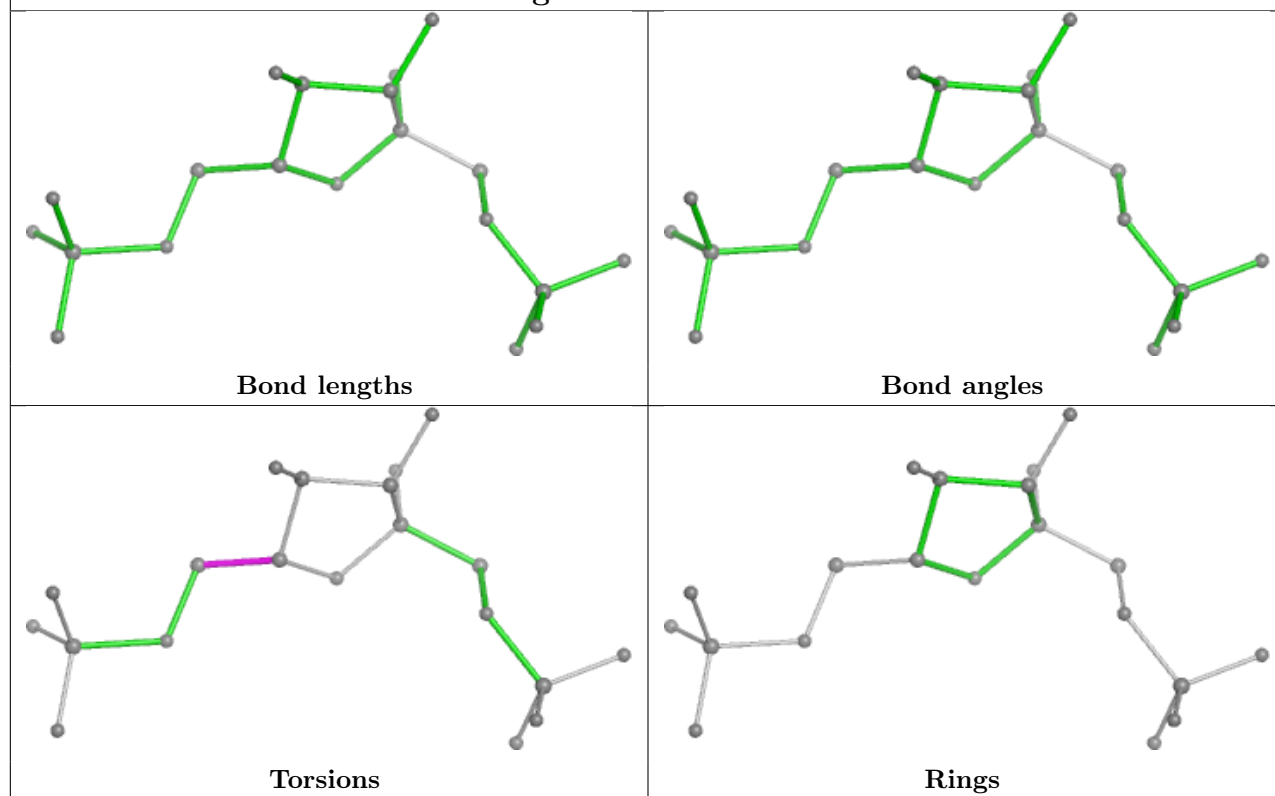
Ligand FBP D 601



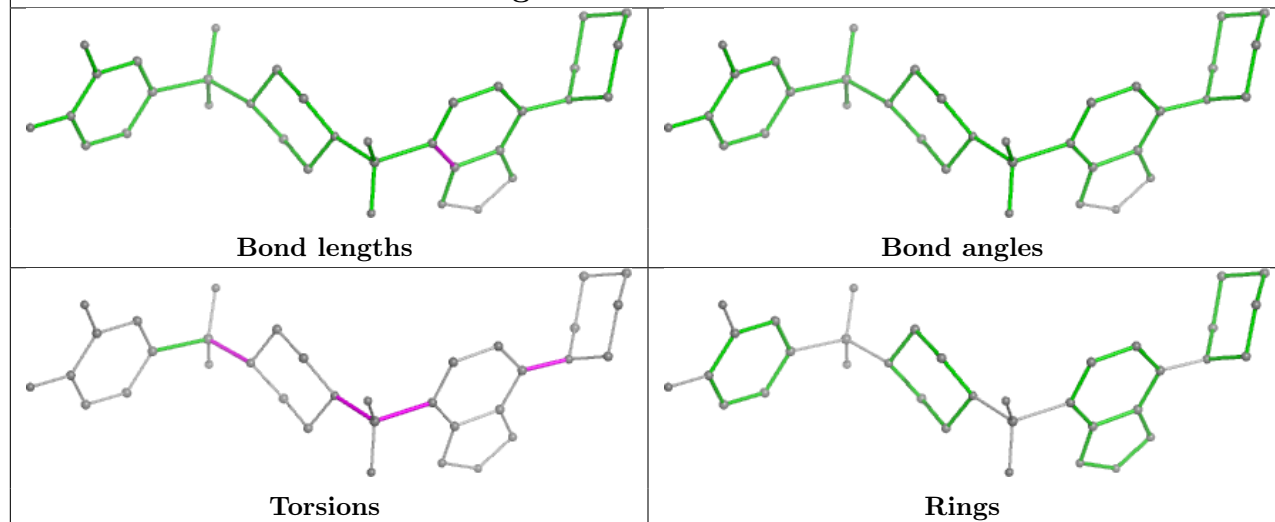
Ligand A1JBZ A 605



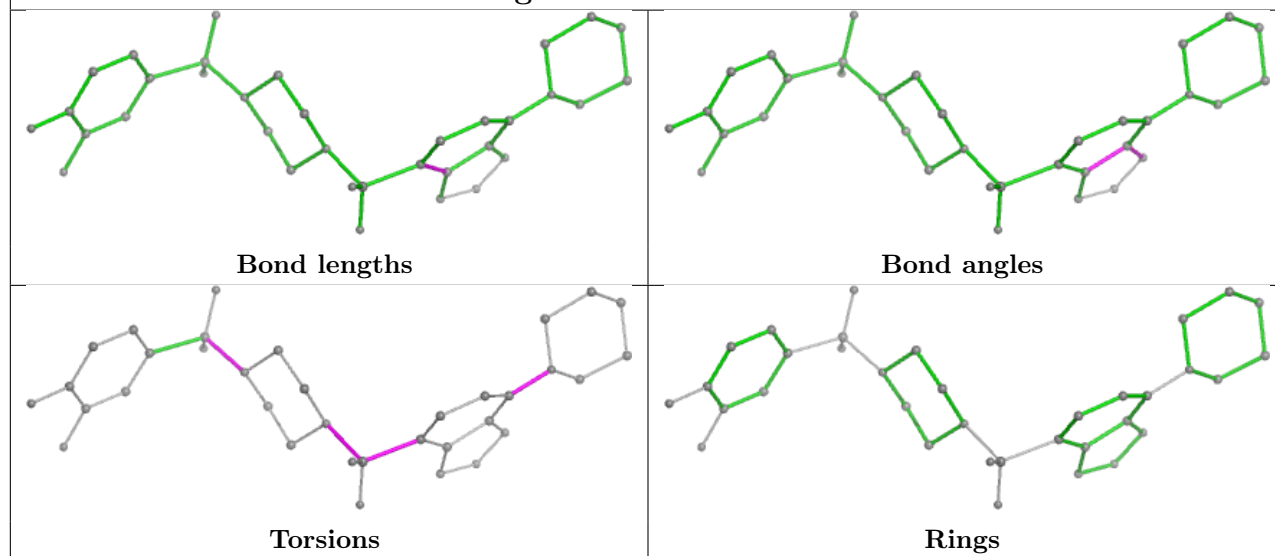
Ligand FBP C 601



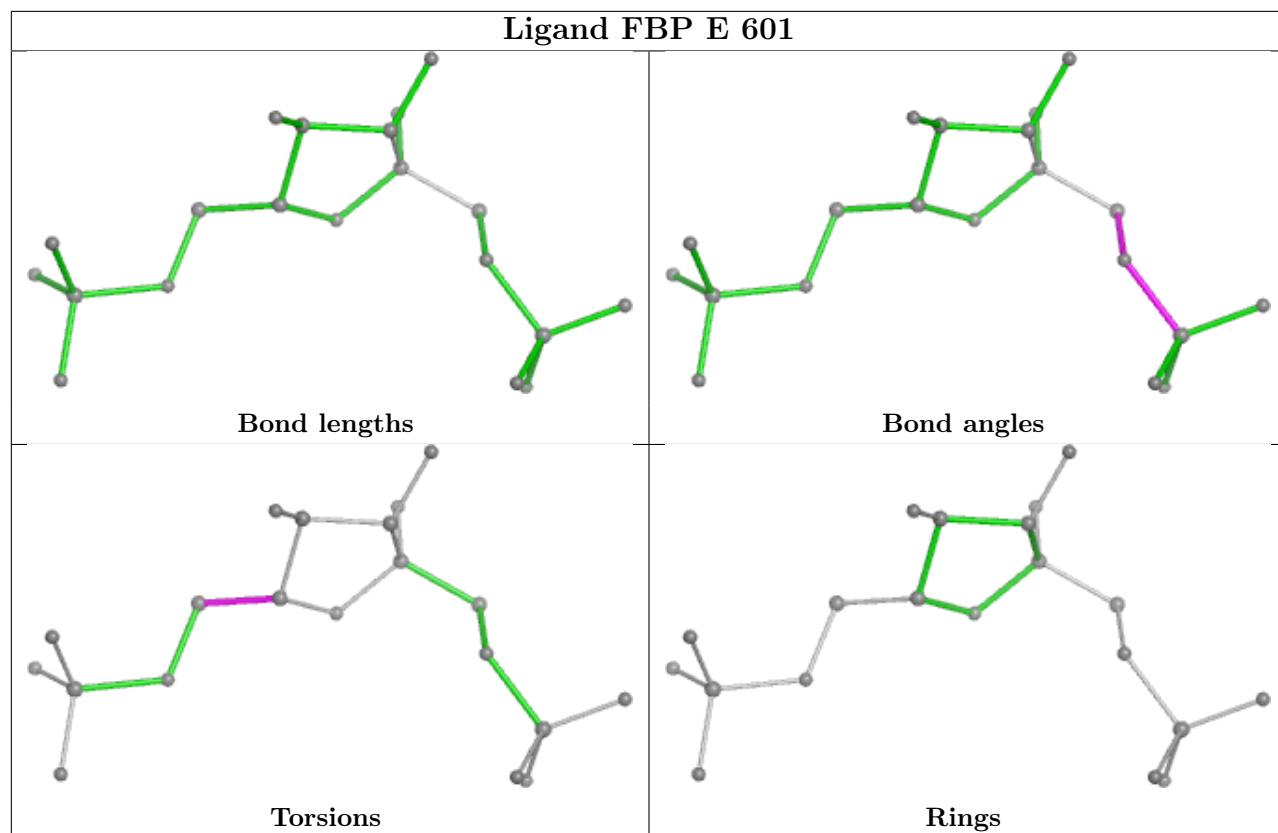
Ligand A1JBZ D 605



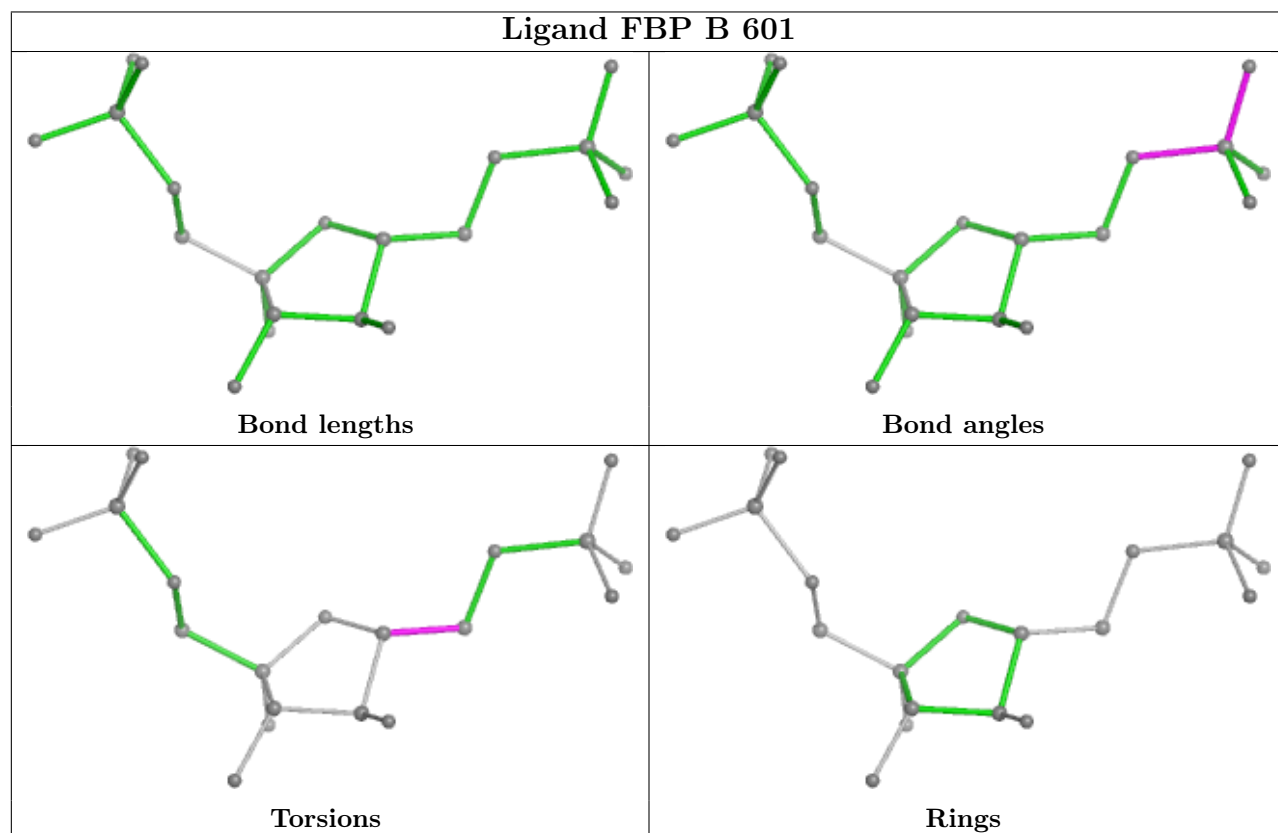
