



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:41 AM UTC

PDB ID : 7QDN / pdb_00007qdn
Title : Structure of human liver pyruvate kinase from which the B domain has been deleted
Authors : Lulla, A.; Hyvonen, M.
Deposited on : 2021-11-27
Resolution : 1.70 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:

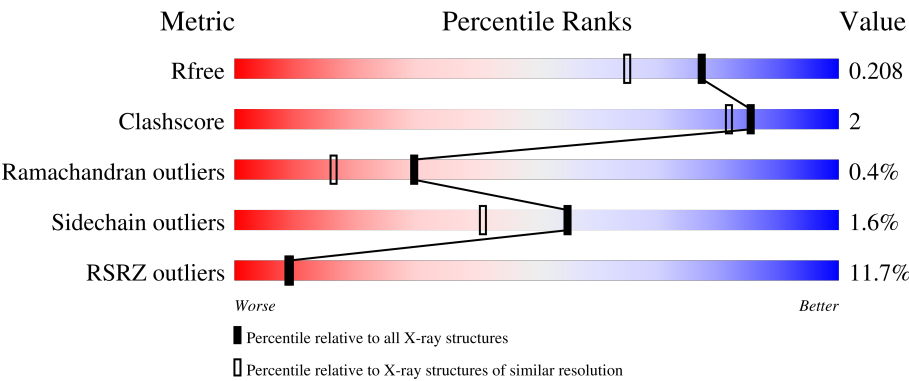
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 1.70 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.



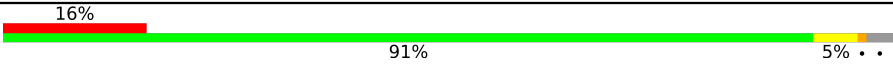
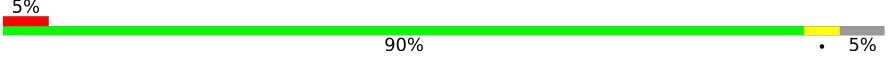
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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% 89% 6% 5%
1	B	447	22% 91% 5% ••
1	C	447	8% 89% 6% •
1	D	447	5% 91% • 5%
1	E	447	13% 88% 6% 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	OXD	A	602	-	X	-	-
3	OXD	B	602	-	X	-	-
3	OXD	C	602	-	X	-	-
3	OXD	D	602	-	X	-	-
3	OXD	E	602	-	X	-	-
3	OXD	F	602	-	X	-	-
3	OXD	G	602	-	X	-	-
3	OXD	H	602	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28811 atoms, of which 0 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 Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	3	0
			3227	2027	586	594	20			
1	B	436	Total	C	N	O	S	0	3	0
			3324	2085	604	615	20			
1	C	427	Total	C	N	O	S	0	1	0
			3242	2035	587	601	19			
1	D	425	Total	C	N	O	S	0	2	0
			3232	2029	587	597	19			
1	E	423	Total	C	N	O	S	0	2	0
			3219	2022	583	594	20			
1	F	435	Total	C	N	O	S	0	3	0
			3313	2079	600	614	20			
1	G	421	Total	C	N	O	S	0	4	0
			3219	2023	581	596	19			
1	H	425	Total	C	N	O	S	0	3	0
			3243	2035	591	598	19			

There are 840 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	ALA	conflict	UNP P30613
A	1	MET	PRO	conflict	UNP P30613
A	2	GLU	GLY	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P30613
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P30613
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	ALA	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	130	GLY	VAL	conflict	UNP P30613
A	131	SER	ASP	conflict	UNP P30613
A	132	GLY	LEU	conflict	UNP P30613
B	0	SER	ALA	conflict	UNP P30613
B	1	MET	PRO	conflict	UNP P30613
B	2	GLU	GLY	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PHE	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
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	conflict	UNP P30613
B	131	SER	ASP	conflict	UNP P30613
B	132	GLY	LEU	conflict	UNP P30613
C	0	SER	ALA	conflict	UNP P30613
C	1	MET	PRO	conflict	UNP P30613
C	2	GLU	GLY	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PRO	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	ALA	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	130	GLY	VAL	conflict	UNP P30613
C	131	SER	ASP	conflict	UNP P30613
C	132	GLY	LEU	conflict	UNP P30613
D	0	SER	ALA	conflict	UNP P30613
D	1	MET	PRO	conflict	UNP P30613
D	2	GLU	GLY	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PHE	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
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	conflict	UNP P30613
D	131	SER	ASP	conflict	UNP P30613
D	132	GLY	LEU	conflict	UNP P30613
E	0	SER	ALA	conflict	UNP P30613
E	1	MET	PRO	conflict	UNP P30613
E	2	GLU	GLY	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
E	130	GLY	VAL	conflict	UNP P30613
E	131	SER	ASP	conflict	UNP P30613
E	132	GLY	LEU	conflict	UNP P30613
F	0	SER	ALA	conflict	UNP P30613
F	1	MET	PRO	conflict	UNP P30613
F	2	GLU	GLY	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	conflict	UNP P30613
F	131	SER	ASP	conflict	UNP P30613
F	132	GLY	LEU	conflict	UNP P30613
G	0	SER	ALA	conflict	UNP P30613
G	1	MET	PRO	conflict	UNP P30613
G	2	GLU	GLY	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP P30613
G	131	SER	ASP	conflict	UNP P30613
G	132	GLY	LEU	conflict	UNP P30613
H	0	SER	ALA	conflict	UNP P30613
H	1	MET	PRO	conflict	UNP P30613
H	2	GLU	GLY	conflict	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

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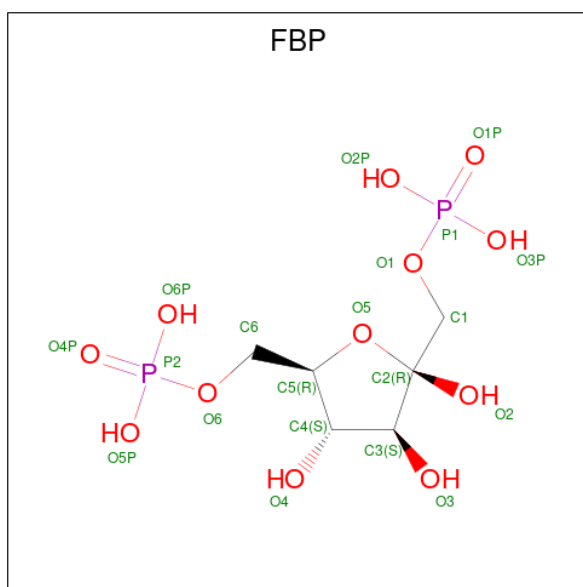
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H	?	-	ARG	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	ALA	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	VAL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

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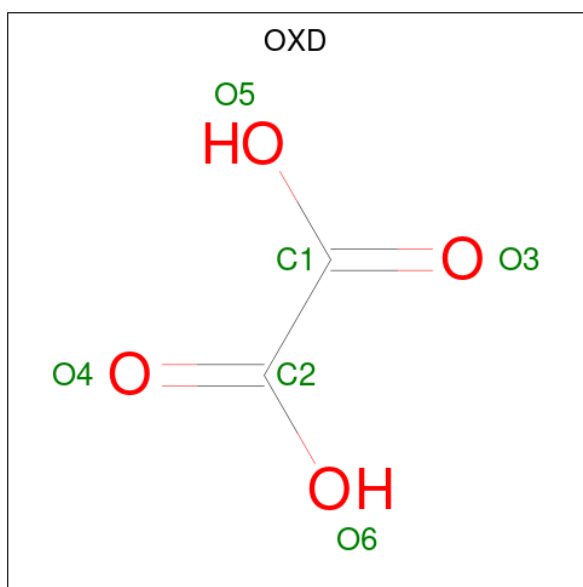
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	PRO	deletion	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	GLN	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	GLU	deletion	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	conflict	UNP P30613
H	131	SER	ASP	conflict	UNP P30613
H	132	GLY	LEU	conflict	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 OXALIC ACID (CCD ID: OXD) (formula: $C_2H_2O_4$).



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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0

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

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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Na 1	0	0
6	C	1	Total 1	Na 1	0	0
6	D	1	Total 1	Na 1	0	0
6	F	1	Total 1	Na 1	0	0
6	G	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total 1	Na 1	0	0

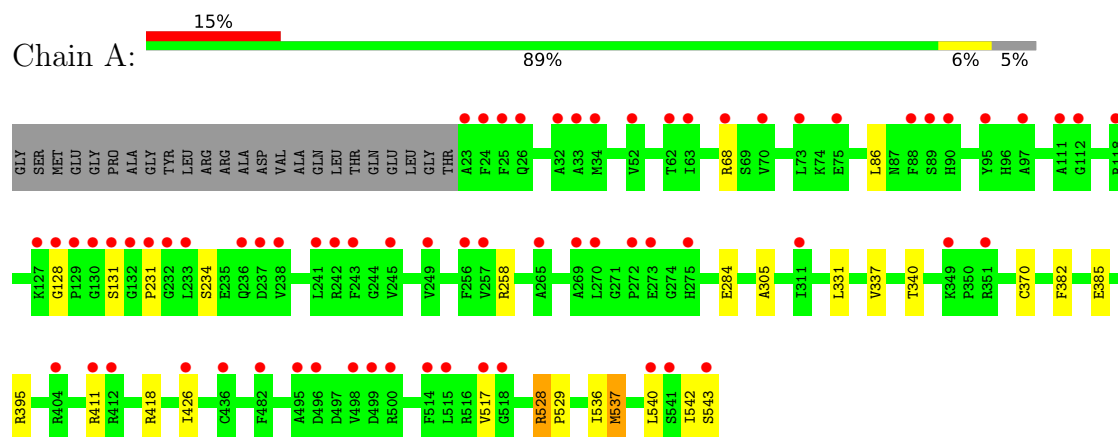
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	258	Total 258	O 258	0	0
7	B	235	Total 235	O 235	0	0
7	C	370	Total 370	O 370	0	0
7	D	383	Total 383	O 383	0	0
7	E	246	Total 246	O 246	0	0
7	F	283	Total 283	O 283	0	0
7	G	368	Total 368	O 368	0	0
7	H	419	Total 419	O 419	0	0

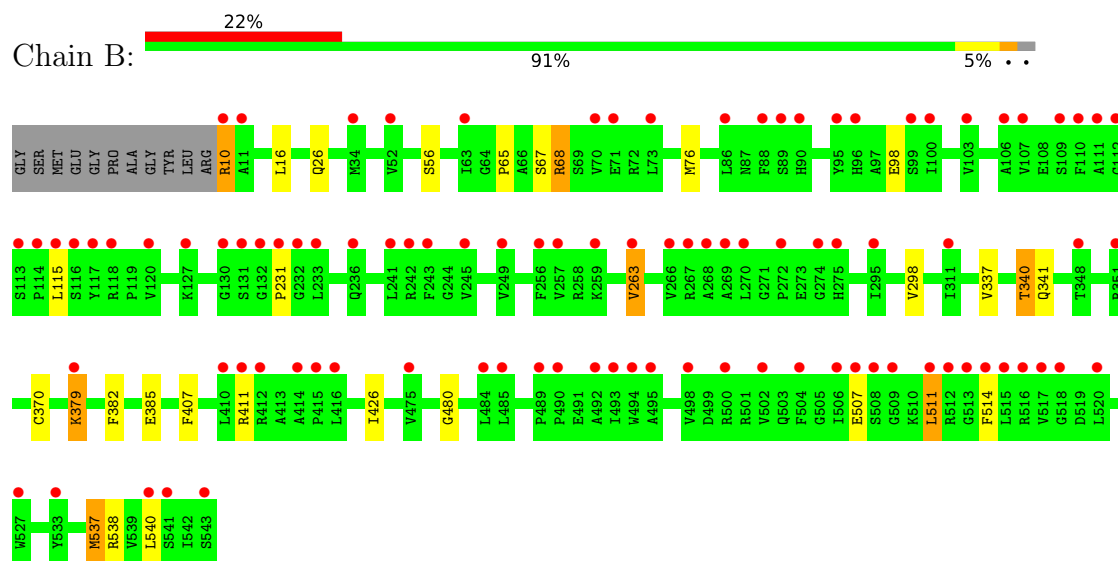
3 Residue-property plots [i](#)

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.

