



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:33 AM UTC

PDB ID : 8TBS / pdb_00008tbs
Title : Structure of human erythrocyte pyruvate kinase in complex with an allosteric activator AG-946
Authors : Jin, L.; Padyana, A.
Deposited on : 2023-06-29
Resolution : 2.35 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

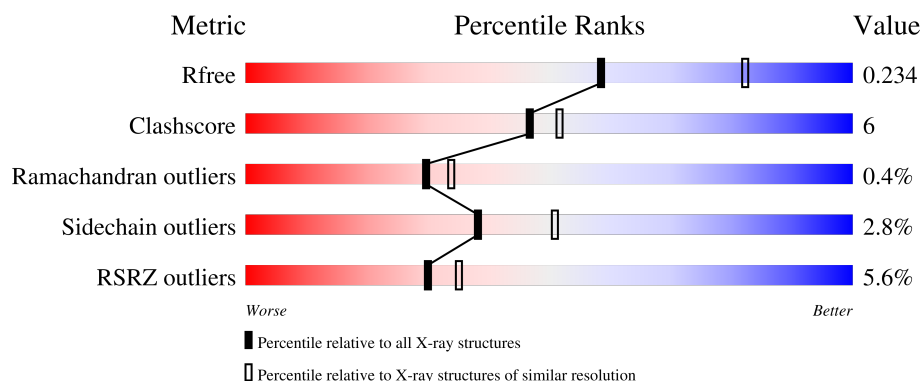
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	544	5% 78% 11% • 11%
1	B	544	6% 85% 10% • 5%
1	C	544	7% 82% 11% • 6%
1	D	544	6% 75% 14% 11%
1	E	544	7% 72% 21% • 5%

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Mol	Chain	Length	Quality of chain
1	F	544	
1	G	544	
1	H	544	

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
5	PYR	E	604	-	X	-	-
5	PYR	H	604	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31741 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	485	Total	C	N	O	S	0	1	0
			3693	2322	670	683	18			
1	B	517	Total	C	N	O	S	0	0	0
			3922	2468	708	728	18			
1	C	512	Total	C	N	O	S	0	2	0
			3895	2450	705	722	18			
1	D	483	Total	C	N	O	S	0	0	0
			3661	2303	664	676	18			
1	E	515	Total	C	N	O	S	0	1	0
			3908	2459	709	722	18			
1	F	520	Total	C	N	O	S	0	0	0
			3941	2479	712	732	18			
1	G	509	Total	C	N	O	S	0	6	0
			3901	2449	709	725	18			
1	H	519	Total	C	N	O	S	0	1	0
			3943	2480	712	733	18			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP P30613
A	32	GLY	-	expression tag	UNP P30613
A	33	SER	-	expression tag	UNP P30613
A	34	SER	-	expression tag	UNP P30613
A	35	HIS	-	expression tag	UNP P30613
A	36	HIS	-	expression tag	UNP P30613
A	37	HIS	-	expression tag	UNP P30613
A	38	HIS	-	expression tag	UNP P30613
A	39	HIS	-	expression tag	UNP P30613
A	40	HIS	-	expression tag	UNP P30613
A	41	SER	-	expression tag	UNP P30613
A	42	SER	-	expression tag	UNP P30613
A	43	GLY	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	44	LEU	-	expression tag	UNP P30613
A	45	VAL	-	expression tag	UNP P30613
A	46	PRO	-	expression tag	UNP P30613
A	47	ARG	-	expression tag	UNP P30613
A	48	GLY	-	expression tag	UNP P30613
A	49	SER	-	expression tag	UNP P30613
B	31	MET	-	initiating methionine	UNP P30613
B	32	GLY	-	expression tag	UNP P30613
B	33	SER	-	expression tag	UNP P30613
B	34	SER	-	expression tag	UNP P30613
B	35	HIS	-	expression tag	UNP P30613
B	36	HIS	-	expression tag	UNP P30613
B	37	HIS	-	expression tag	UNP P30613
B	38	HIS	-	expression tag	UNP P30613
B	39	HIS	-	expression tag	UNP P30613
B	40	HIS	-	expression tag	UNP P30613
B	41	SER	-	expression tag	UNP P30613
B	42	SER	-	expression tag	UNP P30613
B	43	GLY	-	expression tag	UNP P30613
B	44	LEU	-	expression tag	UNP P30613
B	45	VAL	-	expression tag	UNP P30613
B	46	PRO	-	expression tag	UNP P30613
B	47	ARG	-	expression tag	UNP P30613
B	48	GLY	-	expression tag	UNP P30613
B	49	SER	-	expression tag	UNP P30613
C	31	MET	-	initiating methionine	UNP P30613
C	32	GLY	-	expression tag	UNP P30613
C	33	SER	-	expression tag	UNP P30613
C	34	SER	-	expression tag	UNP P30613
C	35	HIS	-	expression tag	UNP P30613
C	36	HIS	-	expression tag	UNP P30613
C	37	HIS	-	expression tag	UNP P30613
C	38	HIS	-	expression tag	UNP P30613
C	39	HIS	-	expression tag	UNP P30613
C	40	HIS	-	expression tag	UNP P30613
C	41	SER	-	expression tag	UNP P30613
C	42	SER	-	expression tag	UNP P30613
C	43	GLY	-	expression tag	UNP P30613
C	44	LEU	-	expression tag	UNP P30613
C	45	VAL	-	expression tag	UNP P30613
C	46	PRO	-	expression tag	UNP P30613
C	47	ARG	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
C	48	GLY	-	expression tag	UNP P30613
C	49	SER	-	expression tag	UNP P30613
D	31	MET	-	initiating methionine	UNP P30613
D	32	GLY	-	expression tag	UNP P30613
D	33	SER	-	expression tag	UNP P30613
D	34	SER	-	expression tag	UNP P30613
D	35	HIS	-	expression tag	UNP P30613
D	36	HIS	-	expression tag	UNP P30613
D	37	HIS	-	expression tag	UNP P30613
D	38	HIS	-	expression tag	UNP P30613
D	39	HIS	-	expression tag	UNP P30613
D	40	HIS	-	expression tag	UNP P30613
D	41	SER	-	expression tag	UNP P30613
D	42	SER	-	expression tag	UNP P30613
D	43	GLY	-	expression tag	UNP P30613
D	44	LEU	-	expression tag	UNP P30613
D	45	VAL	-	expression tag	UNP P30613
D	46	PRO	-	expression tag	UNP P30613
D	47	ARG	-	expression tag	UNP P30613
D	48	GLY	-	expression tag	UNP P30613
D	49	SER	-	expression tag	UNP P30613
E	31	MET	-	initiating methionine	UNP P30613
E	32	GLY	-	expression tag	UNP P30613
E	33	SER	-	expression tag	UNP P30613
E	34	SER	-	expression tag	UNP P30613
E	35	HIS	-	expression tag	UNP P30613
E	36	HIS	-	expression tag	UNP P30613
E	37	HIS	-	expression tag	UNP P30613
E	38	HIS	-	expression tag	UNP P30613
E	39	HIS	-	expression tag	UNP P30613
E	40	HIS	-	expression tag	UNP P30613
E	41	SER	-	expression tag	UNP P30613
E	42	SER	-	expression tag	UNP P30613
E	43	GLY	-	expression tag	UNP P30613
E	44	LEU	-	expression tag	UNP P30613
E	45	VAL	-	expression tag	UNP P30613
E	46	PRO	-	expression tag	UNP P30613
E	47	ARG	-	expression tag	UNP P30613
E	48	GLY	-	expression tag	UNP P30613
E	49	SER	-	expression tag	UNP P30613
F	31	MET	-	initiating methionine	UNP P30613
F	32	GLY	-	expression tag	UNP P30613

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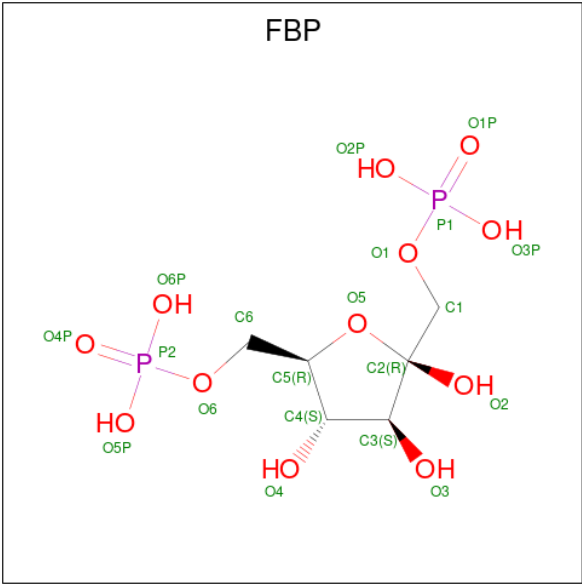
Chain	Residue	Modelled	Actual	Comment	Reference
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F	34	SER	-	expression tag	UNP P30613
F	35	HIS	-	expression tag	UNP P30613
F	36	HIS	-	expression tag	UNP P30613
F	37	HIS	-	expression tag	UNP P30613
F	38	HIS	-	expression tag	UNP P30613
F	39	HIS	-	expression tag	UNP P30613
F	40	HIS	-	expression tag	UNP P30613
F	41	SER	-	expression tag	UNP P30613
F	42	SER	-	expression tag	UNP P30613
F	43	GLY	-	expression tag	UNP P30613
F	44	LEU	-	expression tag	UNP P30613
F	45	VAL	-	expression tag	UNP P30613
F	46	PRO	-	expression tag	UNP P30613
F	47	ARG	-	expression tag	UNP P30613
F	48	GLY	-	expression tag	UNP P30613
F	49	SER	-	expression tag	UNP P30613
G	31	MET	-	initiating methionine	UNP P30613
G	32	GLY	-	expression tag	UNP P30613
G	33	SER	-	expression tag	UNP P30613
G	34	SER	-	expression tag	UNP P30613
G	35	HIS	-	expression tag	UNP P30613
G	36	HIS	-	expression tag	UNP P30613
G	37	HIS	-	expression tag	UNP P30613
G	38	HIS	-	expression tag	UNP P30613
G	39	HIS	-	expression tag	UNP P30613
G	40	HIS	-	expression tag	UNP P30613
G	41	SER	-	expression tag	UNP P30613
G	42	SER	-	expression tag	UNP P30613
G	43	GLY	-	expression tag	UNP P30613
G	44	LEU	-	expression tag	UNP P30613
G	45	VAL	-	expression tag	UNP P30613
G	46	PRO	-	expression tag	UNP P30613
G	47	ARG	-	expression tag	UNP P30613
G	48	GLY	-	expression tag	UNP P30613
G	49	SER	-	expression tag	UNP P30613
H	31	MET	-	initiating methionine	UNP P30613
H	32	GLY	-	expression tag	UNP P30613
H	33	SER	-	expression tag	UNP P30613
H	34	SER	-	expression tag	UNP P30613
H	35	HIS	-	expression tag	UNP P30613
H	36	HIS	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
H	37	HIS	-	expression tag	UNP P30613
H	38	HIS	-	expression tag	UNP P30613
H	39	HIS	-	expression tag	UNP P30613
H	40	HIS	-	expression tag	UNP P30613
H	41	SER	-	expression tag	UNP P30613
H	42	SER	-	expression tag	UNP P30613
H	43	GLY	-	expression tag	UNP P30613
H	44	LEU	-	expression tag	UNP P30613
H	45	VAL	-	expression tag	UNP P30613
H	46	PRO	-	expression tag	UNP P30613
H	47	ARG	-	expression tag	UNP P30613
H	48	GLY	-	expression tag	UNP P30613
H	49	SER	-	expression tag	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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

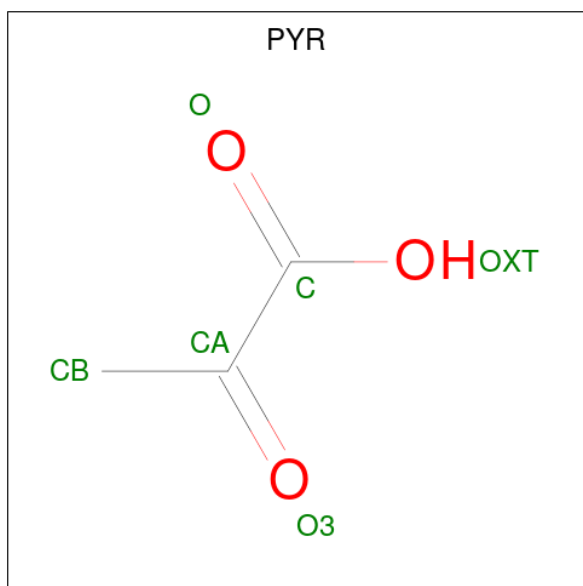
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		

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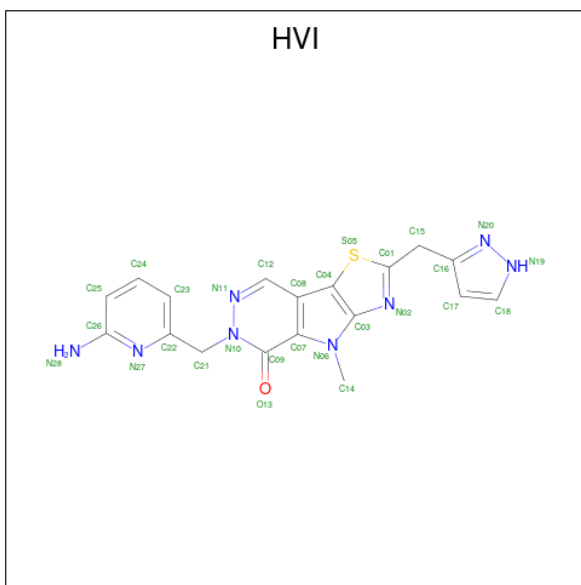
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	K	0	0
			1	1		

- Molecule 5 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 6-[(6-aminopyridin-2-yl)methyl]-4-methyl-2-[(1H-pyrazol-3-yl)methyl]-4,6-dihydro-5H-[1,3]thiazolo[5',4':4,5]pyrrolo[2,3-d]pyridazin-5-one (CCD ID: HVI) (formula: $C_{18}H_{16}N_8OS$) (labeled as "Ligand of Interest" by depositor).