Ligand A1JBZ F 605



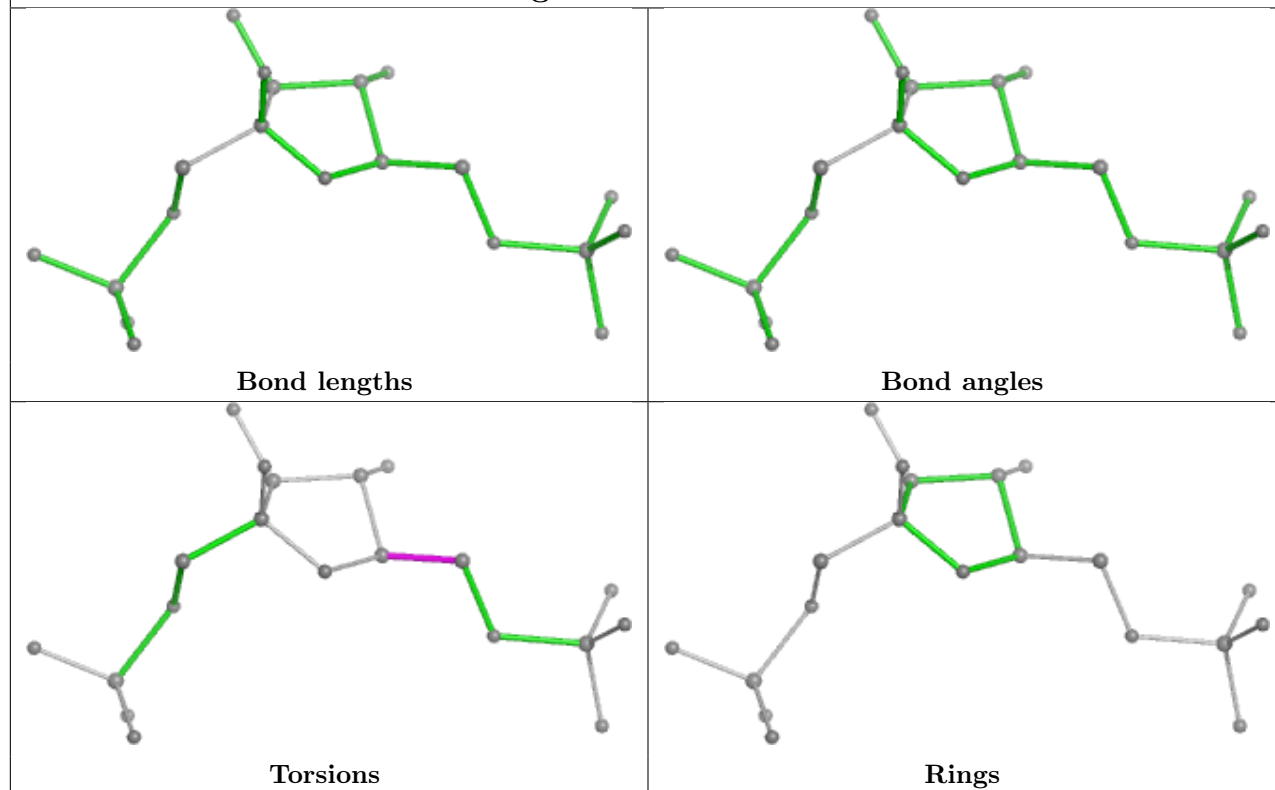
Ligand FBP E 601



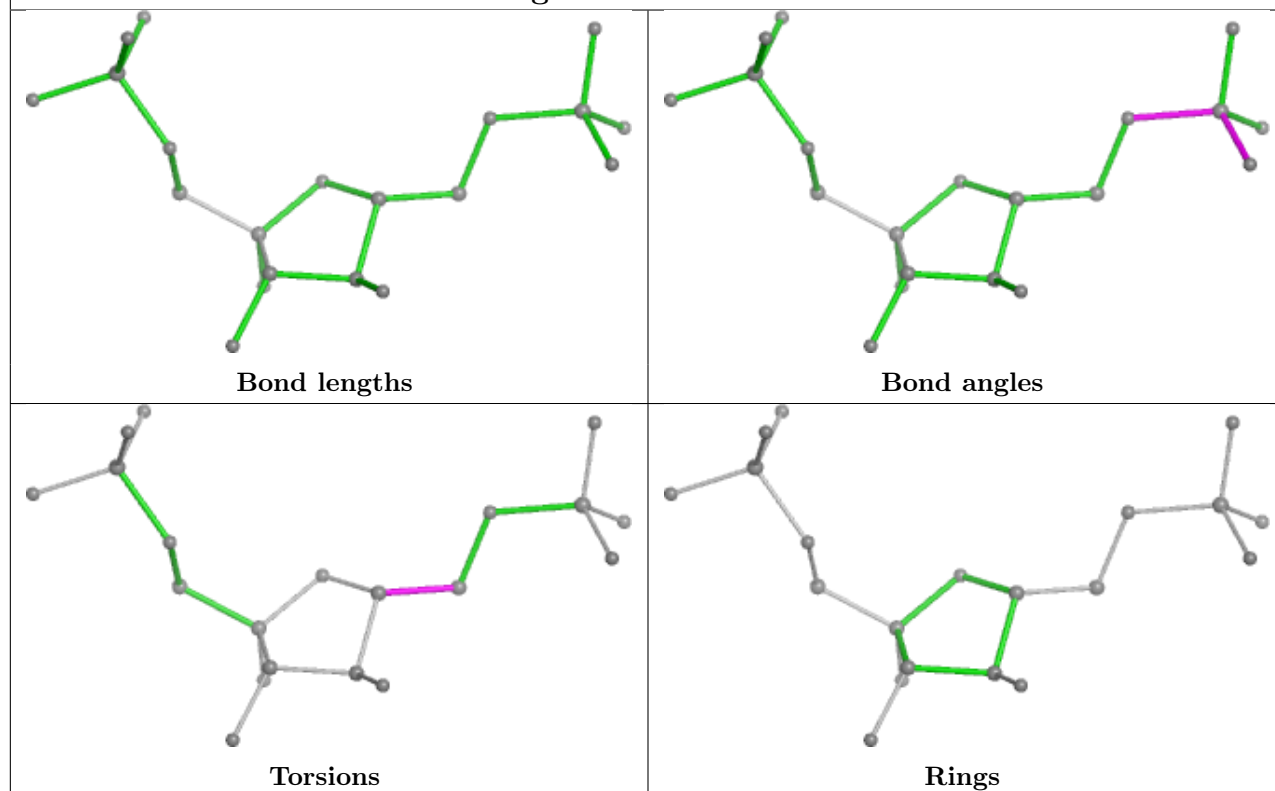
Ligand FBP B 601

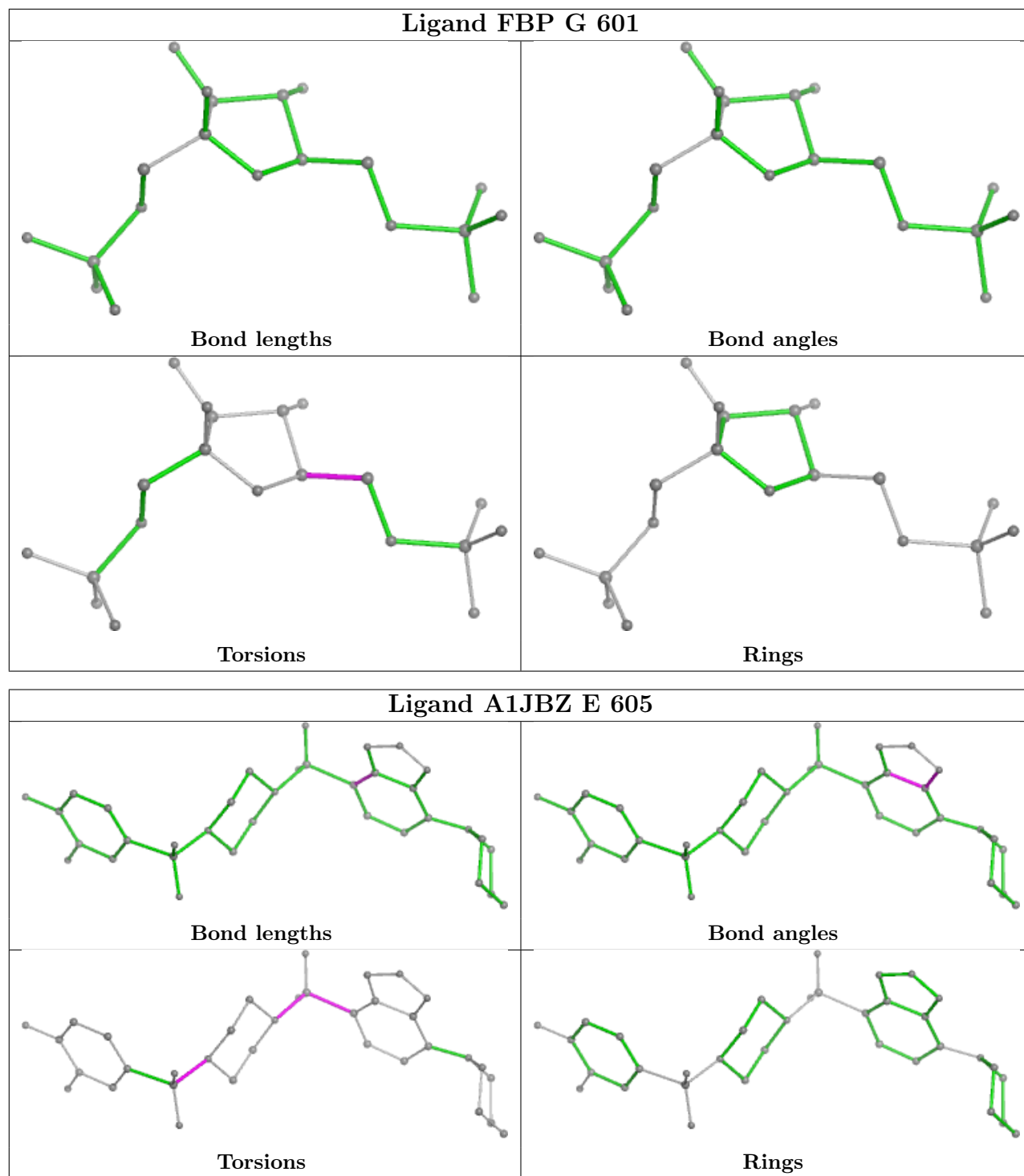


Ligand FBP A 601



Ligand FBP H 601





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.92	48 (11%)	11 12	24, 47, 77, 95	6 (1%)
1	B	436/447 (97%)	1.02	74 (16%)	5 4	22, 46, 78, 94	4 (0%)
1	C	427/447 (95%)	0.12	20 (4%)	37 39	18, 34, 61, 104	4 (0%)
1	D	425/447 (95%)	-0.16	9 (2%)	63 65	14, 28, 54, 101	6 (1%)
1	E	423/447 (94%)	0.80	51 (12%)	10 10	22, 46, 77, 94	5 (1%)
1	F	435/447 (97%)	0.42	31 (7%)	23 25	21, 37, 68, 87	7 (1%)
1	G	423/447 (94%)	-0.08	10 (2%)	59 61	18, 30, 50, 71	7 (1%)
1	H	425/447 (95%)	-0.32	12 (2%)	55 56	13, 25, 48, 85	4 (0%)
All	All	3417/3576 (95%)	0.34	255 (7%)	22 23	13, 37, 70, 104	43 (1%)

