



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 02:42 AM BST

PDB ID : 5X0I
Title : Crystal structure of PKM2 R399E mutant complexed with FBP and serine
Authors : Wang, W.C.; Chen, T.J.
Deposited on : 2017-01-20
Resolution : 2.64 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

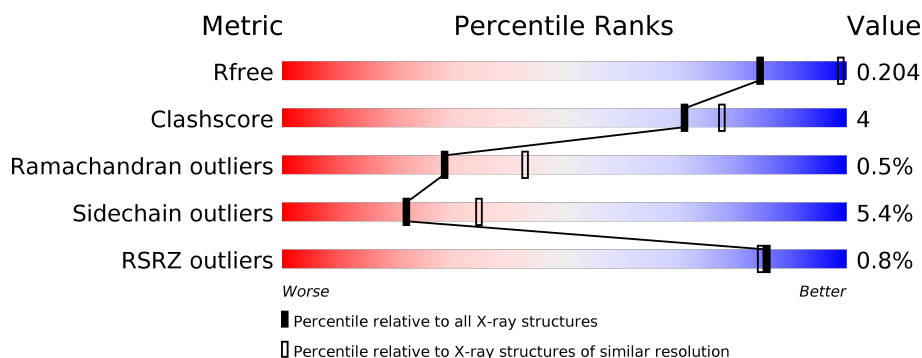
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 on 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	551	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 82%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> </div> <div>82% 12% • 6%</div> </div>
1	B	551	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 79%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 7%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> </div> <div>79% 13% • 7%</div> </div>
1	C	551	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> </div> <div>81% 12% • 6%</div> </div>
1	D	551	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 11%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> </div> <div>81% 11% • 6%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16023 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 PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3963	2491	701	746	25			
1	B	515	Total	C	N	O	S	0	0	0
			3949	2484	698	742	25			
1	C	518	Total	C	N	O	S	0	0	0
			3963	2491	701	746	25			
1	D	518	Total	C	N	O	S	0	0	0
			3963	2491	701	746	25			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P14618
A	-18	GLY	-	expression tag	UNP P14618
A	-17	SER	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	HIS	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	SER	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	GLY	-	expression tag	UNP P14618
A	-6	LEU	-	expression tag	UNP P14618
A	-5	VAL	-	expression tag	UNP P14618
A	-4	PRO	-	expression tag	UNP P14618
A	-3	ARG	-	expression tag	UNP P14618
A	-2	GLY	-	expression tag	UNP P14618
A	-1	SER	-	expression tag	UNP P14618
A	0	HIS	-	expression tag	UNP P14618
A	399	GLU	ARG	engineered mutation	UNP P14618

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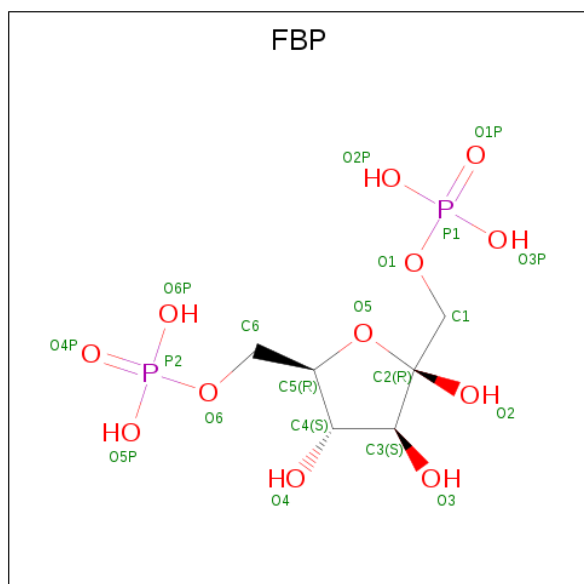
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP P14618
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	SER	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	GLY	-	expression tag	UNP P14618
B	-6	LEU	-	expression tag	UNP P14618
B	-5	VAL	-	expression tag	UNP P14618
B	-4	PRO	-	expression tag	UNP P14618
B	-3	ARG	-	expression tag	UNP P14618
B	-2	GLY	-	expression tag	UNP P14618
B	-1	SER	-	expression tag	UNP P14618
B	0	HIS	-	expression tag	UNP P14618
B	399	GLU	ARG	engineered mutation	UNP P14618
C	-19	MET	-	expression tag	UNP P14618
C	-18	GLY	-	expression tag	UNP P14618
C	-17	SER	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	HIS	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	SER	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	GLY	-	expression tag	UNP P14618
C	-6	LEU	-	expression tag	UNP P14618
C	-5	VAL	-	expression tag	UNP P14618
C	-4	PRO	-	expression tag	UNP P14618
C	-3	ARG	-	expression tag	UNP P14618
C	-2	GLY	-	expression tag	UNP P14618
C	-1	SER	-	expression tag	UNP P14618
C	0	HIS	-	expression tag	UNP P14618
C	399	GLU	ARG	engineered mutation	UNP P14618

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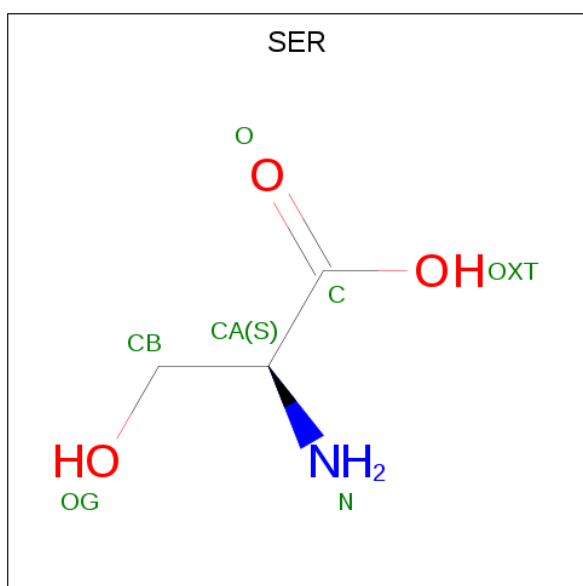
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	SER	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	GLY	-	expression tag	UNP P14618
D	-6	LEU	-	expression tag	UNP P14618
D	-5	VAL	-	expression tag	UNP P14618
D	-4	PRO	-	expression tag	UNP P14618
D	-3	ARG	-	expression tag	UNP P14618
D	-2	GLY	-	expression tag	UNP P14618
D	-1	SER	-	expression tag	UNP P14618
D	0	HIS	-	expression tag	UNP P14618
D	399	GLU	ARG	engineered mutation	UNP P14618