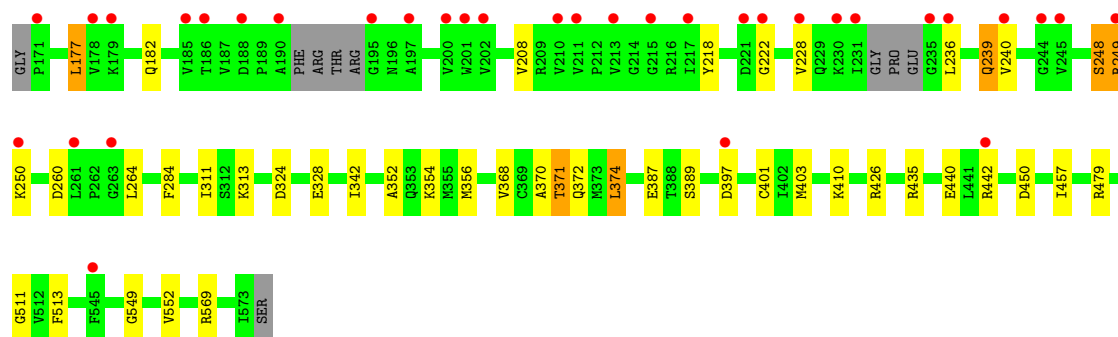
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			28	18	8	1	1		
6	D	1	Total	C	N	O	S	0	0
			28	18	8	1	1		
6	F	1	Total	C	N	O	S	0	0
			28	18	8	1	1		
6	H	1	Total	C	N	O	S	0	0
			28	18	8	1	1		

- Molecule 7 is water.

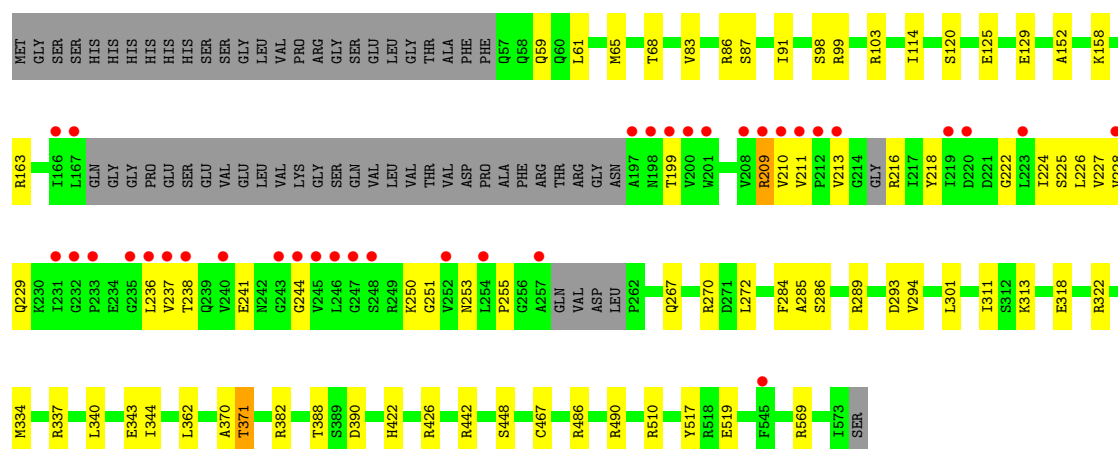
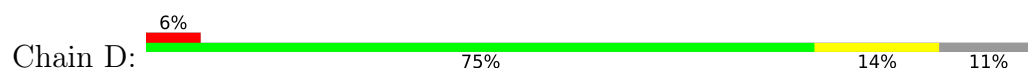
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	73	Total	O	0	0
			73	73		
7	B	64	Total	O	0	0
			64	64		
7	C	62	Total	O	0	0
			62	62		
7	D	55	Total	O	0	0
			55	55		
7	E	41	Total	O	0	0
			41	41		
7	F	91	Total	O	0	0
			91	91		
7	G	48	Total	O	0	0
			48	48		
7	H	109	Total	O	0	0
			109	109		

- Molecule 1: Pyruvate kinase PKLR

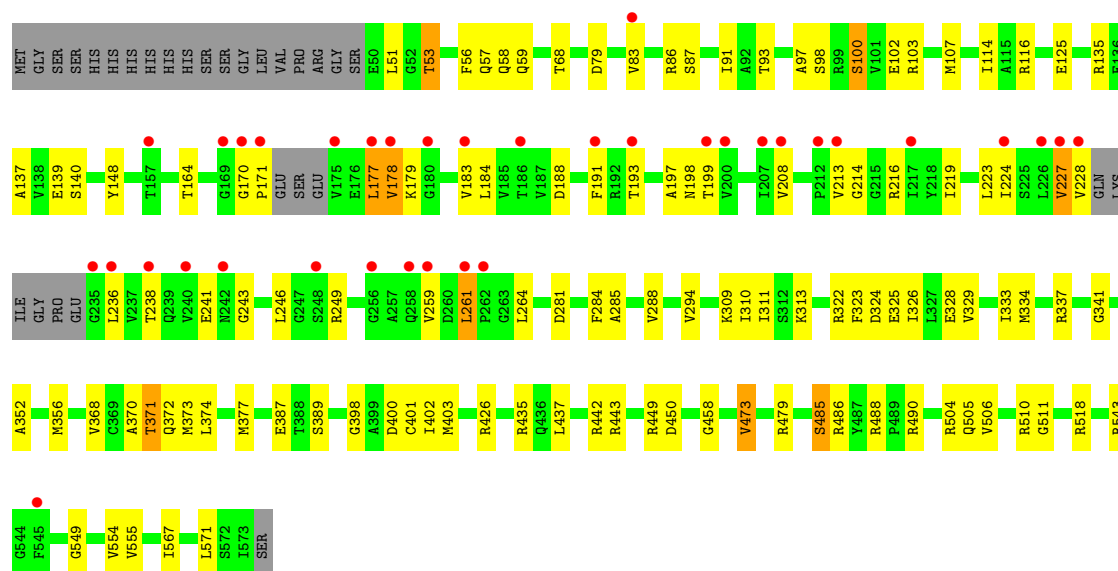




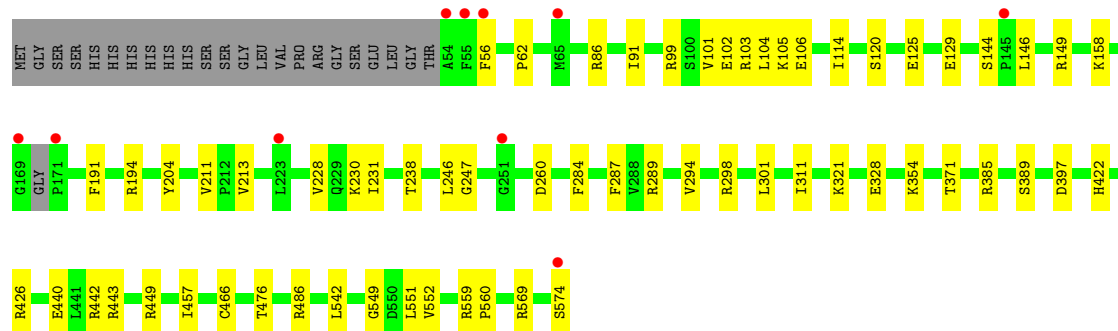
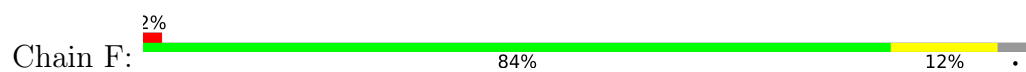
• Molecule 1: Pyruvate kinase PKLR



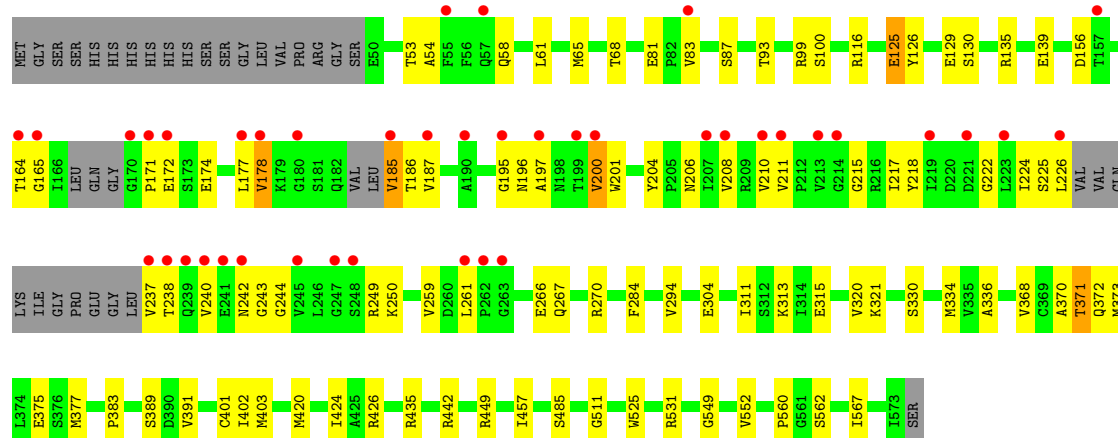
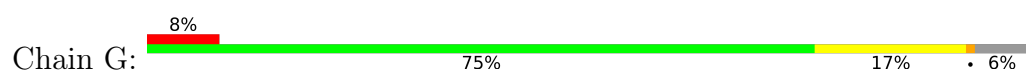
• Molecule 1: Pyruvate kinase PKLR



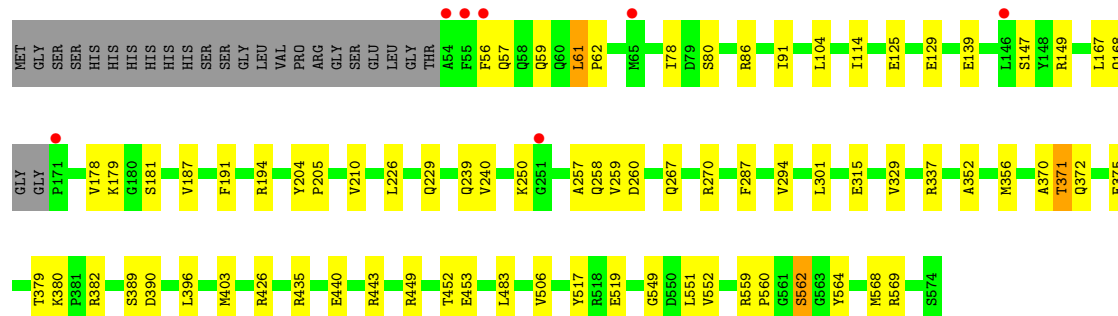
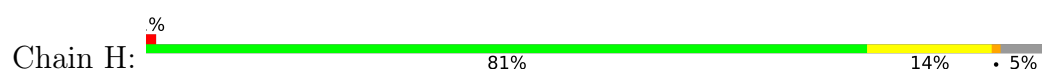
• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.32Å 122.60Å 378.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 2.35 29.44 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.44-2.35) 99.5 (29.44-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.193 , 0.234 0.193 , 0.234	Depositor DCC
R_{free} test set	10643 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31741	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.22 % 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 6.2563e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, PYR, FBP, HVI, MN

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	0.16	0/3750	0.33	0/5076
1	B	0.17	0/3987	0.34	1/5403 (0.0%)
1	C	0.18	0/3956	0.36	0/5357
1	D	0.16	0/3719	0.33	0/5035
1	E	0.17	0/3971	0.34	0/5380
1	F	0.18	0/4006	0.34	0/5428
1	G	0.16	0/3975	0.37	0/5381
1	H	0.17	0/4008	0.36	0/5431
All	All	0.17	0/31372	0.35	1/42491 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	ILE	N-CA-C	-5.25	107.71	112.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3693	0	3766	33	0
1	B	3922	0	3998	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3895	0	3974	43	0
1	D	3661	0	3741	50	0
1	E	3908	0	3987	78	0
1	F	3941	0	4016	39	0
1	G	3901	0	3971	58	1
1	H	3943	0	4018	47	0
2	A	20	0	9	0	0
2	B	20	0	9	0	0
2	C	20	0	9	0	0
2	D	20	0	9	0	0
2	E	20	0	9	0	0
2	F	20	0	9	0	0
2	G	20	0	9	0	0
2	H	20	0	9	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	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	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
5	E	6	0	0	0	0
5	F	6	0	0	0	0
5	G	6	0	0	2	0
5	H	6	0	0	0	0
6	B	28	0	0	0	0
6	D	28	0	0	0	0
6	F	28	0	0	0	0
6	H	28	0	0	0	0
7	A	73	0	0	1	0
7	B	64	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	62	0	0	2	0
7	D	55	0	0	0	0
7	E	41	0	0	3	0
7	F	91	0	0	6	0
7	G	48	0	0	1	0
7	H	109	0	0	0	0
All	All	31741	0	31543	356	1

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 6.

