



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 01:43 PM EDT

PDB ID : 5SCG / pdb\_00005scg  
Title : Structure of liver pyruvate kinase in complex with anthraquinone derivative  
101  
Authors : Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.  
Deposited on : 2021-12-01  
Resolution : 1.94 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](mailto: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>.

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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)  
Xtrriage (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

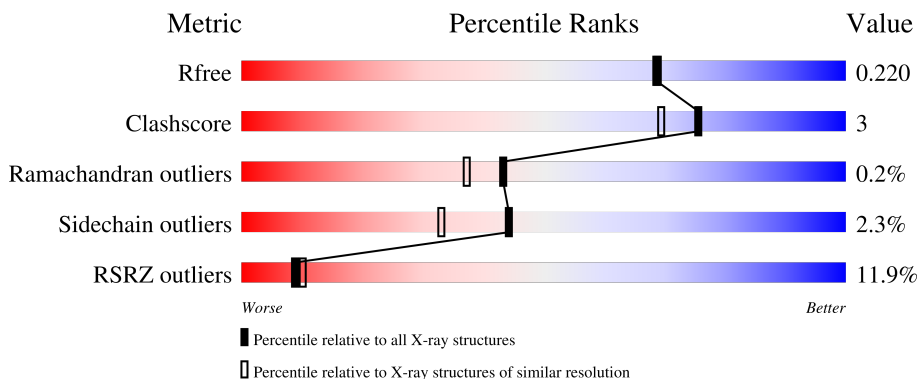
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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  $\geq 3$ , 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	
1	B	447	
1	C	447	
1	D	447	
1	E	447	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	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 [i](#)

There are 7 unique types of molecules in this entry. The entry contains 29025 atoms, of which 102 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
			Total	C	N	O	S			
1	A	418	3238	2033	581	604	20	0	13	0
1	B	436	3350	2104	604	622	20	3	8	0
1	C	424	3260	2051	584	606	19	0	7	0
1	D	425	3261	2048	590	604	19	0	8	0
1	E	419	3257	2049	584	604	20	0	13	0
1	F	432	3327	2094	597	616	20	0	8	0
1	G	422	3257	2048	586	604	19	0	9	0
1	H	425	3277	2057	597	604	19	0	9	0

There are 48 discrepancies between the modelled and reference sequences:

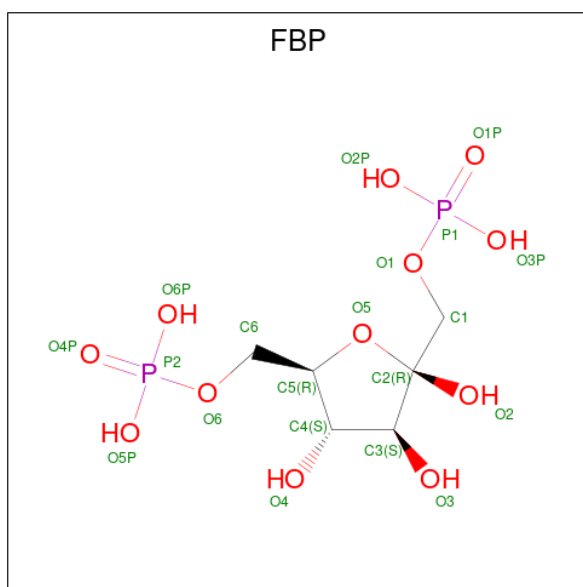
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	230	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression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

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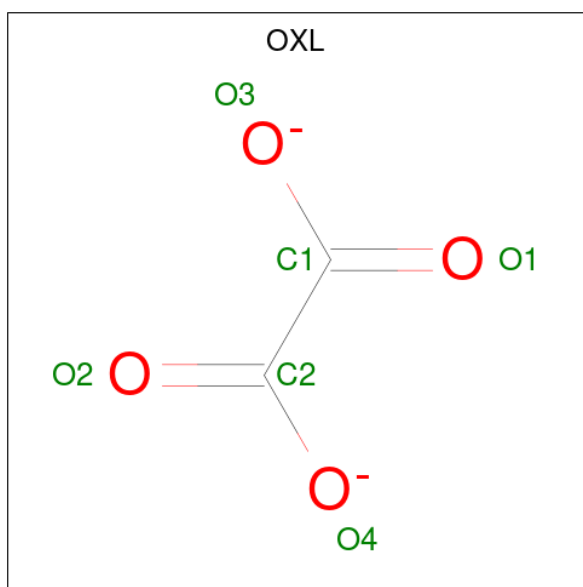
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	228	GLY	-	linker	UNP Q16716
C	229	SER	-	linker	UNP Q16716
C	230	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict	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	228	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	228	GLY	-	linker	UNP Q16716
F	229	SER	-	linker	UNP Q16716
F	230	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:  $C_6H_{14}O_{12}P_2$ ).