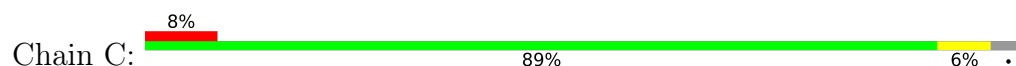
• Molecule 1: Pyruvate kinase PKLR

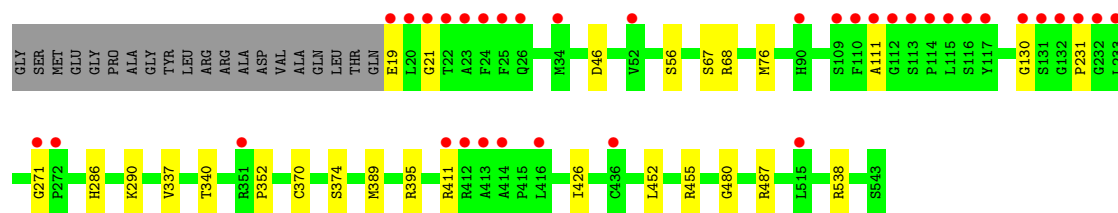


• Molecule 1: Pyruvate kinase PKLR

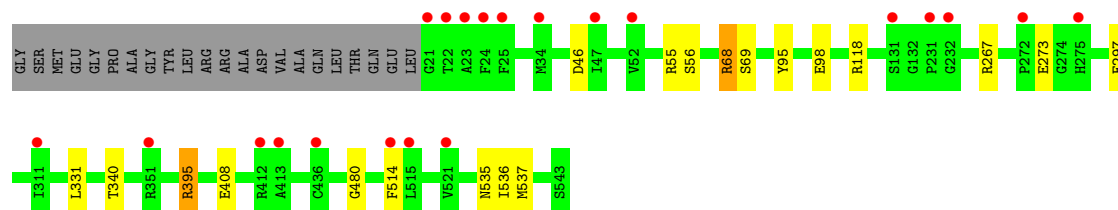
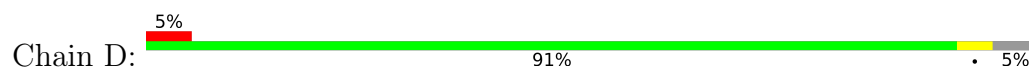


• Molecule 1: Pyruvate kinase PKLR

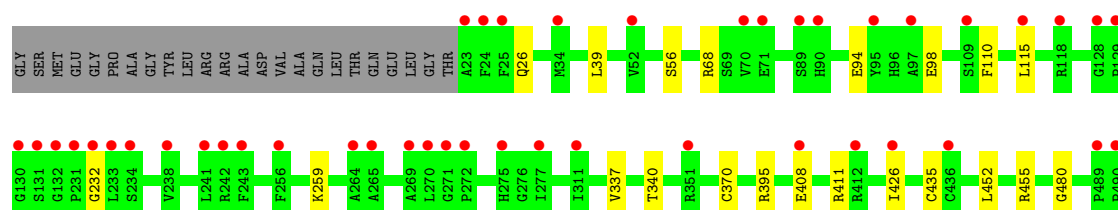
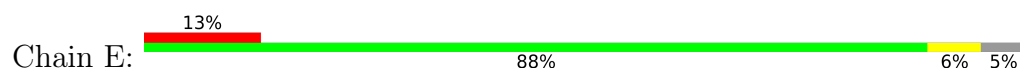




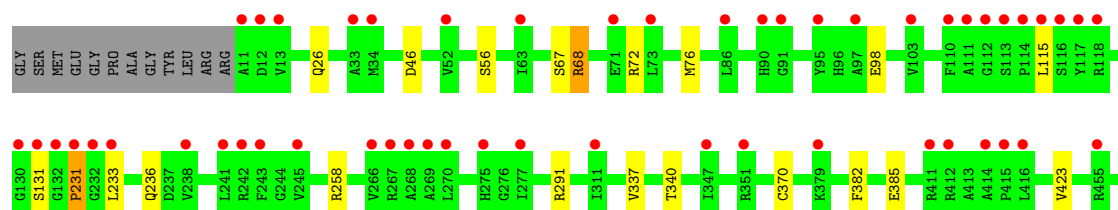
• Molecule 1: Pyruvate kinase PKLR



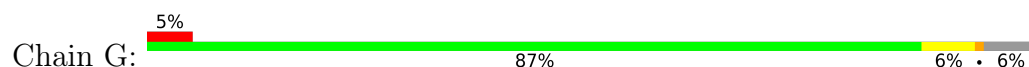
• Molecule 1: Pyruvate kinase PKLR

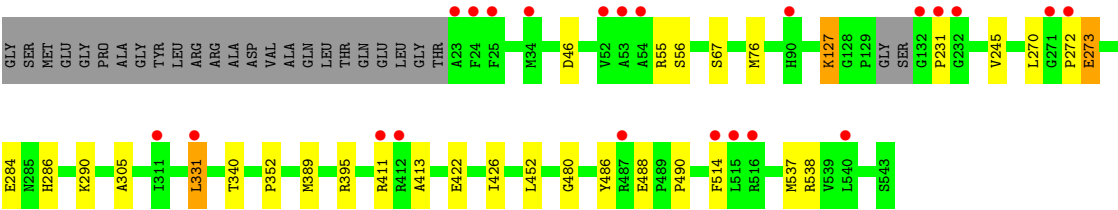


• Molecule 1: Pyruvate kinase PKLR

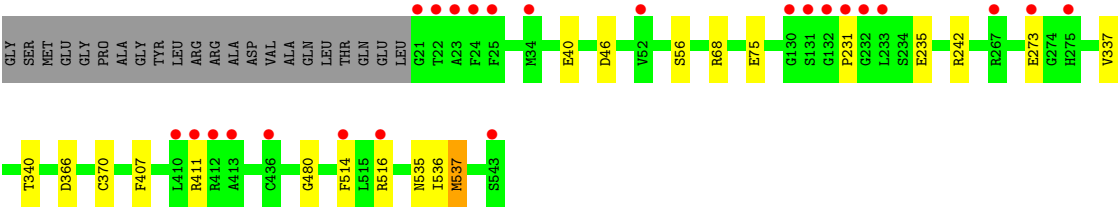
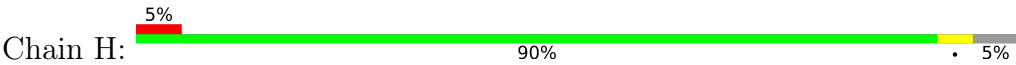


• Molecule 1: Pyruvate kinase PKLR





● Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.45Å 112.69Å 188.33Å 90.00° 91.36° 90.00°	Depositor
Resolution (Å)	103.69 – 1.70 103.69 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.6 (103.69-1.70) 92.6 (103.69-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.70Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.205 , 0.217 0.197 , 0.208	Depositor DCC
R_{free} test set	22295 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28811	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 36.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6746e-04. 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: OXD, MG, K, FBP, NA

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	0.72	0/3291	1.06	4/4449 (0.1%)
1	B	0.70	0/3388	1.06	1/4581 (0.0%)
1	C	0.75	1/3300 (0.0%)	1.01	1/4463 (0.0%)
1	D	0.77	0/3294	1.00	2/4455 (0.0%)
1	E	0.68	0/3280	1.07	2/4435 (0.0%)
1	F	0.71	0/3377	1.05	2/4567 (0.0%)
1	G	0.75	0/3285	1.00	4/4441 (0.1%)
1	H	0.75	0/3305	0.98	3/4469 (0.1%)
All	All	0.73	1/26520 (0.0%)	1.03	19/35860 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	374	SER	CA-C	5.41	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	GLY	N-CA-C	-6.76	104.16	112.68
1	F	131	SER	N-CA-C	-6.69	104.98	113.01
1	E	539	VAL	N-CA-CB	6.01	118.24	111.21
1	G	514	PHE	CA-CB-CG	5.68	119.48	113.80
1	H	514	PHE	CA-CB-CG	5.59	119.39	113.80
1	D	514	PHE	CA-CB-CG	5.53	119.33	113.80
1	B	514	PHE	CA-CB-CG	5.50	119.30	113.80
1	D	46	ASP	CA-CB-CG	5.45	118.05	112.60
1	G	46	ASP	CA-CB-CG	5.45	118.05	112.60
1	G	270	LEU	CA-C-N	5.36	130.28	121.87
1	G	270	LEU	C-N-CA	5.36	130.28	121.87
1	F	46	ASP	CA-CB-CG	5.25	117.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	ILE	CA-C-N	5.21	131.07	121.70
1	A	542	ILE	C-N-CA	5.21	131.07	121.70
1	H	46	ASP	CA-CB-CG	5.12	117.72	112.60
1	H	366	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	46	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	128	GLY	CA-C-N	5.02	124.63	119.56
1	A	128	GLY	C-N-CA	5.02	124.63	119.56