The worst 5 of 356 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:LYS:HB2	1:E:243:GLY:HA3	1.55	0.87
1:G:99:ARG:NH2	1:G:126:TYR:O	2.12	0.82
1:E:59:GLN:O	1:E:490[A]:ARG:NH2	2.10	0.82
1:F:486:ARG:NH1	7:F:701:HOH:O	2.11	0.79
1:G:185:VAL:N	1:G:200:VAL:O	2.18	0.77

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:THR:OG1	1:G:304:GLU:OE1[4_544]	2.16	0.04

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	476/544 (88%)	458 (96%)	16 (3%)	2 (0%)	30 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	513/544 (94%)	498 (97%)	13 (2%)	2 (0%)	30	34
1	C	506/544 (93%)	489 (97%)	12 (2%)	5 (1%)	12	12
1	D	475/544 (87%)	460 (97%)	14 (3%)	1 (0%)	43	52
1	E	510/544 (94%)	491 (96%)	17 (3%)	2 (0%)	30	34
1	F	516/544 (95%)	505 (98%)	10 (2%)	1 (0%)	43	52
1	G	507/544 (93%)	485 (96%)	18 (4%)	4 (1%)	16	17
1	H	516/544 (95%)	507 (98%)	8 (2%)	1 (0%)	43	52
All	All	4019/4352 (92%)	3893 (97%)	108 (3%)	18 (0%)	30	34

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	59	GLN
1	G	178	VAL
1	E	227	VAL
1	G	196	ASN
1	C	164	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	391/436 (90%)	380 (97%)	11 (3%)	38	51
1	B	416/436 (95%)	408 (98%)	8 (2%)	50	65
1	C	412/436 (94%)	405 (98%)	7 (2%)	53	68
1	D	386/436 (88%)	379 (98%)	7 (2%)	51	66
1	E	412/436 (94%)	394 (96%)	18 (4%)	25	33
1	F	417/436 (96%)	409 (98%)	8 (2%)	50	65
1	G	413/436 (95%)	394 (95%)	19 (5%)	24	31
1	H	418/436 (96%)	404 (97%)	14 (3%)	33	44
All	All	3265/3488 (94%)	3173 (97%)	92 (3%)	38	51

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	552	VAL
1	G	389	SER
1	G	100	SER
1	G	200	VAL
1	G	552	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	501	GLN
1	H	258	GLN
1	H	501	GLN
1	H	267	GLN
1	E	57	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 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PYR	B	605	3	5,5,5	3.16	3 (60%)	3,6,6	1.41	0
5	PYR	C	604	3	5,5,5	3.15	3 (60%)	3,6,6	1.50	1 (33%)
6	HVI	B	601	-	31,32,32	1.74	6 (19%)	27,47,47	2.51	11 (40%)
2	FBP	H	602	-	18,20,20	3.42	6 (33%)	21,32,32	0.71	0
5	PYR	D	604	3	5,5,5	3.01	3 (60%)	3,6,6	1.92	1 (33%)
5	PYR	F	605	-	5,5,5	3.07	3 (60%)	3,6,6	1.64	1 (33%)
2	FBP	D	602	-	18,20,20	3.42	5 (27%)	21,32,32	0.73	0
2	FBP	C	601	-	18,20,20	3.58	6 (33%)	21,32,32	1.52	5 (23%)
6	HVI	H	601	-	31,32,32	1.66	8 (25%)	27,47,47	2.52	11 (40%)
5	PYR	A	604	3	5,5,5	3.02	3 (60%)	3,6,6	1.82	2 (66%)
5	PYR	H	604	-	5,5,5	3.05	3 (60%)	3,6,6	1.56	1 (33%)
2	FBP	E	601	-	18,20,20	3.39	6 (33%)	21,32,32	0.79	0
5	PYR	G	604	3	5,5,5	3.02	3 (60%)	3,6,6	1.82	1 (33%)
2	FBP	F	602	-	18,20,20	3.37	5 (27%)	21,32,32	0.69	0
2	FBP	A	601	-	18,20,20	3.41	5 (27%)	21,32,32	0.75	0
6	HVI	D	601	-	31,32,32	1.68	7 (22%)	27,47,47	2.46	11 (40%)
5	PYR	E	604	3	5,5,5	3.02	3 (60%)	3,6,6	1.87	2 (66%)
6	HVI	F	601	-	31,32,32	1.64	6 (19%)	27,47,47	2.46	11 (40%)
2	FBP	B	602	-	18,20,20	3.41	5 (27%)	21,32,32	0.77	0
2	FBP	G	601	-	18,20,20	3.40	5 (27%)	21,32,32	0.83	0

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
5	PYR	B	605	3	-	0/4/4/4	-
5	PYR	C	604	3	-	0/4/4/4	-
6	HVI	B	601	-	-	4/8/8/8	0/5/5/5
2	FBP	H	602	-	-	2/13/32/32	0/1/1/1
5	PYR	D	604	3	-	0/4/4/4	-
5	PYR	F	605	-	-	0/4/4/4	-
2	FBP	D	602	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
6	HVI	H	601	-	-	4/8/8/8	0/5/5/5
5	PYR	A	604	3	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PYR	H	604	-	-	4/4/4/4	-
2	FBP	E	601	-	-	4/13/32/32	0/1/1/1
5	PYR	G	604	3	-	0/4/4/4	-
2	FBP	F	602	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
6	HVI	D	601	-	-	3/8/8/8	0/5/5/5
5	PYR	E	604	3	-	4/4/4/4	-
6	HVI	F	601	-	-	4/8/8/8	0/5/5/5
2	FBP	B	602	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	4/13/32/32	0/1/1/1

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	FBP	O5-C2	-8.74	1.29	1.43
2	C	601	FBP	O5-C5	8.66	1.62	1.43
2	C	601	FBP	O5-C2	-8.38	1.30	1.43
2	A	601	FBP	O5-C5	8.35	1.62	1.43
2	G	601	FBP	O5-C5	8.16	1.61	1.43

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	HVI	C07-N06-C03	7.10	110.17	106.27
6	D	601	HVI	C07-N06-C03	7.04	110.14	106.27
6	H	601	HVI	C07-N06-C03	6.88	110.05	106.27
6	F	601	HVI	C07-N06-C03	6.57	109.88	106.27
6	B	601	HVI	S05-C01-N02	-5.38	108.89	116.18

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

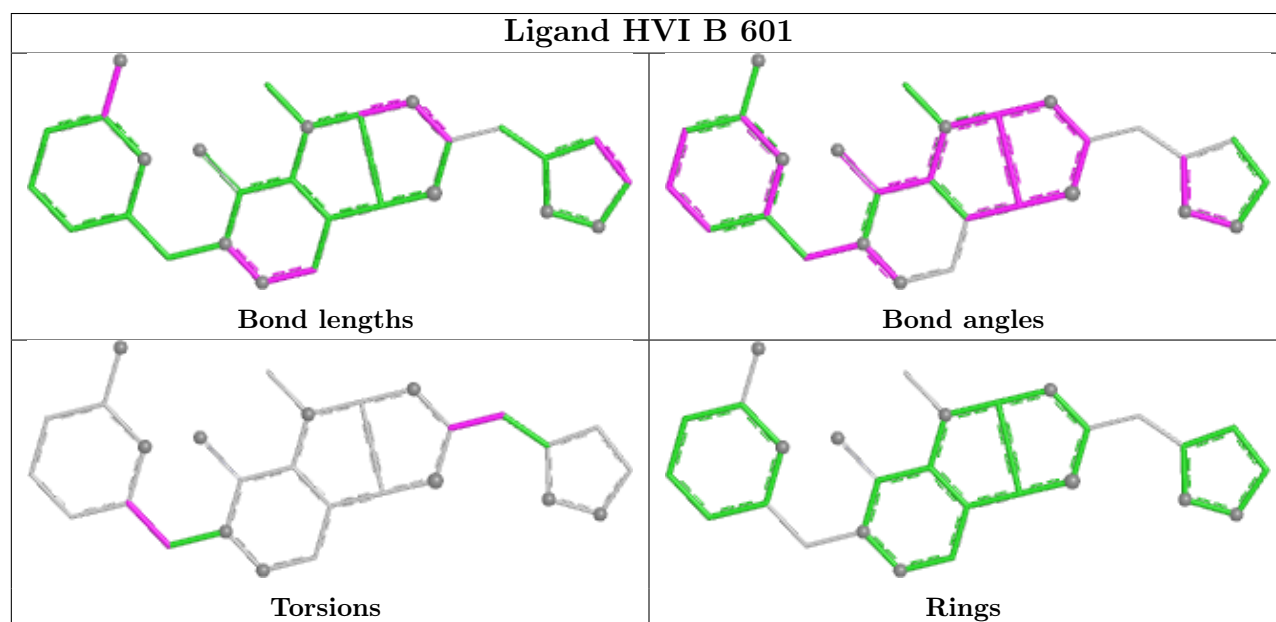
Mol	Chain	Res	Type	Atoms
2	C	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O1-C1-C2-O2
2	E	601	FBP	O1-C1-C2-O5
2	G	601	FBP	O1-C1-C2-O2
5	E	604	PYR	O-C-CA-CB