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



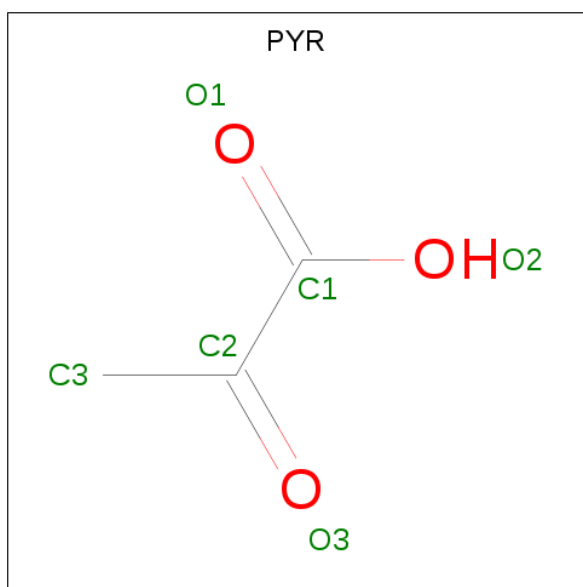
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	3	1	3		
3	B	1	Total	C	N	O	0	0
			7	3	1	3		
3	C	1	Total	C	N	O	0	0
			7	3	1	3		
3	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	C	1	Total 1	K 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total 13	O 13	0	0
7	B	13	Total 13	O 13	0	0
7	C	9	Total 9	O 9	0	0
7	D	10	Total 10	O 10	0	0

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.

Chain A:

Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. A color scale at the top indicates conservation percentage: 82% (green), 12% (yellow), and 6% (red).

Position	Amino Acid	Information Content (bits)
1	Met	0.00
2	Gly	0.00
3	Ser	0.00
4	His	0.00
5	His	0.00
6	His	0.00
7	His	0.00
8	His	0.00
9	Ser	0.00
10	Ser	0.00
11	Gly	0.00
12	Leu	0.00
13	Val	0.00
14	Pro	0.00
15	Arg	0.00
16	Gly	0.00
17	Ser	0.00
18	His	0.00
19	Met	0.00
20	Ser	0.00
21	Lys	0.00
22	Pro	0.00
23	His	0.00
24	Ser	0.00
25	Glu	0.00
26	Ala	0.00
27	Gly	0.00
28	Thr	0.00
29	Ala	0.00
30	Phe	0.00
31	Ile	0.00
32	Gln	0.00
33	Leu	0.00
34	Thr	0.00
35	Thr	0.00
36	Asp	0.00
37	Ser	0.00
38	Pro	0.00
39	Pro	0.00
40	Asp	0.00
41	Pro	0.00
42	Asp	0.00
43	Pro	0.00
44	Asp	0.00
45	Pro	0.00
46	Asp	0.00
47	Pro	0.00
48	Asp	0.00
49	Pro	0.00
50	Asp	0.00
51	Pro	0.00
52	Asp	0.00
53	Pro	0.00
54	Asp	0.00
55	Pro	0.00
56	Asp	0.00
57	Pro	0.00
58	Asp	0.00
59	Pro	0.00
60	Asp	0.00
61	Pro	0.00
62	Asp	0.00
63	Pro	0.00
64	Asp	0.00
65	Pro	0.00
66	Asp	0.00
67	Pro	0.00
68	Asp	0.00
69	Pro	0.00
70	Asp	0.00
71	Pro	0.00
72	Asp	0.00
73	Pro	0.00
74	Asp	0.00
75	Pro	0.00
76	Asp	0.00
77	Pro	0.00
78	Asp	0.00
79	Pro	0.00
80	Asp	0.00
81	Pro	0.00
82	Asp	0.00
83	Pro	0.00
84	Asp	0.00
85	Pro	0.00
86	Asp	0.00
87	Pro	0.00
88	Asp	0.00
89	Pro	0.00
90	Asp	0.00
91	Pro	0.00
92	Asp	0.00
93	Pro	0.00
94	Asp	0.00
95	Pro	0.00
96	Asp	0.00
97	Pro	0.00
98	Asp	0.00
99	Pro	0.00
100	Asp	0.00

Chain B:

79% 13% 7%

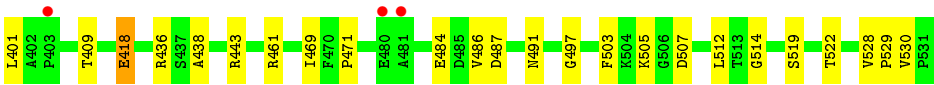
100%

Label	Category
R106	Green
K126	Green
GLY	Green
SER	Green
GLY	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
SER	Green
SER	Green
GLY	Green
LEU	Green
VAL	Green
PRO	Green
ARG	Green
GLY	Green
SER	Green
HIS	Green
HIS	Green
MET	Green
SER	Green
LVS	Green
PRO	Green
HIS	Green
SER	Green
GLU	Green
ALA	Green
GLY	Green
THR	Green
ALA	Green
PHE	Green
ILE	Green
Q14	Green
T25	Green
D36	Green
S37	Green
P38	Green
R43	Green
I48	Green
R56	Green
V71	Green
L74	Green
E82	Green
R92	Green
E96	Green
A99	Green
S100	Green
R106	Green
K126	Green
GLY	Green
SER	Green
GLY	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
SER	Green
SER	Green
GLY	Green
LEU	Green
VAL	Green
PRO	Green
ARG	Green
GLY	Green
SER	Green
HIS	Green
HIS	Green
MET	Green
SER	Green
LVS	Green
PRO	Green
HIS	Green
SER	Green
GLU	Green
ALA	Green
GLY	Green
THR	Green
ALA	Green
PHE	Green
ILE	Green
Q14	Green
T25	Green
D36	Green
S37	Green
P38	Green
R43	Green
I48	Green
R56	Green
V71	Green
L74	Green
E82	Green
R92	Green
E96	Green
A99	Green
S100	Green
R106	Green
K126	Green
GLY	Green
SER	Green
GLY	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
SER	Green
SER	Green
GLY	Green
LEU	Green
VAL	Green
PRO	Green
ARG	Green
GLY	Green
SER	Green
HIS	Green
HIS	Green
MET	Green
SER	Green
LVS	Green
PRO	Green
HIS	Green
SER	Green
GLU	Green
ALA	Green
GLY	Green
THR	Green
ALA	Green
PHE	Green
ILE	Green
Q14	Green
T25	Green
D36	Green
S37	Green
P38	Green
R43	Green
I48	Green
R56	Green
V71	Green
L74	Green
E82	Green
R92	Green
E96	Green
A99	Green
S100	Green
R106	Green
K126	Green
GLY	Green
SER	Green
GLY	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
HIS	Green
SER	Green
SER	Green
GLY	Green
LEU	Green
VAL	Green
PRO	Green
ARG	Green
GLY	Green
SER	Green
HIS	Green
HIS	Green
MET	Green
SER	Green
LVS	Green
PRO	Green
HIS	Green
SER	Green
GLU	Green
ALA	Green
GLY	Green
THR	Green
ALA	Green
PHE	Green
ILE	Green
Q14	Green
T25	Green
D36	Green
S37	Green
P38	Green
R43	Green
I48	Green
R56	Green
V71	Green
L74	Green
E82	Green
R92	Green
E96	Green
A99	Green
S100	Green
R106	Green
K126	Green
GLY	Green
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GLY	Green
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ARG	Green
GLY	Green
SER	Green
HIS	Green
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SER	Green
LVS	Green
PRO	Green
HIS	Green
SER	Green
GLU	Green
ALA	Green
GLY	Green
THR	Green
ALA	Green
PHE	Green
ILE	Green
Q14	Green
T25	Green
D36	Green
S37	Green
P38	Green

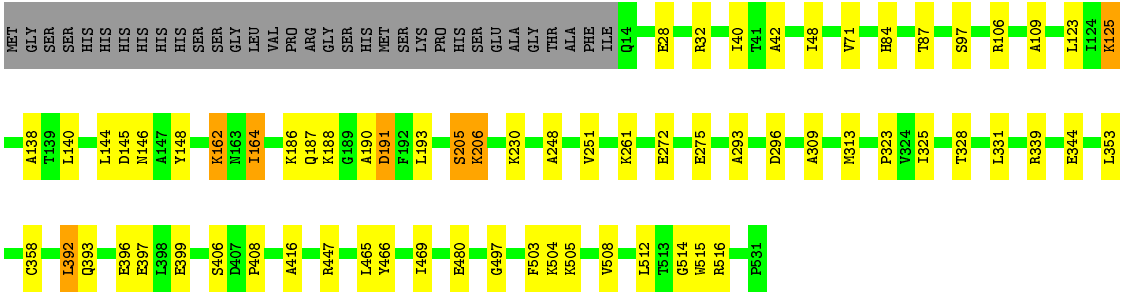
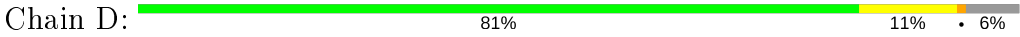
Chain C:

81% 12% 6%

Amino Acid	Frequency (%)
MET	1.0
GLY	1.0
SER	1.0
SER	1.0
HIS	1.0
HIS	1.0
HIS	1.0
HIS	1.0
HIS	1.0
SER	1.0
SER	1.0
GLY	1.0
LEU	1.0
VAL	1.0
PRO	1.0
ARG	1.0
GLY	1.0
SER	1.0
HIS	1.0
MET	1.0
SER	1.0
LYS	1.0
PRO	1.0
SER	1.0
SER	1.0
GLU	1.0
ALA	1.0
GLY	1.0
THR	1.0
ALA	1.0
PHE	1.0
ILE	1.0
Q14	1.0
M22	1.0
A23	1.0
D24	1.0
I48	1.0
R56	1.0
E59	1.0
V71	1.0
R106	1.0
K125	1.0
G126	1.0
S127	1.0
G128	1.0
T129	1.0
A130	1.0
K135	1.0
T143	1.0
I144	1.0
E154	1.0
N155	1.0
I156	1.0
K162	1.0
C165	1.0
V168	1.0
K173	1.0
K186	1.0
Q187	1.0
K188	1.0
D191	1.0
S202	1.0
L218	1.0
P219	1.0
E223	1.0
I226	1.0
D238	1.0
K256	1.0
E272	1.0
D288	1.0
L297	1.0
I301	1.0
K311	1.0
G321	1.0
K322	1.0
P323	1.0
V324	1.0
I325	1.0
T328	1.0
E332	1.0
S346	1.0
C358	1.0
Q393	1.0
E397	1.0



● Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.60Å 137.88Å 149.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.64 29.68 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.64) 100.0 (29.68-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.180 , 0.218 0.185 , 0.204	Depositor DCC
R_{free} test set	3616 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16023	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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, MG, FBP, PYR

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	0.87	0/4027	0.76	3/5439 (0.1%)
1	B	0.84	0/4012	0.74	2/5418 (0.0%)
1	C	0.81	0/4027	0.73	0/5439
1	D	0.82	1/4027 (0.0%)	0.73	3/5439 (0.1%)
All	All	0.83	1/16093 (0.0%)	0.74	8/21735 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	399	GLU	CG-CD	5.76	1.60	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	106	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	180	LEU	CA-CB-CG	6.26	129.69	115.30
1	D	447	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	106	ARG	NE-CZ-NH2	-5.91	117.34	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	GLY	Peptide

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	3963	0	4041	30	0
1	B	3949	0	4029	35	0
1	C	3963	0	4041	28	0
1	D	3963	0	4041	29	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	1	0
2	D	20	0	10	1	0
3	A	7	0	4	0	0
3	B	7	0	4	1	0
3	C	7	0	4	0	0
3	D	7	0	4	0	0
4	A	6	0	3	0	0
4	B	6	0	3	0	0
4	C	6	0	3	0	0
4	D	6	0	3	1	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
6	A	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
7	A	13	0	0	0	0
7	B	13	0	0	0	0
7	C	9	0	0	0	0
7	D	10	0	0	0	0
All	All	16023	0	16220	114	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 4.