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	3227	0	3286	10	0
1	B	3324	0	3383	21	0
1	C	3242	0	3290	18	0
1	D	3232	0	3280	12	0
1	E	3219	0	3273	17	0
1	F	3313	0	3369	17	0
1	G	3219	0	3271	20	0
1	H	3243	0	3292	13	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	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	258	0	0	1	0
7	B	235	0	0	3	0
7	C	370	0	0	9	0
7	D	383	0	0	3	0
7	E	246	0	0	4	0
7	F	283	0	0	3	0
7	G	368	0	0	2	0
7	H	419	0	0	5	0
All	All	28811	0	26524	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (116) 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:D:297:GLU:HG3	7:D:1007:HOH:O	1.53	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:75:GLU:HG3	7:H:1050:HOH:O	1.57	1.04
1:D:273:GLU:HB2	7:D:719:HOH:O	1.58	1.01
1:C:111:ALA:HB1	7:C:919:HOH:O	1.71	0.89
1:B:231:PRO:HG2	7:B:778:HOH:O	1.77	0.84
1:D:267:ARG:HD2	7:D:1020:HOH:O	1.79	0.82
1:E:39:LEU:HD21	1:G:331:LEU:HD23	1.62	0.82
1:H:516:ARG:HB2	7:H:925:HOH:O	1.81	0.80
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.62	0.80
1:E:537[B]:MET:HE3	1:F:537[B]:MET:HE3	1.63	0.80
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.65	0.79
1:C:538:ARG:HD3	7:C:765:HOH:O	1.81	0.78
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.67	0.77
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.68	0.75
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.67	0.75
1:C:111:ALA:CB	7:C:919:HOH:O	2.33	0.74
1:F:26:GLN:NE2	7:F:701:HOH:O	2.21	0.73
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.69	0.73
1:C:21:GLY:HA3	7:C:707:HOH:O	1.88	0.72
1:H:516:ARG:CB	7:H:925:HOH:O	2.40	0.70
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.09	0.68
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.75	0.68
1:A:528:ARG:HD2	1:A:529:PRO:O	1.93	0.67
1:C:21:GLY:CA	7:C:707:HOH:O	2.42	0.66
1:F:236:GLN:HG3	7:F:838:HOH:O	1.94	0.66
1:C:21:GLY:C	7:C:707:HOH:O	2.40	0.64
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.62	0.64
1:G:331:LEU:HD21	1:G:413:ALA:CB	2.28	0.64
1:E:26:GLN:C	7:E:720:HOH:O	2.42	0.62
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.82	0.61
1:B:26:GLN:HG3	7:B:751:HOH:O	2.01	0.60
1:B:263:VAL:HG21	1:B:298:VAL:HG23	1.84	0.59
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.85	0.59
1:G:331:LEU:HD21	1:G:413:ALA:HB1	1.86	0.57
1:B:10:ARG:O	1:B:10:ARG:HG2	2.03	0.56
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.06	0.56
1:E:26:GLN:CB	7:E:720:HOH:O	2.53	0.55
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.88	0.55
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.89	0.55
1:F:231:PRO:C	7:F:709:HOH:O	2.50	0.54
1:B:407:PHE:CZ	1:B:411:ARG:HD2	2.43	0.54
1:B:507:GLU:O	1:B:511:LEU:HD22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ARG:HB2	1:G:395:ARG:HG3	1.89	0.53
1:E:39:LEU:CD2	1:G:331:LEU:HD23	2.34	0.52
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.90	0.52
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.92	0.52
1:G:537:MET:HE3	1:H:537:MET:HG2	1.92	0.51
1:E:452:LEU:O	1:E:455:ARG:HG2	2.11	0.51
1:B:65:PRO:HG2	1:B:379:LYS:HG2	1.94	0.50
1:D:68:ARG:HD2	1:D:95:TYR:OH	2.11	0.50
1:B:26:GLN:CG	7:B:751:HOH:O	2.56	0.49
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.95	0.49
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.95	0.49
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.95	0.49
1:H:235:GLU:HG2	7:H:1047:HOH:O	2.13	0.49
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.94	0.48
1:F:507:GLU:O	1:F:511:LEU:HG	2.13	0.48
1:H:407:PHE:O	1:H:411:ARG:HG3	2.14	0.48
1:A:284:GLU:HG2	1:A:305:ALA:HB3	1.95	0.48
1:D:56:SER:HB2	1:D:480:GLY:CA	2.44	0.48
1:F:511:LEU:HD23	1:F:511:LEU:N	2.28	0.48
1:G:127:LYS:NZ	7:G:706:HOH:O	2.47	0.48
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.30	0.47
1:H:56:SER:HB2	1:H:480:GLY:CA	2.44	0.47
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.98	0.46
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.51	0.46
1:B:67:SER:HB2	1:B:76[B]:MET:SD	2.55	0.46
1:E:68:ARG:NH2	1:E:98:GLU:HB3	2.31	0.46
1:H:40:GLU:HB2	7:H:978:HOH:O	2.17	0.45
1:F:231:PRO:O	1:F:258:ARG:NH2	2.50	0.45
1:H:535:ASN:OD1	1:H:536:ILE:HG13	2.15	0.45
1:D:55:ARG:HB2	1:D:395:ARG:HG3	1.99	0.45
1:F:67:SER:HB2	1:F:76[B]:MET:SD	2.56	0.45
1:G:56:SER:HB2	1:G:480:GLY:CA	2.46	0.45
1:B:56:SER:HB2	1:B:480:GLY:CA	2.48	0.44
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.48	0.44
1:C:271:GLY:HA3	7:C:837:HOH:O	2.17	0.44
1:D:535:ASN:OD1	1:D:536:ILE:HG13	2.18	0.44
1:E:110:PHE:HB3	7:E:726:HOH:O	2.18	0.43
1:G:490:PRO:HB3	7:G:1021:HOH:O	2.17	0.43
1:B:68:ARG:NH2	1:B:98:GLU:HB3	2.33	0.43
1:B:538:ARG:NH1	1:B:540:LEU:HD11	2.34	0.43
1:F:56:SER:HB2	1:F:480:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:SER:HB2	1:C:76[B]:MET:SD	2.59	0.43
1:E:491:GLU:OE2	1:E:500:ARG:HD2	2.18	0.43
1:F:382:PHE:HB3	1:F:385:GLU:HB2	2.00	0.43
1:C:271:GLY:HA2	7:C:717:HOH:O	2.19	0.43
1:C:286:HIS:CE1	1:C:290:LYS:HG3	2.54	0.43
1:E:94:GLU:HB2	7:E:884:HOH:O	2.17	0.43
1:C:56:SER:HB2	1:C:480:GLY:CA	2.49	0.43
1:A:68:ARG:NH1	7:A:702:HOH:O	2.51	0.42
1:G:284:GLU:HG2	1:G:305:ALA:HB3	2.02	0.42
1:A:411:ARG:HG3	1:A:426:ILE:HD11	2.02	0.42
1:G:352:PRO:HG3	1:G:389:MET:HG2	2.01	0.42
1:C:337:VAL:HG22	1:C:370:CYS:HB2	2.02	0.42
1:G:411:ARG:HG3	1:G:426:ILE:HD11	2.01	0.42
1:A:537[B]:MET:HE3	1:B:537[B]:MET:HE3	2.01	0.42
1:D:68:ARG:NH2	1:D:95:TYR:O	2.53	0.42
1:E:337:VAL:HG22	1:E:370:CYS:HB2	2.01	0.42
1:B:340:THR:HG22	1:B:341:GLN:HG3	2.02	0.42
1:B:507:GLU:O	1:B:511:LEU:CD2	2.67	0.41
1:B:337:VAL:HG22	1:B:370:CYS:HB2	2.01	0.41
1:C:452:LEU:O	1:C:455:ARG:HG2	2.20	0.41
1:F:337:VAL:HG22	1:F:370:CYS:HB2	2.02	0.41
1:F:56:SER:HB2	1:F:480:GLY:CA	2.50	0.41
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.03	0.41
1:A:382:PHE:HB3	1:A:385:GLU:HB2	2.02	0.41
1:E:56:SER:HB2	1:E:480:GLY:CA	2.50	0.41
1:H:537:MET:O	1:H:537:MET:HG3	2.19	0.41
1:E:435:CYS:HB3	1:F:423:VAL:HG21	2.03	0.41
1:G:67:SER:HB2	1:G:76[B]:MET:SD	2.60	0.41
1:G:286:HIS:CE1	1:G:290:LYS:HG3	2.56	0.41
1:C:352:PRO:HG3	1:C:389:MET:HG2	2.03	0.41
1:C:487:ARG:CD	7:C:758:HOH:O	2.68	0.41
1:F:233:LEU:HD12	1:F:233:LEU:HA	1.88	0.40
1:A:337:VAL:HG22	1:A:370:CYS:HB2	2.02	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	424/447 (95%)	417 (98%)	4 (1%)	3 (1%)	18	7
1	B	437/447 (98%)	430 (98%)	6 (1%)	1 (0%)	43	28
1	C	426/447 (95%)	416 (98%)	7 (2%)	3 (1%)	18	7
1	D	425/447 (95%)	422 (99%)	2 (0%)	1 (0%)	43	28
1	E	423/447 (95%)	417 (99%)	5 (1%)	1 (0%)	43	28
1	F	436/447 (98%)	430 (99%)	4 (1%)	2 (0%)	24	12
1	G	421/447 (94%)	413 (98%)	6 (1%)	2 (0%)	24	12
1	H	426/447 (95%)	421 (99%)	3 (1%)	2 (0%)	24	12
All	All	3418/3576 (96%)	3366 (98%)	37 (1%)	15 (0%)	30	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	PRO
1	F	231	PRO
1	G	231	PRO
1	A	131	SER
1	C	130	GLY
1	C	231	PRO
1	H	231	PRO
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	338/352 (96%)	329 (97%)	9 (3%)	39	23
1	B	348/352 (99%)	340 (98%)	8 (2%)	44	27
1	C	339/352 (96%)	336 (99%)	3 (1%)	70	62
1	D	338/352 (96%)	331 (98%)	7 (2%)	47	30
1	E	337/352 (96%)	329 (98%)	8 (2%)	43	26
1	F	347/352 (99%)	342 (99%)	5 (1%)	59	46
1	G	338/352 (96%)	335 (99%)	3 (1%)	70	62
1	H	339/352 (96%)	335 (99%)	4 (1%)	63	51
All	All	2724/2816 (97%)	2677 (98%)	47 (2%)	55	38

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	234	SER
1	A	258	ARG
1	A	331	LEU
1	A	395	ARG
1	A	528	ARG
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	68	ARG
1	B	115	LEU
1	B	263	VAL
1	B	379	LYS
1	B	511	LEU
1	B	537[A]	MET
1	B	537[B]	MET
1	C	19	GLU
1	C	68	ARG

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Mol	Chain	Res	Type
1	C	395	ARG
1	D	68	ARG
1	D	69	SER
1	D	118	ARG
1	D	331	LEU
1	D	395	ARG
1	D	408	GLU
1	D	537	MET
1	E	115	LEU
1	E	259	LYS
1	E	395	ARG
1	E	408	GLU
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	68	ARG
1	F	72	ARG
1	F	115	LEU
1	F	291	ARG
1	F	511	LEU
1	G	127	LYS
1	G	273	GLU
1	G	331	LEU
1	H	68	ARG
1	H	242	ARG
1	H	273	GLU
1	H	537	MET

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	405	GLN
1	B	405	GLN
1	C	90	HIS
1	C	405	GLN
1	D	405	GLN
1	E	405	GLN
1	F	236	GLN
1	F	405	GLN
1	G	275	HIS
1	G	405	GLN

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Mol	Chain	Res	Type
1	G	470	GLN
1	H	28	GLN
1	H	405	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 22 are monoatomic - leaving 16 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	$\# Z > 2$
3	OXD	H	602	4	5,5,5	2.02	2 (40%)	6,6,6	1.43	1 (16%)
2	FBP	A	601	-	18,20,20	0.61	0	21,32,32	0.66	0
3	OXD	B	602	4	5,5,5	2.15	2 (40%)	6,6,6	1.37	1 (16%)
2	FBP	H	601	-	18,20,20	0.77	0	21,32,32	0.83	1 (4%)
2	FBP	G	601	-	18,20,20	0.57	0	21,32,32	0.69	0
2	FBP	B	601	-	18,20,20	0.75	0	21,32,32	0.80	1 (4%)
2	FBP	E	601	-	18,20,20	0.62	0	21,32,32	0.60	0
3	OXD	A	602	4	5,5,5	1.93	2 (40%)	6,6,6	2.20	3 (50%)
3	OXD	E	602	4	5,5,5	2.09	2 (40%)	6,6,6	1.67	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXD	D	602	4	5,5,5	2.08	2 (40%)	6,6,6	2.33	2 (33%)
2	FBP	D	601	-	18,20,20	0.45	0	21,32,32	0.76	1 (4%)
3	OXD	F	602	4	5,5,5	2.73	4 (80%)	6,6,6	2.43	3 (50%)
2	FBP	F	601	-	18,20,20	0.46	0	21,32,32	0.52	0
2	FBP	C	601	-	18,20,20	0.51	0	21,32,32	0.61	0
3	OXD	G	602	4	5,5,5	1.89	2 (40%)	6,6,6	2.47	3 (50%)
3	OXD	C	602	4	5,5,5	1.91	2 (40%)	6,6,6	1.70	1 (16%)

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
3	OXD	H	602	4	-	4/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXD	B	602	4	-	4/4/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
3	OXD	A	602	4	-	4/4/4/4	-
3	OXD	E	602	4	-	4/4/4/4	-
3	OXD	D	602	4	-	4/4/4/4	-
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXD	F	602	4	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	OXD	G	602	4	-	4/4/4/4	-
3	OXD	C	602	4	-	4/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXD	O4-C2	3.79	1.31	1.22
3	E	602	OXD	O3-C1	3.77	1.31	1.22
3	A	602	OXD	O4-C2	3.41	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	OXD	O5-C1	-3.40	1.21	1.30
3	D	602	OXD	O4-C2	3.37	1.30	1.22
3	H	602	OXD	O4-C2	3.26	1.30	1.22
3	F	602	OXD	O3-C1	3.25	1.30	1.22
3	F	602	OXD	O4-C2	3.09	1.30	1.22
3	C	602	OXD	O3-C1	3.07	1.30	1.22
3	G	602	OXD	O3-C1	2.95	1.29	1.22
3	G	602	OXD	O5-C1	-2.91	1.22	1.30
3	E	602	OXD	O5-C1	-2.77	1.23	1.30
3	C	602	OXD	O5-C1	-2.74	1.23	1.30
3	D	602	OXD	O6-C2	-2.71	1.23	1.30
3	H	602	OXD	O6-C2	-2.69	1.23	1.30
3	B	602	OXD	O6-C2	-2.69	1.23	1.30
3	A	602	OXD	O6-C2	-2.53	1.23	1.30
3	F	602	OXD	O6-C2	-2.23	1.24	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	OXD	O5-C1-C2	4.54	121.63	112.83
3	F	602	OXD	O6-C2-C1	4.37	121.30	112.83
3	A	602	OXD	O6-C2-C1	4.10	120.78	112.83
3	D	602	OXD	O6-C2-C1	4.09	120.77	112.83
3	C	602	OXD	O5-C1-C2	3.62	119.85	112.83
3	H	602	OXD	O6-C2-C1	3.14	118.93	112.83
3	D	602	OXD	O5-C1-C2	3.13	118.90	112.83
3	F	602	OXD	O5-C1-C2	2.98	118.61	112.83
3	E	602	OXD	O5-C1-C2	2.91	118.47	112.83
3	G	602	OXD	O6-C2-C1	2.86	118.38	112.83
3	B	602	OXD	O6-C2-C1	2.61	117.88	112.83
3	F	602	OXD	O4-C2-C1	-2.50	115.42	120.63
3	A	602	OXD	O5-C1-C2	2.49	117.66	112.83
3	G	602	OXD	O3-C1-C2	-2.45	115.52	120.63
2	D	601	FBP	O5P-P2-O6	2.44	113.04	106.67
3	E	602	OXD	O6-C2-C1	2.42	117.53	112.83
3	A	602	OXD	O4-C2-C1	-2.34	115.75	120.63
2	H	601	FBP	O5P-P2-O6	2.13	112.23	106.67
2	B	601	FBP	O3P-P1-O2P	2.02	115.38	107.80

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	G	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
3	H	602	OXD	O5-C1-C2-O6
3	E	602	OXD	O5-C1-C2-O6
3	F	602	OXD	O5-C1-C2-O6
3	G	602	OXD	O5-C1-C2-O6
3	C	602	OXD	O5-C1-C2-O6
3	F	602	OXD	O3-C1-C2-O4
3	A	602	OXD	O5-C1-C2-O6
3	B	602	OXD	O5-C1-C2-O6
3	D	602	OXD	O5-C1-C2-O6
3	A	602	OXD	O3-C1-C2-O4
3	B	602	OXD	O3-C1-C2-O4
3	D	602	OXD	O3-C1-C2-O4
3	G	602	OXD	O3-C1-C2-O4
3	C	602	OXD	O3-C1-C2-O4
3	E	602	OXD	O3-C1-C2-O4
3	H	602	OXD	O3-C1-C2-O4
3	H	602	OXD	O5-C1-C2-O4
3	F	602	OXD	O3-C1-C2-O6
3	F	602	OXD	O5-C1-C2-O4
3	G	602	OXD	O3-C1-C2-O6
3	G	602	OXD	O5-C1-C2-O4
3	A	602	OXD	O5-C1-C2-O4
3	B	602	OXD	O5-C1-C2-O4
3	C	602	OXD	O5-C1-C2-O4
3	D	602	OXD	O5-C1-C2-O4
3	E	602	OXD	O3-C1-C2-O6
3	E	602	OXD	O5-C1-C2-O4