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	6.5
1	E	23	ALA	5.9
1	H	21	GLY	5.5
1	A	25	PHE	5.4
1	B	511	LEU	5.3
1	D	25	PHE	4.9
1	G	25	PHE	4.7
1	F	115	LEU	4.7
1	E	25	PHE	4.6
1	B	507	GLU	4.6
1	F	511	LEU	4.5
1	D	22	THR	4.5
1	A	231	PRO	4.2
1	C	25	PHE	4.2
1	B	114	PRO	4.0
1	D	21	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	271	GLY	4.0
1	A	238	VAL	3.9
1	D	23	ALA	3.9
1	C	271	GLY	3.9
1	E	490	PRO	3.8
1	B	267[A]	ARG	3.8
1	E	514	PHE	3.7
1	A	63	ILE	3.7
1	F	516	ARG	3.7
1	B	490	PRO	3.6
1	H	232	GLY	3.5
1	A	23	ALA	3.5
1	C	117	TYR	3.5
1	A	543	SER	3.5
1	C	22	THR	3.4
1	F	114	PRO	3.4
1	C	229	SER	3.4
1	F	230	GLY	3.4
1	B	543	SER	3.3
1	C	111	ALA	3.3
1	B	493	ILE	3.3
1	H	231	PRO	3.3
1	C	21	GLY	3.3
1	B	348	THR	3.3
1	F	512	ARG	3.3
1	B	269	ALA	3.3
1	A	70	VAL	3.3
1	B	61	ALA	3.2
1	E	232	GLY	3.2
1	B	241	LEU	3.2
1	C	20	LEU	3.2
1	E	249	VAL	3.2
1	A	95	TYR	3.1
1	E	233	LEU	3.1
1	B	238	VAL	3.1
1	B	485	LEU	3.1
1	B	513	GLY	3.1
1	C	26	GLN	3.1
1	D	24	PHE	3.1
1	A	233	LEU	3.0
1	B	484	LEU	3.0
1	C	230	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	493	ILE	3.0
1	F	493	ILE	3.0
1	H	22	THR	3.0
1	F	231	PRO	3.0
1	A	482	PHE	3.0
1	A	514	PHE	3.0
1	A	68	ARG	3.0
1	C	130	GLY	3.0
1	F	490	PRO	3.0
1	F	233	LEU	3.0
1	A	24	PHE	3.0
1	B	88	PHE	3.0
1	B	512	ARG	3.0
1	B	122	ILE	2.9
1	A	114	PRO	2.9
1	F	267[A]	ARG	2.9
1	B	111	ALA	2.9
1	B	268	ALA	2.9
1	E	114	PRO	2.9
1	E	129	PRO	2.9
1	G	23	ALA	2.9
1	E	231	PRO	2.9
1	C	115	LEU	2.9
1	B	91	GLY	2.9
1	E	70	VAL	2.8
1	B	495	ALA	2.8
1	E	271	GLY	2.8
1	A	73	LEU	2.8
1	E	270	LEU	2.8
1	A	61	ALA	2.8
1	G	24	PHE	2.8
1	E	234	SER	2.8
1	B	379	LYS	2.8
1	B	70	VAL	2.8
1	B	107	VAL	2.8
1	F	112	GLY	2.8
1	A	241	LEU	2.8
1	E	502	VAL	2.8
1	B	100	ILE	2.7
1	A	28	GLN	2.7
1	G	52	VAL	2.7
1	A	232	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	489	PRO	2.7
1	B	540[A]	LEU	2.7
1	E	238	VAL	2.7
1	B	230	GLY	2.7
1	B	382	PHE	2.7
1	H	25	PHE	2.7
1	B	118	ARG	2.7
1	A	270	LEU	2.7
1	B	416	LEU	2.7
1	A	488[A]	GLU	2.7
1	E	115	LEU	2.6
1	D	275[A]	HIS	2.6
1	E	504	PHE	2.6
1	F	415	PRO	2.6
1	B	508	SER	2.6
1	A	30	LEU	2.6
1	B	270	LEU	2.6
1	E	511	LEU	2.6
1	C	23	ALA	2.6
1	F	411	ARG	2.6
1	H	411	ARG	2.6
1	B	97	ALA	2.6
1	A	496	ASP	2.6
1	C	24	PHE	2.6
1	G	272	PRO	2.6
1	F	416	LEU	2.6
1	B	84	ALA	2.5
1	B	106	ALA	2.5
1	D	231	PRO	2.5
1	E	275	HIS	2.5
1	F	270	LEU	2.5
1	E	274	GLY	2.5
1	F	128	GLY	2.5
1	E	269	ALA	2.5
1	F	240	ASP	2.5
1	C	114	PRO	2.5
1	G	63	ILE	2.5
1	E	101	ALA	2.5
1	A	236	GLN	2.5
1	A	475	VAL	2.5
1	F	507	GLU	2.4
1	B	231	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	24	PHE	2.4
1	A	34	MET	2.4
1	D	232	GLY	2.4
1	F	232	GLY	2.4
1	B	73	LEU	2.4
1	E	95	TYR	2.4
1	A	118	ARG	2.4
1	B	10	ARG	2.4
1	C	34	MET	2.4
1	E	487	ARG	2.4
1	F	351	ARG	2.4
1	H	514	PHE	2.4
1	B	542	ILE	2.4
1	E	237	ASP	2.4
1	E	241	LEU	2.4
1	E	485	LEU	2.4
1	B	90	HIS	2.4
1	B	120	VAL	2.4
1	B	245	VAL	2.4
1	F	489	PRO	2.4
1	A	110	PHE	2.4
1	B	243	PHE	2.4
1	E	236	GLN	2.4
1	E	30	LEU	2.3
1	B	498	VAL	2.3
1	C	272	PRO	2.3
1	E	109	SER	2.3
1	A	527	TRP	2.3
1	E	26	GLN	2.3
1	B	232	GLY	2.3
1	B	256	PHE	2.3
1	A	90	HIS	2.3
1	A	269	ALA	2.3
1	A	263	VAL	2.3
1	A	130	GLY	2.3
1	E	540	LEU	2.3
1	E	242	ARG	2.3
1	D	26	GLN	2.3
1	F	517	VAL	2.3
1	A	112	GLY	2.3
1	A	378	ALA	2.3
1	F	11	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	95	TYR	2.2
1	E	515	LEU	2.2
1	E	106	ALA	2.2
1	E	111	ALA	2.2
1	B	504	PHE	2.2
1	A	277	ILE	2.2
1	B	77	ILE	2.2
1	B	62	THR	2.2
1	E	97	ALA	2.2
1	B	237	ASP	2.2
1	G	230	GLY	2.2
1	B	516	ARG	2.2
1	E	124	LEU	2.2
1	C	116	SER	2.2
1	F	229	SER	2.2
1	B	129	PRO	2.2
1	F	129	PRO	2.2
1	E	244	GLY	2.2
1	A	498	VAL	2.2
1	B	514	PHE	2.1
1	G	514	PHE	2.1
1	B	63	ILE	2.1
1	B	494	TRP	2.1
1	A	242	ARG	2.1
1	B	260	ALA	2.1
1	B	264	ALA	2.1
1	F	492	ALA	2.1
1	H	23	ALA	2.1
1	H	412	ARG	2.1
1	G	231	PRO	2.1
1	B	503	GLN	2.1
1	C	107	VAL	2.1
1	A	426	ILE	2.1
1	B	233	LEU	2.1
1	B	347	ILE	2.1
1	E	351	ARG	2.1
1	A	251	ILE	2.1
1	B	86	LEU	2.1
1	B	279	ILE	2.1
1	E	90	HIS	2.1
1	H	275[A]	HIS	2.1
1	A	106	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	530	GLY	2.1
1	B	236	GLN	2.1
1	E	103	VAL	2.1
1	F	245	VAL	2.1
1	E	499	ASP	2.1
1	A	89	SER	2.1
1	B	109	SER	2.1
1	A	311	ILE	2.1
1	B	110	PHE	2.1
1	B	482	PHE	2.1
1	E	277	ILE	2.1
1	F	514	PHE	2.1
1	H	24	PHE	2.1
1	A	111	ALA	2.0
1	E	128	GLY	2.0
1	F	274	GLY	2.0
1	H	516	ARG	2.0
1	B	266	VAL	2.0
1	E	245	VAL	2.0
1	C	113	SER	2.0
1	A	243	PHE	2.0
1	E	110	PHE	2.0
1	A	91	GLY	2.0
1	A	265	ALA	2.0
1	B	378	ALA	2.0
1	B	415	PRO	2.0
1	B	242	ARG	2.0
1	A	237	ASP	2.0
1	E	403	HIS	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 ⓘ

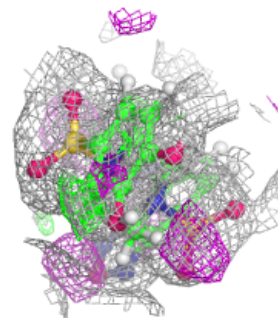
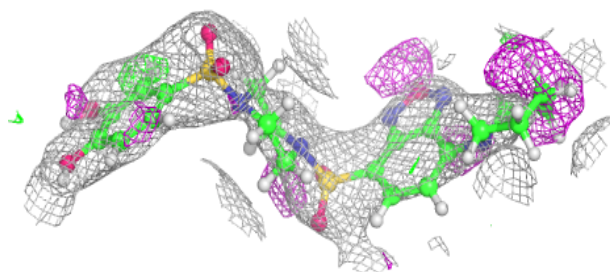
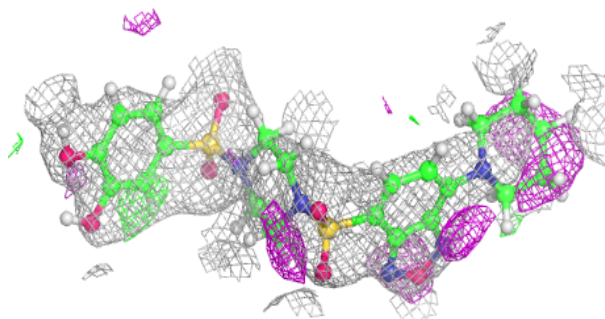
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
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.