The worst 5 of 114 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:136:LYS:HG3	1:A:198:GLU:O	1.89	0.72
1:C:106:ARG:NH2	1:C:471:PRO:O	2.24	0.71
1:A:133:GLU:HG2	1:A:133:GLU:O	1.92	0.68
1:B:412:THR:HG22	1:B:512:LEU:HD21	1.74	0.68
1:C:218:LEU:O	1:C:219:PRO:C	2.37	0.62

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	516/551 (94%)	493 (96%)	22 (4%)	1 (0%)	47	64
1	B	511/551 (93%)	490 (96%)	19 (4%)	2 (0%)	34	48
1	C	516/551 (94%)	494 (96%)	19 (4%)	3 (1%)	25	37
1	D	516/551 (94%)	487 (94%)	25 (5%)	4 (1%)	19	28
All	All	2059/2204 (93%)	1964 (95%)	85 (4%)	10 (0%)	29	43

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	D	191	ASP
1	C	125	LYS
1	D	138	ALA
1	B	191	ASP

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	426/453 (94%)	404 (95%)	22 (5%)	23	36
1	B	425/453 (94%)	400 (94%)	25 (6%)	19	30
1	C	426/453 (94%)	400 (94%)	26 (6%)	18	29
1	D	426/453 (94%)	406 (95%)	20 (5%)	26	40
All	All	1703/1812 (94%)	1610 (94%)	93 (6%)	22	33

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	436	ARG
1	C	154	GLU
1	D	275	GLU
1	B	443	ARG
1	C	14	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	184	GLN
1	D	479	GLN
1	D	187	GLN
1	C	155	ASN
1	D	146	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\# Z > 2$
4	PYR	C	603	5	2,5,5	1.00	0	2,6,6	1.17	0
2	FBP	A	601	-	18,20,20	0.67	0	23,32,32	1.38	3 (13%)
4	PYR	D	603	5	2,5,5	0.24	0	2,6,6	2.77	1 (50%)
4	PYR	A	603	5	2,5,5	0.57	0	2,6,6	1.16	0
4	PYR	B	603	5	2,5,5	0.60	0	2,6,6	1.32	0
2	FBP	D	601	-	18,20,20	1.03	1 (5%)	23,32,32	1.19	3 (13%)
2	FBP	C	601	-	18,20,20	0.76	0	23,32,32	1.24	4 (17%)
2	FBP	B	601	-	18,20,20	0.75	0	23,32,32	1.13	3 (13%)

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
4	PYR	C	603	5	-	0/0/4/4	-
2	FBP	A	601	-	-	9/13/32/32	0/1/1/1
4	PYR	D	603	5	-	0/0/4/4	-
4	PYR	A	603	5	-	0/0/4/4	-
4	PYR	B	603	5	-	0/0/4/4	-
2	FBP	D	601	-	-	3/13/32/32	0/1/1/1
2	FBP	C	601	-	-	5/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FBP	O5-C2	2.46	1.47	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	PYR	O3-C2-C3	3.45	127.93	120.17
2	A	601	FBP	O6P-P2-O5P	3.31	120.31	107.64
2	D	601	FBP	O3P-P1-O1	-2.76	99.39	106.73
2	A	601	FBP	O5P-P2-O6	-2.64	99.70	106.73
2	B	601	FBP	O3P-P1-O1	-2.58	99.87	106.73

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C1-O1-P1-O1P
2	A	601	FBP	C1-O1-P1-O2P
2	A	601	FBP	C1-O1-P1-O3P
2	A	601	FBP	O1-C1-C2-O2
2	A	601	FBP	O1-C1-C2-C3