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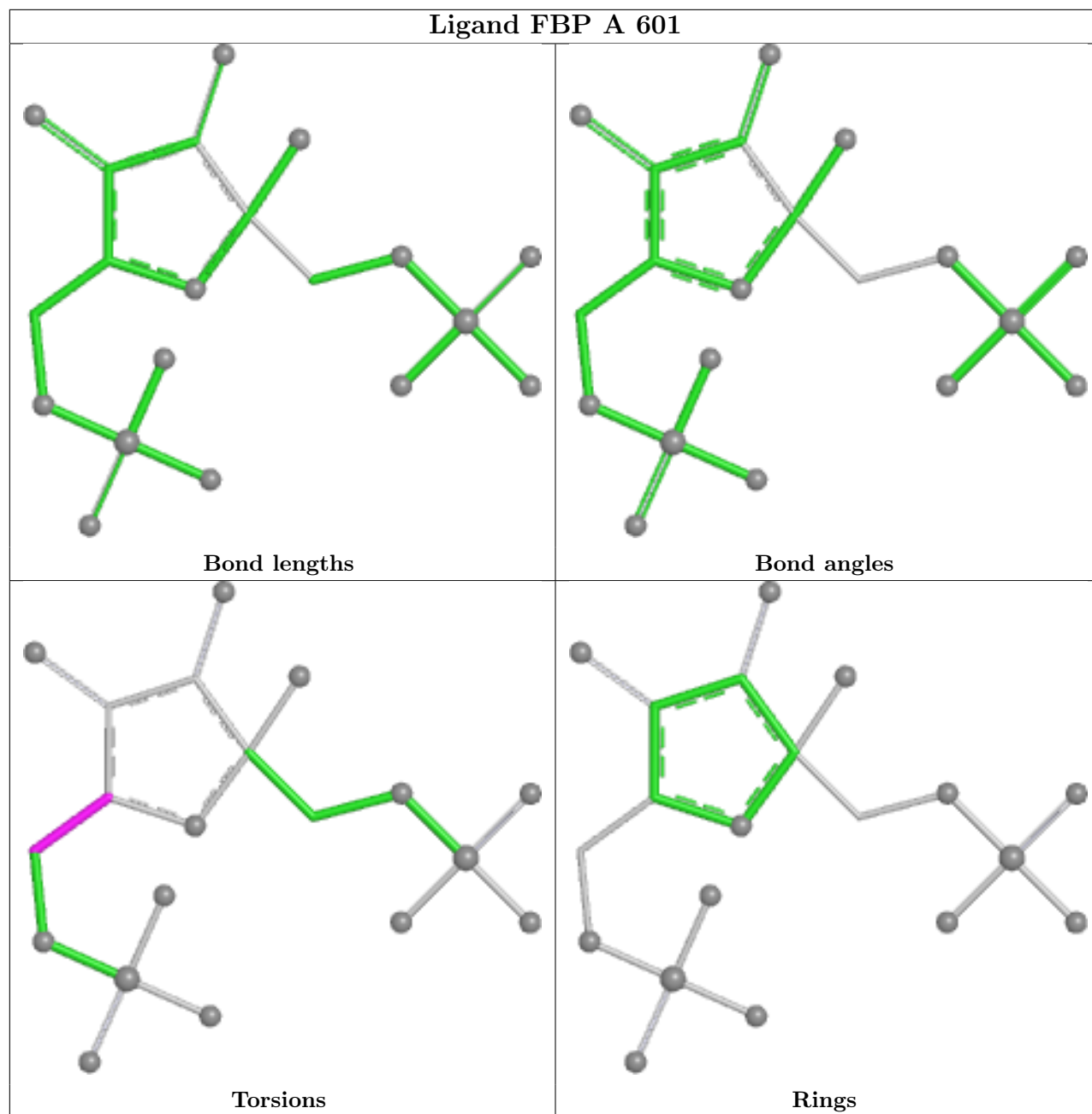
Continued from previous page...

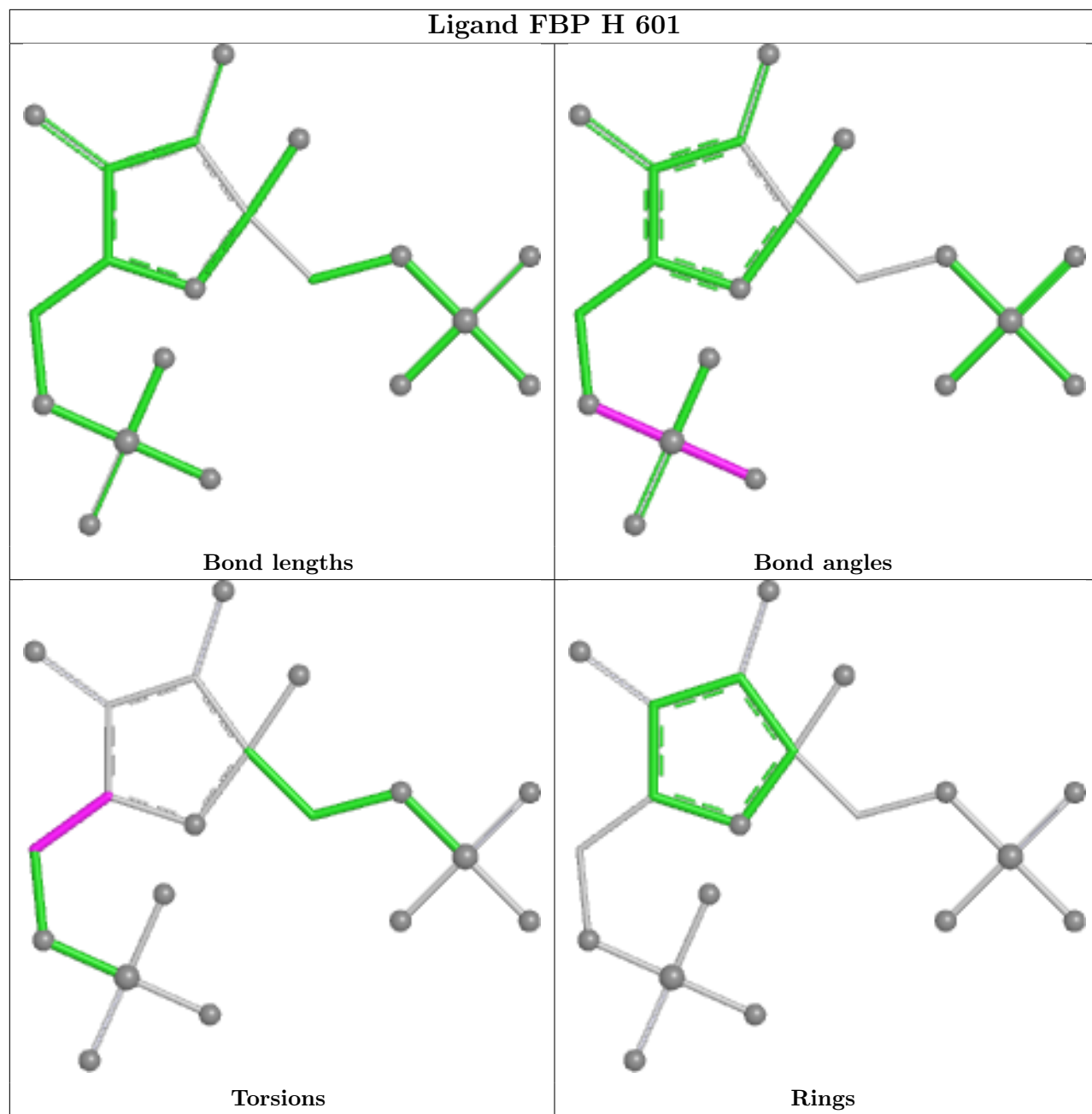
Mol	Chain	Res	Type	Atoms
3	A	602	OXD	O3-C1-C2-O6
3	B	602	OXD	O3-C1-C2-O6
3	C	602	OXD	O3-C1-C2-O6
3	D	602	OXD	O3-C1-C2-O6
3	H	602	OXD	O3-C1-C2-O6

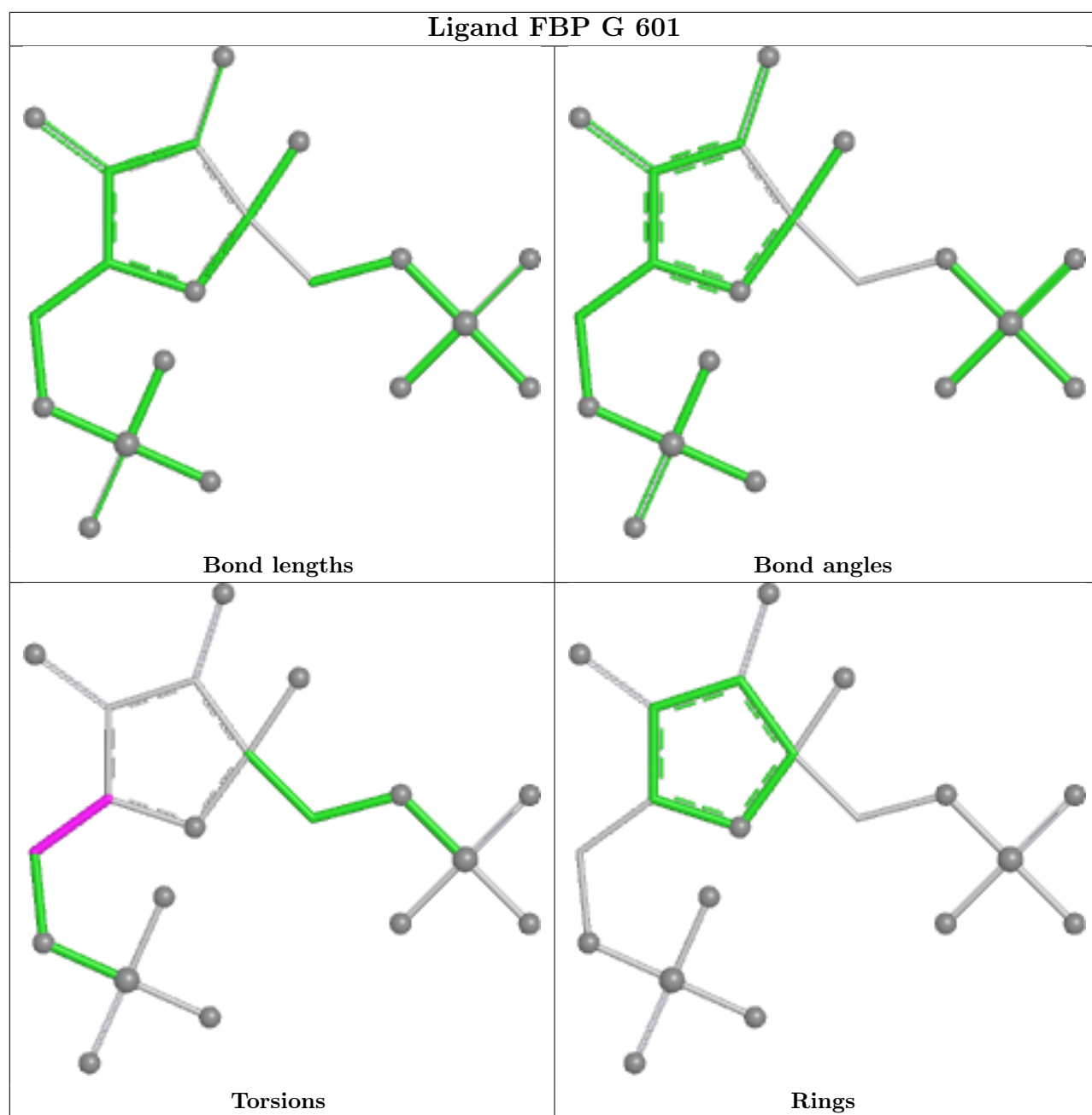
There are no ring outliers.