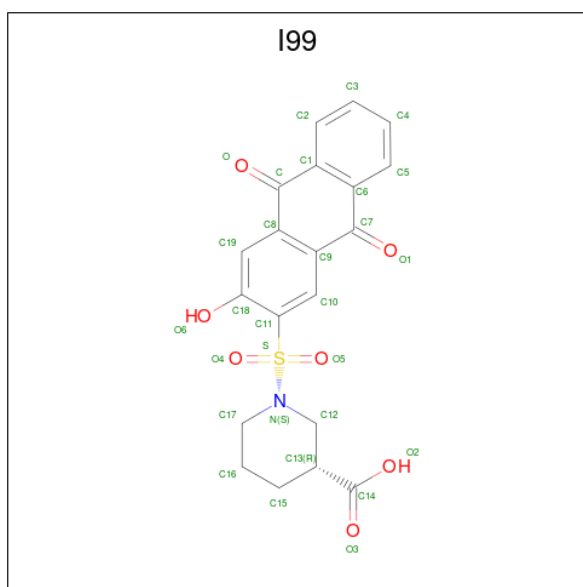
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	20	6	12	2	0	0
2	B	1	20	6	12	2	0	0
2	C	1	20	6	12	2	0	0
2	D	1	20	6	12	2	0	0
2	E	1	20	6	12	2	0	0
2	F	1	20	6	12	2	0	0
2	G	1	20	6	12	2	0	0
2	H	1	20	6	12	2	0	0

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C<sub>2</sub>O<sub>4</sub>).



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

- Molecule 4 is (3R)-1-(3-hydroxy-9,10-dioxo-9,10-dihydroanthracene-2-sulfonyl)piperidine-3-carboxylic acid (CCD ID: I99) (formula: C<sub>20</sub>H<sub>17</sub>NO<sub>7</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
4	A	1	Total	C	H	N	O	S	17	0
			46	20	17	1	7	1		
4	B	1	Total	C	H	N	O	S	17	0
			46	20	17	1	7	1		
4	C	1	Total	C	H	N	O	S	17	0
			46	20	17	1	7	1		
4	E	1	Total	C	H	N	O	S	17	0
			46	20	17	1	7	1		
4	F	1	Total	C	H	N	O	S	17	0
			46	20	17	1	7	1		
4	G	1	Total	C	H	N	O	S	17	0
			46	20	17	1	7	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	206	Total O 206 206	0	0
7	B	186	Total O 186 186	0	0
7	C	319	Total O 319 319	0	0
7	D	367	Total O 367 367	0	0
7	E	208	Total O 208 208	0	0
7	F	273	Total O 273 273	0	0
7	G	347	Total O 347 347	0	0

