



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 01:09 AM UTC

PDB ID : 5SCE / pdb_00005sce
Title : Structure of liver pyruvate kinase in complex with anthraquinone derivative
55
Authors : Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.
Deposited on : 2021-12-01
Resolution : 2.15 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

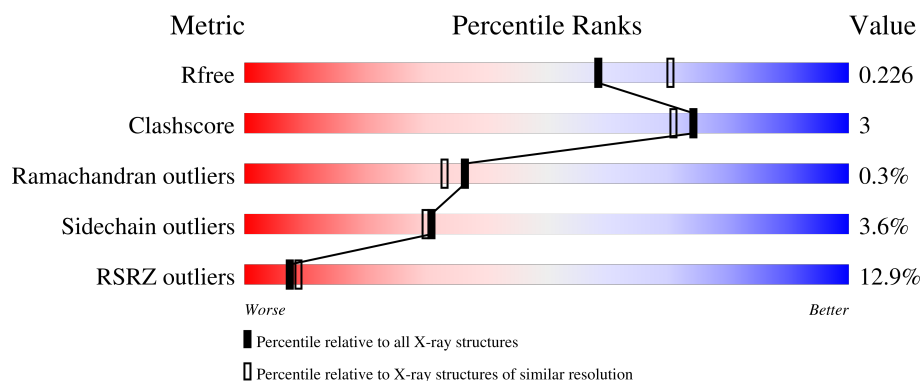
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	31% 83% 9% 6%
1	B	447	15% 87% 10% 6%
1	C	447	10% 86% 9% 5%
1	D	447	4% 85% 9% 5%
1	E	447	22% 83% 9% 6%

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	602	-	X	-	-
3	OXL	B	602	-	X	-	-
3	OXL	C	602	-	X	-	-
3	OXL	D	602	-	X	-	-
3	OXL	E	602	-	X	-	-
3	OXL	F	602	-	X	-	-
3	OXL	G	602	-	X	-	-
3	OXL	H	602	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27888 atoms, of which 36 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	13	0
			3238	2033	581	604	20			
1	B	436	Total	C	N	O	S	0	7	0
			3347	2102	604	621	20			
1	C	424	Total	C	N	O	S	0	8	0
			3263	2053	584	607	19			
1	D	425	Total	C	N	O	S	0	8	0
			3261	2048	590	604	19			
1	E	420	Total	C	N	O	S	0	13	0
			3261	2051	585	605	20			
1	F	434	Total	C	N	O	S	0	8	0
			3335	2098	599	618	20			
1	G	422	Total	C	N	O	S	0	8	0
			3246	2042	582	603	19			
1	H	425	Total	C	N	O	S	0	9	0
			3277	2057	597	604	19			

There are 48 discrepancies between the modelled and reference sequences:

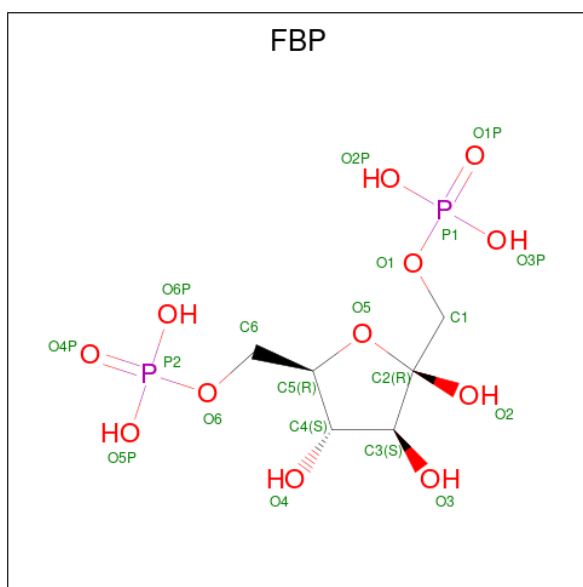
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	230	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression tag	UNP Q16716
B	12	ASP	SER	conflict	UNP Q16716
B	130	GLY	-	linker	UNP Q16716
B	131	SER	-	linker	UNP Q16716
B	132	GLY	-	linker	UNP Q16716
C	-1	GLY	-	expression tag	UNP Q16716

Continued on next page...

Continued from previous page...

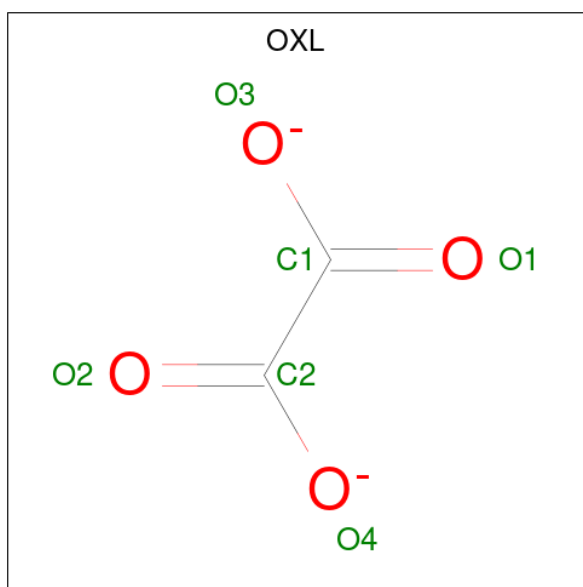
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	228	GLY	-	linker	UNP Q16716
C	229	SER	-	linker	UNP Q16716
C	230	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict	UNP Q16716
D	130	GLY	-	linker	UNP Q16716
D	131	SER	-	linker	UNP Q16716
D	132	GLY	-	linker	UNP Q16716
E	-1	GLY	-	expression tag	UNP Q16716
E	0	SER	-	expression tag	UNP Q16716
E	12	ASP	SER	conflict	UNP Q16716
E	130	GLY	-	linker	UNP Q16716
E	229	SER	-	linker	UNP Q16716
E	230	GLY	-	linker	UNP Q16716
F	-1	GLY	-	expression tag	UNP Q16716
F	0	SER	-	expression tag	UNP Q16716
F	12	ASP	SER	conflict	UNP Q16716
F	130	GLY	-	linker	UNP Q16716
F	131	SER	-	linker	UNP Q16716
F	132	GLY	-	linker	UNP Q16716
G	-1	GLY	-	expression tag	UNP Q16716
G	0	SER	-	expression tag	UNP Q16716
G	12	ASP	SER	conflict	UNP Q16716
G	228	GLY	-	linker	UNP Q16716
G	229	SER	-	linker	UNP Q16716
G	230	GLY	-	linker	UNP Q16716
H	-1	GLY	-	expression tag	UNP Q16716
H	0	SER	-	expression tag	UNP Q16716
H	12	ASP	SER	conflict	UNP Q16716
H	130	GLY	-	linker	UNP Q16716
H	131	SER	-	linker	UNP Q16716
H	132	GLY	-	linker	UNP Q16716

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



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

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



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

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

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

Continued on next page...

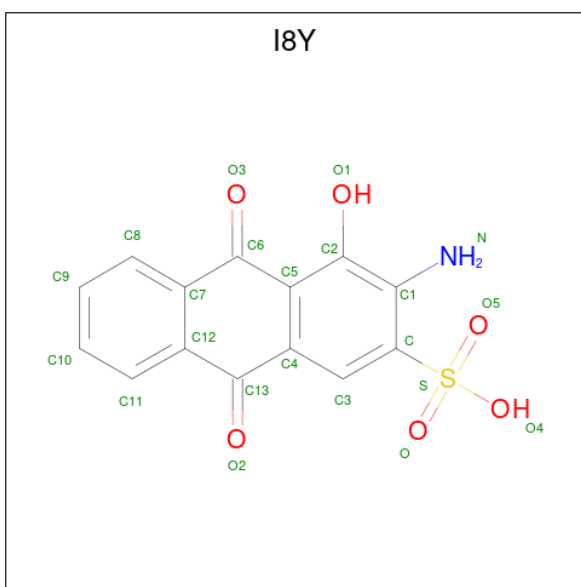
Continued from previous page...

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 3-amino-4-hydroxy-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (CCD ID: I8Y) (formula: C₁₄H₉NO₆S) (labeled as "Ligand of Interest" by depositor).

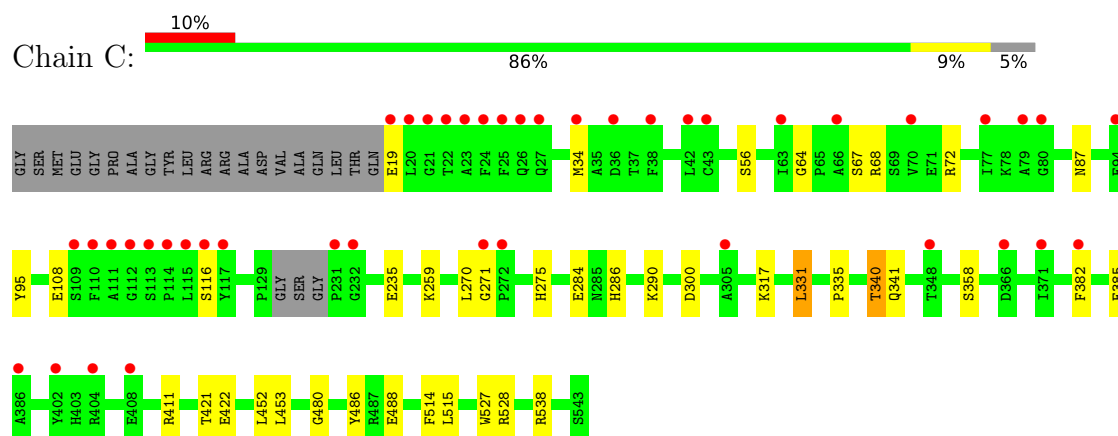


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	S	
			31	14	9	1	6	1	9 0
6	C	1	Total	C	H	N	O	S	
			31	14	9	1	6	1	9 0
6	F	1	Total	C	H	N	O	S	
			31	14	9	1	6	1	9 0
6	G	1	Total	C	H	N	O	S	
			31	14	9	1	6	1	9 0

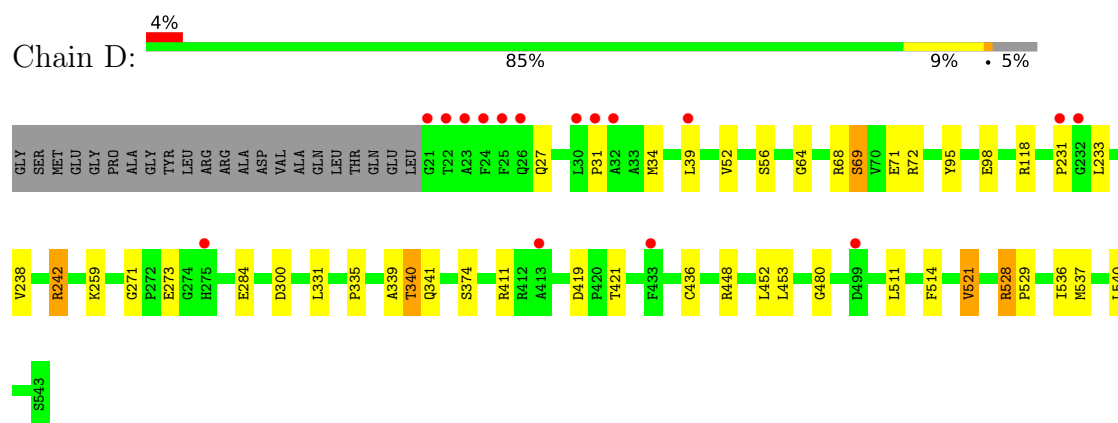
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	48	Total	O		
			48	48	0	0
7	B	101	Total	O		
			101	101	0	0
7	C	181	Total	O		
			181	181	0	0
7	D	239	Total	O		
			239	239	0	0
7	E	90	Total	O		
			90	90	0	0
7	F	153	Total	O		
			153	153	0	0
7	G	226	Total	O		
			226	226	0	0
7	H	274	Total	O		
			274	274	0	0