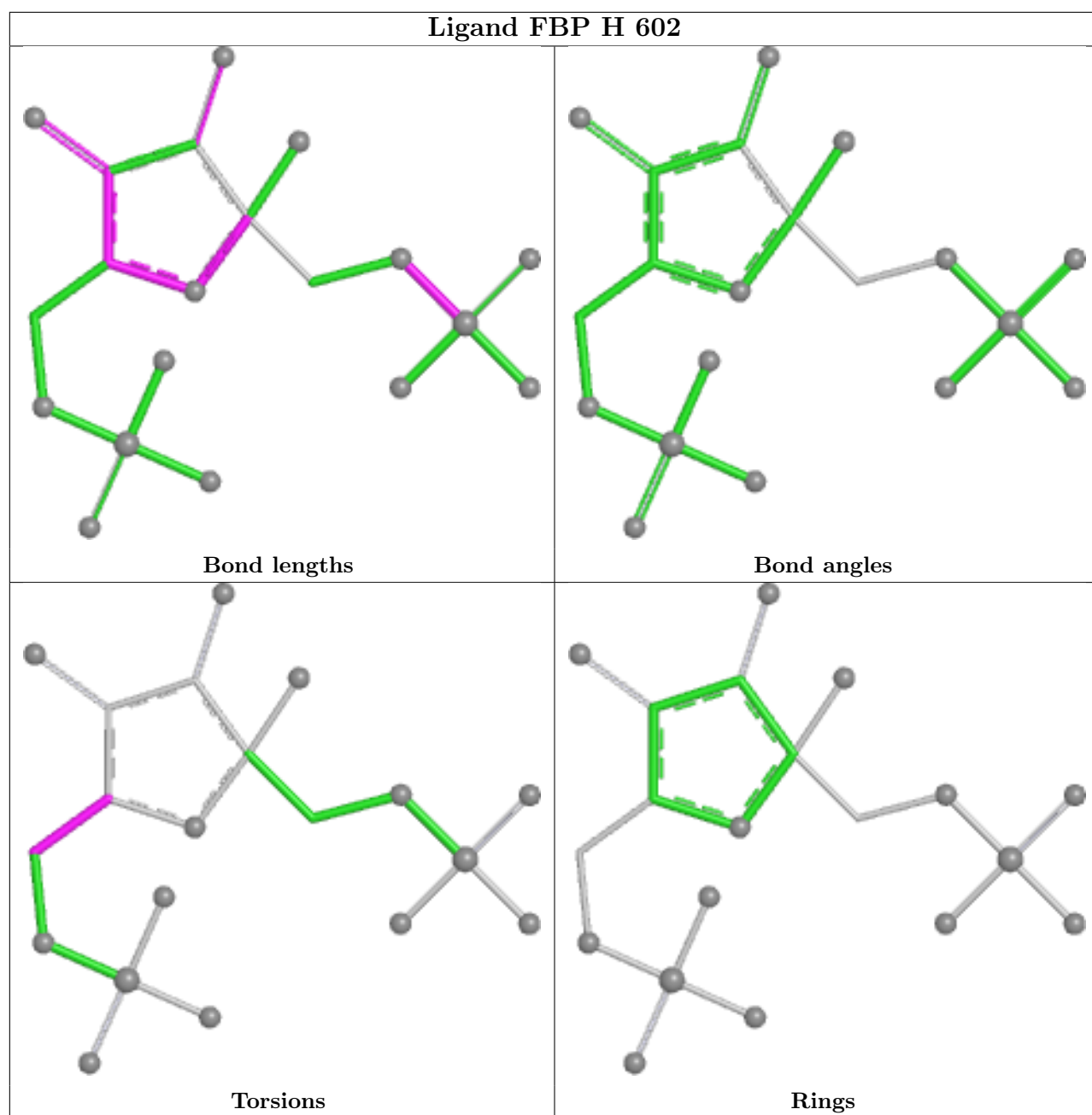
There are no ring outliers.

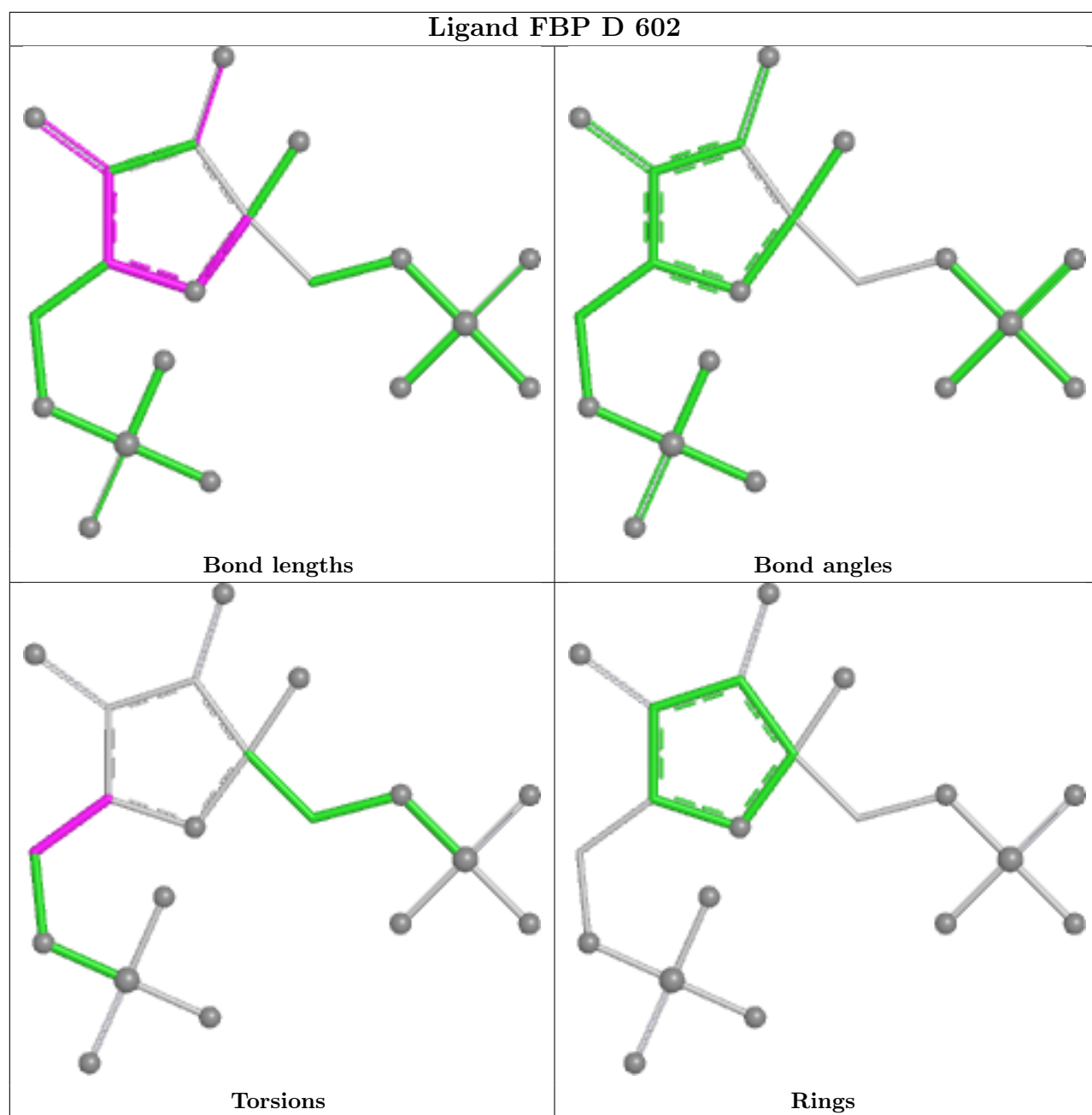
2 monomers are involved in 3 short contacts:

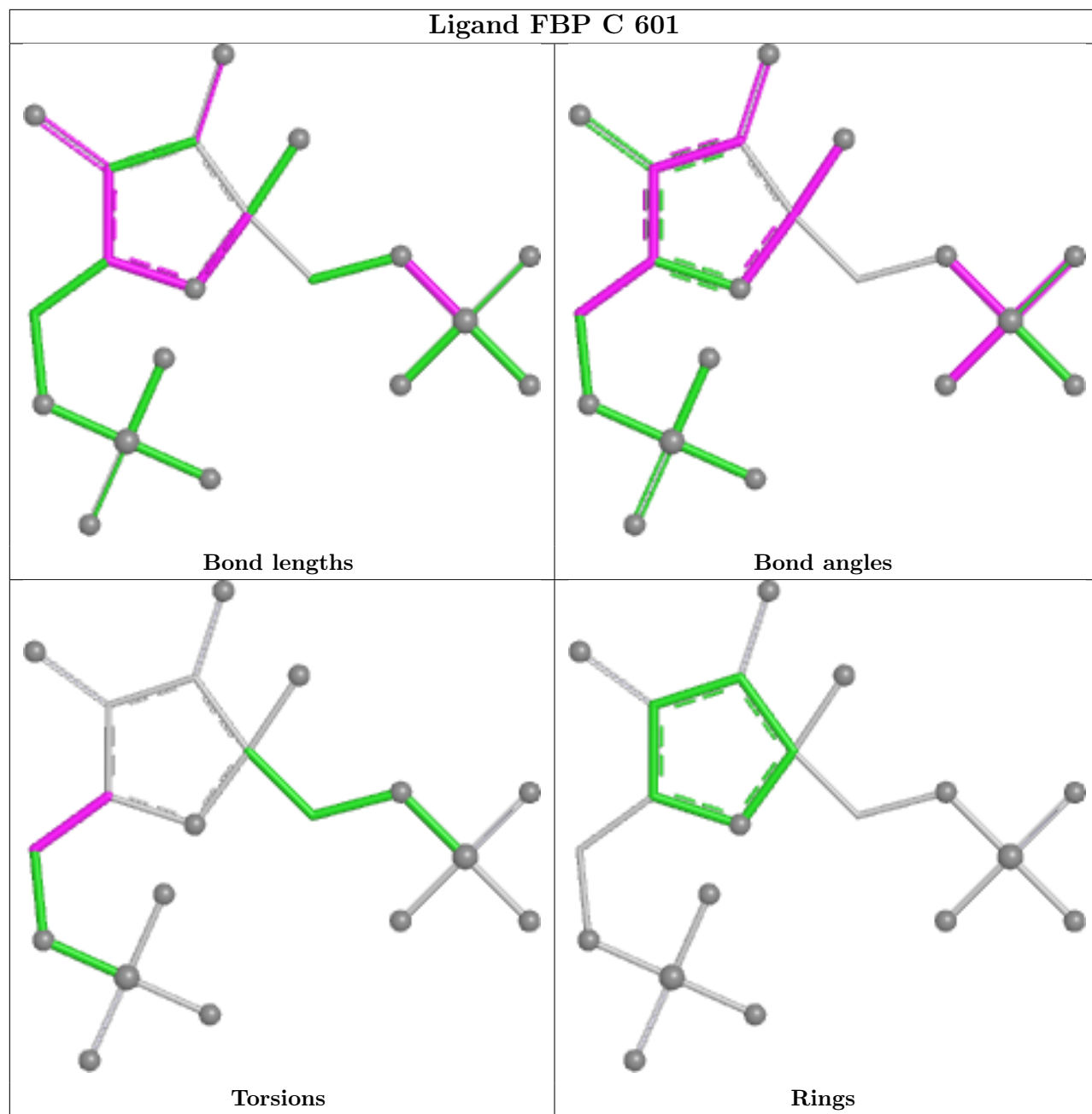
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	602	FBP	1	0
5	G	604	PYR	2	0

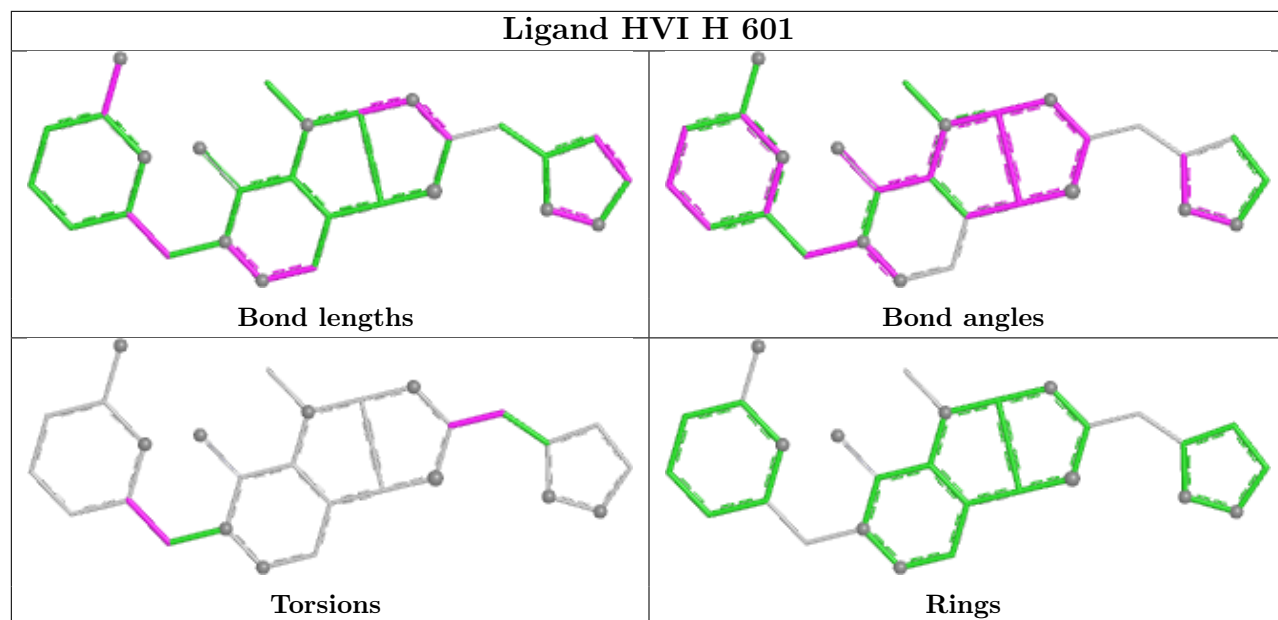
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