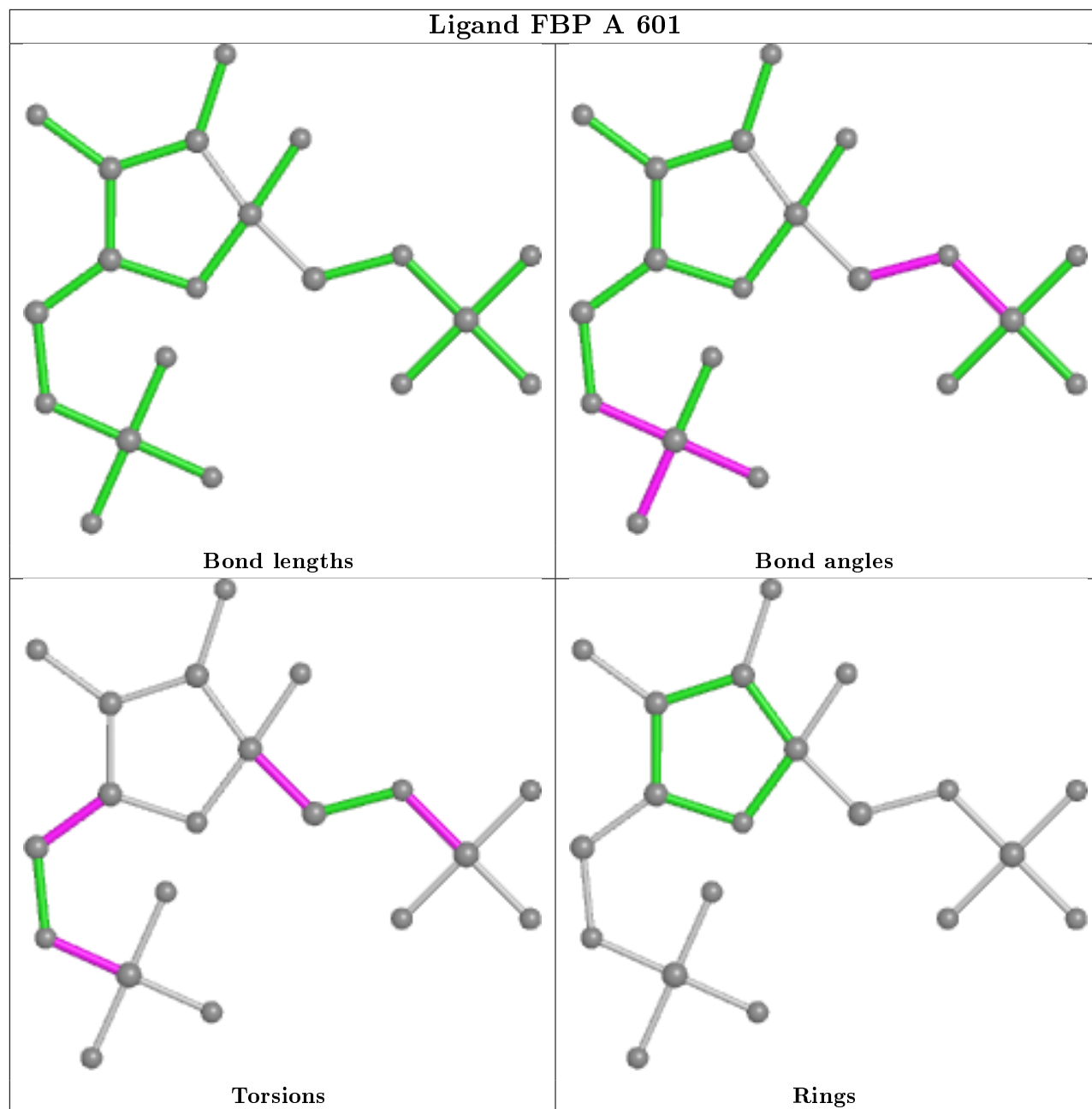
There are no ring outliers.

3 monomers are involved in 3 short contacts:

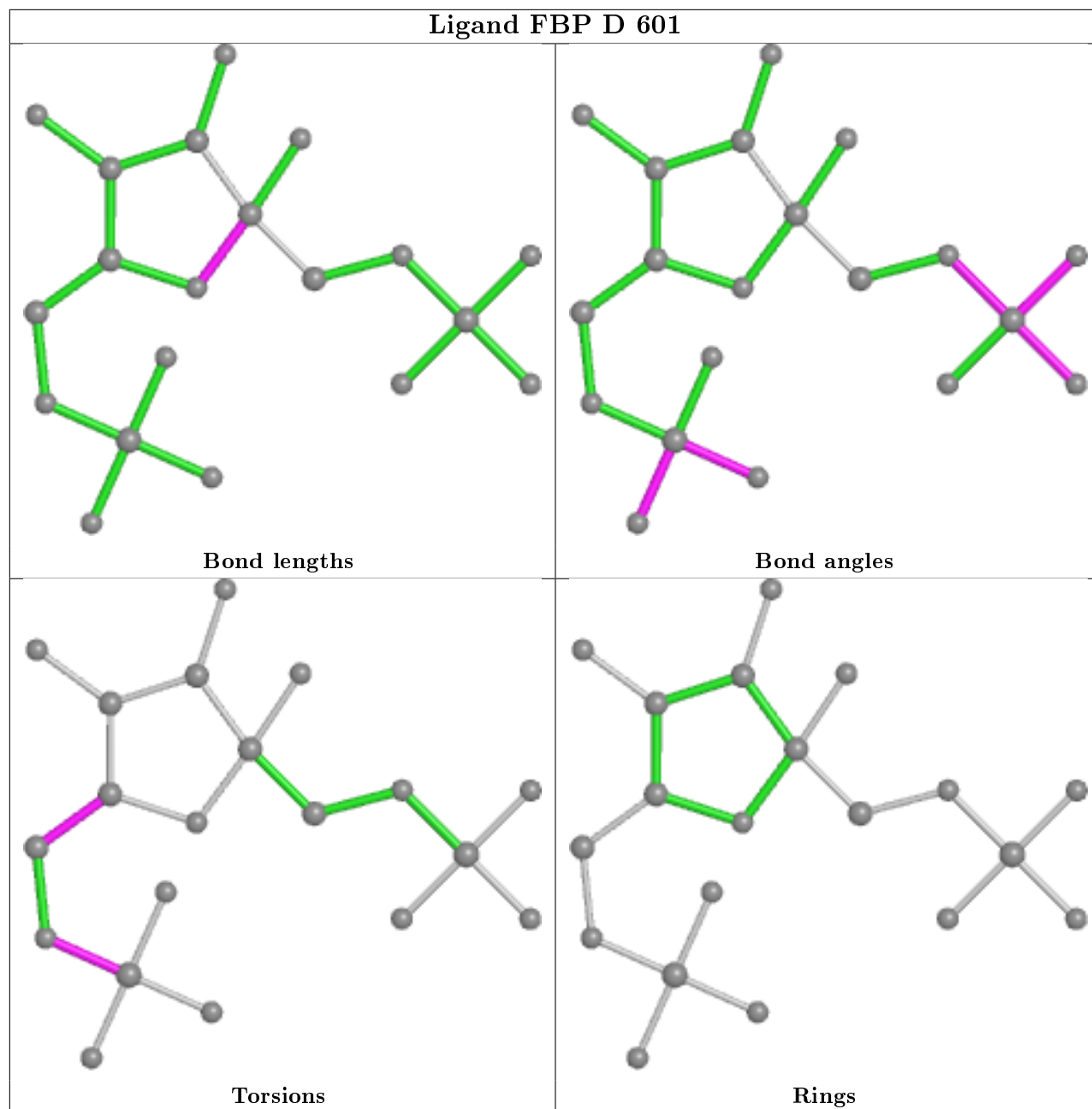
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	PYR	1	0
2	D	601	FBP	1	0
2	C	601	FBP	1	0

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.