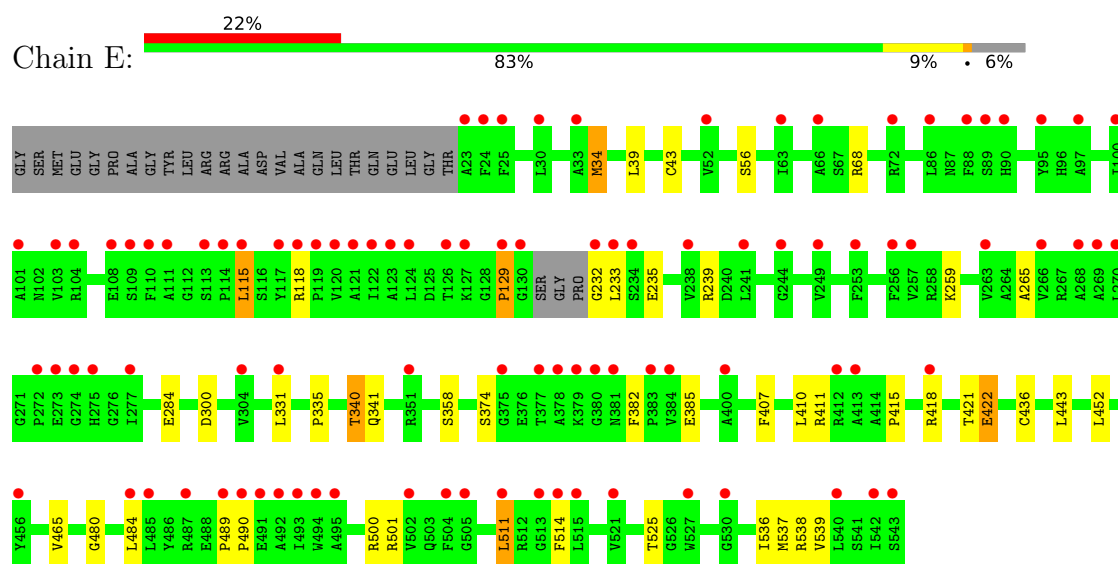
- Molecule 1: Pyruvate kinase



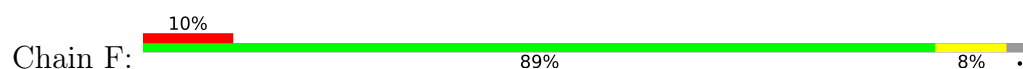
- Molecule 1: Pyruvate kinase

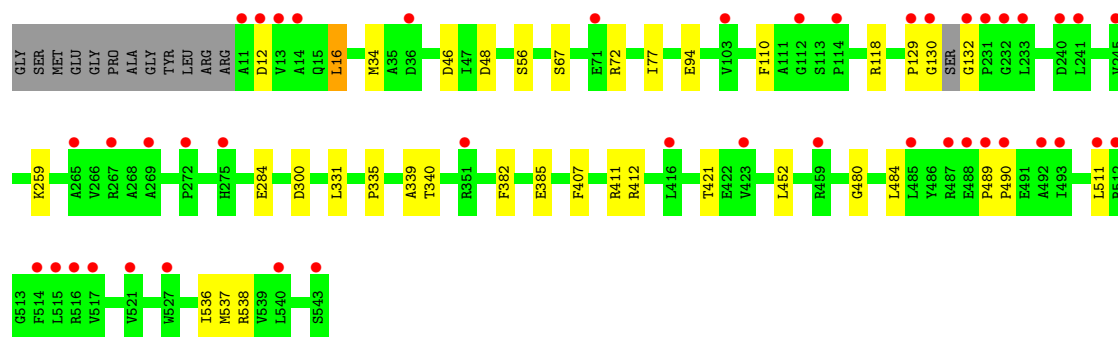


- Molecule 1: Pyruvate kinase

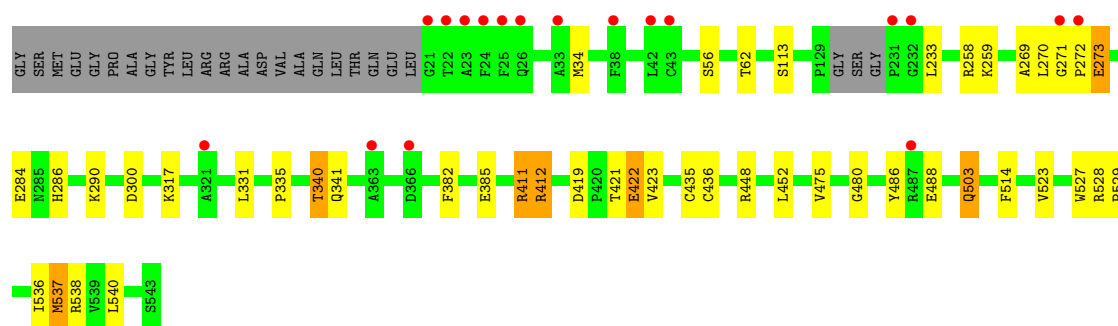
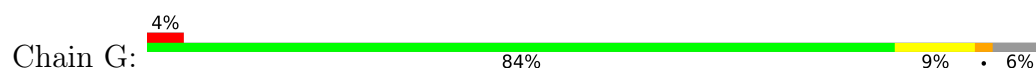


- Molecule 1: Pyruvate kinase

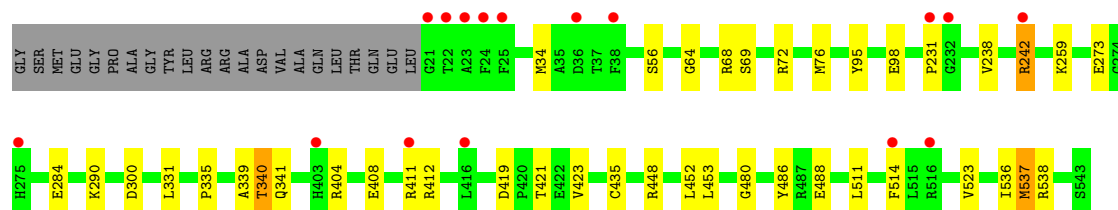
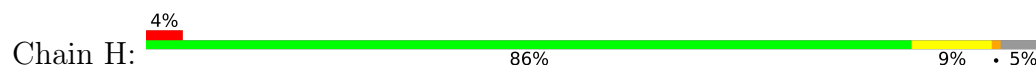




● Molecule 1: Pyruvate kinase



● Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.15Å 113.10Å 189.30Å 90.00° 91.49° 90.00°	Depositor
Resolution (Å)	104.04 – 2.15 104.04 – 2.15	Depositor EDS
% Data completeness (in resolution range)	66.9 (104.04-2.15) 67.0 (104.04-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.14Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.206 , 0.236 0.200 , 0.226	Depositor DCC
R_{free} test set	8277 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27888	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 61.97 % 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 1.2095e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: FBP, OXL, MG, K, I8Y

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	0/3328	1.05	3/4497 (0.1%)
1	B	0.71	0/3423	1.05	4/4628 (0.1%)
1	C	0.76	0/3341	1.06	4/4516 (0.1%)
1	D	0.80	1/3341 (0.0%)	1.07	5/4517 (0.1%)
1	E	0.67	1/3354 (0.0%)	1.02	3/4532 (0.1%)
1	F	0.73	0/3413	1.05	3/4614 (0.1%)
1	G	0.80	1/3324 (0.0%)	1.05	4/4493 (0.1%)
1	H	0.81	0/3357	1.05	5/4537 (0.1%)
All	All	0.75	3/26881 (0.0%)	1.05	31/36334 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	374	SER	CA-C	7.54	1.56	1.52
1	E	374	SER	CA-C	6.02	1.55	1.52
1	G	537	MET	SD-CE	-5.39	1.66	1.79

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	514	PHE	CA-CB-CG	5.99	119.79	113.80
1	C	514	PHE	CA-CB-CG	5.92	119.72	113.80
1	G	270	LEU	CA-C-N	5.91	131.15	121.87
1	G	270	LEU	C-N-CA	5.91	131.15	121.87
1	F	46	ASP	CA-CB-CG	5.82	118.42	112.60

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	3238	0	3312	25	0
1	B	3347	0	3412	28	0
1	C	3263	0	3325	24	0
1	D	3261	0	3322	24	0
1	E	3261	0	3326	24	0
1	F	3335	0	3404	19	0
1	G	3246	0	3308	29	0
1	H	3277	0	3342	24	0
2	A	20	0	10	2	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	1	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	B	22	9	0	1	0
6	C	22	9	0	1	0
6	F	22	9	0	0	0
6	G	22	9	0	1	0
7	A	48	0	0	1	0
7	B	101	0	0	2	0
7	C	181	0	0	1	0
7	D	239	0	0	2	0
7	E	90	0	0	0	0
7	F	153	0	0	0	0
7	G	226	0	0	2	0
7	H	274	0	0	1	0
All	All	27852	36	26831	166	0

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

The worst 5 of 166 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:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.68	0.76
1:A:528:ARG:HD2	1:A:529:PRO:O	1.87	0.75
1:E:415:PRO:HB3	1:F:12:ASP:HA	1.68	0.73
1:E:418[B]:ARG:HG3	1:F:16:LEU:HD11	1.70	0.73
1:C:64:GLY:O	1:C:68:ARG:HG3	1.89	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/447 (96%)	422 (99%)	4 (1%)	1 (0%)	43	42
1	B	441/447 (99%)	435 (99%)	5 (1%)	1 (0%)	43	42
1	C	428/447 (96%)	422 (99%)	5 (1%)	1 (0%)	43	42
1	D	431/447 (96%)	425 (99%)	4 (1%)	2 (0%)	24	19
1	E	429/447 (96%)	425 (99%)	2 (0%)	2 (0%)	24	19
1	F	438/447 (98%)	433 (99%)	4 (1%)	1 (0%)	43	42
1	G	426/447 (95%)	420 (99%)	5 (1%)	1 (0%)	43	42
1	H	432/447 (97%)	428 (99%)	2 (0%)	2 (0%)	24	19
All	All	3452/3576 (96%)	3410 (99%)	31 (1%)	11 (0%)	36	33

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	129	PRO
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	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	345/352 (98%)	325 (94%)	20 (6%)	18	13
1	B	352/352 (100%)	336 (96%)	16 (4%)	24	21
1	C	345/352 (98%)	335 (97%)	10 (3%)	37	38
1	D	344/352 (98%)	331 (96%)	13 (4%)	29	28
1	E	346/352 (98%)	331 (96%)	15 (4%)	26	23
1	F	351/352 (100%)	340 (97%)	11 (3%)	35	35
1	G	343/352 (97%)	331 (96%)	12 (4%)	32	31
1	H	345/352 (98%)	334 (97%)	11 (3%)	34	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2771/2816 (98%)	2663 (96%)	108 (4%)	31 26

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	528	ARG
1	E	537[A]	MET
1	H	242[A]	ARG
1	E	34	MET
1	E	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	390	GLN
1	G	405	GLN
1	E	390	GLN
1	G	390	GLN
1	D	405	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	I8Y	B	603	-	23,24,24	0.86	1 (4%)	34,38,38	0.47	0
3	OXL	D	602	4	5,5,5	2.16	2 (40%)	6,6,6	2.41	3 (50%)
3	OXL	F	602	4	5,5,5	2.73	4 (80%)	6,6,6	3.05	4 (66%)
2	FBP	H	601	-	18,20,20	0.74	0	21,32,32	0.82	1 (4%)
3	OXL	G	602	4	5,5,5	2.12	2 (40%)	6,6,6	2.56	4 (66%)
2	FBP	C	601	-	18,20,20	0.70	1 (5%)	21,32,32	0.69	0
6	I8Y	C	603	-	23,24,24	0.86	1 (4%)	34,38,38	0.51	0
2	FBP	F	601	-	18,20,20	0.50	0	21,32,32	0.60	0
2	FBP	A	601	-	18,20,20	0.64	0	21,32,32	0.89	0
2	FBP	B	601	-	18,20,20	0.72	0	21,32,32	0.86	1 (4%)
3	OXL	B	602	4	5,5,5	2.71	3 (60%)	6,6,6	1.10	1 (16%)
3	OXL	H	602	4	5,5,5	1.99	2 (40%)	6,6,6	1.65	1 (16%)
6	I8Y	F	603	-	23,24,24	0.67	1 (4%)	34,38,38	0.49	0
2	FBP	G	601	-	18,20,20	0.48	0	21,32,32	0.64	0
6	I8Y	G	603	-	23,24,24	0.72	1 (4%)	34,38,38	0.43	0
3	OXL	E	602	4	5,5,5	2.23	2 (40%)	6,6,6	1.17	1 (16%)
2	FBP	D	601	-	18,20,20	0.61	0	21,32,32	0.76	1 (4%)
3	OXL	A	602	4	5,5,5	2.00	2 (40%)	6,6,6	2.29	3 (50%)
2	FBP	E	601	-	18,20,20	0.46	0	21,32,32	0.71	1 (4%)
3	OXL	C	602	4	5,5,5	2.04	2 (40%)	6,6,6	0.98	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
6	I8Y	B	603	-	-	4/6/22/22	0/3/3/3
3	OXL	D	602	4	-	4/4/4/4	-
3	OXL	F	602	4	-	4/4/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	G	602	4	-	4/4/4/4	-
2	FBP	C	601	-	-	4/13/32/32	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	I8Y	C	603	-	-	6/6/22/22	0/3/3/3
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	5/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	H	602	4	-	4/4/4/4	-
6	I8Y	F	603	-	-	0/6/22/22	0/3/3/3
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
6	I8Y	G	603	-	-	6/6/22/22	0/3/3/3
3	OXL	E	602	4	-	4/4/4/4	-
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	4	-	4/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
3	OXL	C	602	4	-	4/4/4/4	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXL	O2-C2	4.74	1.34	1.22
3	E	602	OXL	O1-C1	4.13	1.32	1.22
6	C	603	I8Y	C-S	-3.89	1.67	1.77
6	B	603	I8Y	C-S	-3.73	1.67	1.77
3	A	602	OXL	O2-C2	3.59	1.31	1.22

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	OXL	O4-C2-C1	5.00	122.52	112.83
3	A	602	OXL	O4-C2-C1	4.34	121.25	112.83
3	F	602	OXL	O3-C1-C2	3.93	120.46	112.83
3	G	602	OXL	O4-C2-C1	3.84	120.29	112.83
3	G	602	OXL	O3-C1-C2	3.83	120.27	112.83

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C6-O6-P2-O5P

Continued on next page...