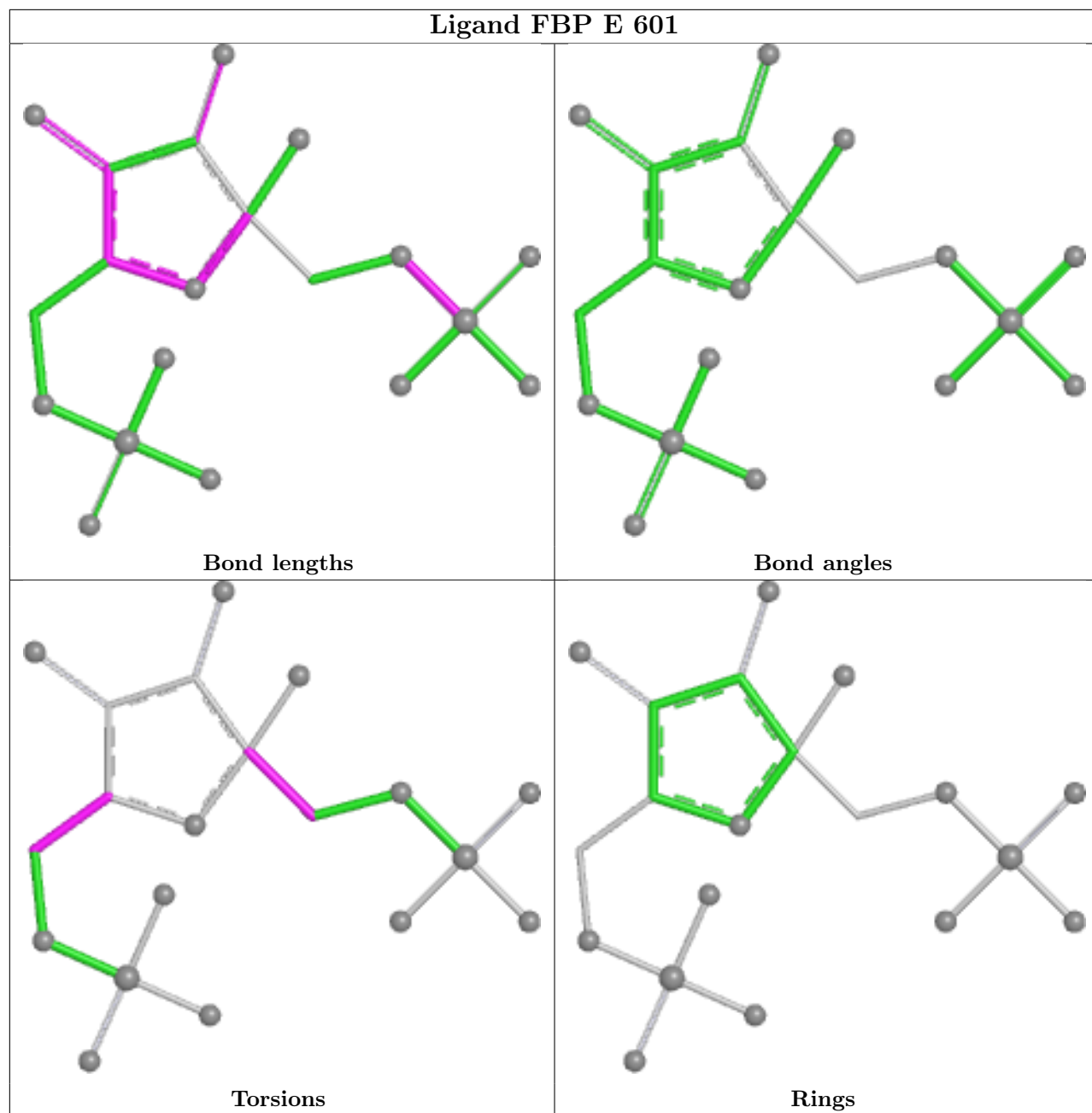




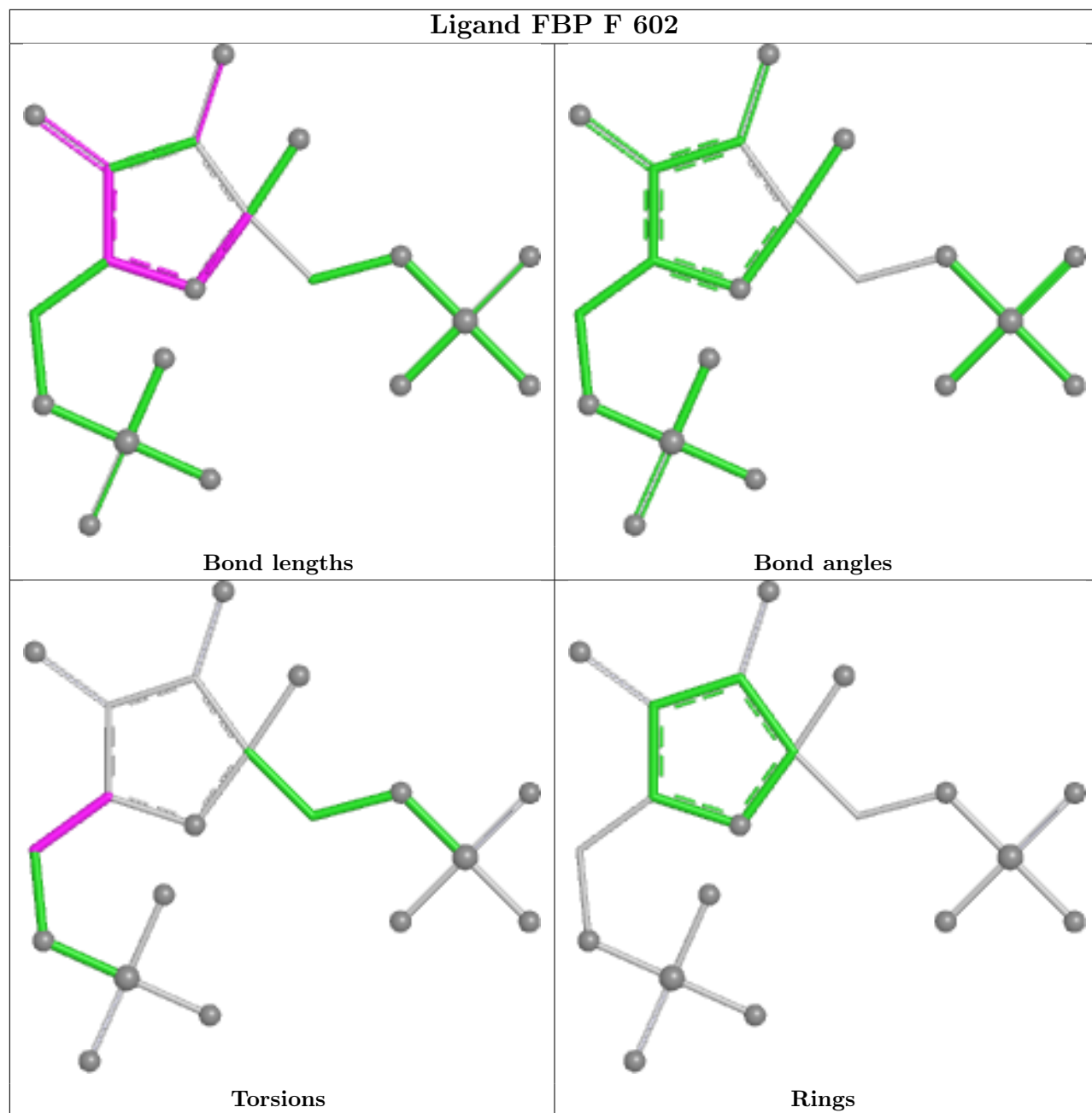


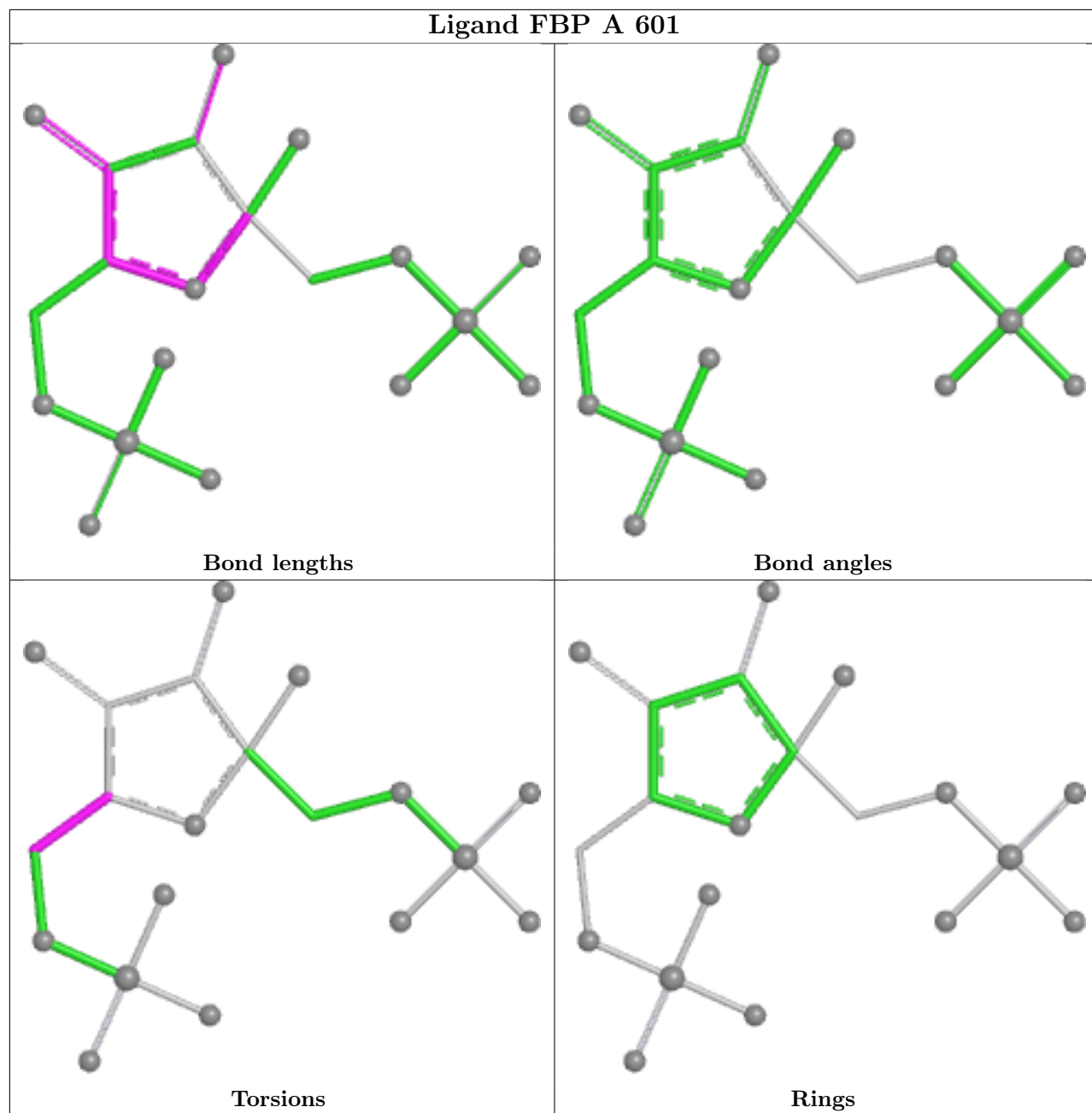


Ligand FBP E 601

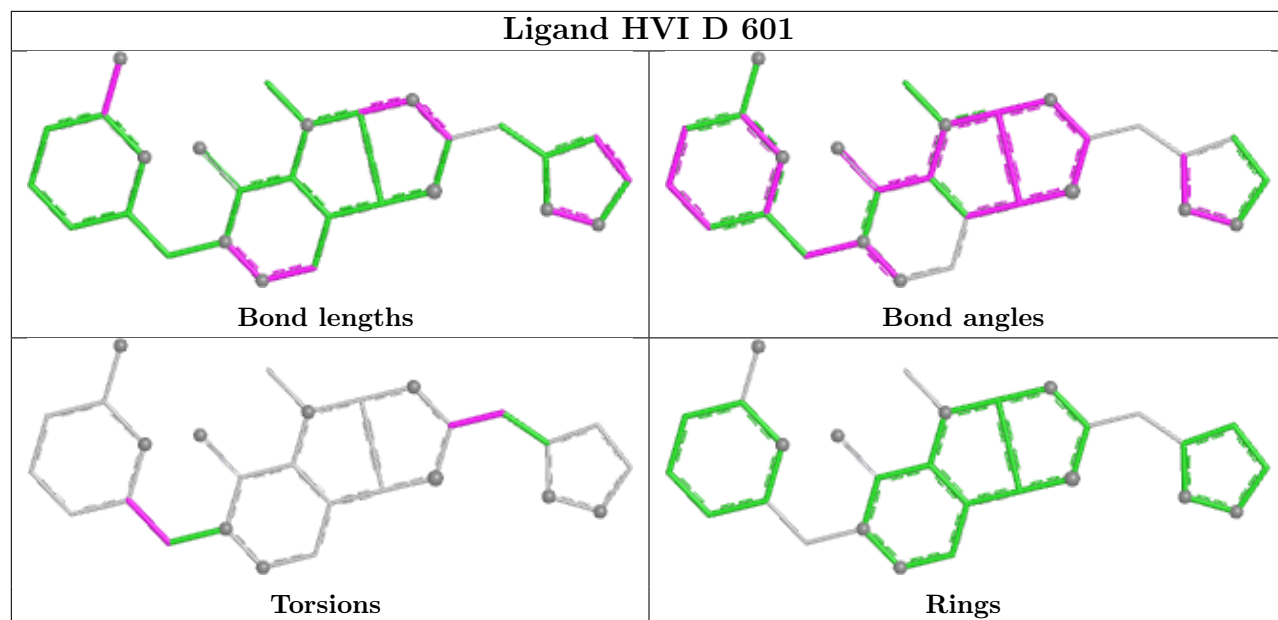


Ligand FBP F 602

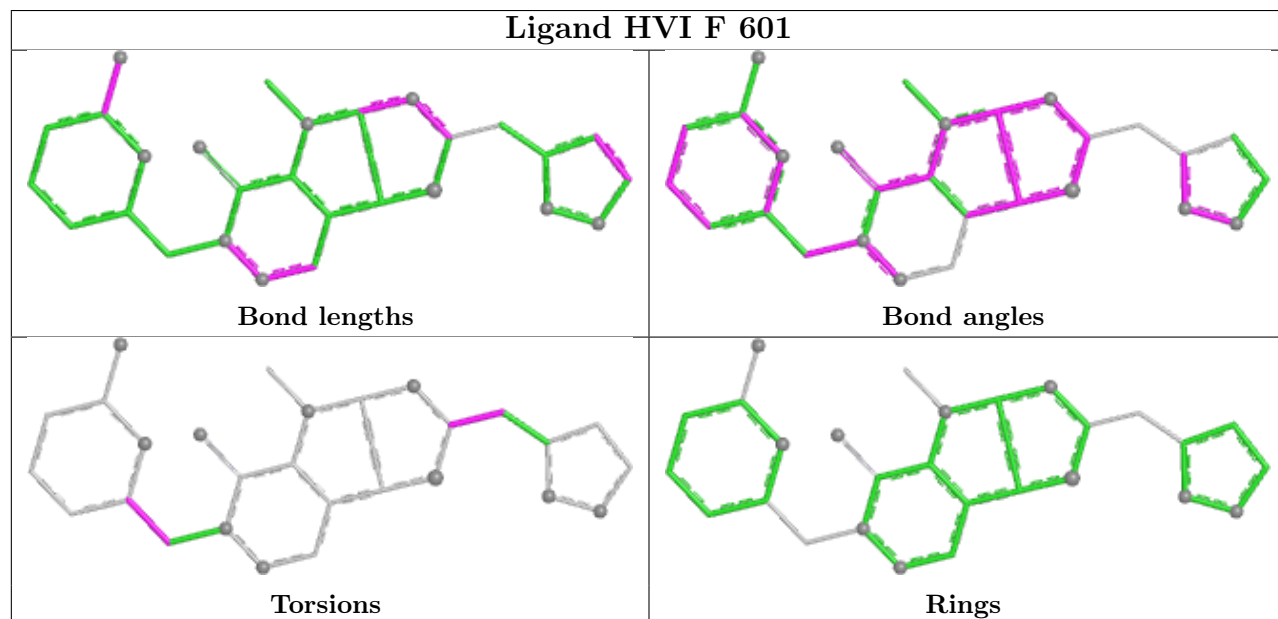




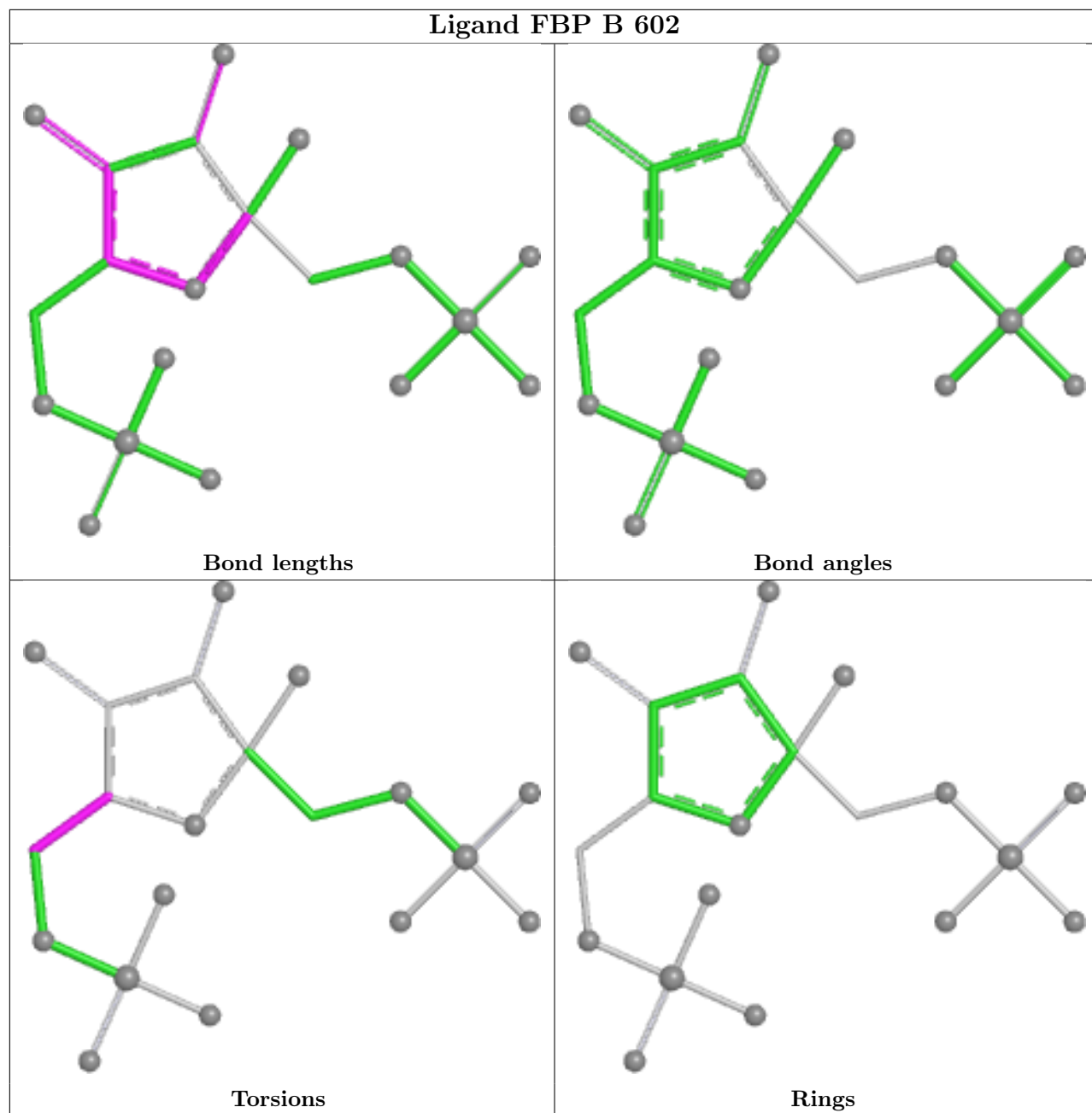
Ligand HVI D 601

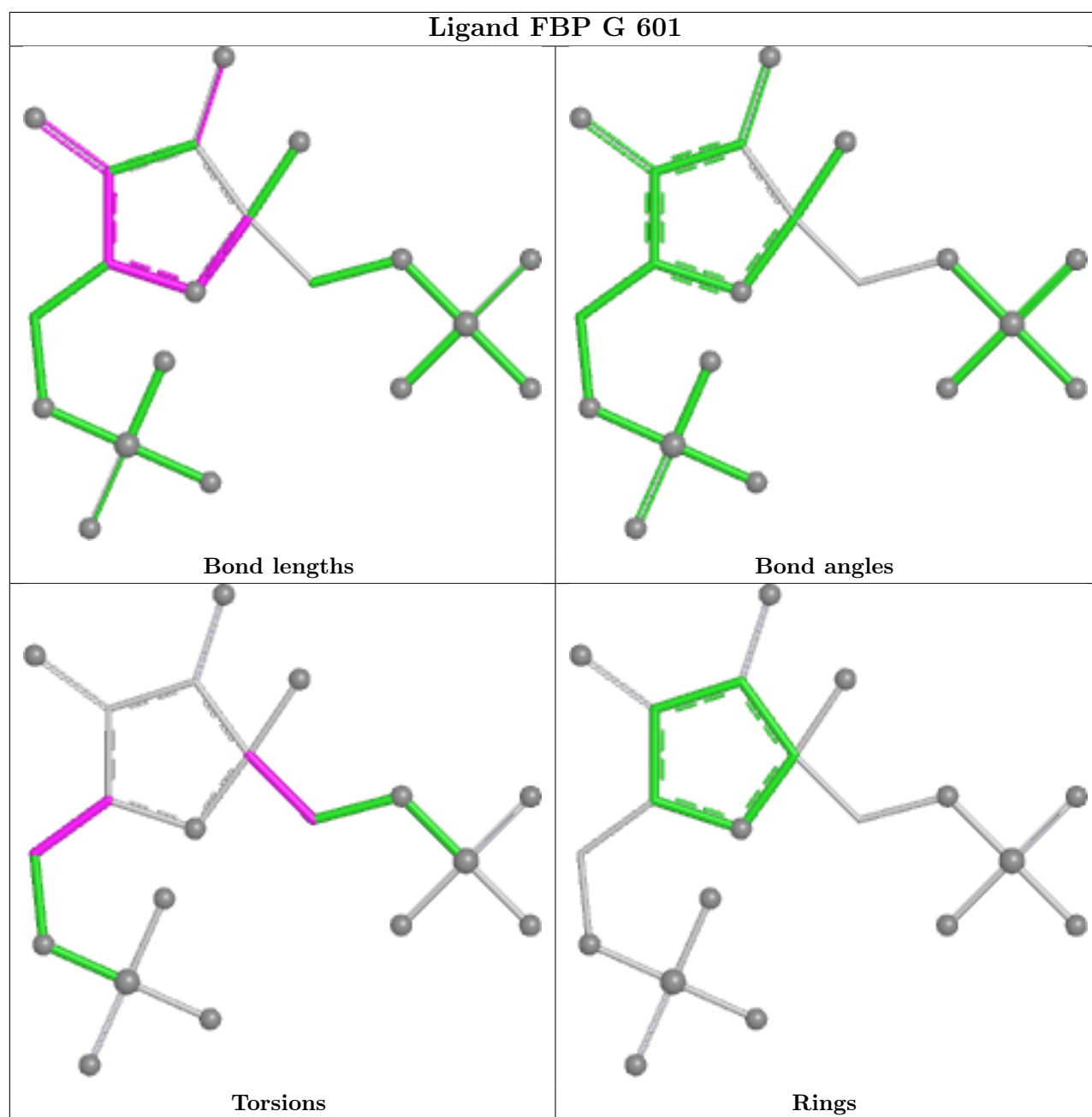


Ligand HVI F 601



Ligand FBP B 602





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	485/544 (89%)	0.16	26 (5%) 31 37	26, 51, 124, 158	1 (0%)
1	B	517/544 (95%)	0.18	32 (6%) 26 30	35, 51, 132, 162	0
1	C	512/544 (94%)	0.19	39 (7%) 20 22	24, 50, 135, 181	2 (0%)
1	D	483/544 (88%)	0.20	35 (7%) 21 24	36, 50, 110, 153	0
1	E	515/544 (94%)	0.39	36 (6%) 22 25	23, 62, 102, 155	1 (0%)
1	F	520/544 (95%)	-0.11	10 (1%) 66 71	31, 46, 75, 138	0
1	G	509/544 (93%)	0.38	41 (8%) 18 20	26, 61, 109, 155	6 (1%)
1	H	519/544 (95%)	-0.11	7 (1%) 75 79	29, 45, 73, 124	1 (0%)
All	All	4060/4352 (93%)	0.16	226 (5%) 30 35	23, 51, 116, 181	11 (0%)

The worst 5 of 226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	246	LEU	6.7
1	D	245	VAL	6.2
1	A	245	VAL	5.8
1	G	185	VAL	5.8
1	D	208	VAL	5.4