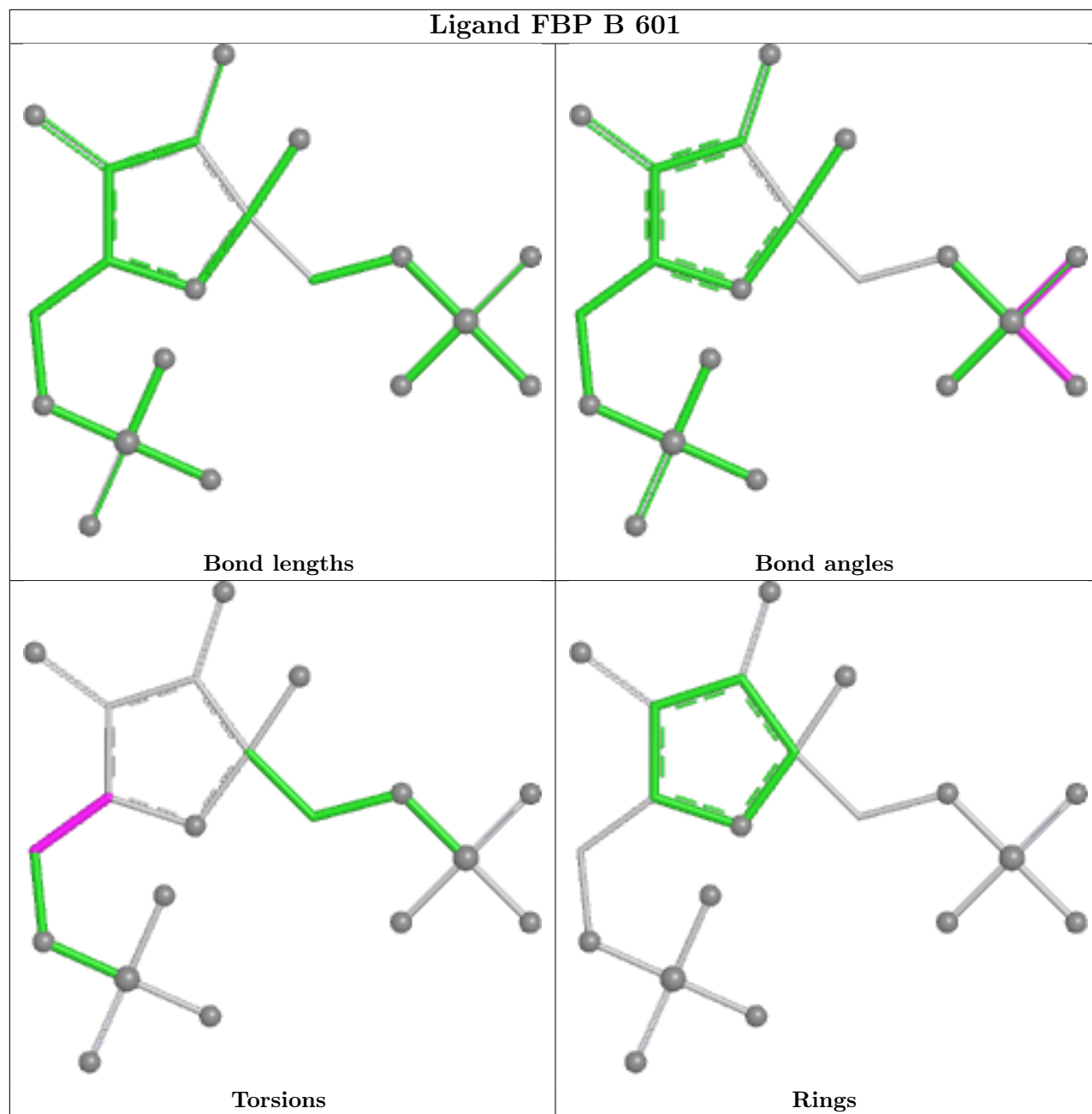
No monomer is involved in short contacts.

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.