Continued from previous page...

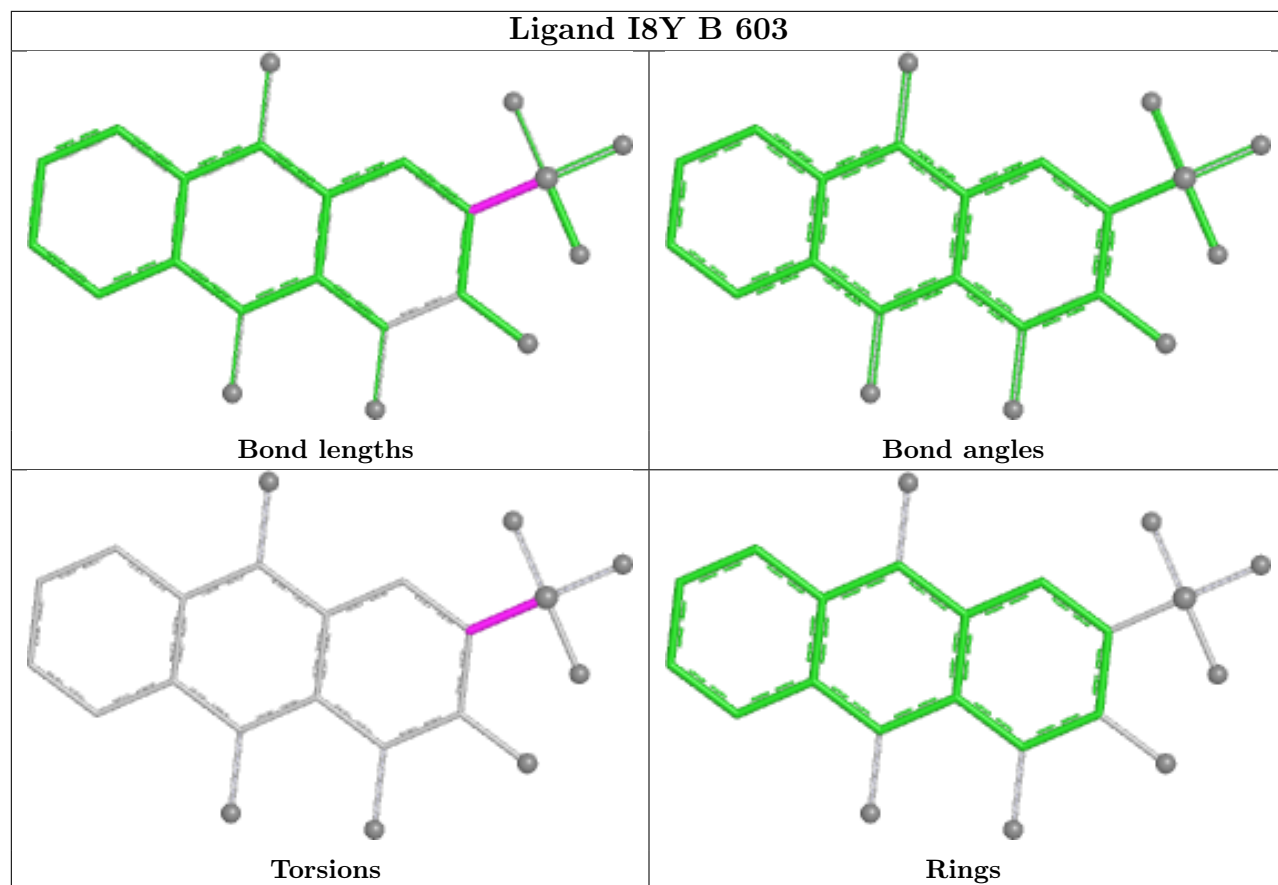
Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C6-O6-P2-O6P
6	B	603	I8Y	C3-C-S-O5
6	B	603	I8Y	C1-C-S-O4
6	B	603	I8Y	C3-C-S-O4

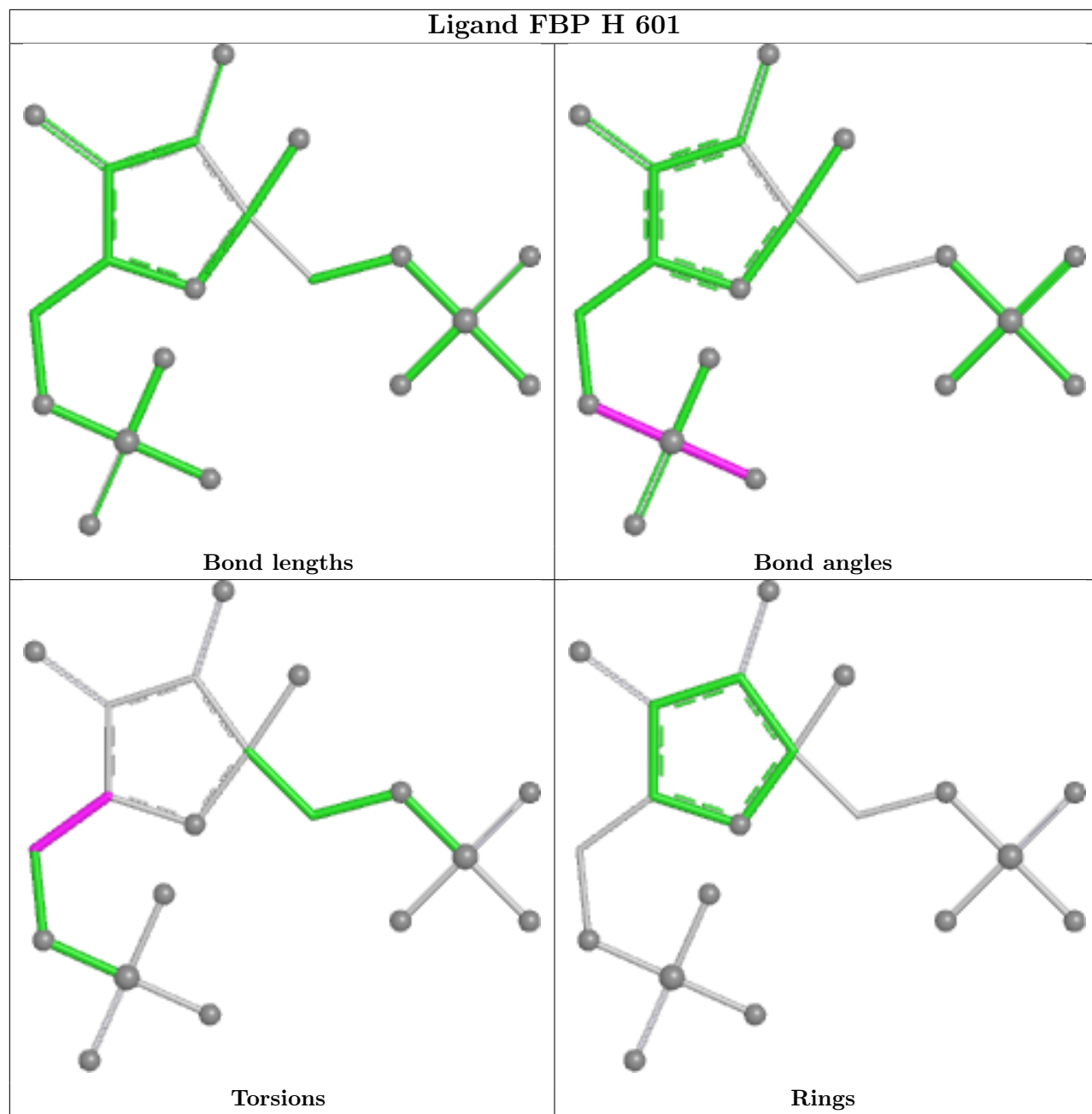
There are no ring outliers.

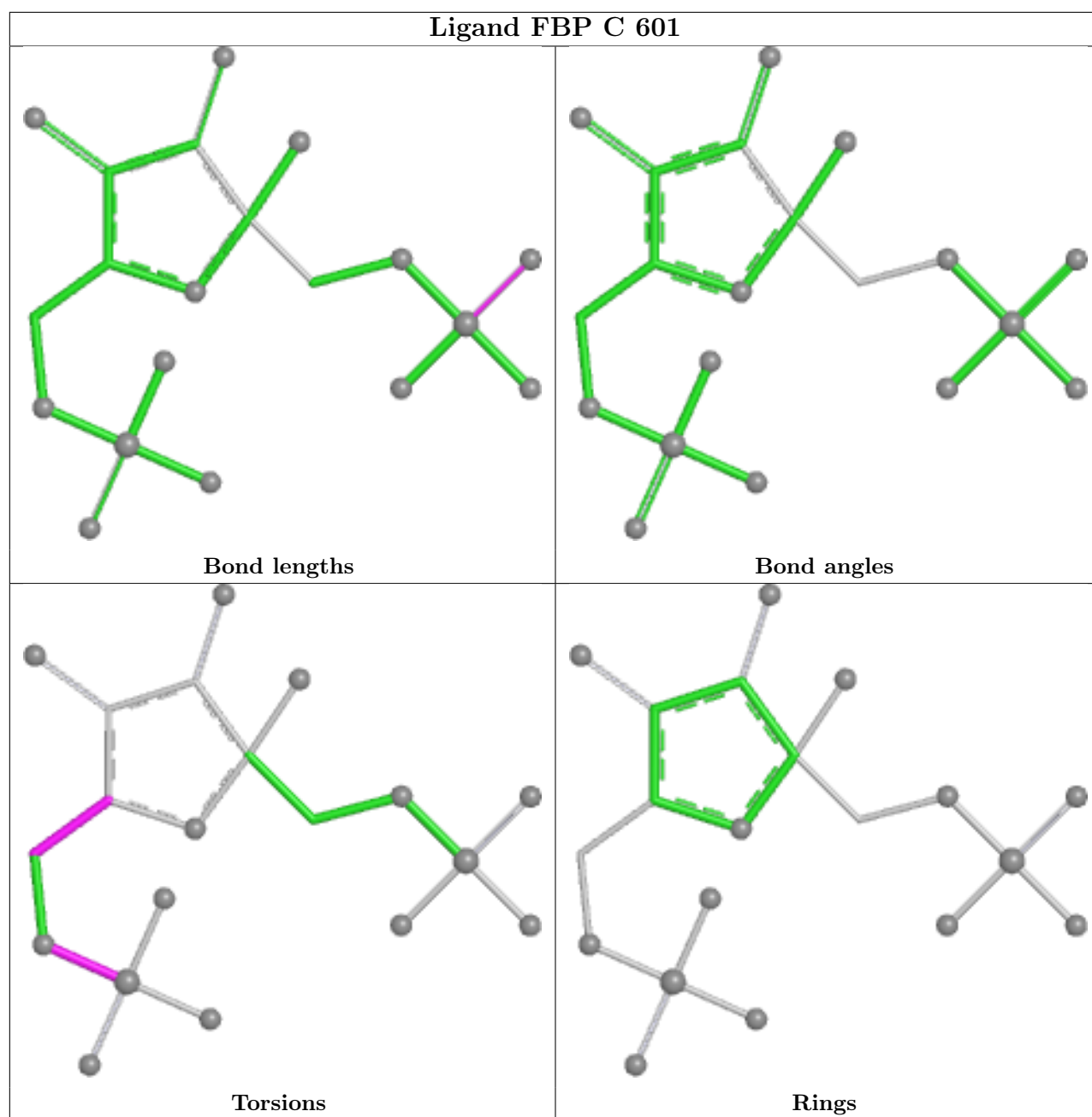
5 monomers are involved in 6 short contacts:

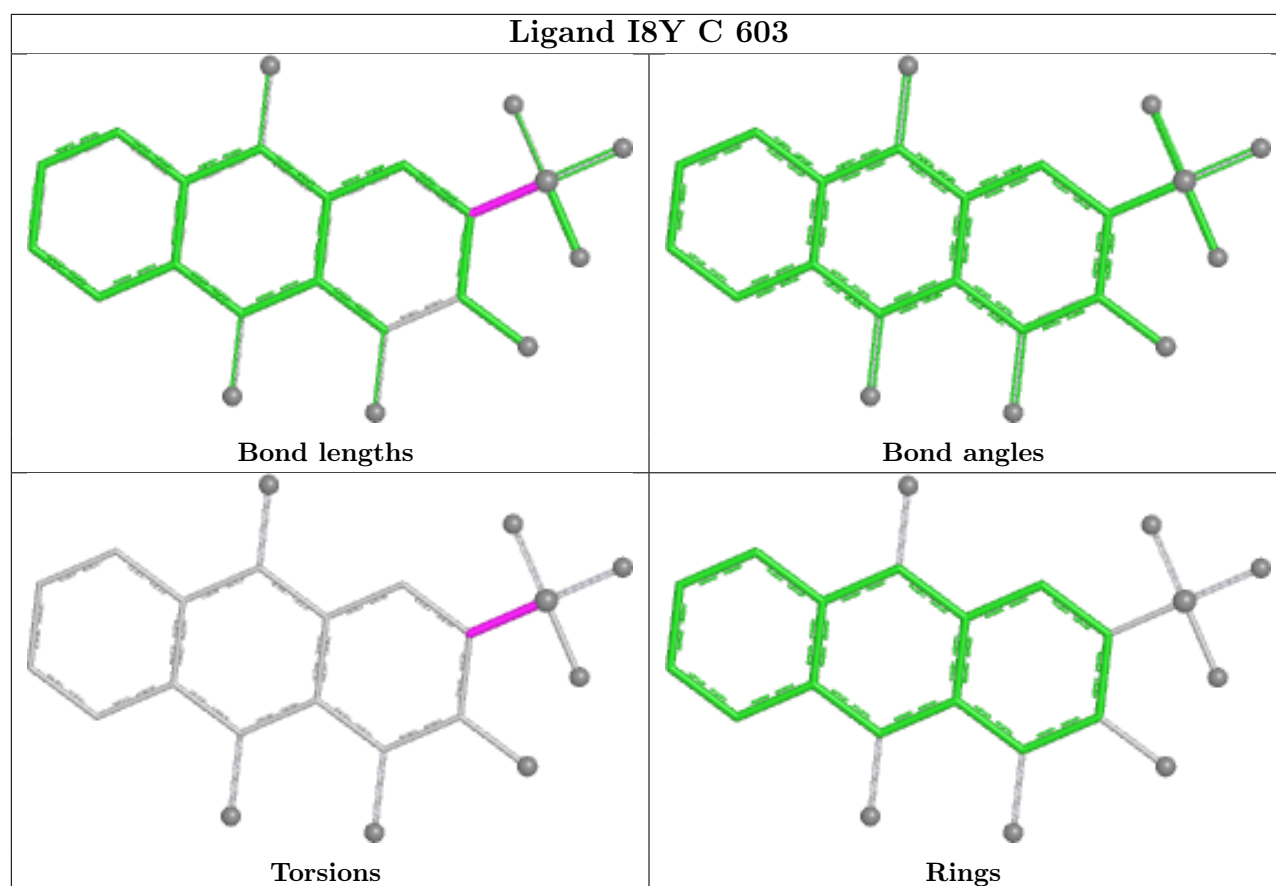
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	603	I8Y	1	0
6	C	603	I8Y	1	0
2	A	601	FBP	2	0
6	G	603	I8Y	1	0
2	E	601	FBP	1	0

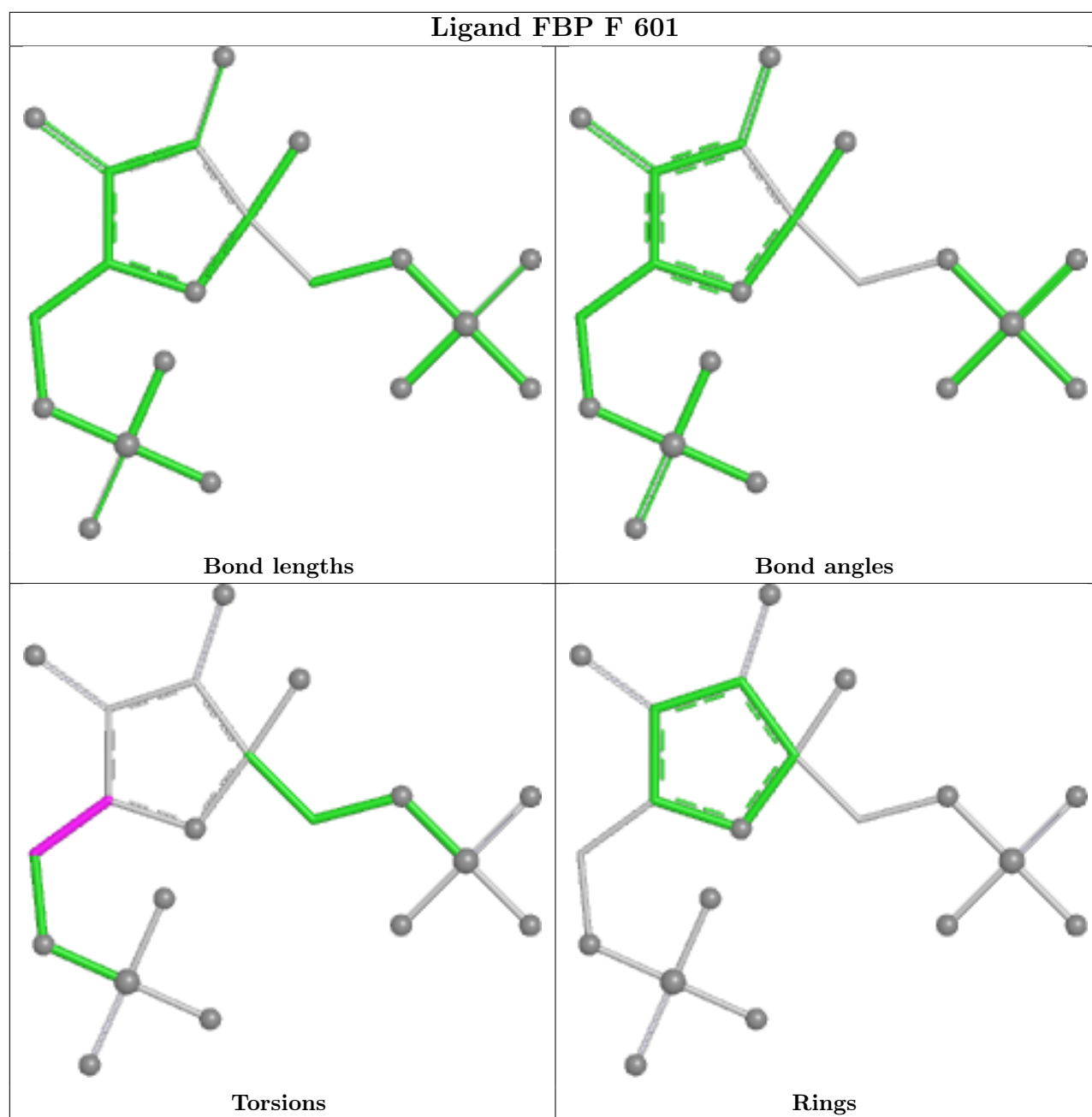
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