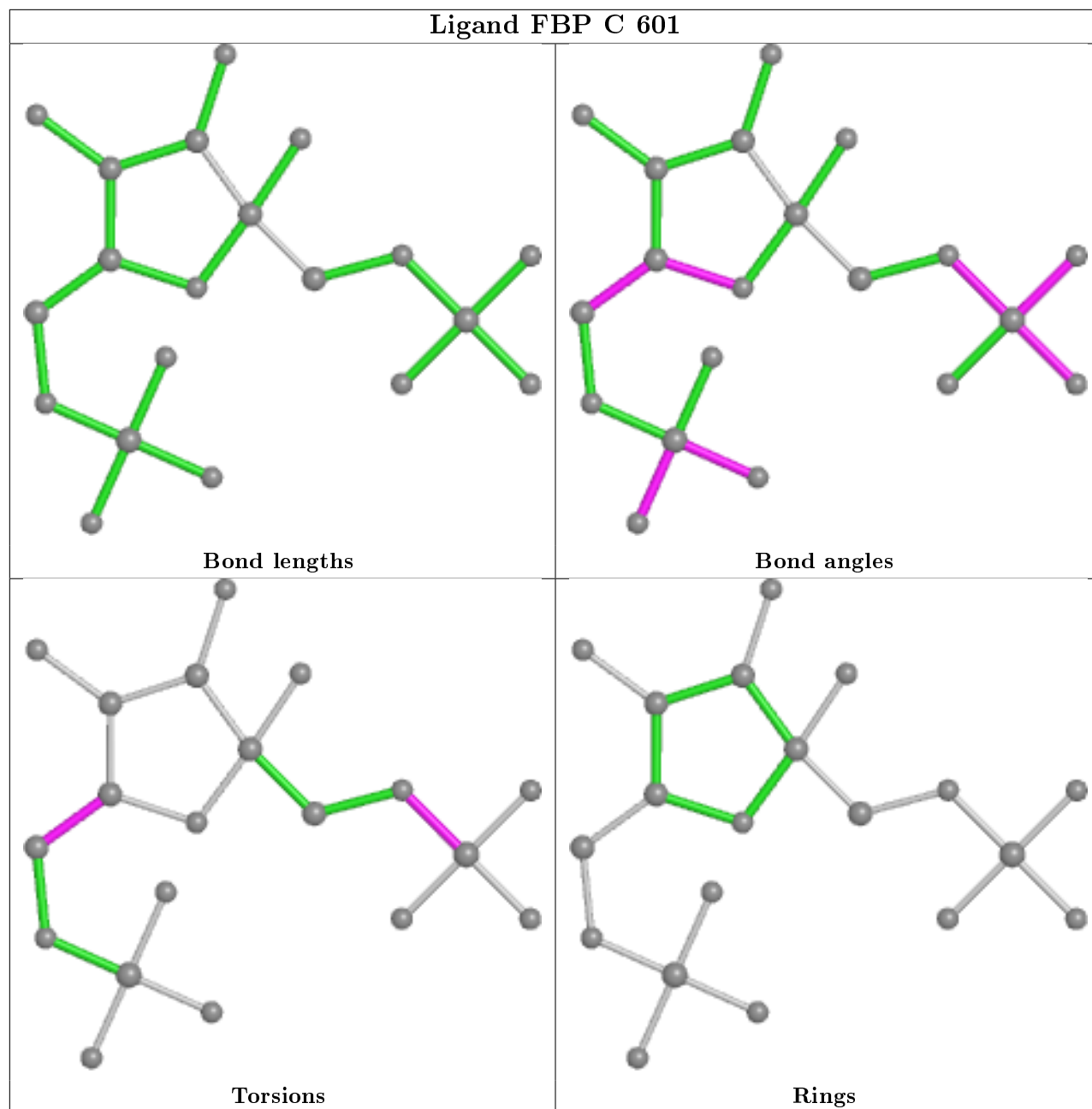
Ligand FBP A 601

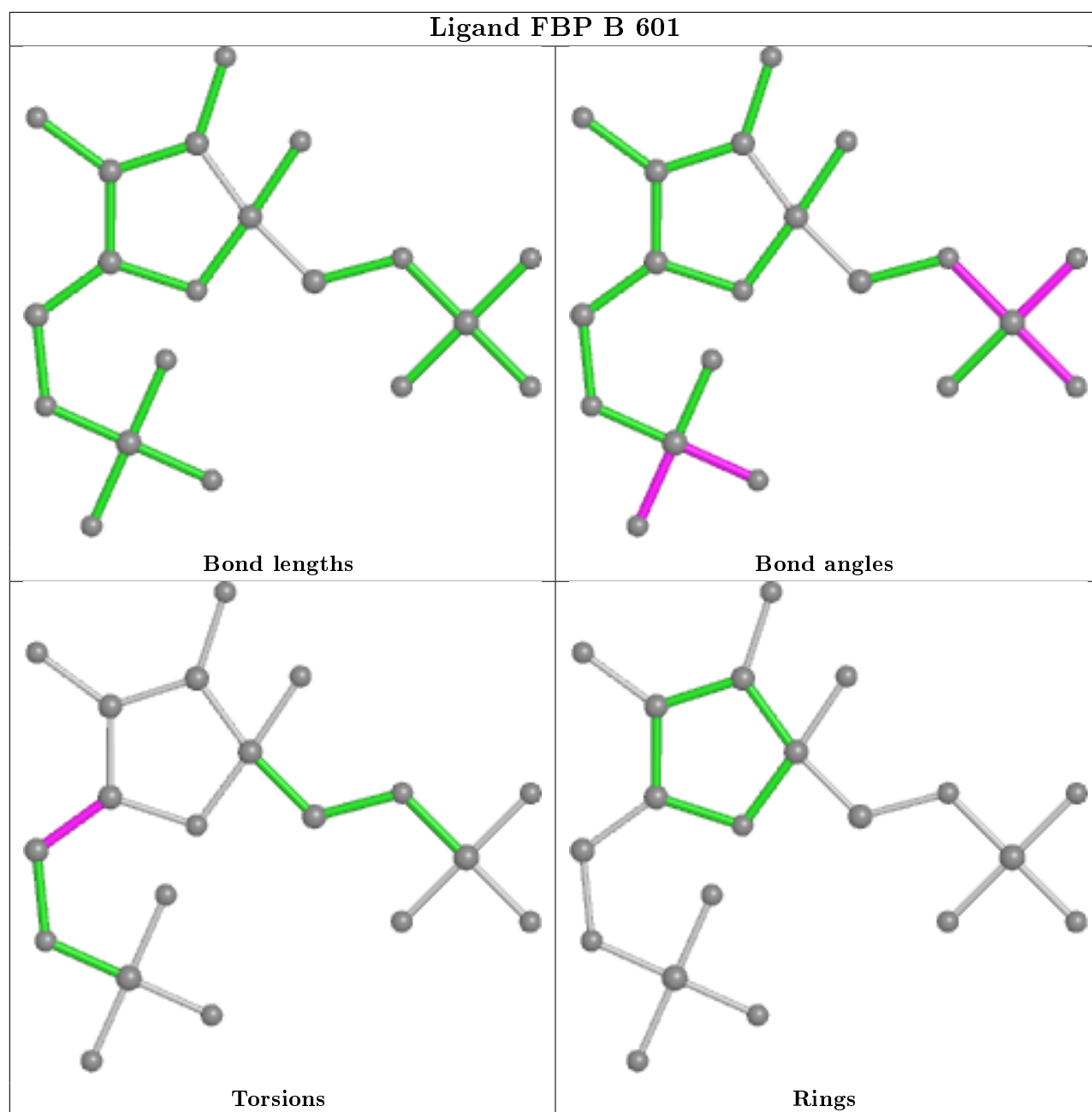


Ligand FBP D 601



Ligand FBP C 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	518/551 (94%)	-0.55	3 (0%) 89 88	19, 35, 61, 102	0
1	B	515/551 (93%)	-0.50	7 (1%) 75 73	23, 35, 81, 119	0
1	C	518/551 (94%)	-0.43	7 (1%) 75 73	23, 40, 77, 108	0
1	D	518/551 (94%)	-0.39	0 100 100	23, 41, 79, 100	0
All	All	2069/2204 (93%)	-0.47	17 (0%) 86 85	19, 38, 77, 119	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	ASP	3.5
1	C	403	PRO	3.2
1	B	191	ASP	3.1
1	B	215	ALA	3.0
1	A	133	GLU	2.8

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 monosaccharides in this entry.

6.4 Ligands [i](#)

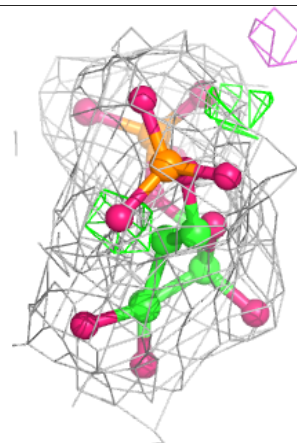
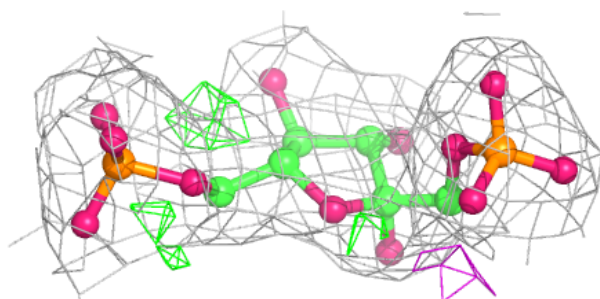
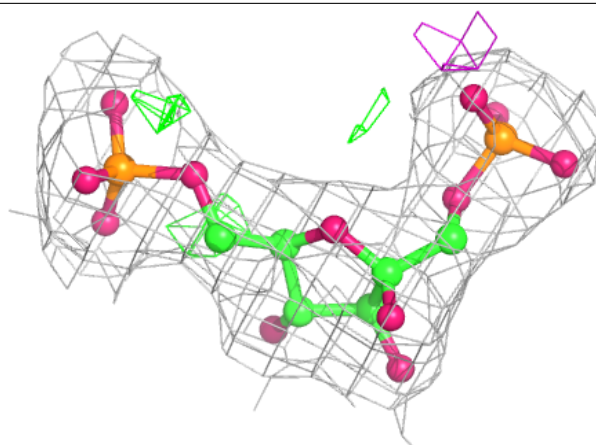