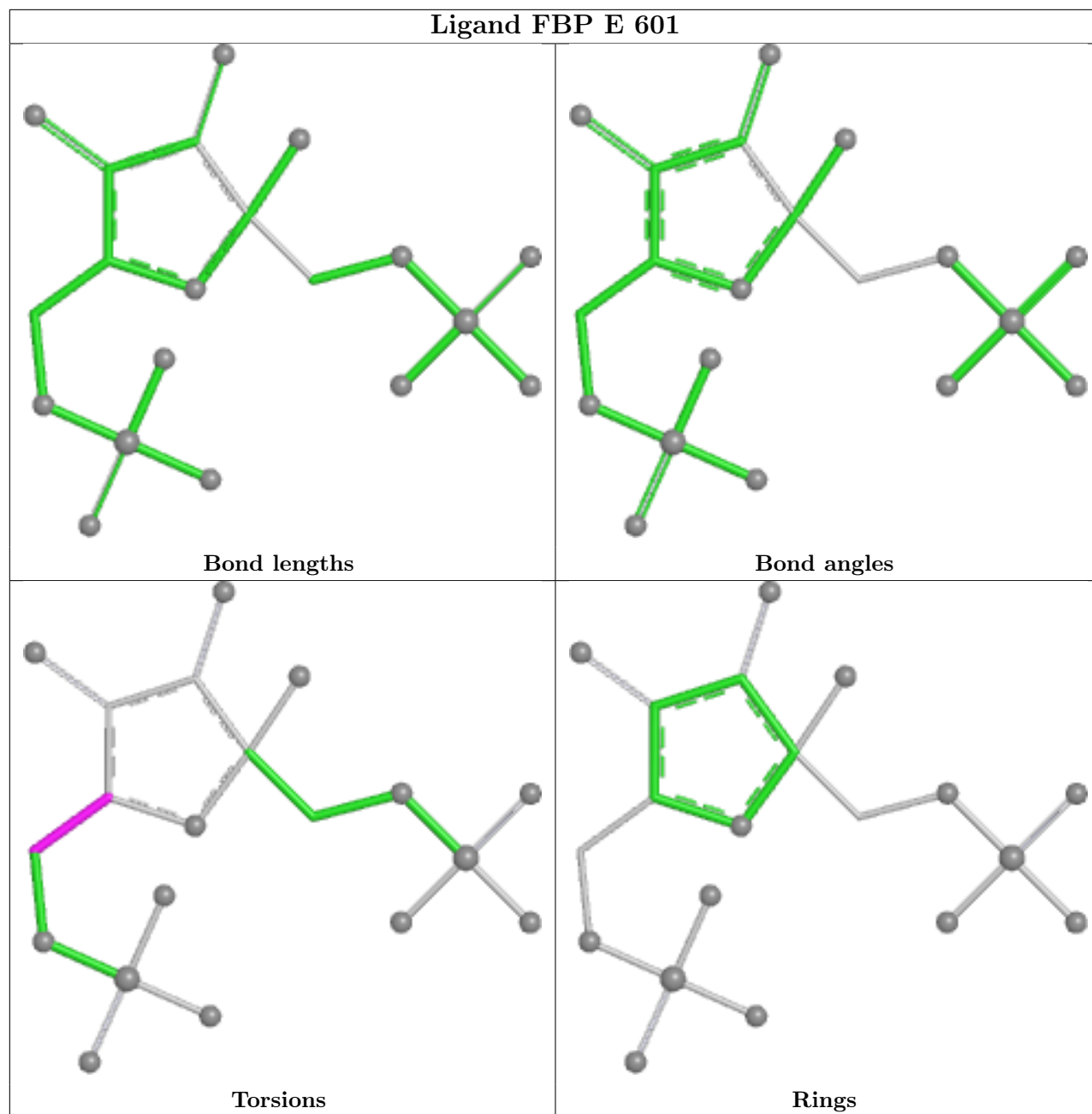


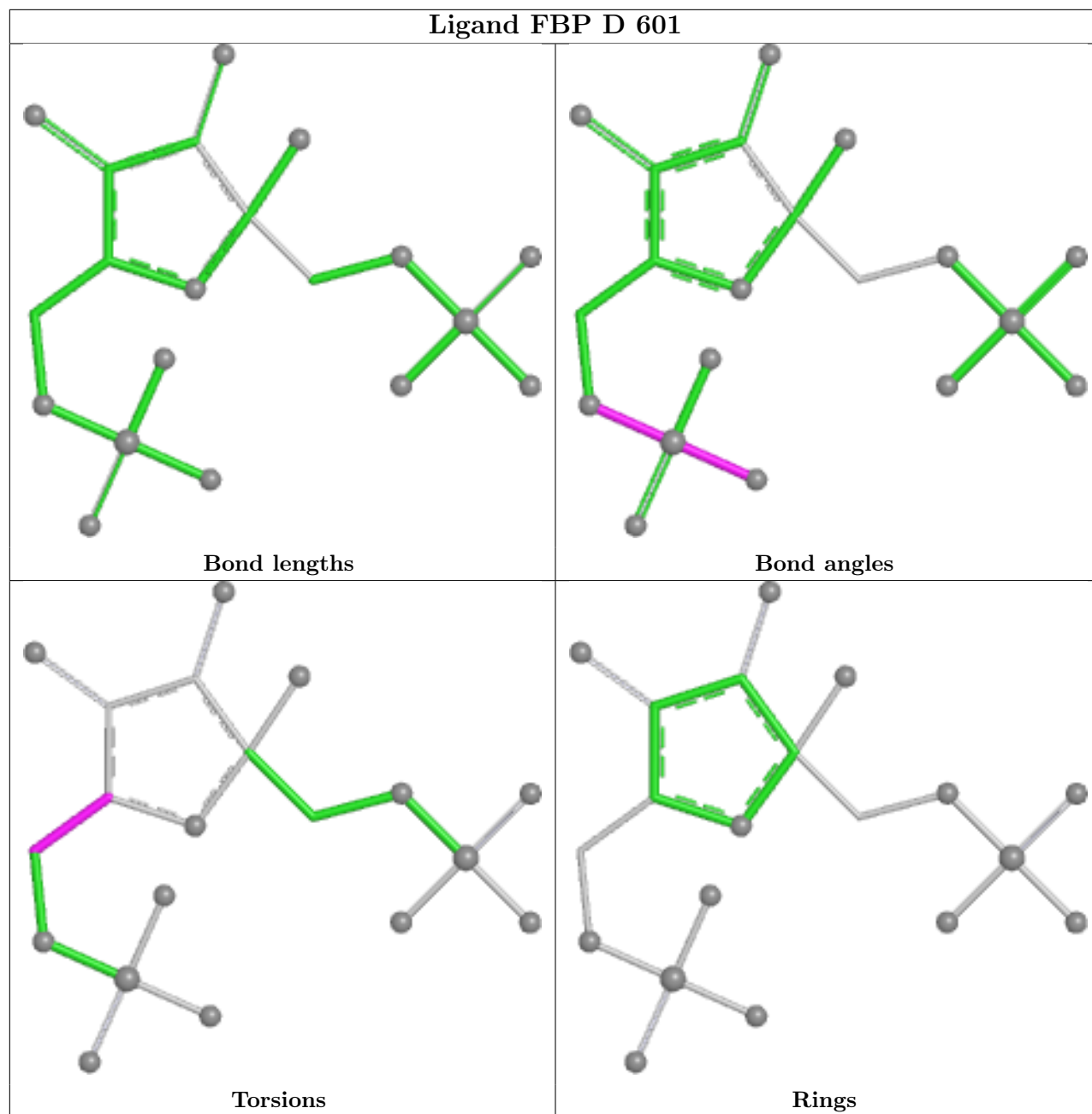




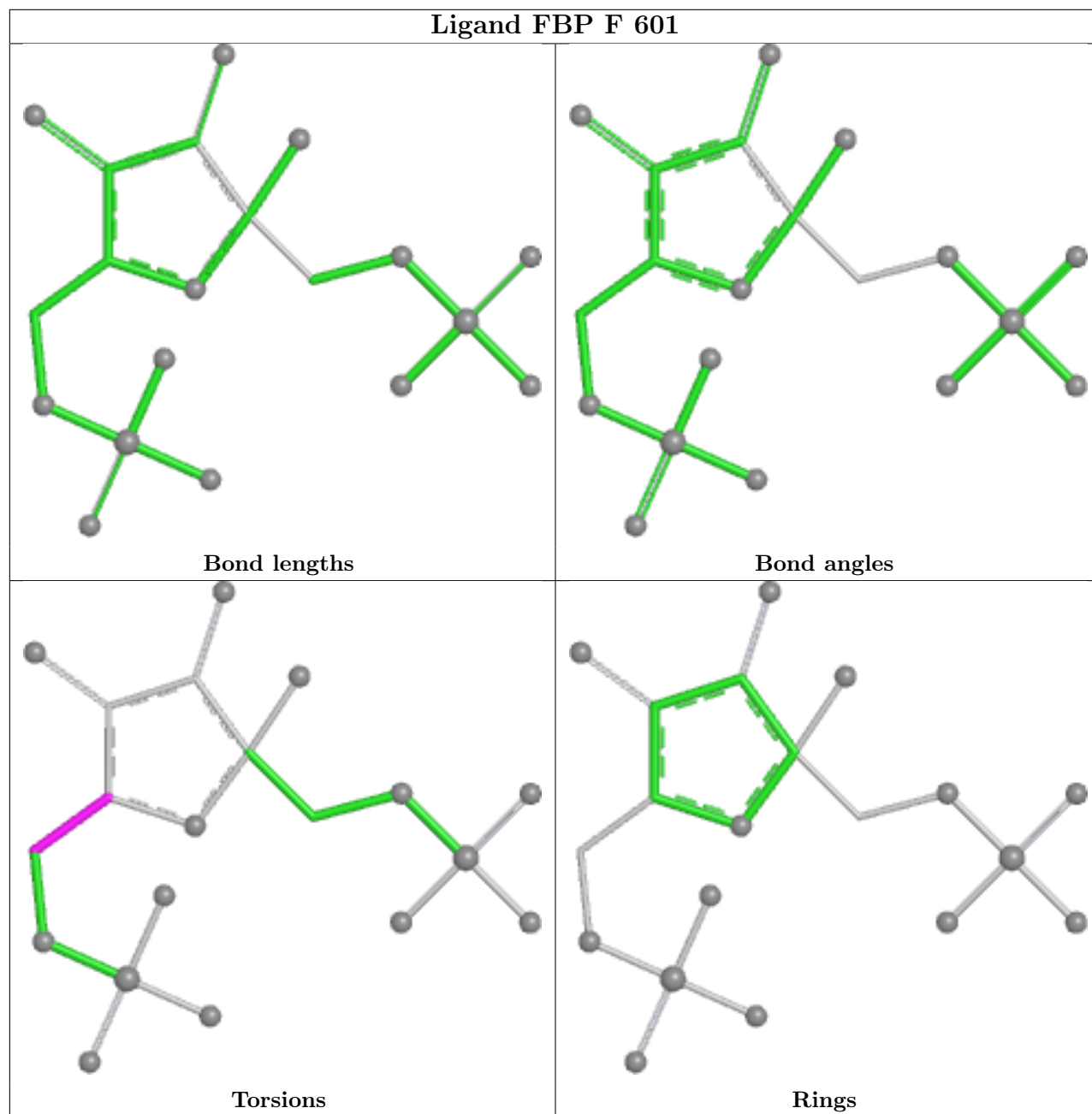


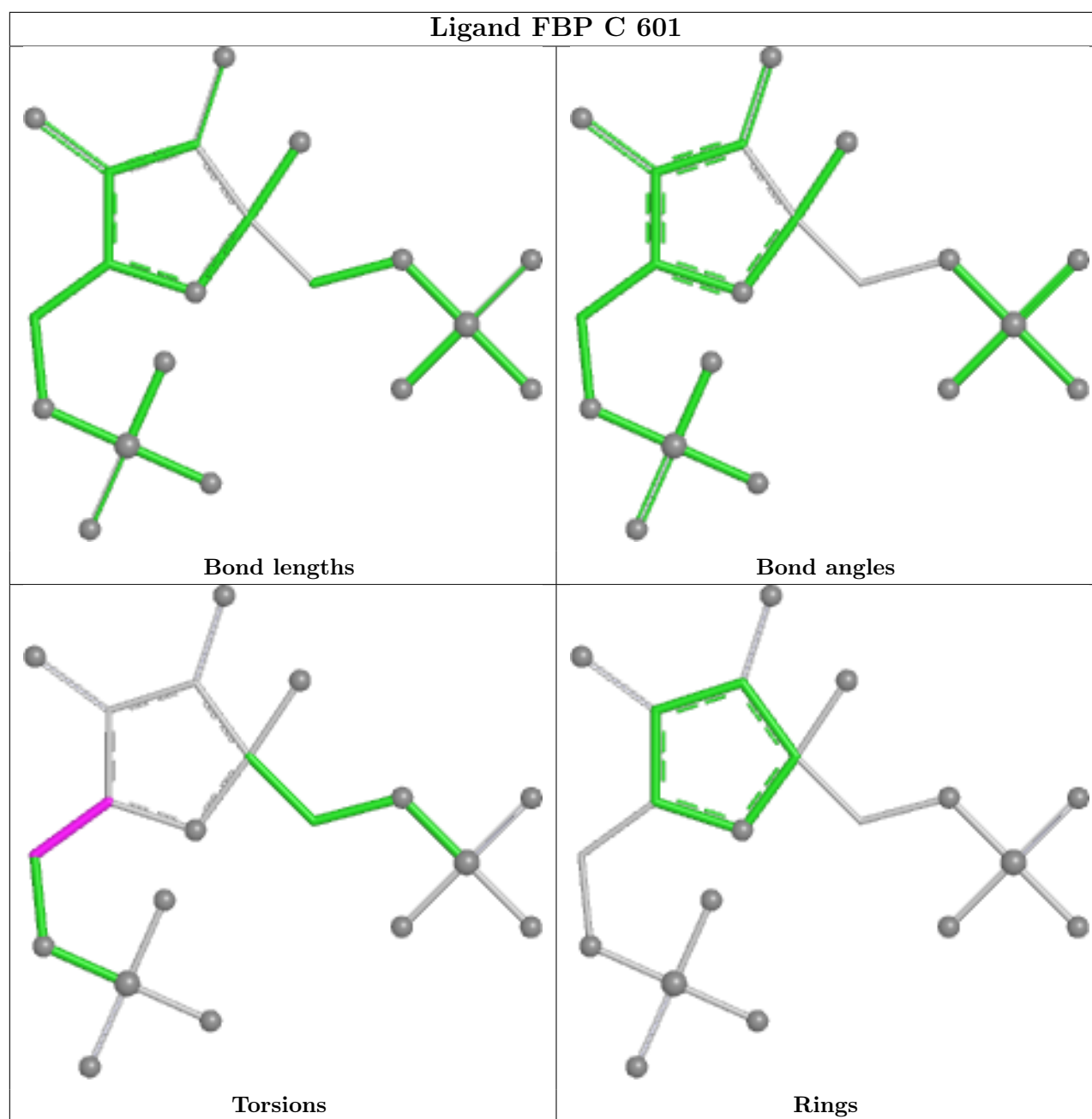
Ligand FBP E 601





Ligand FBP F 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	423/447 (94%)	1.02	68 (16%) 4 4	22, 42, 68, 88	3 (0%)
1	B	436/447 (97%)	1.19	97 (22%) 2 2	24, 42, 75, 92	3 (0%)
1	C	427/447 (95%)	0.45	36 (8%) 17 18	24, 34, 58, 81	1 (0%)
1	D	425/447 (95%)	0.22	21 (4%) 35 38	17, 31, 52, 80	2 (0%)
1	E	423/447 (94%)	1.04	60 (14%) 6 5	27, 45, 69, 91	2 (0%)
1	F	435/447 (97%)	0.98	70 (16%) 4 4	25, 41, 71, 85	3 (0%)
1	G	421/447 (94%)	0.29	22 (5%) 33 36	20, 33, 51, 75	5 (1%)
1	H	425/447 (95%)	0.19	24 (5%) 30 33	17, 30, 52, 79	3 (0%)
All	All	3415/3576 (95%)	0.67	398 (11%) 9 9	17, 37, 66, 92	22 (0%)