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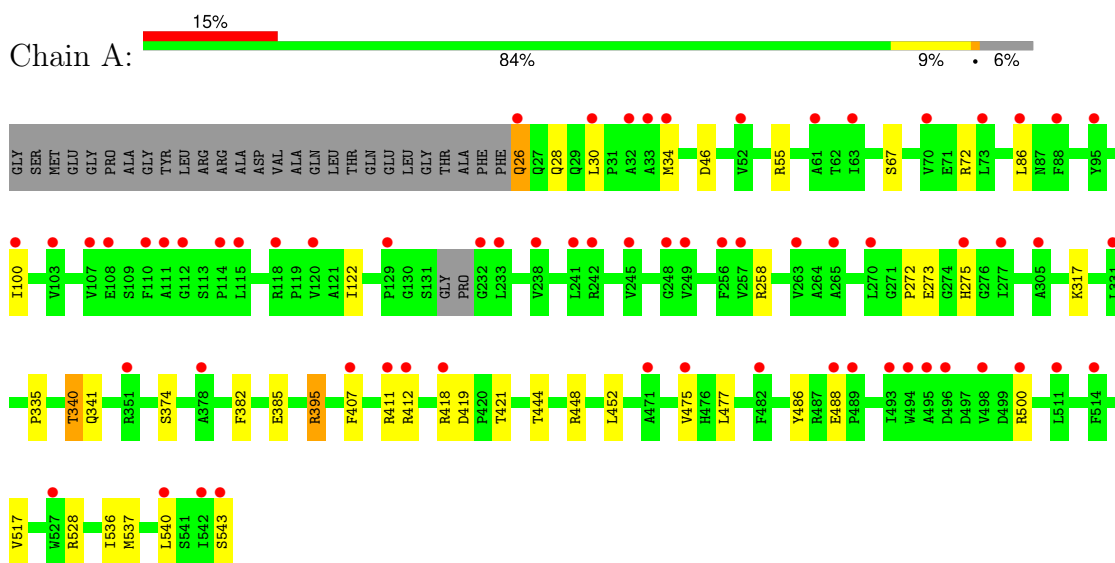
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	H	392	Total 392	O 392	0	0

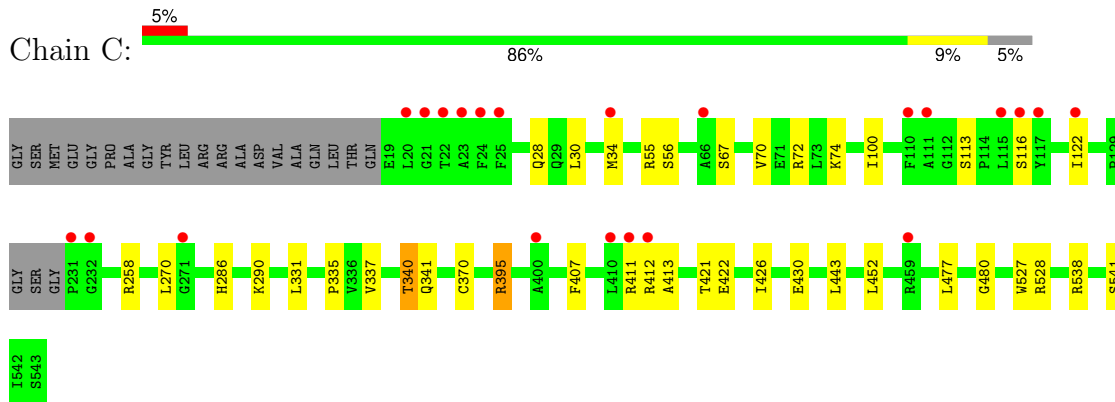
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