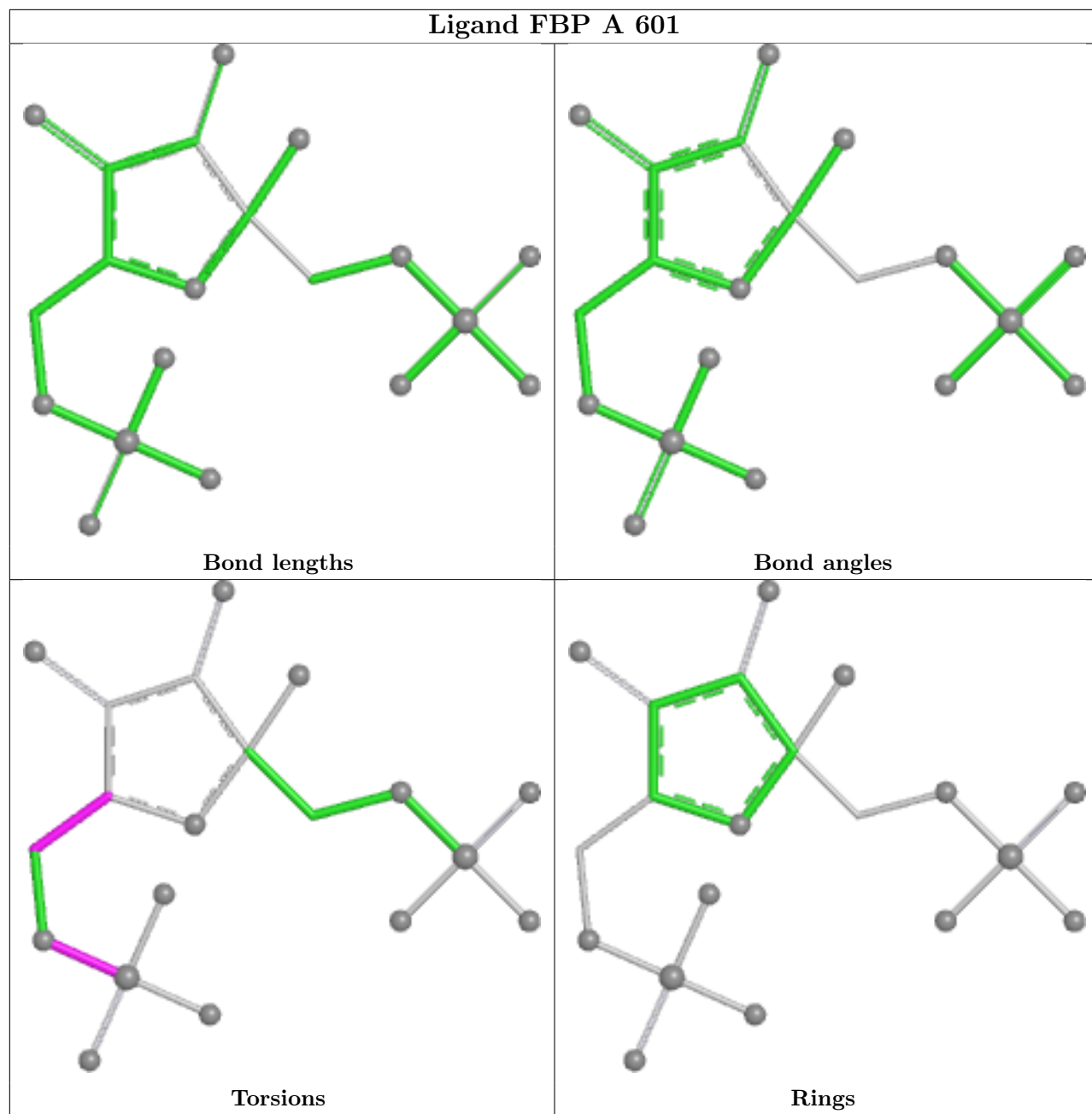


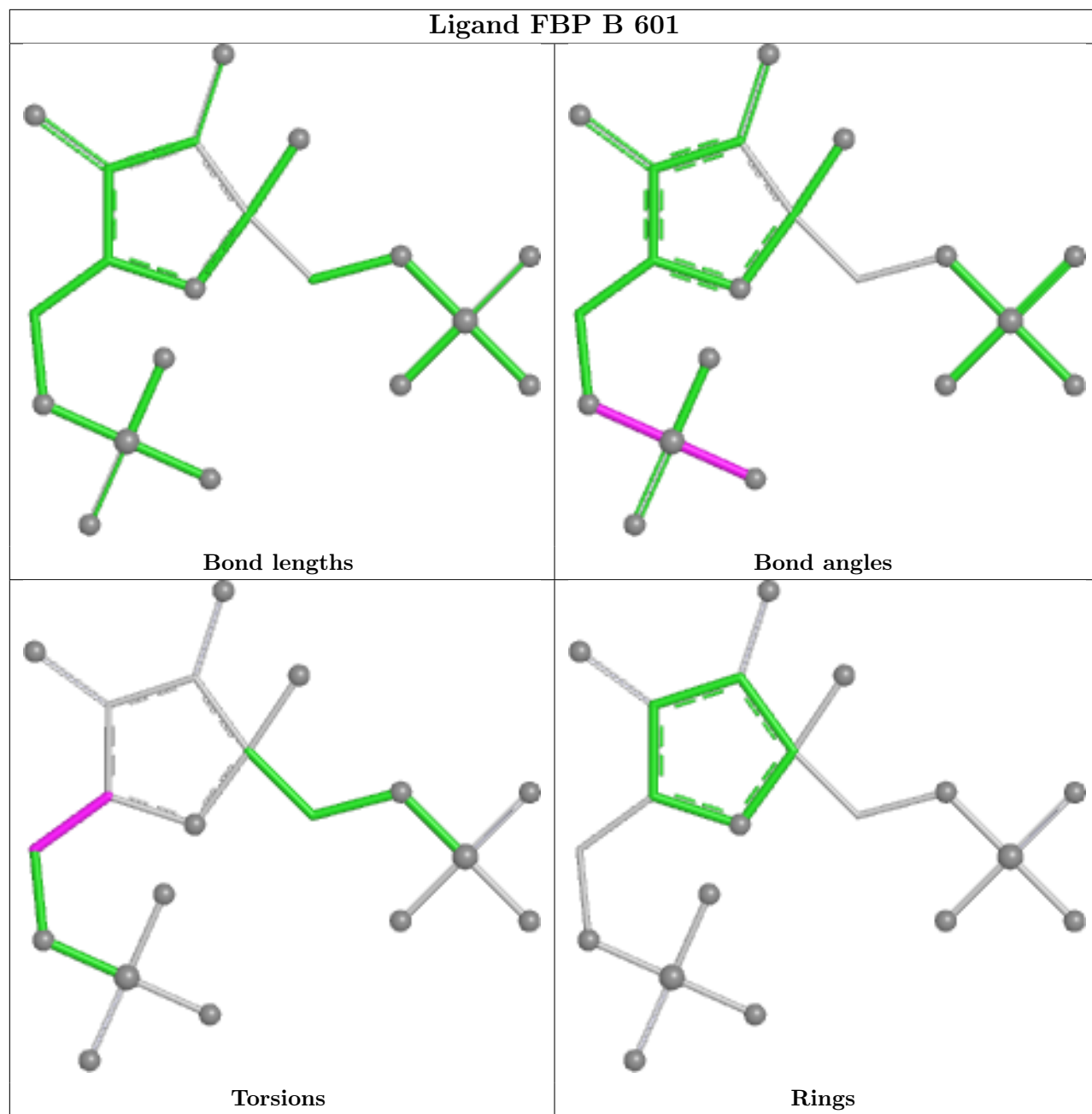


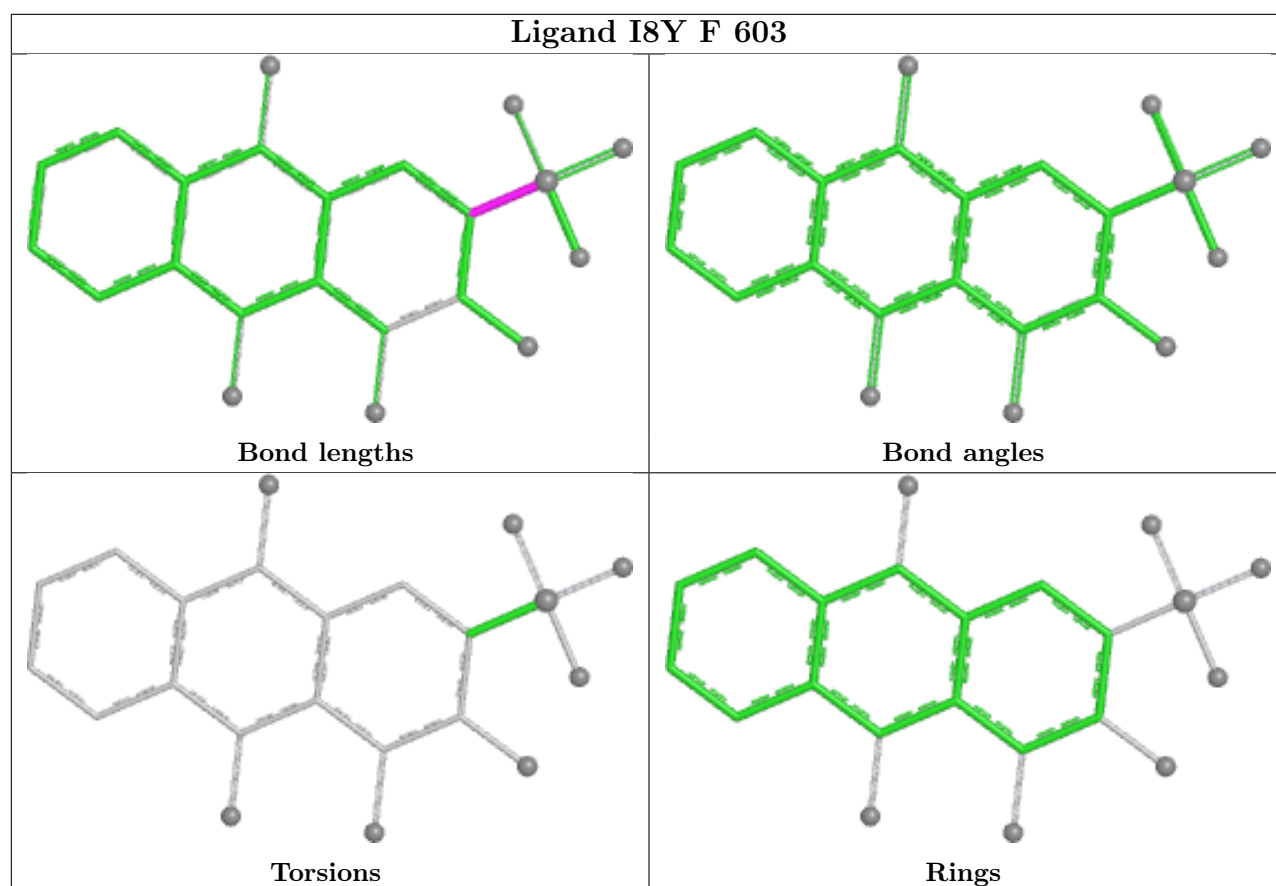


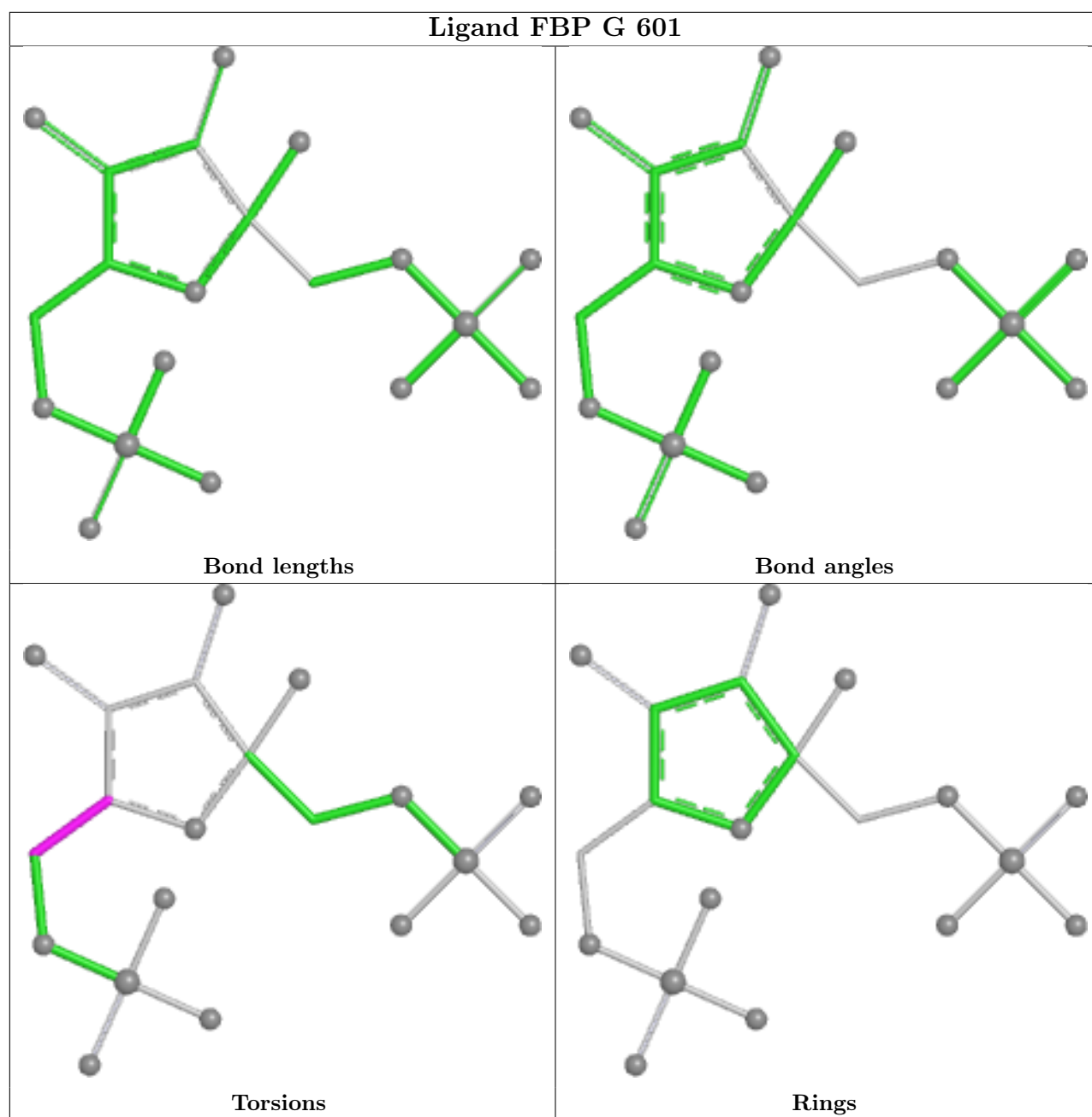


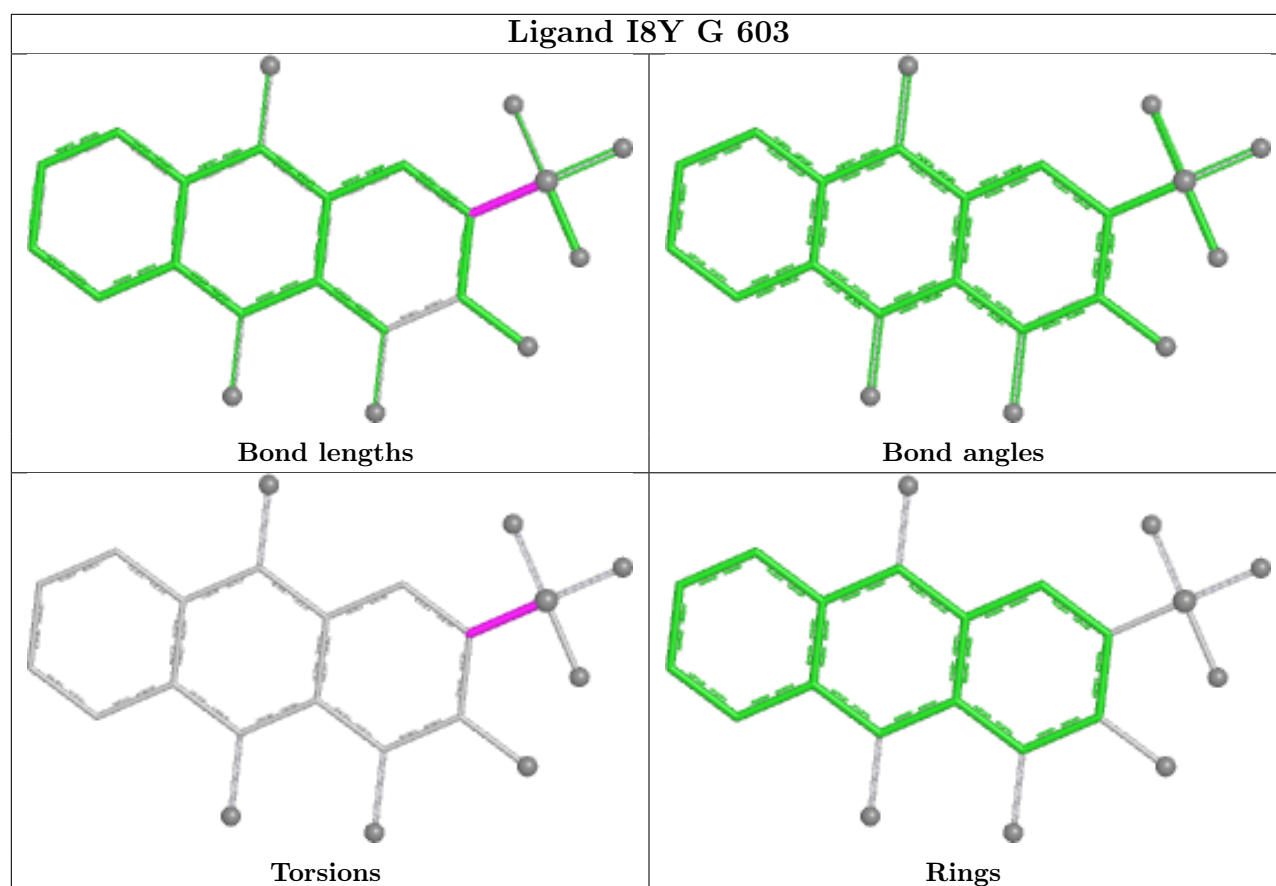


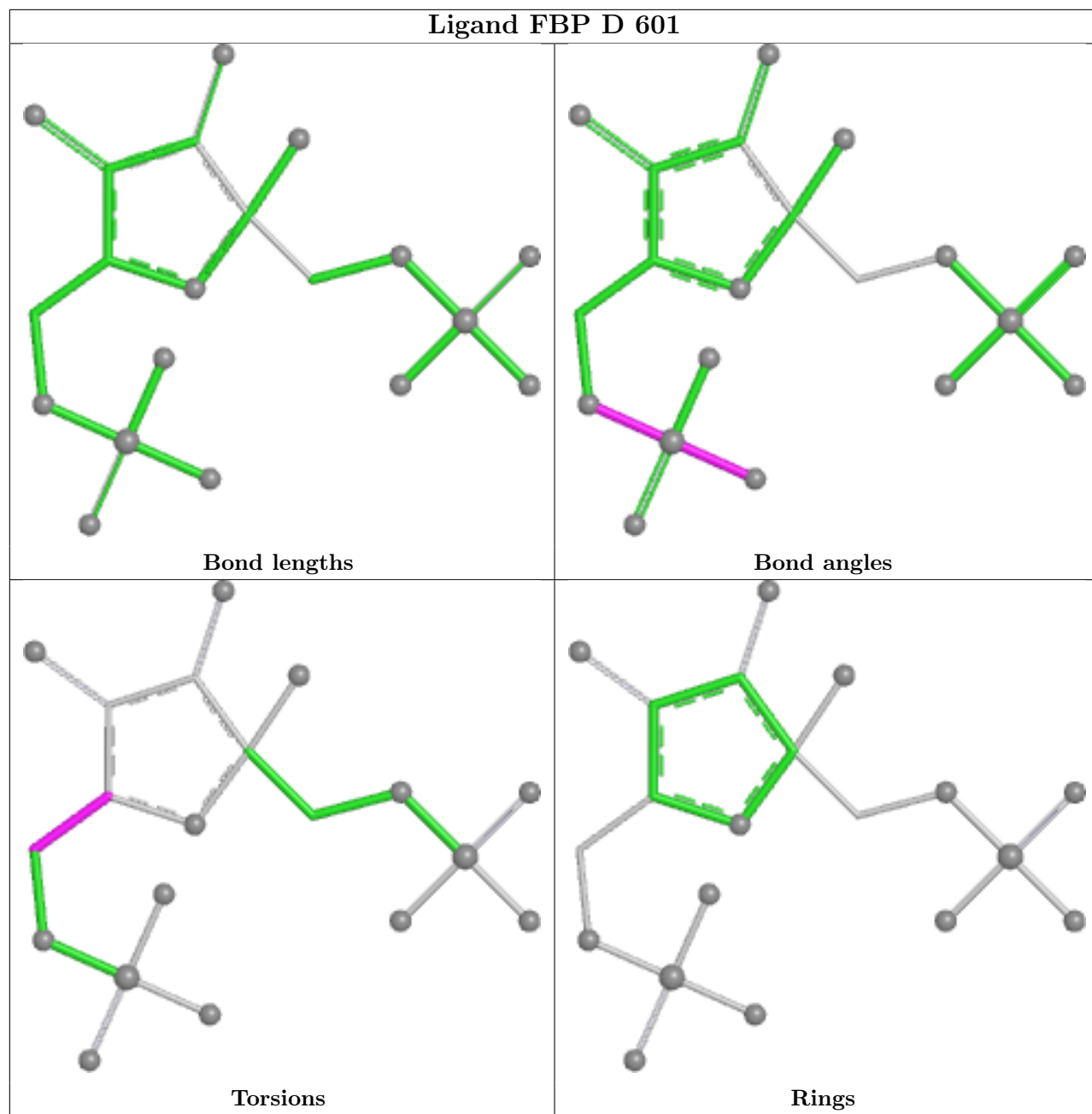


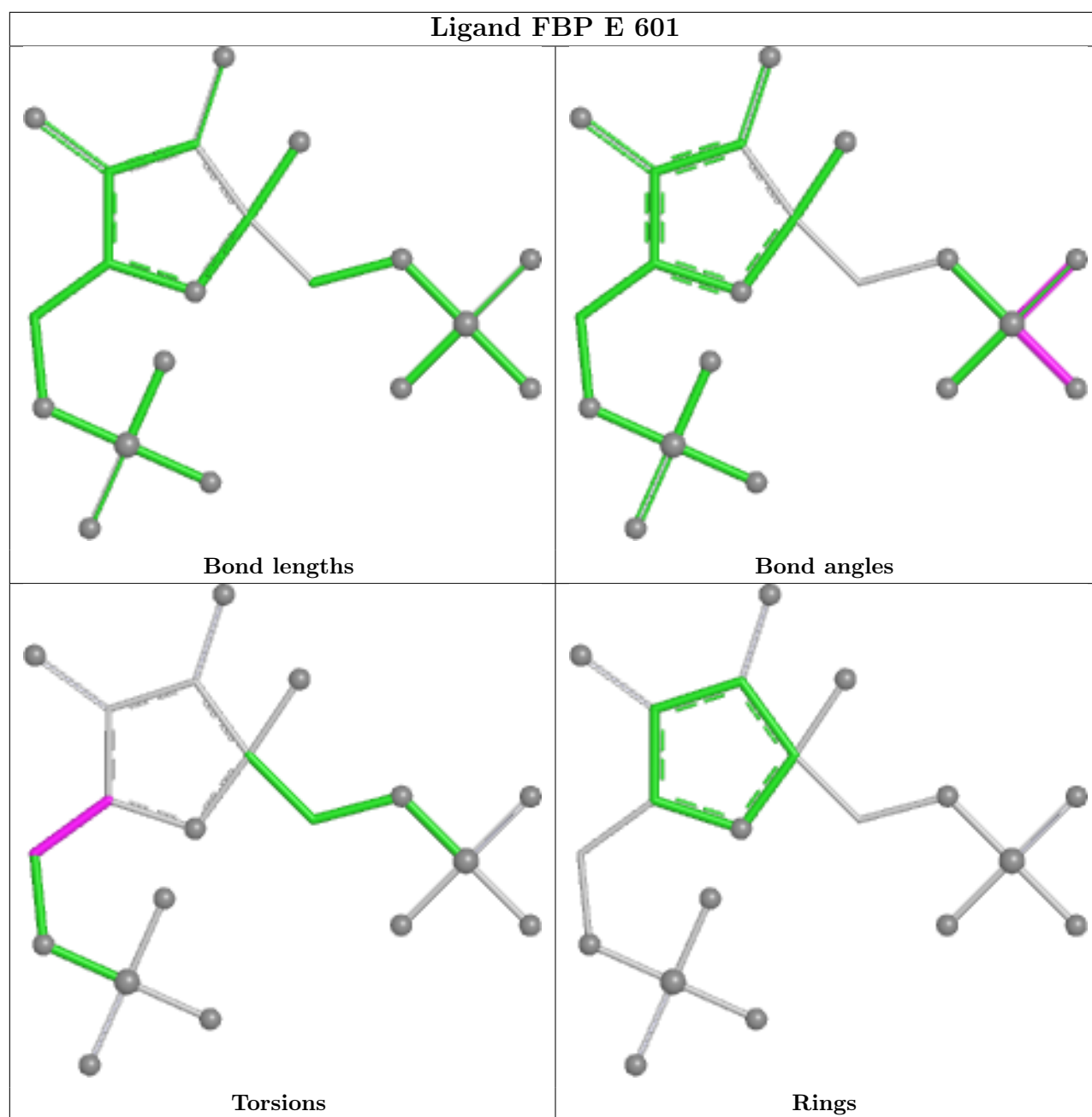












5.7 Other polymers [i](#)

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	418/447 (93%)	1.69	137 (32%) 1 1	37, 75, 106, 123	13 (3%)
1	B	436/447 (97%)	1.04	68 (15%) 5 6	31, 60, 92, 110	7 (1%)
1	C	424/447 (94%)	0.63	43 (10%) 12 14	27, 50, 81, 138	8 (1%)
1	D	425/447 (95%)	0.20	16 (3%) 44 49	21, 40, 70, 126	8 (1%)
1	E	420/447 (93%)	1.34	97 (23%) 2 2	30, 67, 100, 116	13 (3%)
1	F	434/447 (97%)	0.72	44 (10%) 12 14	30, 53, 84, 102	8 (1%)
1	G	422/447 (94%)	0.28	18 (4%) 40 45	21, 44, 69, 120	9 (2%)
1	H	425/447 (95%)	0.03	16 (3%) 44 49	17, 37, 66, 113	9 (2%)
All	All	3404/3576 (95%)	0.74	439 (12%) 7 9	17, 53, 93, 138	75 (2%)

The worst 5 of 439 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	21	GLY	6.9
1	C	20	LEU	6.9
1	D	25	PHE	6.8
1	A	543	SER	6.5
1	E	275[A]	HIS	6.3