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	271	GLY	8.1
1	B	511	LEU	7.9
1	C	271	GLY	7.1
1	H	21	GLY	6.8
1	C	22	THR	6.3
1	A	25	PHE	6.2
1	C	130	GLY	6.2
1	A	231	PRO	6.2
1	E	231	PRO	6.1
1	A	543	SER	5.8
1	E	23	ALA	5.6
1	H	232	GLY	5.2
1	E	25	PHE	5.1
1	D	21	GLY	5.1
1	F	115	LEU	5.1
1	F	131	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	231	PRO	4.9
1	F	114	PRO	4.9
1	E	232	GLY	4.9
1	B	233	LEU	4.8
1	A	232	GLY	4.8
1	A	132	GLY	4.7
1	C	114	PRO	4.7
1	A	24	PHE	4.7
1	F	231	PRO	4.5
1	A	514	PHE	4.5
1	A	233	LEU	4.5
1	H	231	PRO	4.5
1	F	111	ALA	4.4
1	B	113	SER	4.4
1	B	543	SER	4.4
1	G	132	GLY	4.4
1	B	132	GLY	4.2
1	F	232	GLY	4.2
1	C	117	TYR	4.2
1	D	275[A]	HIS	4.2
1	F	511	LEU	4.2
1	D	311	ILE	4.2
1	B	515	LEU	4.1
1	D	22	THR	4.1
1	H	267[A]	ARG	4.1
1	F	112	GLY	4.1
1	F	233	LEU	4.1
1	H	411	ARG	4.0
1	A	540	LEU	4.0
1	B	517	VAL	4.0
1	C	412	ARG	4.0
1	C	232	GLY	4.0
1	E	514	PHE	3.9
1	F	130	GLY	3.9
1	G	514	PHE	3.9
1	F	516	ARG	3.9
1	B	267[A]	ARG	3.9
1	D	25	PHE	3.9
1	F	493	ILE	3.9
1	B	493	ILE	3.8
1	A	270	LEU	3.8
1	B	516	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	232	GLY	3.8
1	E	540	LEU	3.8
1	F	245	VAL	3.8
1	B	231	PRO	3.8
1	B	489	PRO	3.8
1	D	24	PHE	3.7
1	E	24	PHE	3.7
1	G	52	VAL	3.7
1	D	23	ALA	3.7
1	D	231	PRO	3.7
1	C	20	LEU	3.7
1	F	113	SER	3.7
1	C	21	GLY	3.6
1	A	499	ASP	3.6
1	A	131	SER	3.6
1	G	23	ALA	3.6
1	E	52	VAL	3.6
1	B	10	ARG	3.5
1	B	115	LEU	3.5
1	B	275	HIS	3.5
1	A	95	TYR	3.5
1	G	231	PRO	3.5
1	D	514	PHE	3.5
1	E	233	LEU	3.5
1	E	541	SER	3.5
1	E	132	GLY	3.5
1	C	411	ARG	3.5
1	C	25	PHE	3.5
1	F	514	PHE	3.5
1	H	514	PHE	3.5
1	B	272	PRO	3.4
1	D	131	SER	3.4
1	E	311	ILE	3.4
1	E	90	HIS	3.4
1	F	90	HIS	3.4
1	B	514	PHE	3.4
1	C	112	GLY	3.4
1	B	131	SER	3.4
1	A	34	MET	3.4
1	B	268	ALA	3.3
1	G	232	GLY	3.3
1	A	52	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	11	ALA	3.3
1	H	275[A]	HIS	3.3
1	E	351	ARG	3.3
1	E	493	ILE	3.3
1	F	311	ILE	3.3
1	B	270	LEU	3.3
1	E	256	PHE	3.3
1	F	542	ILE	3.2
1	E	272	PRO	3.2
1	A	351	ARG	3.2
1	A	70	VAL	3.2
1	B	232	GLY	3.2
1	B	509	GLY	3.2
1	F	379	LYS	3.2
1	B	112	GLY	3.2
1	A	238	VAL	3.2
1	E	238	VAL	3.2
1	B	512	ARG	3.2
1	E	275	HIS	3.2
1	F	270	LEU	3.2
1	B	109	SER	3.2
1	B	110	PHE	3.2
1	B	490	PRO	3.1
1	B	416	LEU	3.1
1	C	113	SER	3.1
1	C	116	SER	3.1
1	B	245	VAL	3.1
1	A	242	ARG	3.1
1	F	267[A]	ARG	3.1
1	B	414	ALA	3.1
1	E	130	GLY	3.1
1	C	115	LEU	3.1
1	B	269	ALA	3.1
1	B	256	PHE	3.1
1	C	131	SER	3.1
1	A	272	PRO	3.0
1	B	475	VAL	3.0
1	A	23	ALA	3.0
1	B	348	THR	3.0
1	F	275	HIS	3.0
1	G	272	PRO	3.0
1	D	412	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	52	VAL	3.0
1	F	351	ARG	3.0
1	C	413	ALA	3.0
1	E	511	LEU	3.0
1	E	131	SER	2.9
1	C	34	MET	2.9
1	B	506	ILE	2.9
1	F	490	PRO	2.9
1	H	25	PHE	2.9
1	H	22	THR	2.9
1	C	414	ALA	2.9
1	F	117	TYR	2.9
1	A	436	CYS	2.9
1	B	70	VAL	2.9
1	B	90	HIS	2.9
1	F	116	SER	2.9
1	B	527	TRP	2.9
1	A	256	PHE	2.8
1	E	34	MET	2.8
1	A	541	SER	2.8
1	E	115	LEU	2.8
1	E	129	PRO	2.8
1	C	110	PHE	2.8
1	B	263	VAL	2.8
1	B	117	TYR	2.8
1	F	416	LEU	2.8
1	D	436	CYS	2.8
1	A	63	ILE	2.8
1	A	311	ILE	2.8
1	E	269	ALA	2.8
1	F	492	ALA	2.8
1	F	118	ARG	2.8
1	F	498	VAL	2.8
1	F	517	VAL	2.8
1	H	131	SER	2.8
1	B	114	PRO	2.7
1	E	490	PRO	2.7
1	B	103	VAL	2.7
1	B	116	SER	2.7
1	A	518	GLY	2.7
1	F	91	GLY	2.7
1	F	411	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	243	PHE	2.7
1	B	533	TYR	2.7
1	C	233	LEU	2.7
1	A	273	GLU	2.7
1	B	63	ILE	2.7
1	A	128	GLY	2.7
1	B	379	LYS	2.7
1	B	111	ALA	2.7
1	C	111	ALA	2.7
1	E	265	ALA	2.7
1	B	415	PRO	2.7
1	A	482	PHE	2.7
1	A	515	LEU	2.7
1	F	238	VAL	2.7
1	A	90	HIS	2.6
1	G	90	HIS	2.6
1	G	25	PHE	2.6
1	H	132	GLY	2.6
1	F	266	VAL	2.6
1	B	100	ILE	2.6
1	F	63	ILE	2.6
1	B	118	ARG	2.6
1	G	412	ARG	2.6
1	H	412	ARG	2.6
1	B	508	SER	2.6
1	G	34	MET	2.6
1	B	88	PHE	2.6
1	B	274	GLY	2.6
1	E	505	GLY	2.6
1	F	412	ARG	2.6
1	B	107	VAL	2.6
1	F	506	ILE	2.6
1	A	111	ALA	2.6
1	B	89	SER	2.6
1	C	23	ALA	2.6
1	F	415	PRO	2.6
1	A	75	GLU	2.6
1	B	241	LEU	2.6
1	G	515	LEU	2.6
1	E	242	ARG	2.6
1	H	130	GLY	2.5
1	C	24	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	436	CYS	2.5
1	D	515	LEU	2.5
1	G	331	LEU	2.5
1	H	273	GLU	2.5
1	A	236	GLN	2.5
1	A	130	GLY	2.5
1	F	132	GLY	2.5
1	A	275	HIS	2.5
1	E	504	PHE	2.5
1	A	73	LEU	2.5
1	B	540	LEU	2.5
1	B	120	VAL	2.5
1	E	97	ALA	2.5
1	B	411	ARG	2.5
1	B	507	GLU	2.5
1	E	234	SER	2.5
1	E	270	LEU	2.5
1	E	515	LEU	2.5
1	F	110	PHE	2.5
1	H	24	PHE	2.5
1	E	264	ALA	2.5
1	F	268	ALA	2.5
1	B	311	ILE	2.5
1	A	411	ARG	2.5
1	E	408	GLU	2.5
1	E	543	SER	2.5
1	A	496	ASP	2.4
1	B	243	PHE	2.4
1	B	484	LEU	2.4
1	G	411	ARG	2.4
1	F	95	TYR	2.4
1	E	70	VAL	2.4
1	G	516	ARG	2.4
1	C	272	PRO	2.4
1	E	489	PRO	2.4
1	F	73	LEU	2.4
1	B	266	VAL	2.4
1	D	52	VAL	2.4
1	F	521	VAL	2.4
1	E	71	GLU	2.4
1	D	34	MET	2.4
1	H	34	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	241	LEU	2.4
1	G	540	LEU	2.4
1	A	68	ARG	2.4
1	A	500	ARG	2.4
1	B	95	TYR	2.4
1	B	236	GLN	2.3
1	C	132	GLY	2.3
1	C	19	GLU	2.3
1	A	495	ALA	2.3
1	B	492	ALA	2.3
1	F	455	ARG	2.3
1	G	487	ARG	2.3
1	H	410	LEU	2.3
1	A	349	LYS	2.3
1	A	257	VAL	2.3
1	F	530	GLY	2.3
1	B	351	ARG	2.3
1	D	351	ARG	2.3
1	F	512	ARG	2.3
1	E	243	PHE	2.3
1	B	295	ILE	2.3
1	B	99	SER	2.3
1	B	52	VAL	2.3
1	E	517	VAL	2.3
1	B	127	LYS	2.3
1	F	34	MET	2.3
1	C	515	LEU	2.3
1	B	504	PHE	2.3
1	F	504	PHE	2.3
1	A	426	ILE	2.3
1	E	499	ASP	2.3
1	A	33	ALA	2.2
1	B	495	ALA	2.2
1	F	97	ALA	2.2
1	G	53	ALA	2.2
1	H	413	ALA	2.2
1	B	242	ARG	2.2
1	E	412	ARG	2.2
1	B	520	LEU	2.2
1	H	233	LEU	2.2
1	E	271	GLY	2.2
1	C	90	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	521	VAL	2.2
1	F	489	PRO	2.2
1	A	62	THR	2.2
1	B	494	TRP	2.2
1	A	97	ALA	2.2
1	A	265	ALA	2.2
1	G	54	ALA	2.2
1	A	127	LYS	2.2
1	F	12	ASP	2.2
1	C	26	GLN	2.2
1	G	24	PHE	2.2
1	A	118	ARG	2.2
1	E	95	TYR	2.2
1	D	47	ILE	2.2
1	E	426	ILE	2.2
1	E	506	ILE	2.2
1	B	259	LYS	2.2
1	B	502	VAL	2.2
1	H	52	VAL	2.2
1	B	11	ALA	2.2
1	F	269	ALA	2.2
1	F	414	ALA	2.2
1	H	23	ALA	2.2
1	H	436	CYS	2.2
1	A	112	GLY	2.2
1	F	241	LEU	2.2
1	F	485	LEU	2.2
1	B	96	HIS	2.2
1	E	118	ARG	2.2
1	A	243	PHE	2.2
1	A	129	PRO	2.2
1	E	277	ILE	2.2
1	C	52	VAL	2.1
1	F	33	ALA	2.1
1	E	516	ARG	2.1
1	E	128	GLY	2.1
1	B	73	LEU	2.1
1	B	410	LEU	2.1
1	B	485	LEU	2.1
1	E	89	SER	2.1
1	A	88	PHE	2.1
1	A	404	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	242	ARG	2.1
1	H	516	ARG	2.1
1	B	249	VAL	2.1
1	F	103	VAL	2.1
1	B	518	GLY	2.1
1	C	436	CYS	2.1
1	F	515	LEU	2.1
1	B	71	GLU	2.1
1	C	351	ARG	2.1
1	E	542	ILE	2.1
1	F	277	ILE	2.1
1	G	311	ILE	2.1
1	B	106	ALA	2.1
1	B	513	GLY	2.1
1	D	413	ALA	2.1
1	A	245	VAL	2.1
1	B	498	VAL	2.1
1	A	412	ARG	2.1
1	C	416	LEU	2.1
1	F	86	LEU	2.1
1	F	71	GLU	2.0
1	B	34	MET	2.0
1	A	26	GLN	2.0
1	A	89	SER	2.0
1	A	249	VAL	2.0
1	A	517	VAL	2.0
1	C	109	SER	2.0
1	E	109	SER	2.0
1	F	543	SER	2.0
1	B	86	LEU	2.0
1	E	241	LEU	2.0
1	D	272	PRO	2.0
1	B	130	GLY	2.0
1	E	513	GLY	2.0
1	B	412	ARG	2.0
1	B	500	ARG	2.0
1	E	536	ILE	2.0
1	F	347	ILE	2.0
1	A	32	ALA	2.0
1	A	237	ASP	2.0
1	A	269	ALA	2.0
1	B	541	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	543	SER	2.0
1	A	498	VAL	2.0
1	B	257	VAL	2.0
1	F	13	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NA	B	605	1/1	0.89	0.17	40,40,40,40	0
5	K	E	604	1/1	0.90	0.20	62,62,62,62	0
5	K	B	604	1/1	0.91	0.14	52,52,52,52	0
3	OXD	E	602	6/6	0.93	0.09	48,49,49,49	0
6	NA	H	605	1/1	0.93	0.14	39,39,39,39	0
3	OXD	B	602	6/6	0.94	0.08	39,40,41,41	0
5	K	A	604	1/1	0.94	0.14	54,54,54,54	0
2	FBP	F	601	20/20	0.95	0.08	37,41,44,44	0
3	OXD	C	602	6/6	0.95	0.06	35,36,37,38	0
3	OXD	A	602	6/6	0.95	0.08	48,49,49,50	0
3	OXD	F	602	6/6	0.95	0.07	40,41,42,43	0
6	NA	C	605	1/1	0.95	0.12	37,37,37,37	0
6	NA	G	605	1/1	0.95	0.16	36,36,36,36	0
3	OXD	H	602	6/6	0.95	0.07	32,33,33,35	0
3	OXD	D	602	6/6	0.96	0.06	31,32,33,33	0
6	NA	F	605	1/1	0.96	0.13	39,39,39,39	0
5	K	F	604	1/1	0.96	0.13	52,52,52,52	0
2	FBP	B	601	20/20	0.96	0.07	40,42,45,45	0
3	OXD	G	602	6/6	0.97	0.05	32,33,34,35	0

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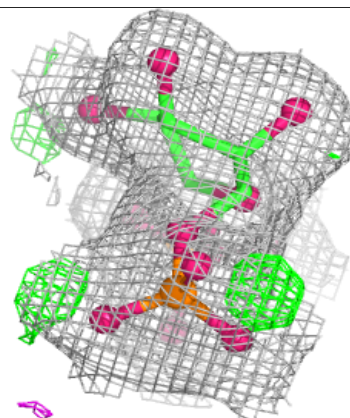
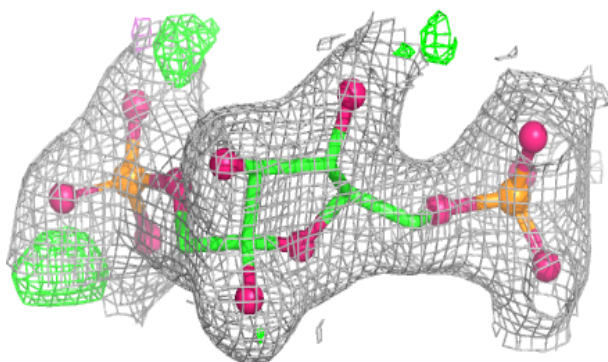
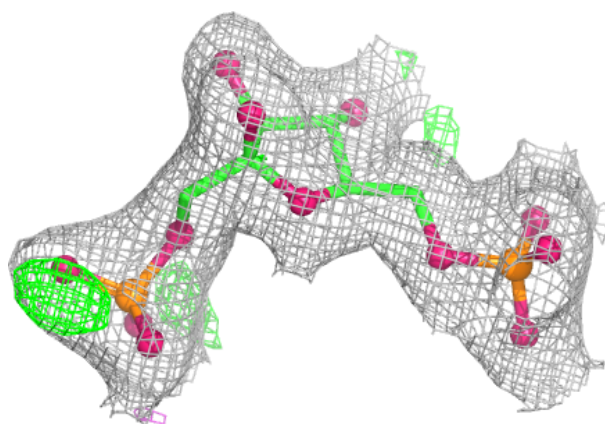
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FBP	E	601	20/20	0.97	0.07	38,39,44,44	0
4	MG	B	603	1/1	0.97	0.06	42,42,42,42	0
5	K	H	604	1/1	0.98	0.07	36,36,36,36	0
2	FBP	A	601	20/20	0.98	0.06	34,35,36,36	0
5	K	C	604	1/1	0.98	0.11	39,39,39,39	0
6	NA	D	605	1/1	0.98	0.13	38,38,38,38	0
4	MG	C	603	1/1	0.98	0.03	34,34,34,34	0
2	FBP	G	601	20/20	0.98	0.04	26,27,29,31	0
5	K	G	604	1/1	0.98	0.13	40,40,40,40	0
4	MG	E	603	1/1	0.99	0.04	47,47,47,47	0
4	MG	F	603	1/1	0.99	0.03	39,39,39,39	0
4	MG	G	603	1/1	0.99	0.02	31,31,31,31	0
4	MG	H	603	1/1	0.99	0.04	33,33,33,33	0
2	FBP	C	601	20/20	0.99	0.04	26,28,30,31	0
4	MG	A	603	1/1	0.99	0.03	48,48,48,48	0
2	FBP	H	601	20/20	0.99	0.04	24,26,28,30	0
5	K	D	604	1/1	0.99	0.06	33,33,33,33	0
2	FBP	D	601	20/20	0.99	0.04	25,27,29,31	0
4	MG	D	603	1/1	1.00	0.02	30,30,30,30	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.