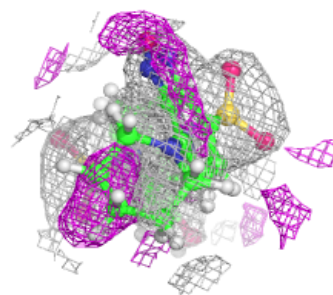
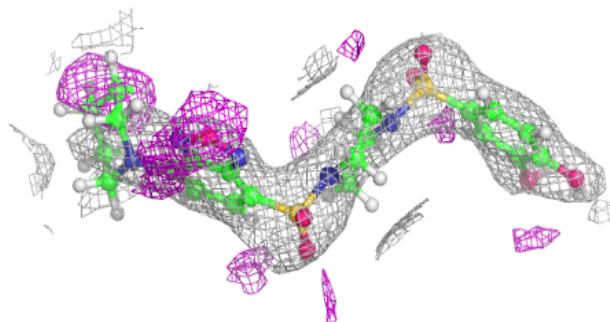
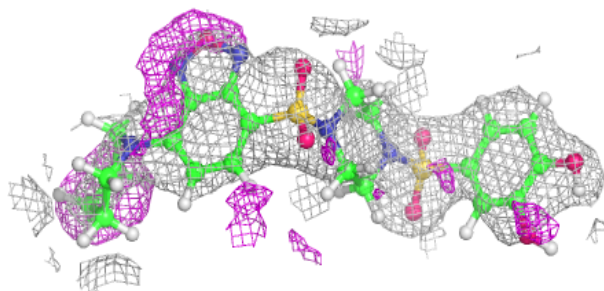
Electron density around A1JBZ F 605:

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

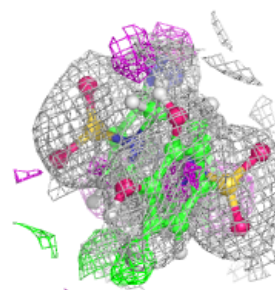
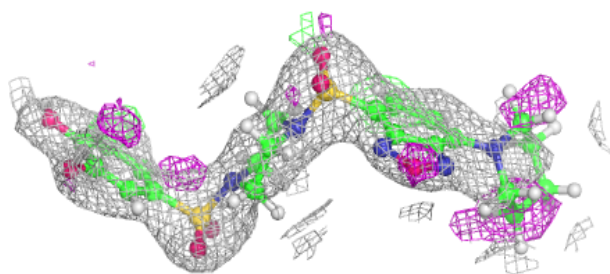
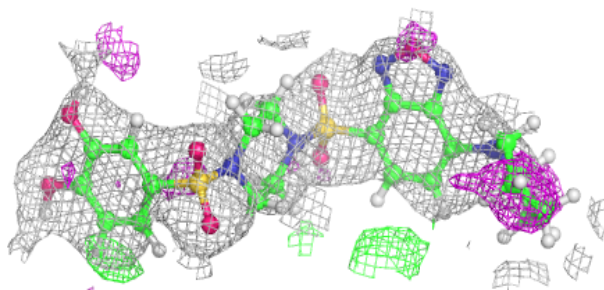


Electron density around A1JBZ E 605:

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

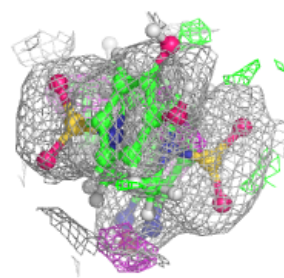
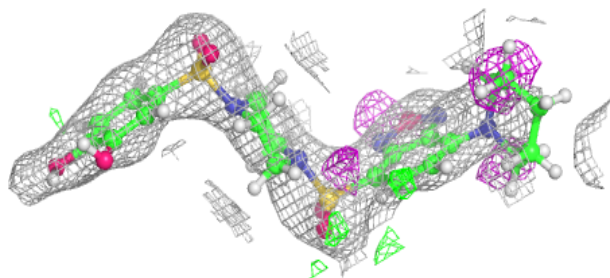
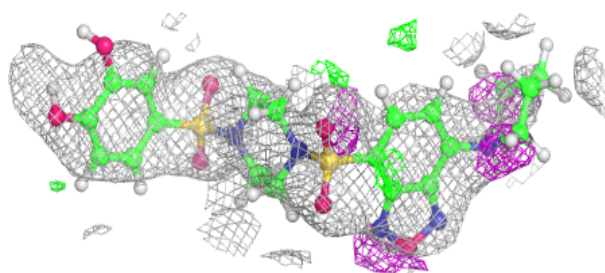
**Electron density around A1JBZ A 605:**

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

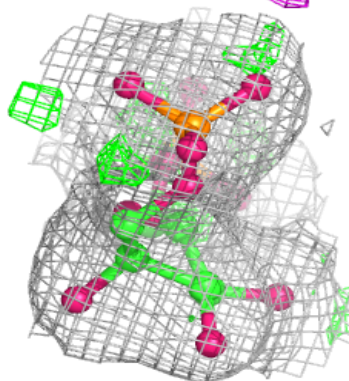
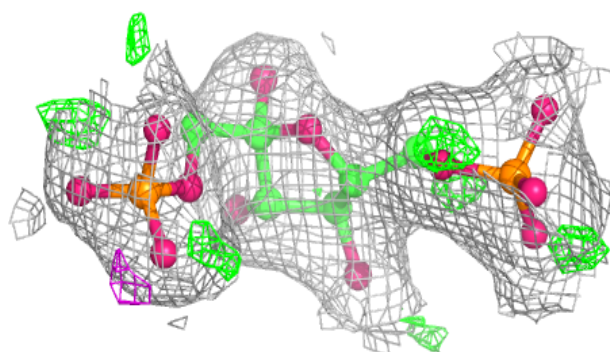
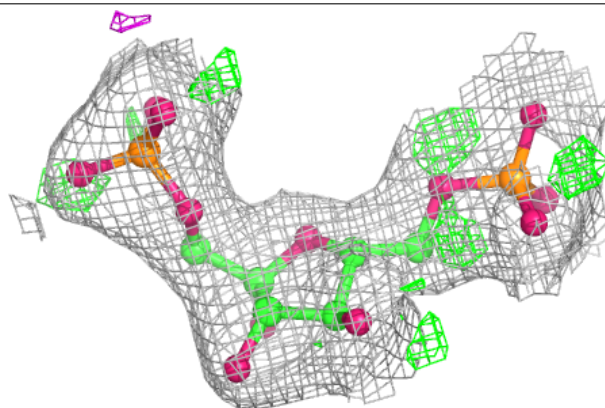


Electron density around A1JBZ D 605:

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

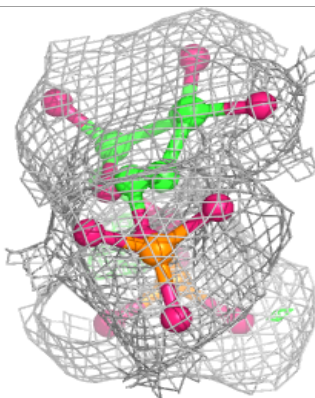
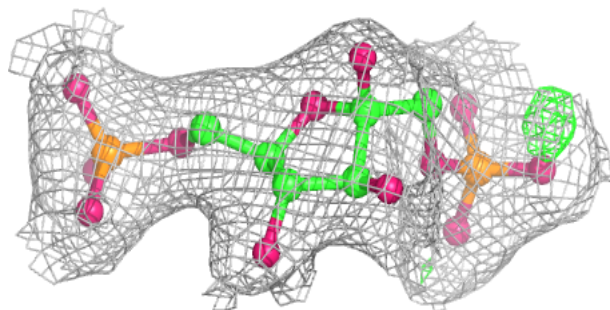
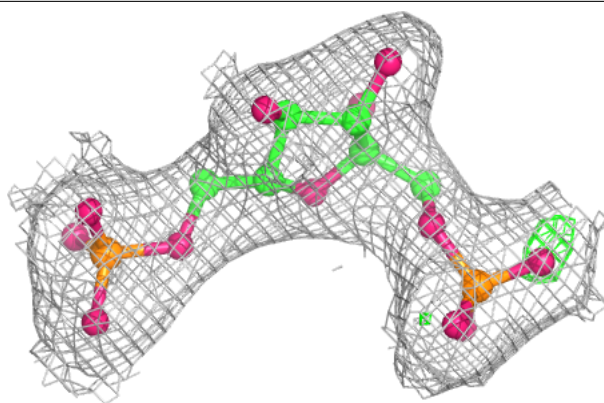
**Electron density around FBP B 601:**