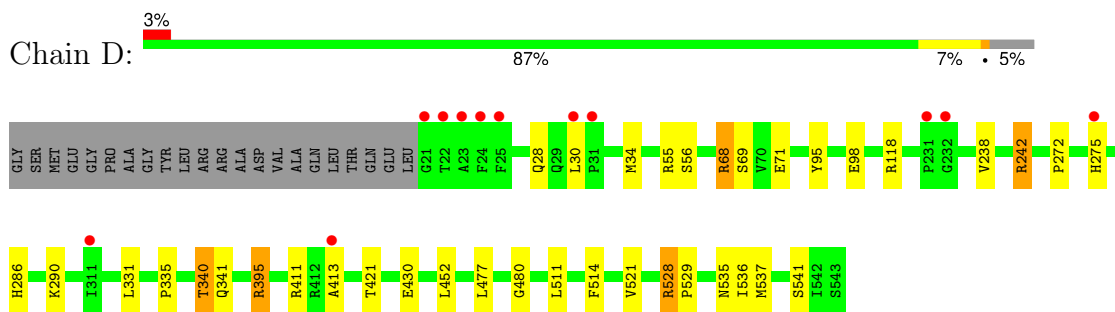
- Molecule 1: Pyruvate kinase



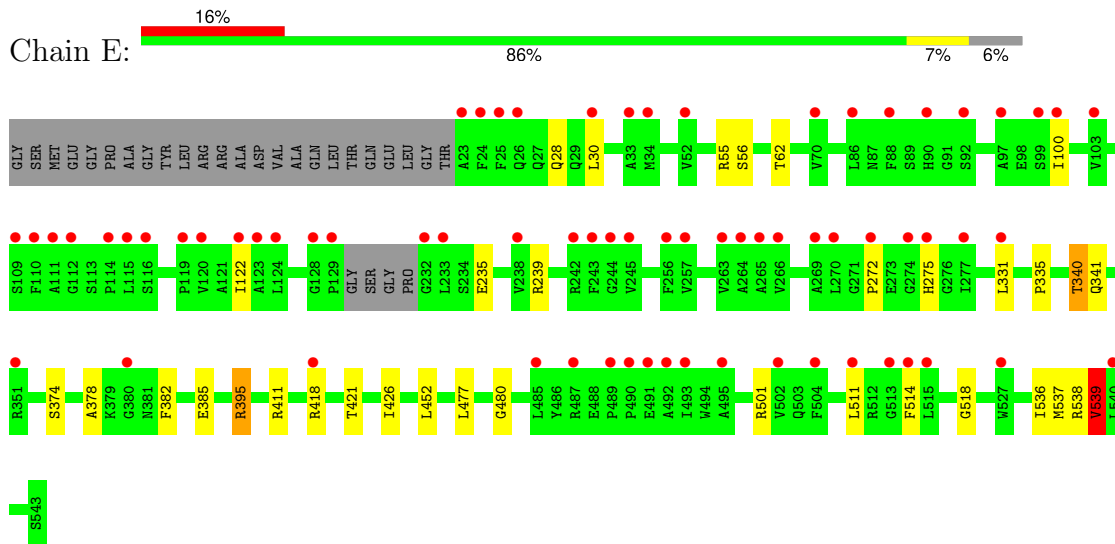
- Molecule 1: Pyruvate kinase



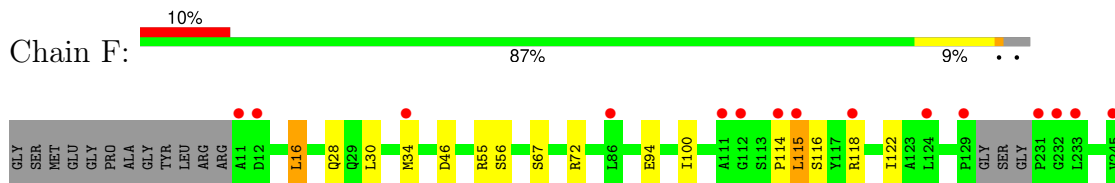
- Molecule 1: Pyruvate kinase

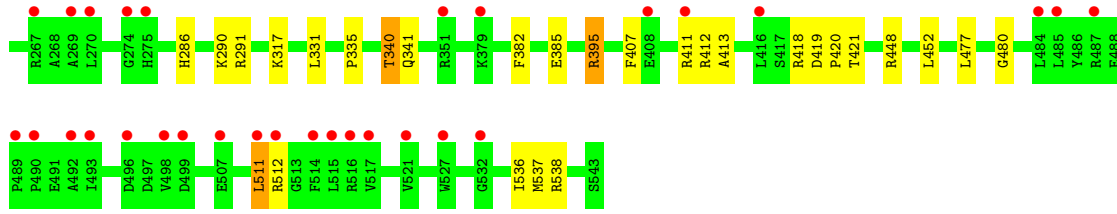


- Molecule 1: Pyruvate kinase

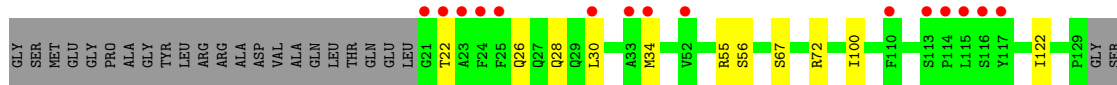
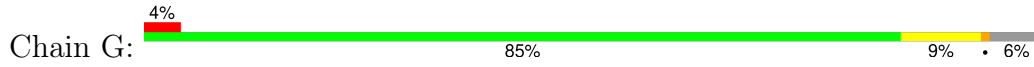