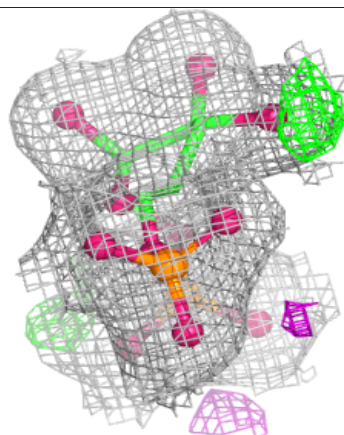
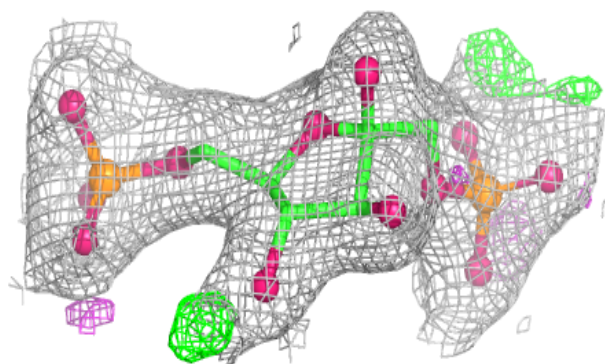
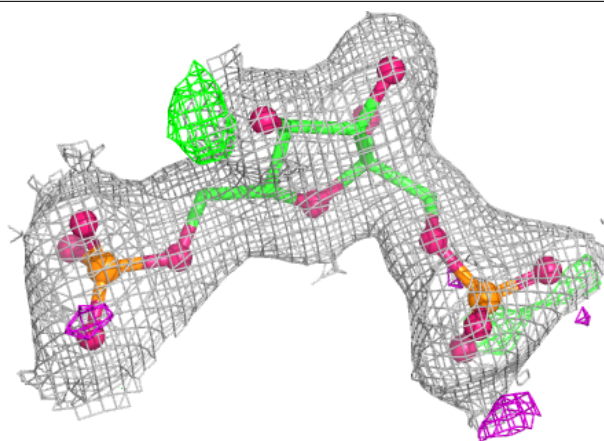
Electron density around FBP F 601:

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

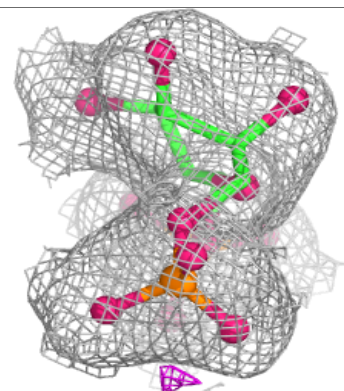
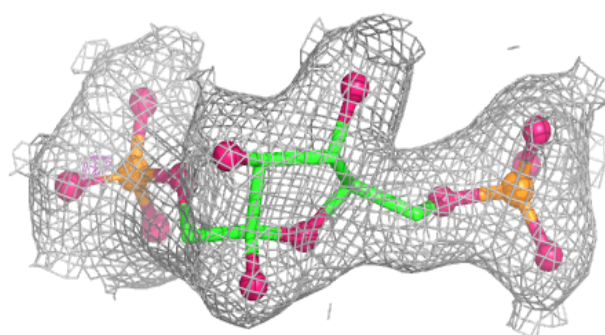
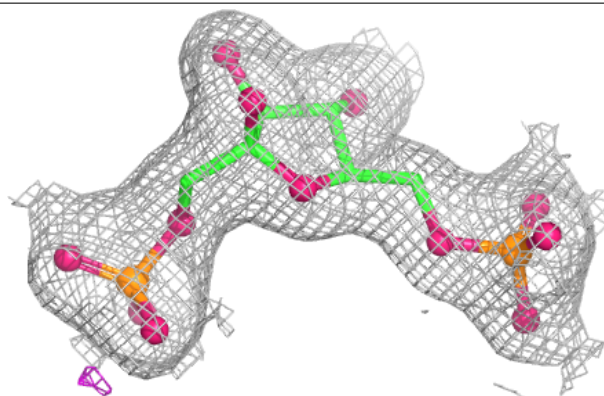


Electron density around FBP B 601:

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

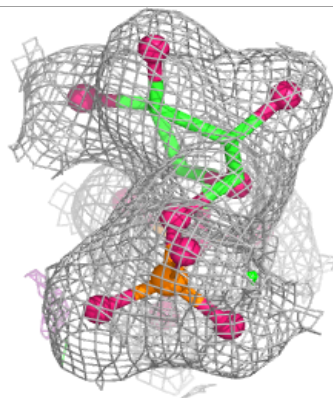
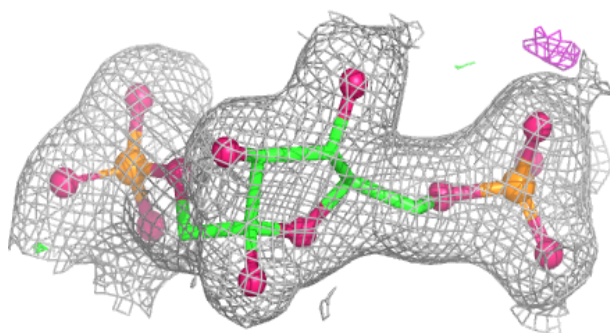
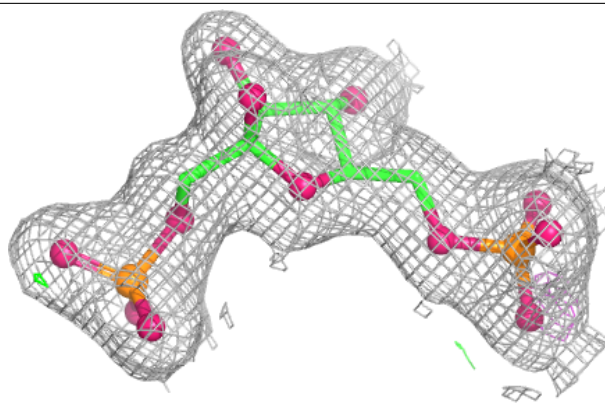
**Electron density around FBP E 601:**

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

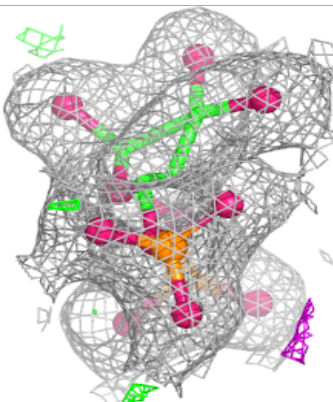
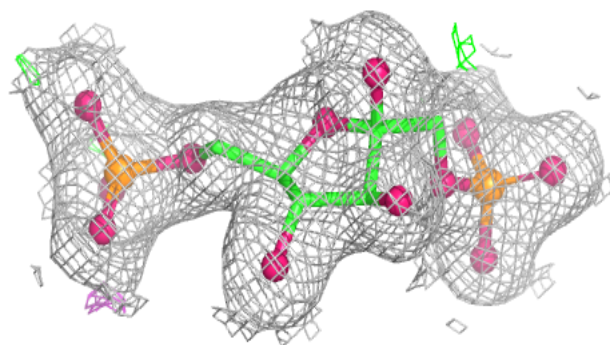
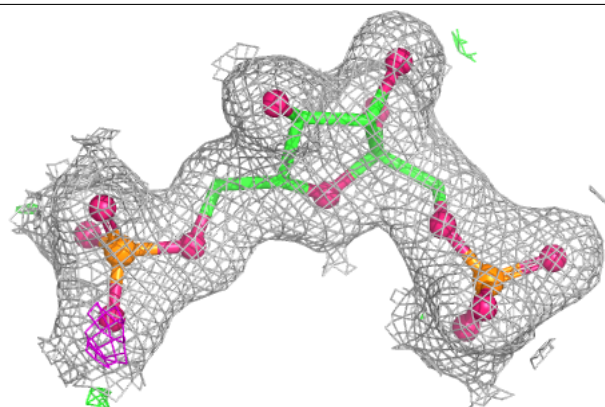


Electron density around FBP A 601:

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

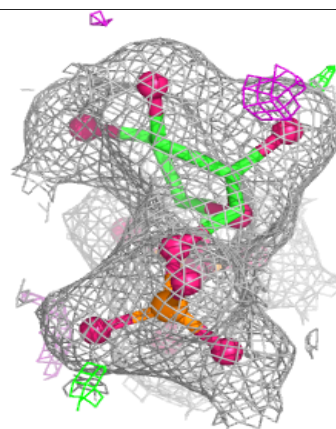
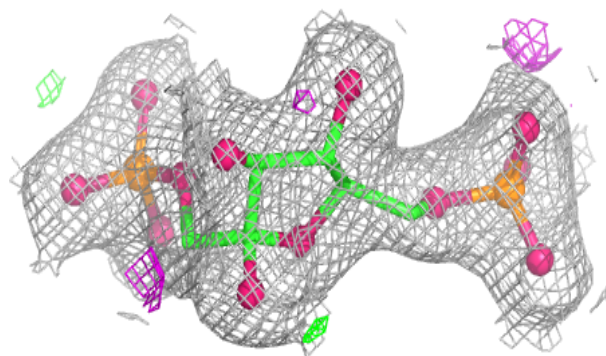
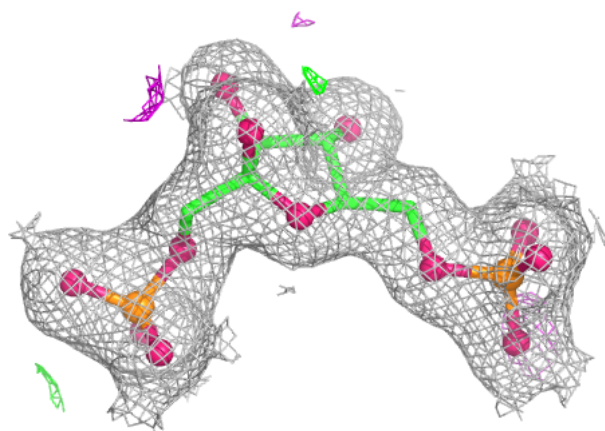
**Electron density around FBP G 601:**

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



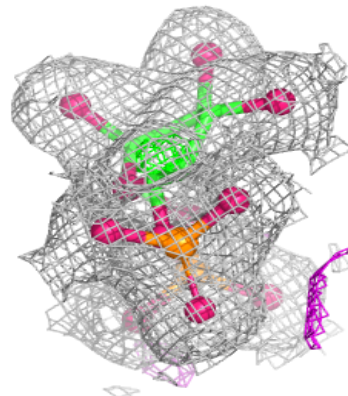
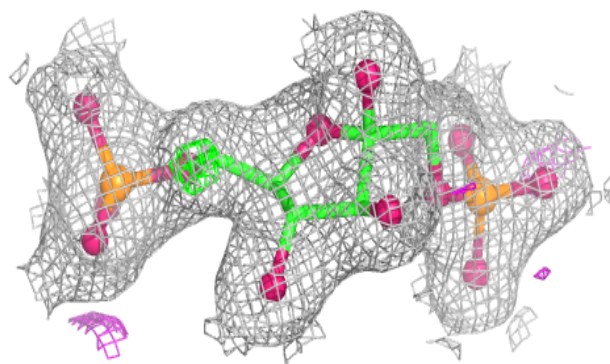
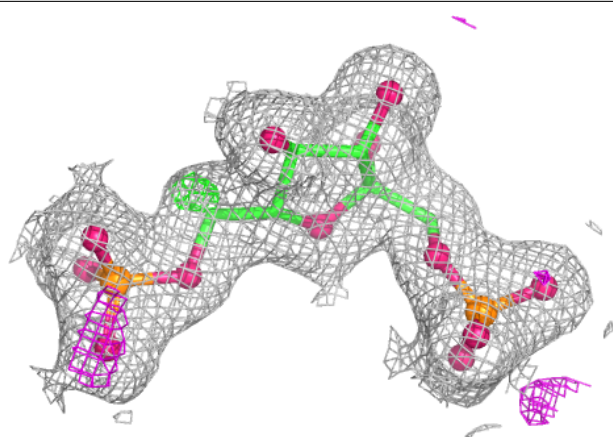
Electron density around FBP C 601:

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

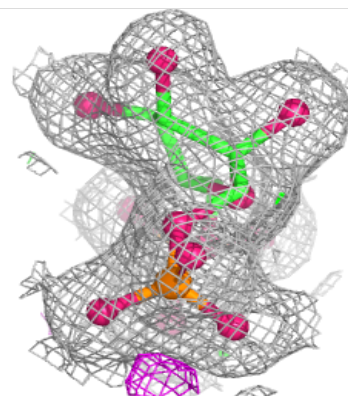
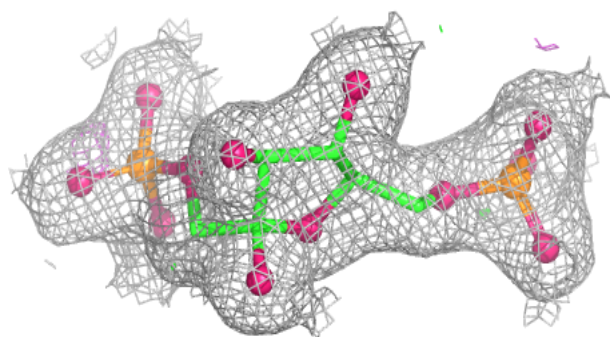
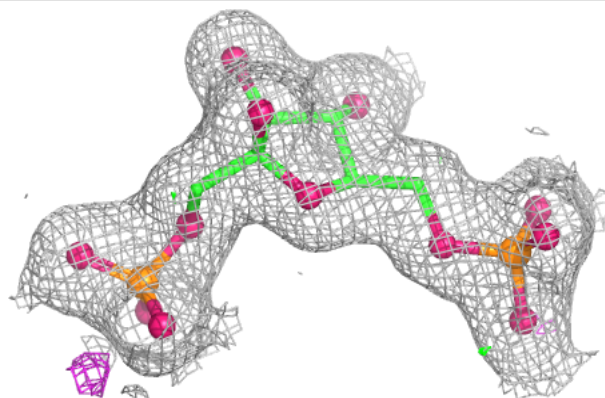


Electron density around FBP H 601:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.