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

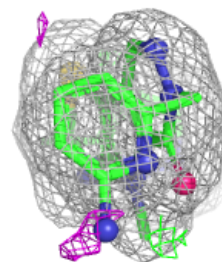
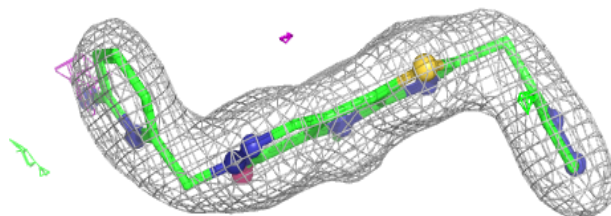
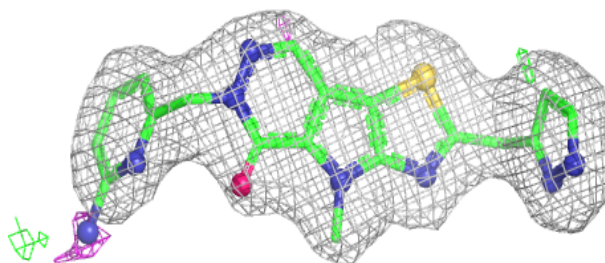
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MN	H	603	1/1	0.58	0.31	210,210,210,210	0
5	PYR	F	605	6/6	0.70	0.16	74,75,85,90	0
4	K	G	603	1/1	0.71	0.13	119,119,119,119	0
4	K	E	603	1/1	0.71	0.19	140,140,140,140	0
4	K	C	603	1/1	0.78	0.14	102,102,102,102	0
4	K	B	604	1/1	0.78	0.16	98,98,98,98	0
5	PYR	H	604	6/6	0.81	0.13	80,81,83,86	0
5	PYR	E	604	6/6	0.83	0.12	61,75,77,84	0
3	MN	F	603	1/1	0.84	0.24	160,160,160,160	0
4	K	F	604	1/1	0.85	0.21	107,107,107,107	0
5	PYR	D	604	6/6	0.86	0.12	58,68,78,84	0
4	K	A	603	1/1	0.89	0.12	90,90,90,90	0
5	PYR	B	605	6/6	0.89	0.14	51,72,77,78	0
5	PYR	C	604	6/6	0.91	0.11	52,60,68,72	0
5	PYR	G	604	6/6	0.92	0.10	63,70,75,78	0
6	HVI	B	601	28/28	0.93	0.08	31,46,52,58	0
3	MN	G	602	1/1	0.94	0.12	133,133,133,133	0
2	FBP	C	601	20/20	0.94	0.09	37,42,56,57	0
3	MN	D	603	1/1	0.95	0.07	99,99,99,99	0
2	FBP	E	601	20/20	0.95	0.07	41,48,56,61	0
2	FBP	G	601	20/20	0.95	0.08	38,47,58,61	0
6	HVI	H	601	28/28	0.95	0.08	31,38,45,48	0
6	HVI	D	601	28/28	0.96	0.07	33,45,55,59	0
6	HVI	F	601	28/28	0.96	0.07	31,38,46,50	0
2	FBP	D	602	20/20	0.96	0.07	40,49,55,62	0
5	PYR	A	604	6/6	0.97	0.14	50,59,65,65	0
2	FBP	A	601	20/20	0.97	0.05	39,46,56,61	0
2	FBP	F	602	20/20	0.97	0.06	31,41,47,48	0
3	MN	E	602	1/1	0.97	0.08	93,93,93,93	0
3	MN	B	603	1/1	0.98	0.06	87,87,87,87	0
2	FBP	B	602	20/20	0.98	0.04	32,39,44,47	0
2	FBP	H	602	20/20	0.98	0.06	35,41,51,51	0
3	MN	C	602	1/1	0.99	0.05	67,67,67,67	0
3	MN	A	602	1/1	0.99	0.04	61,61,61,61	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.

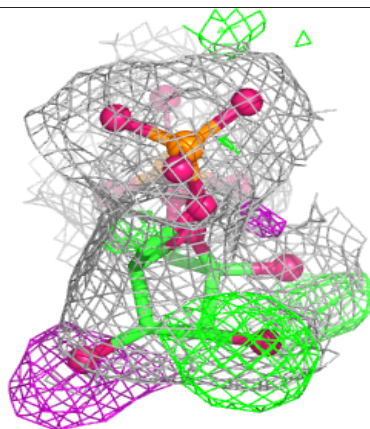
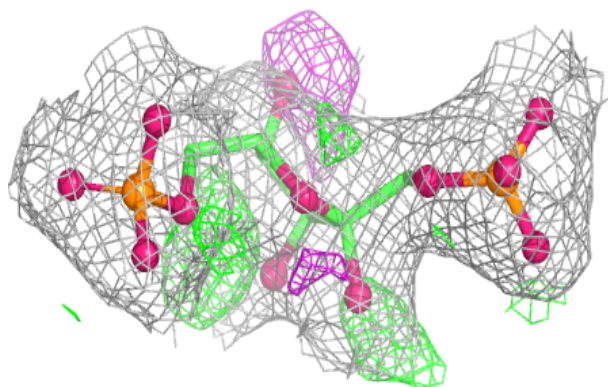
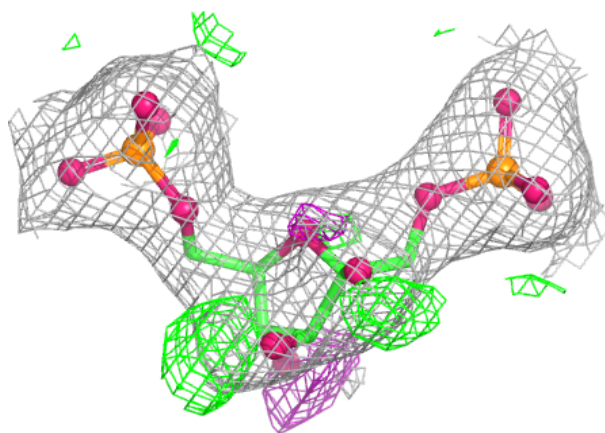
Electron density around HVI B 601:

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

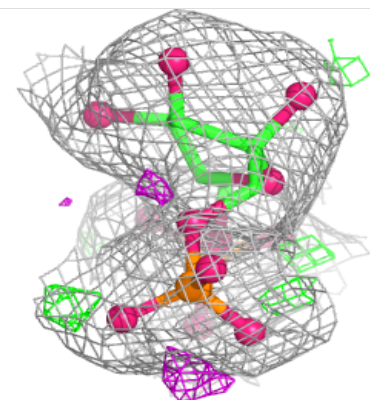
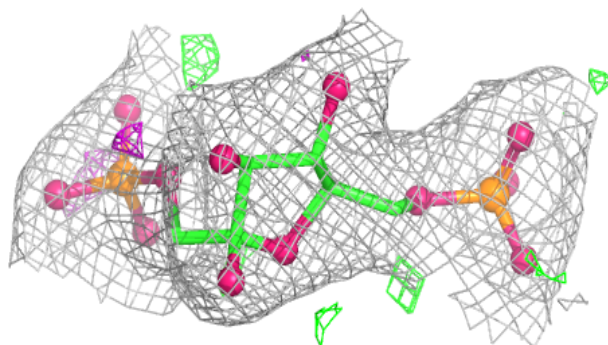
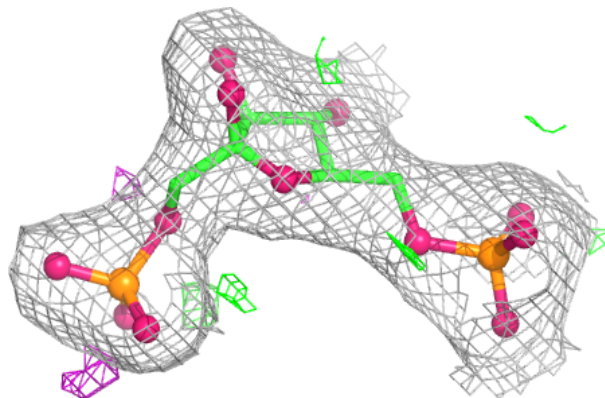


Electron density around FBP C 601:

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

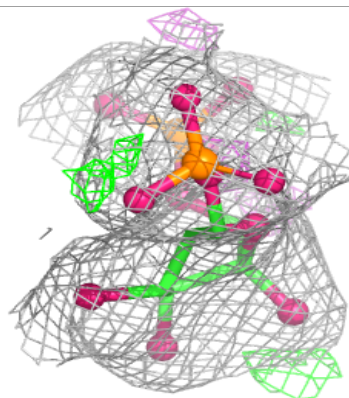
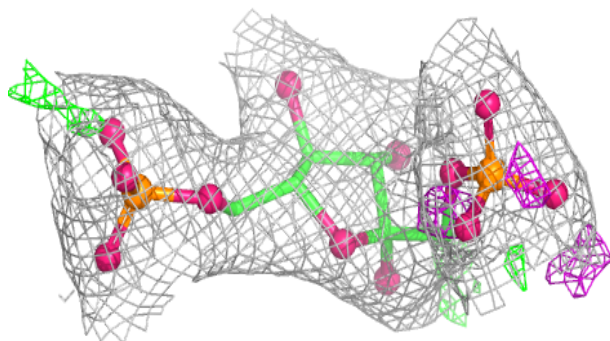
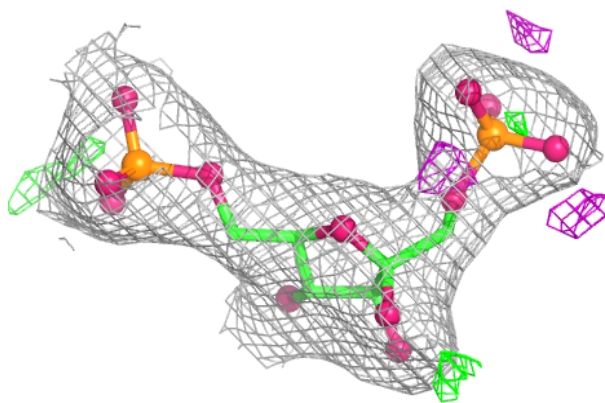
**Electron density around FBP E 601:**

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

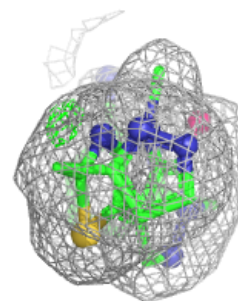
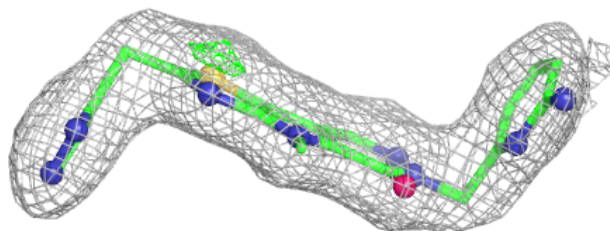
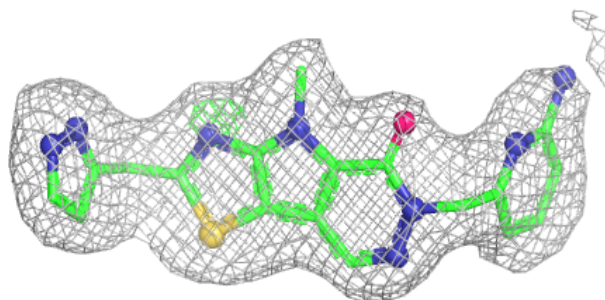


Electron density around FBP G 601:

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

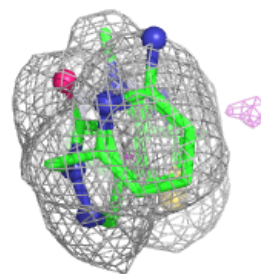
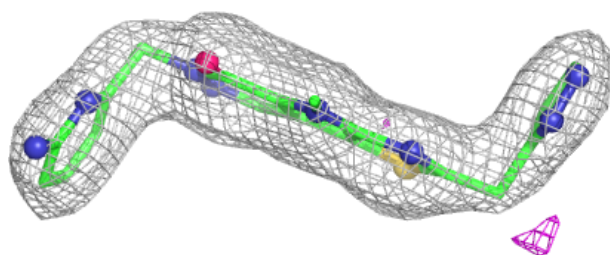
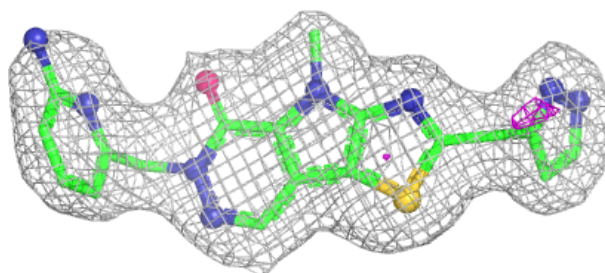
**Electron density around HVI H 601:**