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

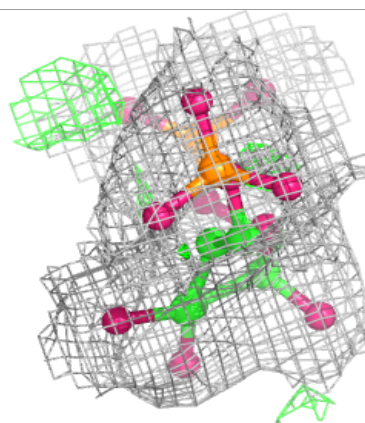
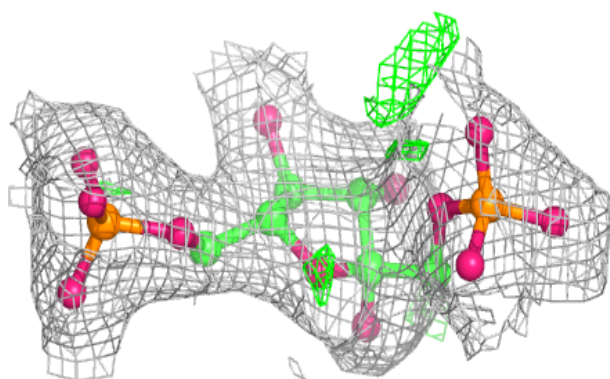
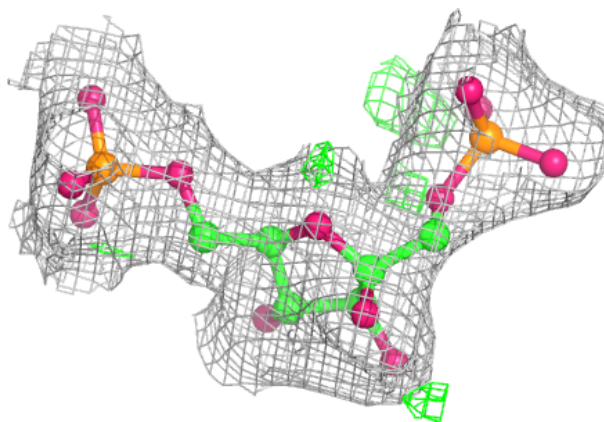


Electron density around FBP E 601:

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

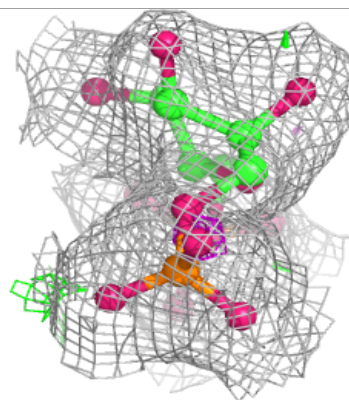
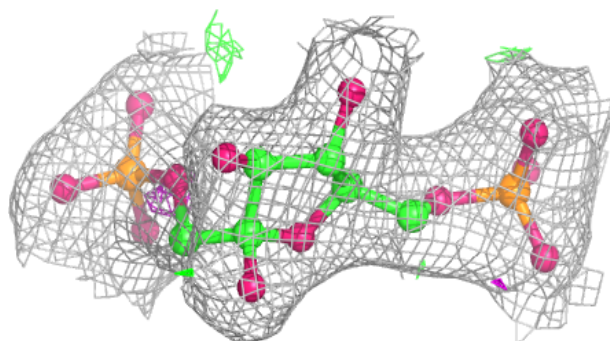
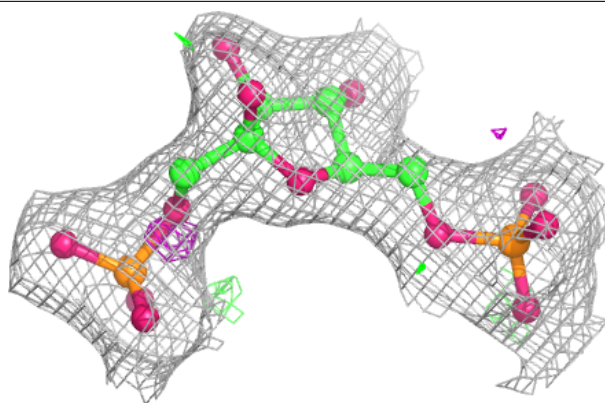
**Electron density around FBP F 601:**

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

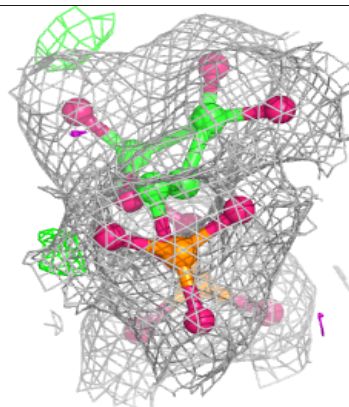
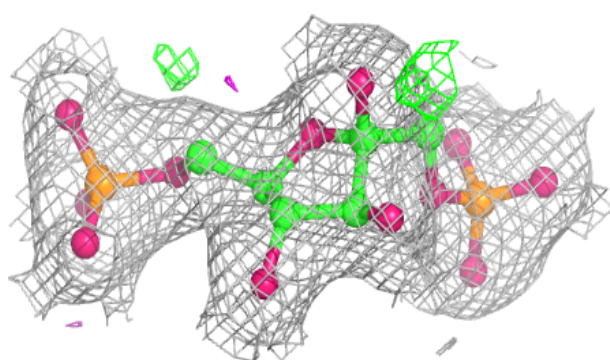
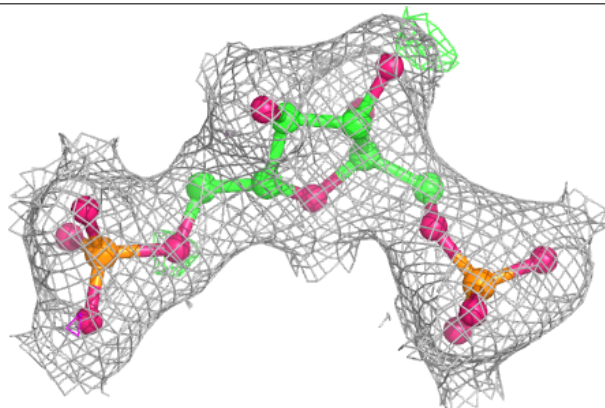


Electron density around FBP A 601:

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

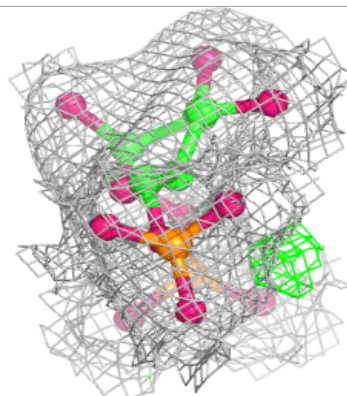
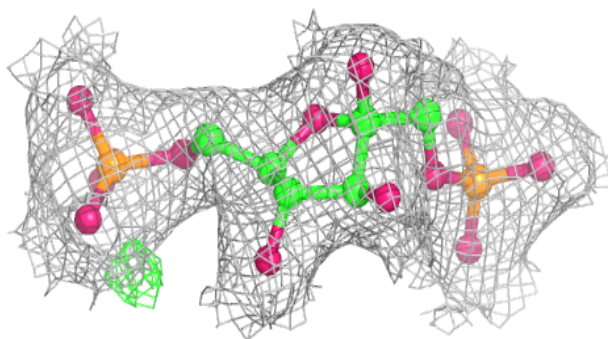
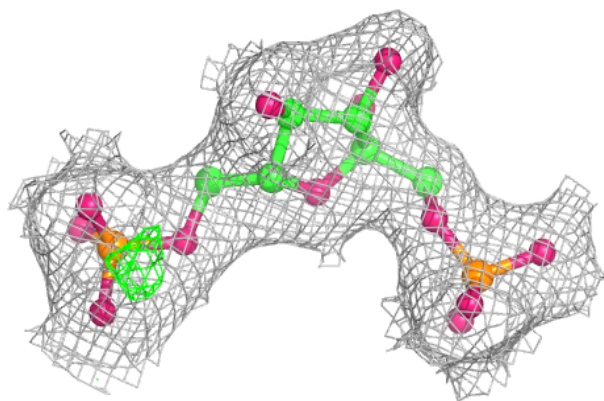
**Electron density around FBP C 601:**

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

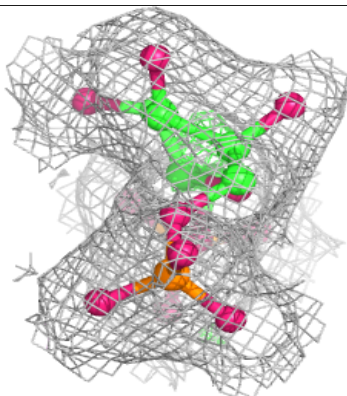
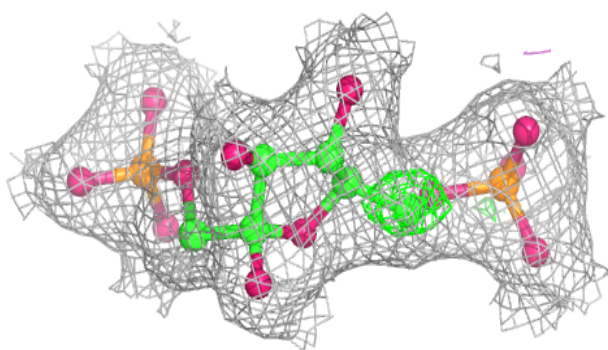
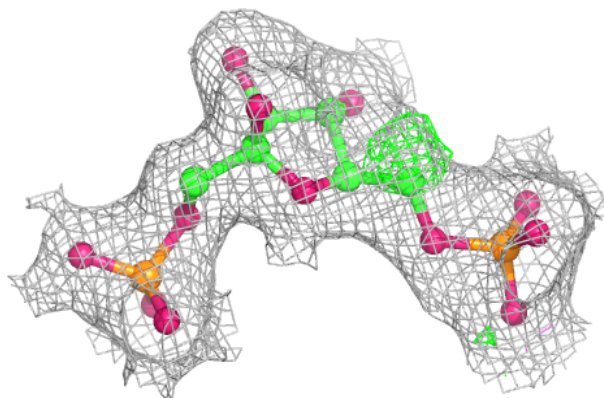


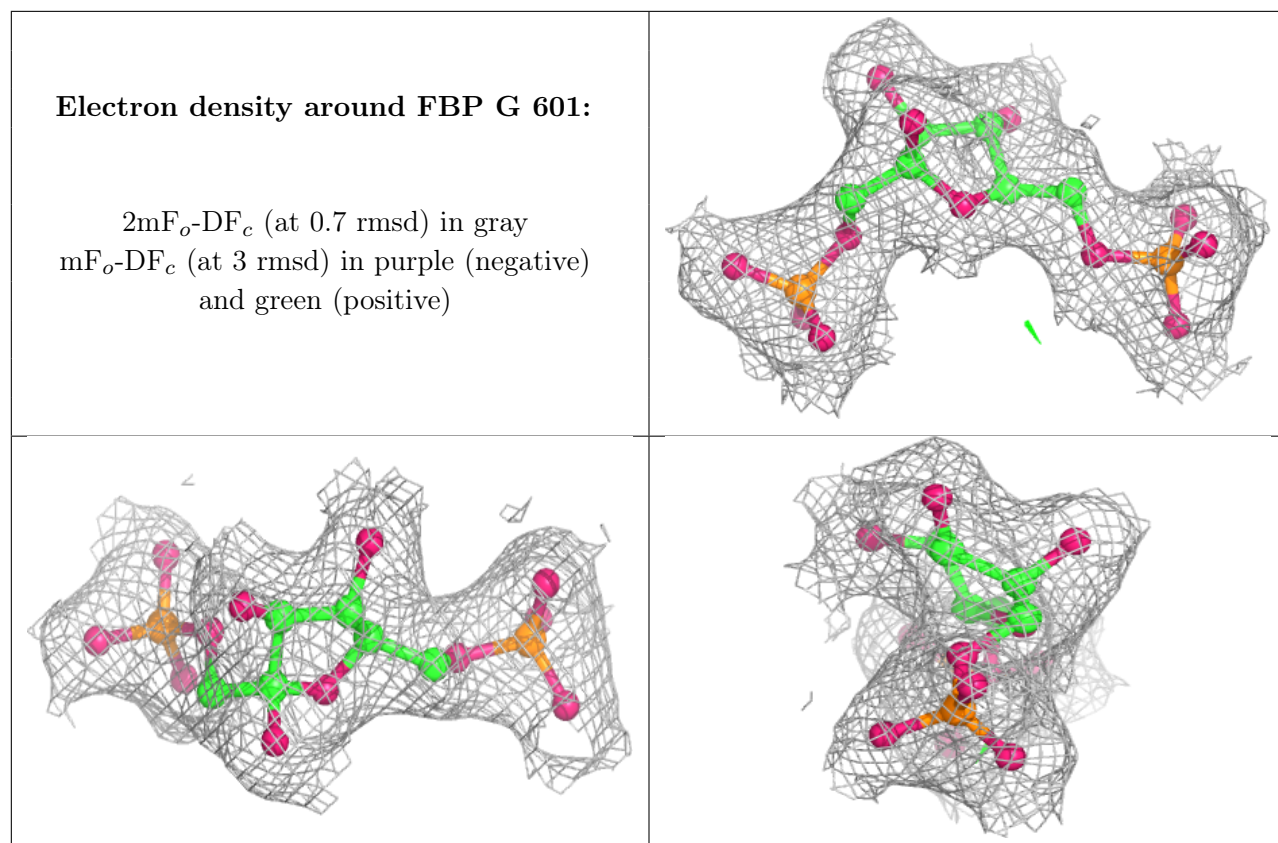
Electron density around FBP D 601:

$2mF_o-DF_c$ (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.