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SER	B	602	7/7	0.91	0.25	39,44,47,47	0
3	SER	A	602	7/7	0.91	0.19	31,37,38,39	0
6	K	C	605	1/1	0.92	0.13	44,44,44,44	0
3	SER	C	602	7/7	0.93	0.21	44,44,50,51	0
4	PYR	D	603	6/6	0.94	0.21	40,41,45,46	0
3	SER	D	602	7/7	0.95	0.31	42,46,50,55	0
5	MG	B	604	1/1	0.96	0.24	33,33,33,33	0
5	MG	D	604	1/1	0.96	0.27	46,46,46,46	0
5	MG	A	604	1/1	0.96	0.23	28,28,28,28	0
4	PYR	C	603	6/6	0.96	0.17	30,34,36,38	0
4	PYR	B	603	6/6	0.97	0.17	24,25,32,35	0
6	K	B	605	1/1	0.97	0.07	42,42,42,42	0
6	K	A	605	1/1	0.97	0.14	44,44,44,44	0
6	K	D	605	1/1	0.97	0.08	52,52,52,52	0
2	FBP	D	601	20/20	0.98	0.09	20,26,31,31	0
4	PYR	A	603	6/6	0.98	0.19	36,38,38,41	0
5	MG	C	604	1/1	0.98	0.23	35,35,35,35	0
2	FBP	A	601	20/20	0.98	0.09	22,28,33,36	0
2	FBP	C	601	20/20	0.98	0.10	27,31,40,41	0
2	FBP	B	601	20/20	0.99	0.09	21,25,32,34	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.