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

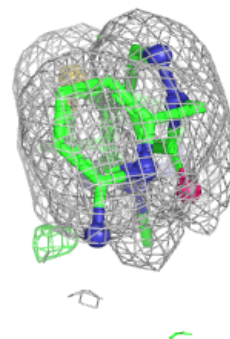
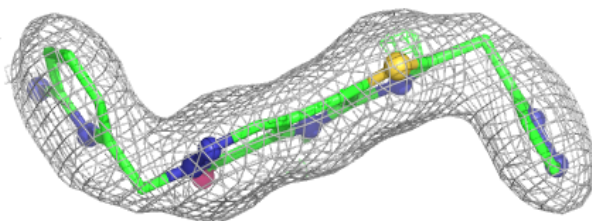
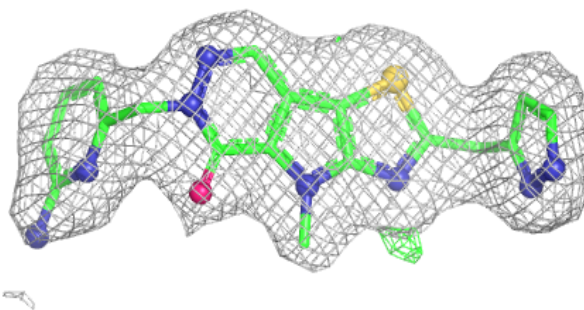


Electron density around HVI D 601:

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

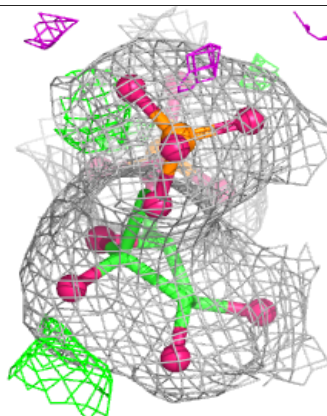
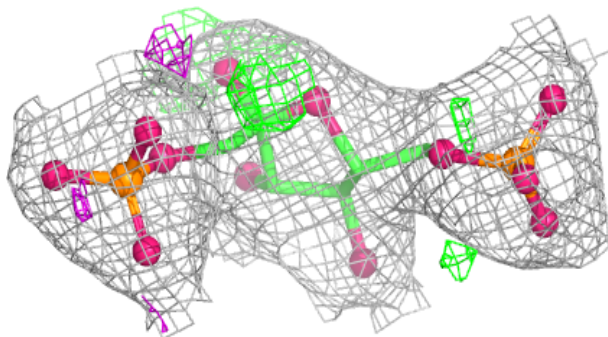
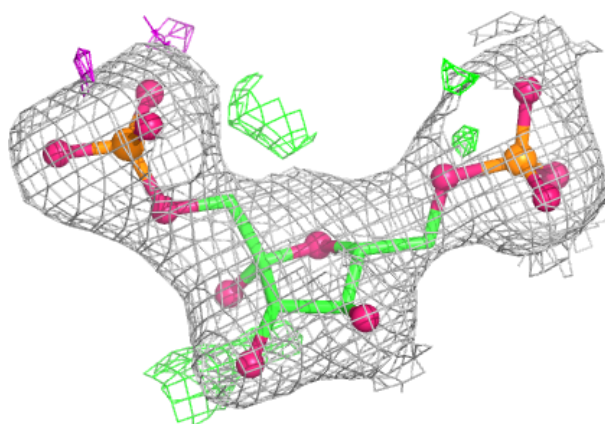
**Electron density around HVI F 601:**

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

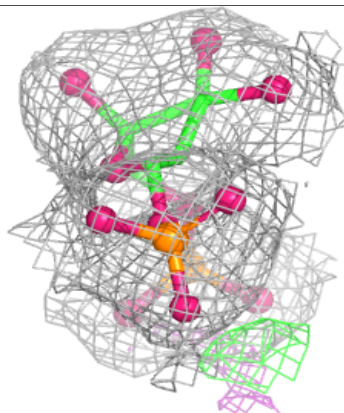
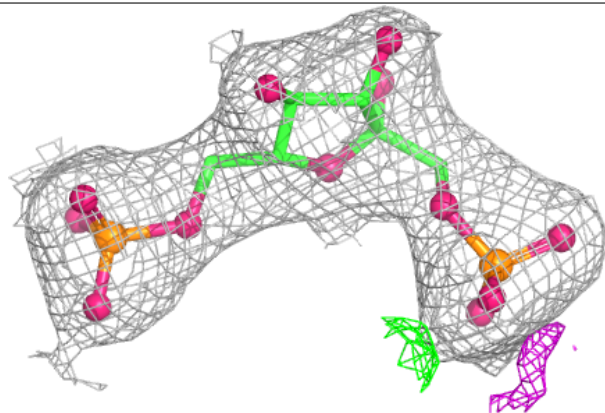


Electron density around FBP D 602:

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

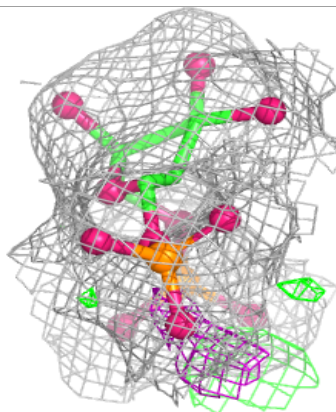
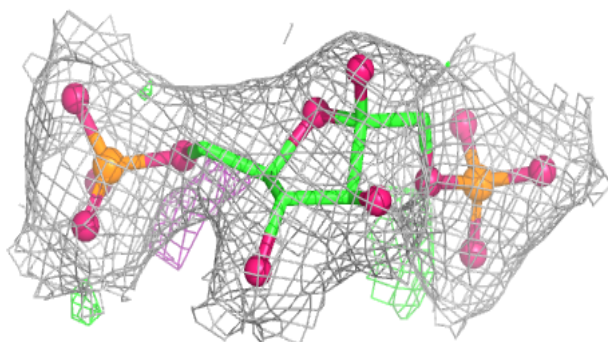
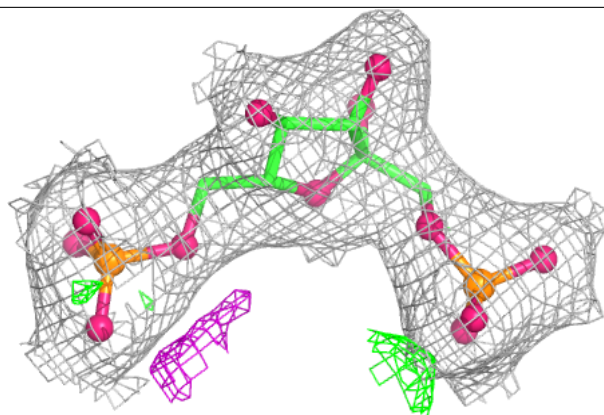
**Electron density around FBP A 601:**

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

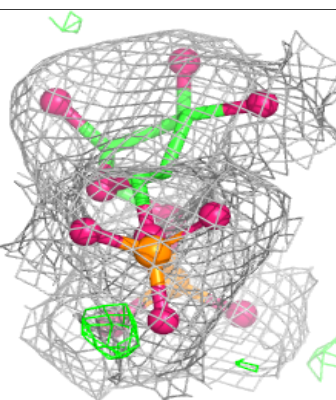
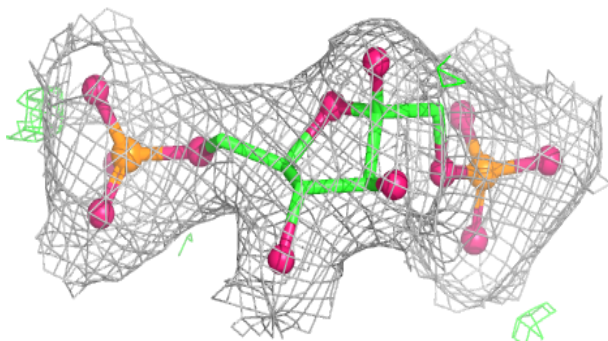
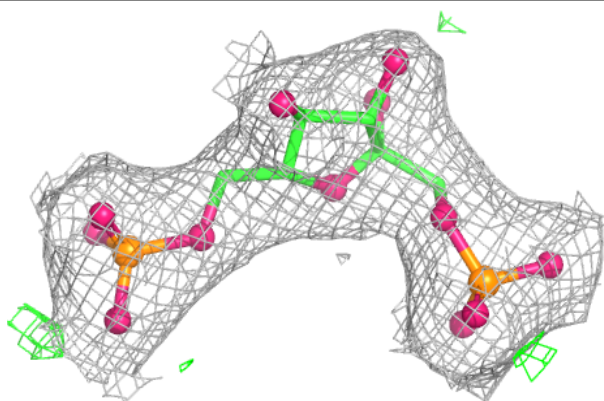


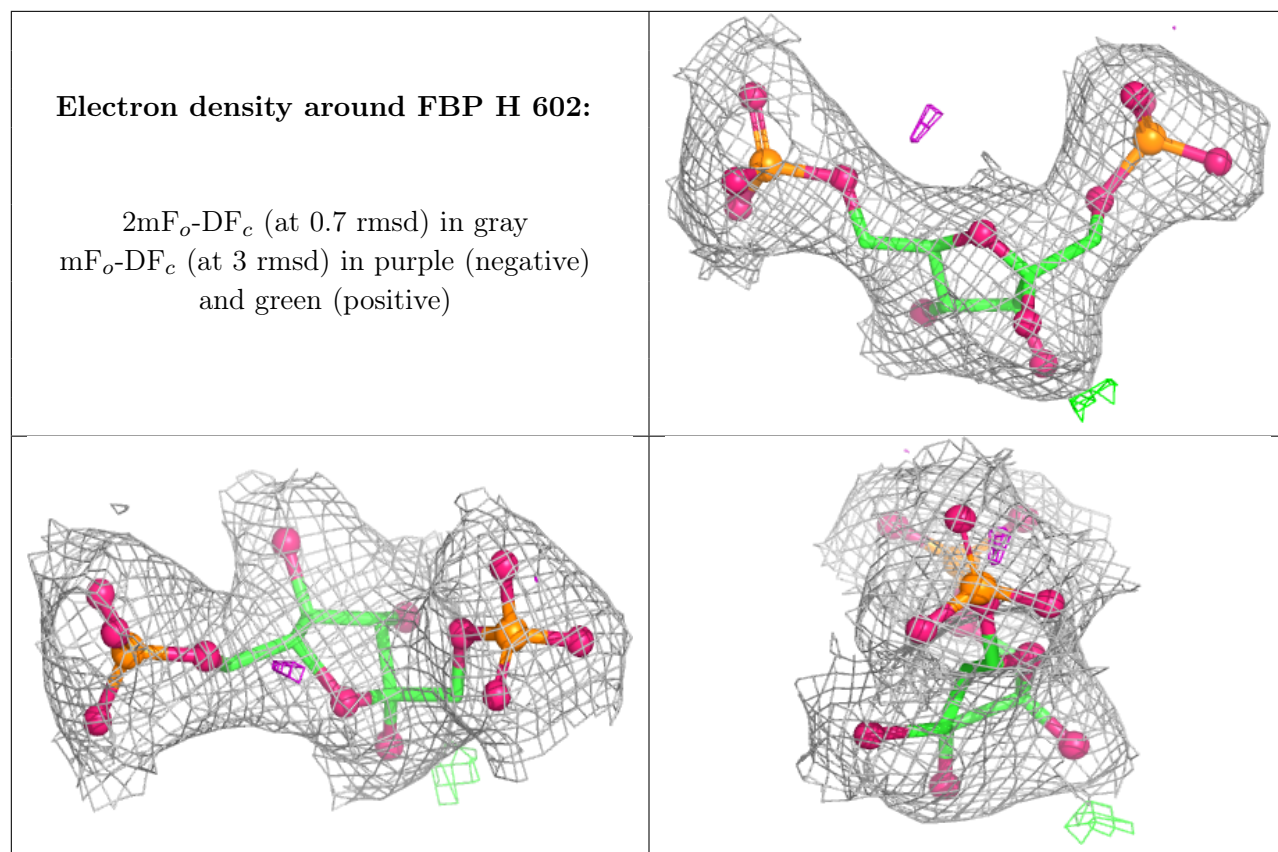
Electron density around FBP F 602:

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

**Electron density around FBP B 602:**

$2mF_o - DF_c$ (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.