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

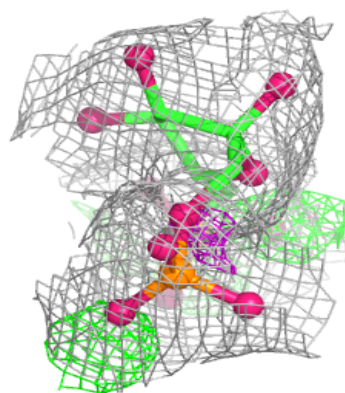
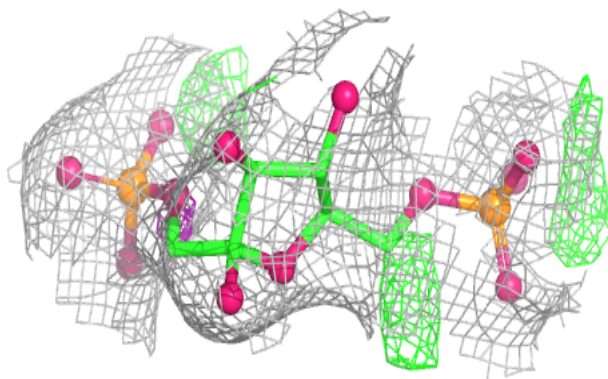
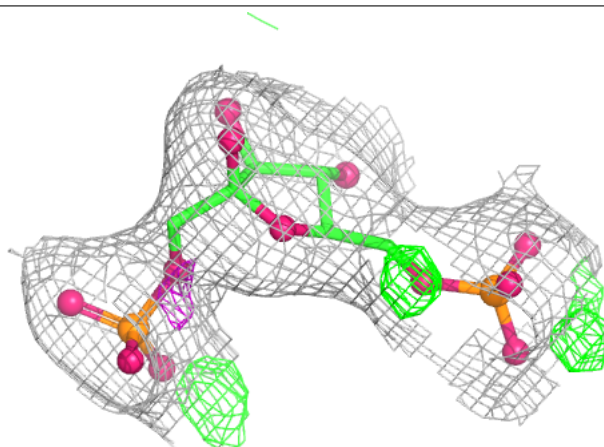
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	K	E	604	1/1	0.79	0.28	116,116,116,116	0
3	OXL	E	602	6/6	0.85	0.12	77,78,78,78	0
3	OXL	A	602	6/6	0.85	0.10	79,80,80,80	0
4	MG	A	603	1/1	0.86	0.08	90,90,90,90	0
5	K	A	604	1/1	0.87	0.12	121,121,121,121	0
2	FBP	A	601	20/20	0.87	0.12	73,74,75,75	0
6	I8Y	G	603	22/22	0.87	0.13	72,74,75,76	9
3	OXL	B	602	6/6	0.89	0.10	58,59,61,62	0
6	I8Y	B	603	22/22	0.90	0.12	96,98,98,98	9
5	K	B	605	1/1	0.90	0.10	97,97,97,97	0
6	I8Y	C	603	22/22	0.91	0.10	86,87,87,88	9
5	K	F	605	1/1	0.91	0.07	87,87,87,87	0
6	I8Y	F	603	22/22	0.92	0.09	68,69,69,70	9
2	FBP	F	601	20/20	0.92	0.09	54,59,63,63	0
3	OXL	C	602	6/6	0.93	0.08	62,62,63,63	0
5	K	C	605	1/1	0.93	0.11	78,78,78,78	0
4	MG	E	603	1/1	0.93	0.13	76,76,76,76	0
2	FBP	E	601	20/20	0.93	0.08	63,64,65,65	0
2	FBP	B	601	20/20	0.94	0.09	66,69,71,71	0
3	OXL	F	602	6/6	0.94	0.09	65,66,67,68	0
4	MG	F	604	1/1	0.94	0.10	60,60,60,60	0
3	OXL	G	602	6/6	0.94	0.08	49,50,51,51	0
4	MG	H	603	1/1	0.95	0.11	45,45,45,45	0
5	K	G	605	1/1	0.95	0.16	68,68,68,68	0
3	OXL	D	602	6/6	0.96	0.07	51,52,53,54	0
3	OXL	H	602	6/6	0.96	0.07	40,41,42,42	0
4	MG	B	604	1/1	0.97	0.06	53,53,53,53	0
2	FBP	H	601	20/20	0.98	0.05	30,32,34,34	0
4	MG	G	604	1/1	0.98	0.06	41,41,41,41	0
5	K	D	604	1/1	0.98	0.10	62,62,62,62	0
2	FBP	C	601	20/20	0.98	0.05	34,35,38,38	0
2	FBP	D	601	20/20	0.98	0.04	33,35,38,38	0
2	FBP	G	601	20/20	0.99	0.04	30,32,33,34	0
5	K	H	604	1/1	0.99	0.11	62,62,62,62	0
4	MG	D	603	1/1	0.99	0.03	46,46,46,46	0
4	MG	C	604	1/1	1.00	0.04	53,53,53,53	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.

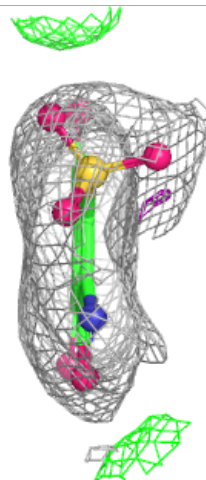
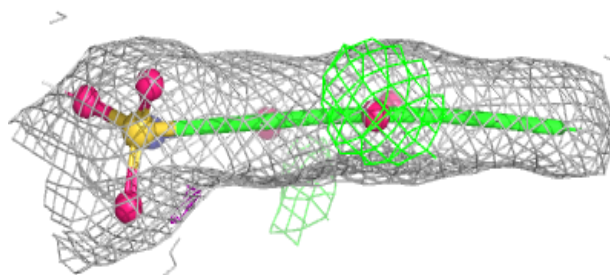
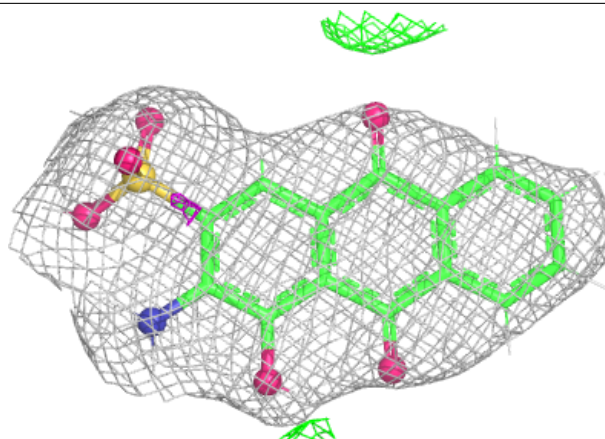
Electron density around FBP A 601:

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



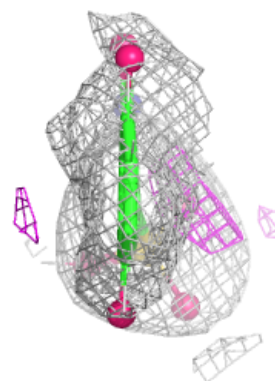
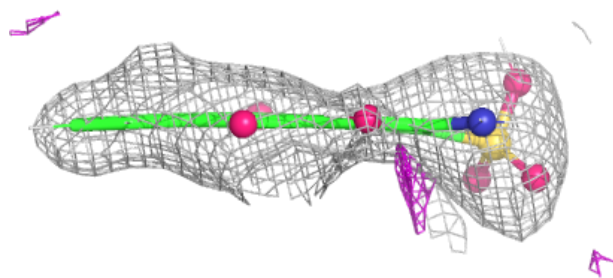
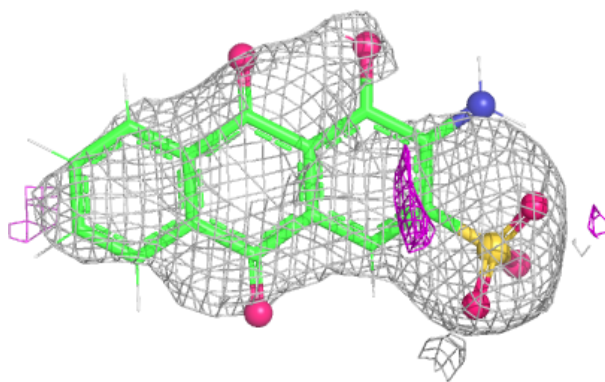
Electron density around I8Y G 603:

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



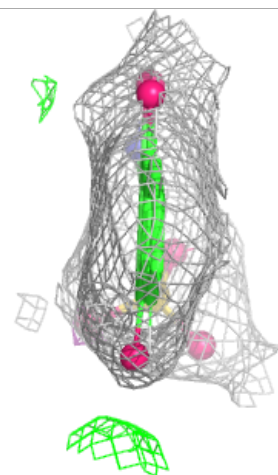
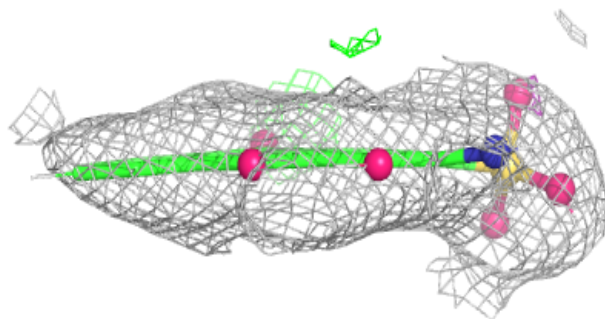
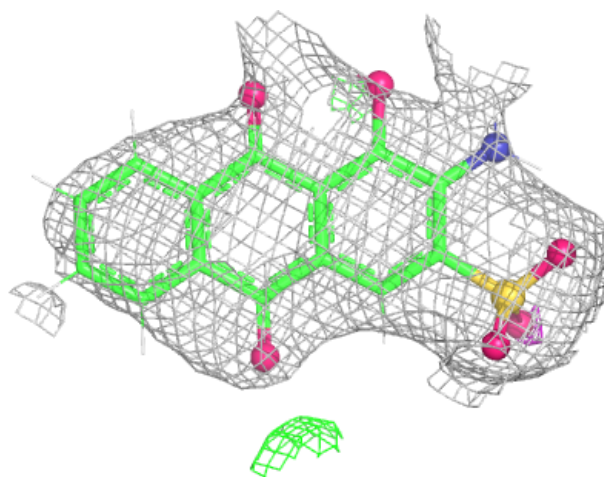
Electron density around I8Y B 603:

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



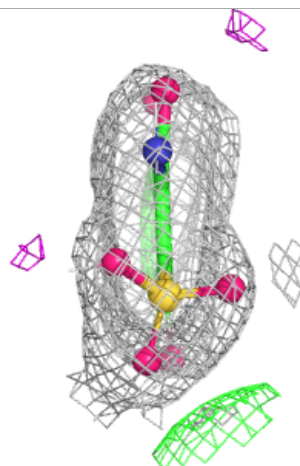
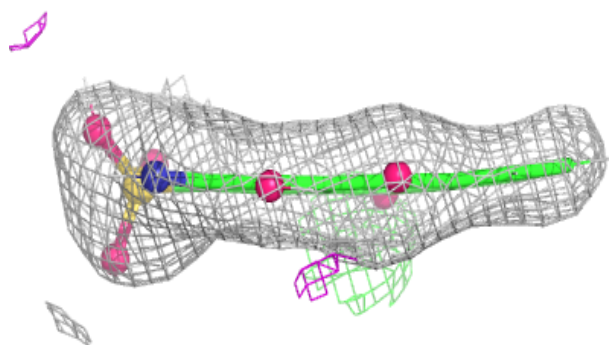
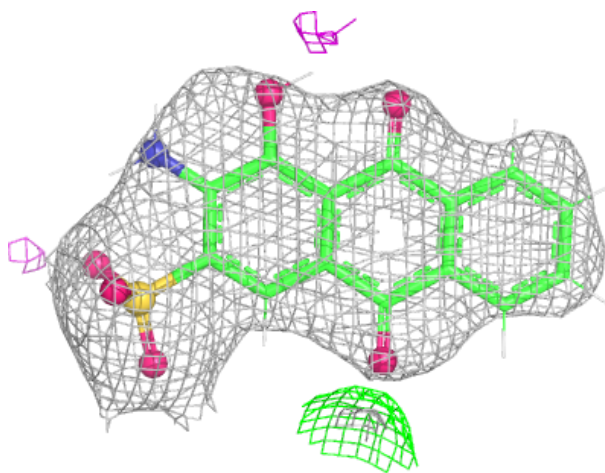
Electron density around I8Y C 603:

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



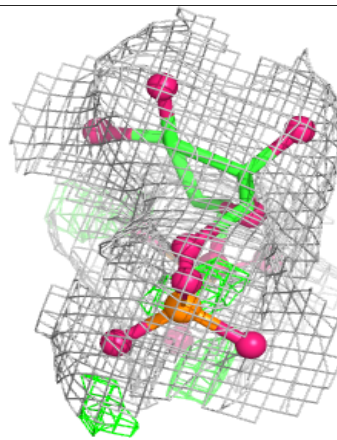
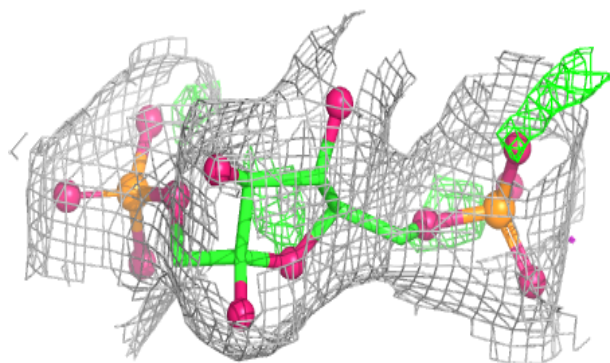
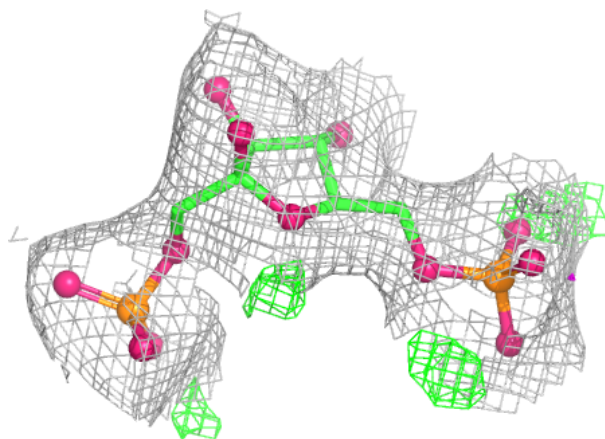
Electron density around I8Y F 603:

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



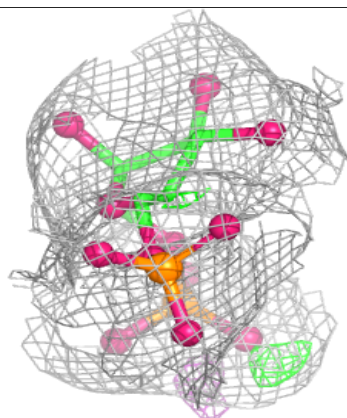
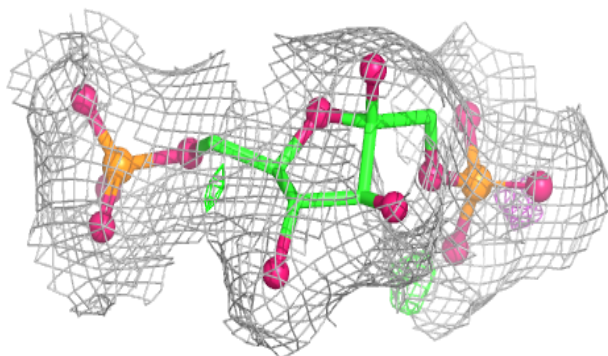
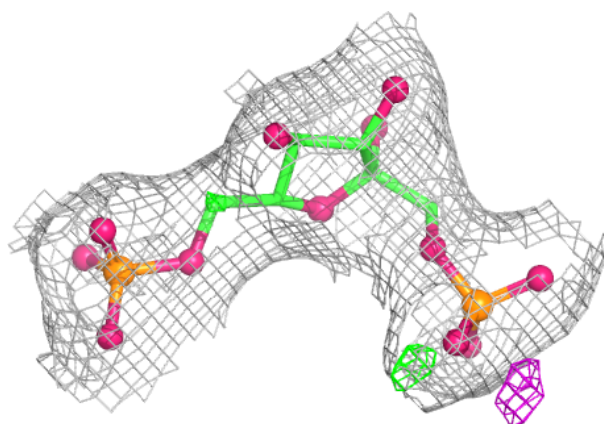
Electron density around FBP F 601:

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

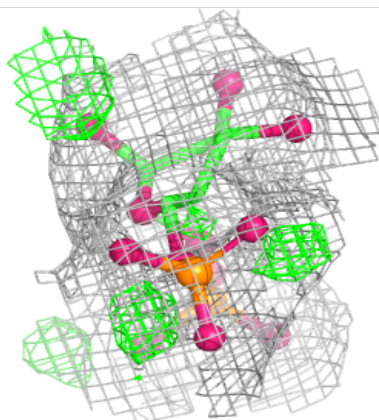
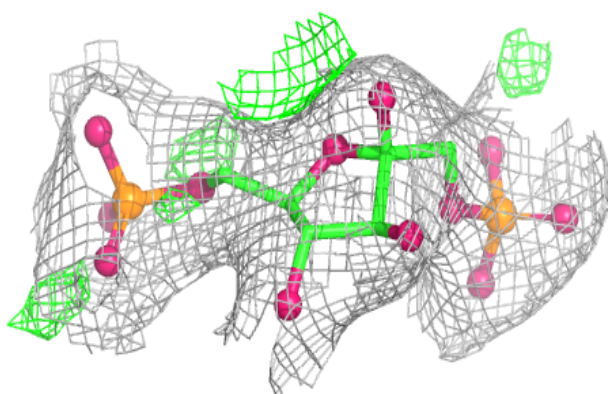
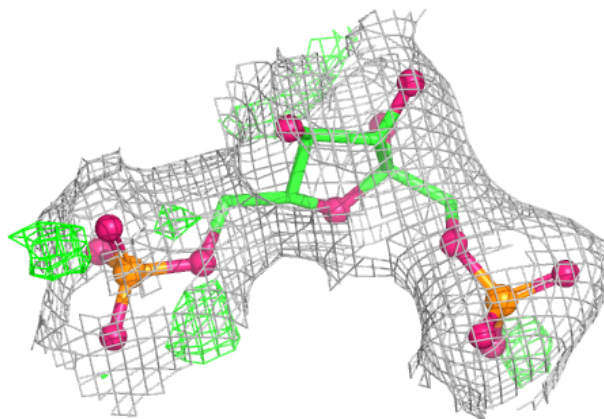


Electron density around FBP E 601:

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

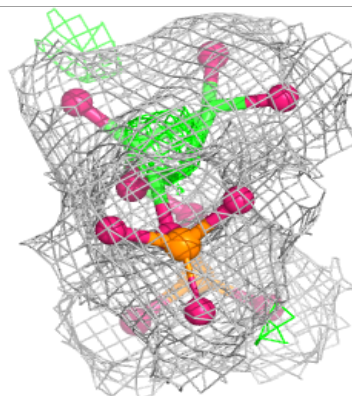
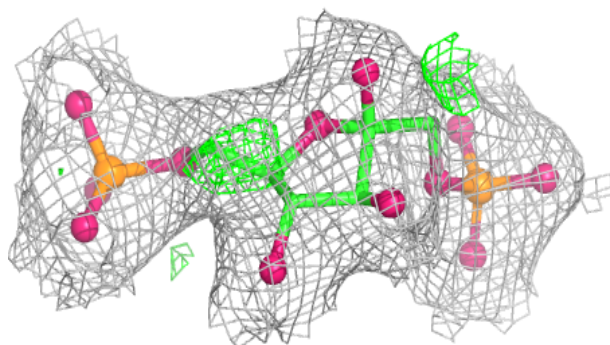
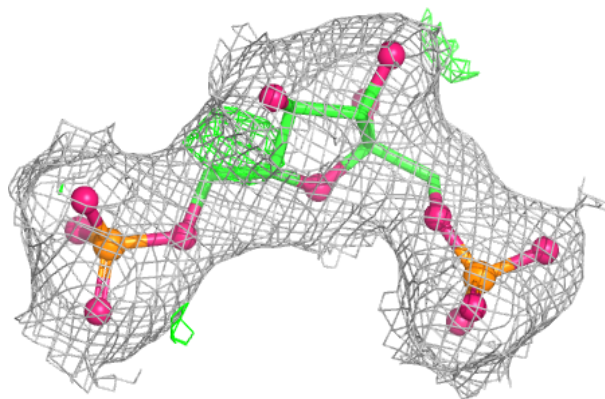
**Electron density around FBP B 601:**

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

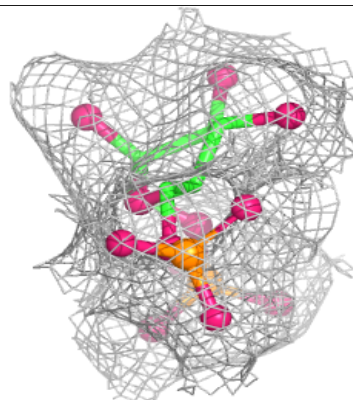
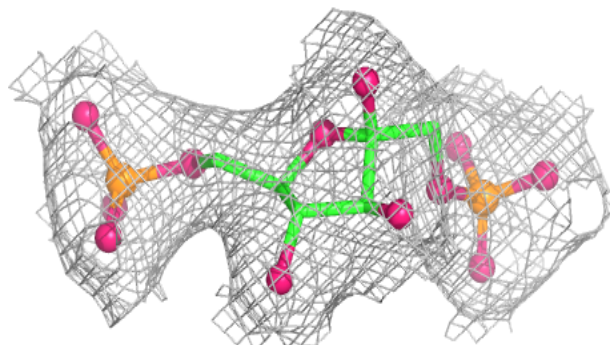
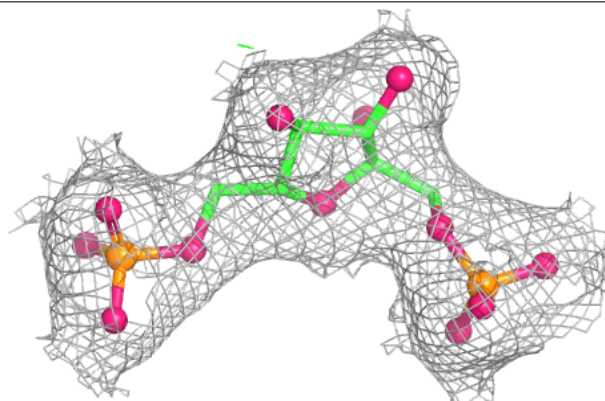


Electron density around FBP H 601:

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

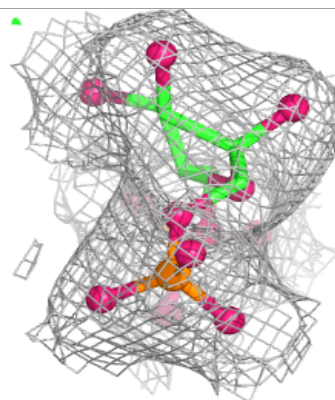
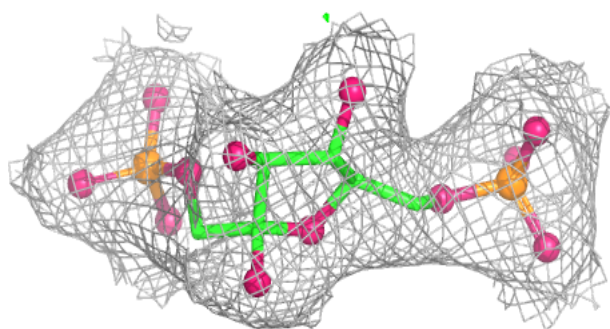
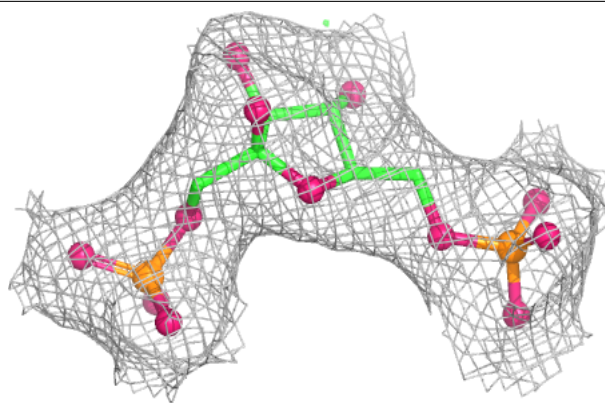
**Electron density around FBP C 601:**

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

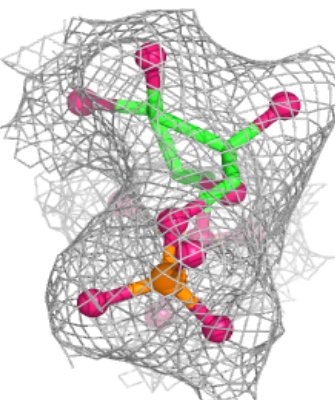
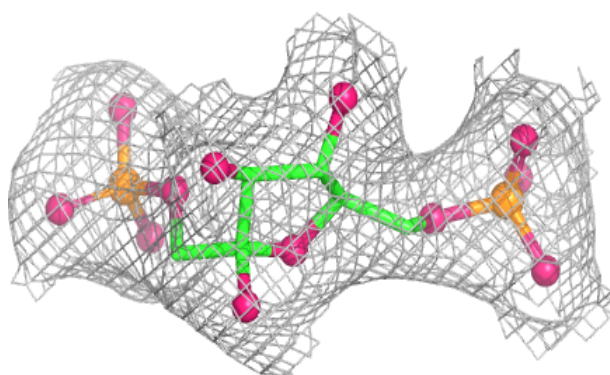
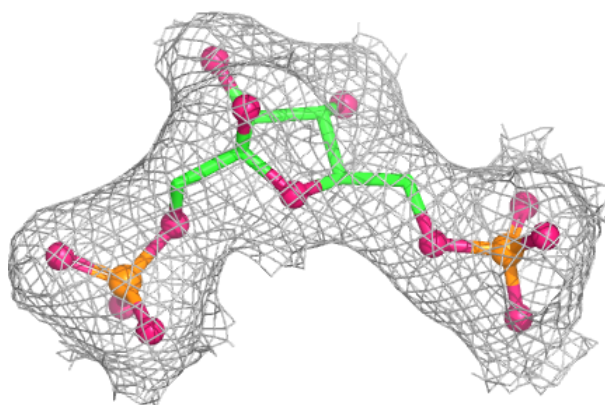


Electron density around FBP D 601:

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

**Electron density around FBP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.