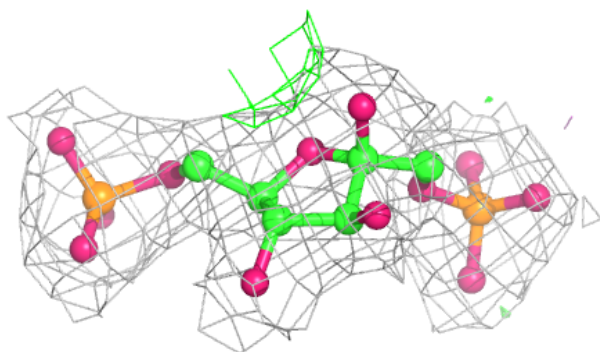
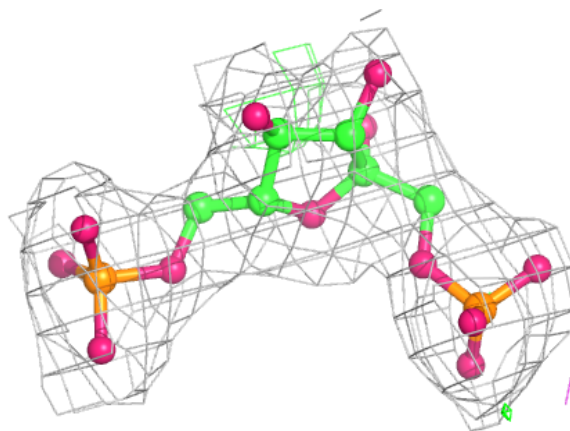
Electron density around FBP D 601:

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

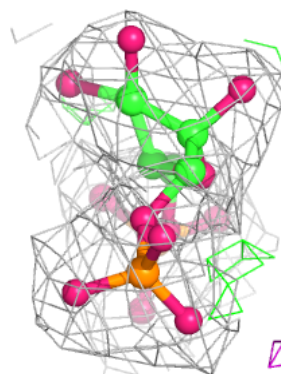
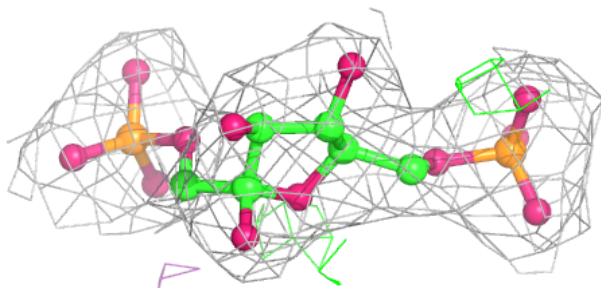
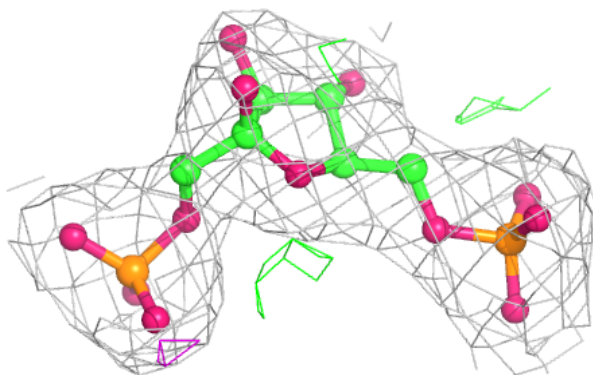


Electron density around FBP A 601:

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

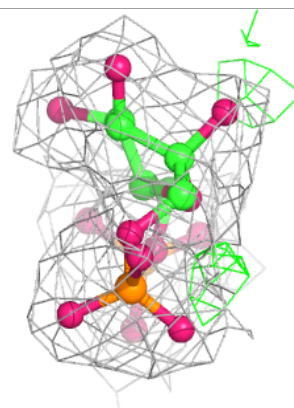
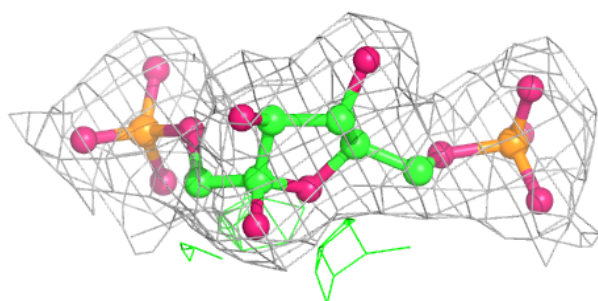
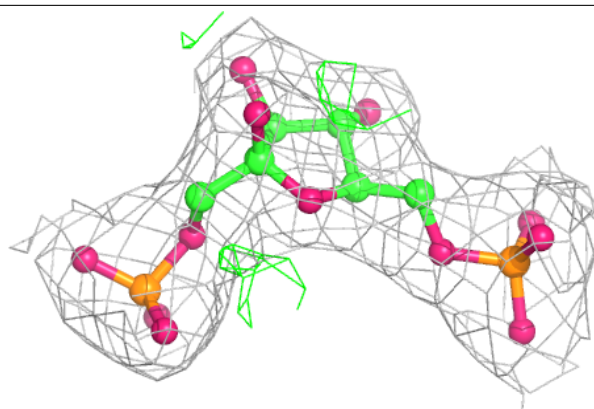
**Electron density around FBP C 601:**

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



Electron density around FBP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.