- Molecule 1: Pyruvate kinase

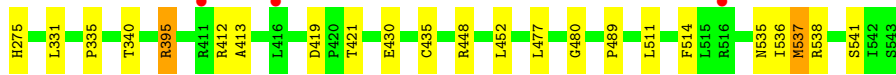
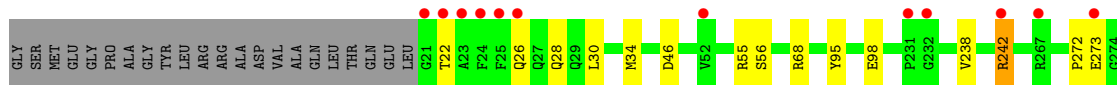
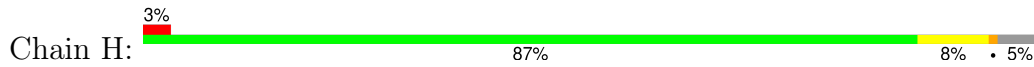




● Molecule 1: Pyruvate kinase



● Molecule 1: Pyruvate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.97Å 113.10Å 188.63Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	188.54 – 1.94 188.54 – 1.94	Depositor EDS
% Data completeness (in resolution range)	77.3 (188.54-1.94) 77.3 (188.54-1.94)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 1.94Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, $R_{free}$	0.200 , 0.229 0.192 , 0.220	Depositor DCC
$R_{free}$ test set	12493 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtrriage
Anisotropy	0.009	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	29025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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 39.99 % 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 2.9250e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: I99, MG, FBP, OXL, K

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	0.69	1/3328 (0.0%)	1.00	3/4497 (0.1%)
1	B	0.72	0/3429	1.00	1/4636 (0.0%)
1	C	0.77	0/3335	1.01	0/4508
1	D	0.80	0/3341	1.03	1/4517 (0.0%)
1	E	0.67	1/3350 (0.0%)	0.99	2/4527 (0.0%)
1	F	0.71	0/3405	1.00	1/4603 (0.0%)
1	G	0.79	2/3335 (0.1%)	1.00	2/4507 (0.0%)
1	H	0.79	1/3357 (0.0%)	1.00	2/4537 (0.0%)
All	All	0.74	5/26880 (0.0%)	1.00	12/36332 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	489	PRO	CA-C	5.51	1.55	1.52
1	G	303	MET	SD-CE	-5.50	1.65	1.79
1	A	374	SER	CA-C	5.46	1.55	1.52
1	G	489	PRO	CA-C	5.15	1.54	1.51
1	E	374	SER	CA-C	5.01	1.54	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	G	273	GLU	CB-CG-CD	7.06	124.60	112.60
1	E	539	VAL	N-CA-CB	5.77	117.96	111.21
1	G	514	PHE	CA-CB-CG	5.71	119.51	113.80
1	H	46	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	26	GLN	CA-C-N	5.50	130.74	120.95

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	19	0
1	B	3350	0	3417	23	0
1	C	3260	0	3320	24	0
1	D	3261	0	3321	22	0
1	E	3257	0	3323	19	0
1	F	3327	0	3399	24	0
1	G	3257	0	3320	27	0
1	H	3277	0	3341	22	0
2	A	20	0	10	1	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	29	17	0	0	0
4	B	29	17	0	0	0
4	C	29	17	0	0	0
4	E	29	17	0	0	0
4	F	29	17	0	0	0
4	G	29	17	0	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
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	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
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	206	0	0	1	0
7	B	186	0	0	0	0
7	C	319	0	0	1	0
7	D	367	0	0	0	0
7	E	208	0	0	0	0
7	F	273	0	0	1	0
7	G	347	0	0	3	0
7	H	392	0	0	0	0
All	All	28923	102	26833	162	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 162 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:C:411:ARG:HG2	1:C:426:ILE:HD11	1.66	0.76
1:H:68:ARG:NH2	1:H:95:TYR:O	2.19	0.75
1:E:418[B]:ARG:HG3	1:F:16:LEU:HD11	1.69	0.74
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.71	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	37
1	B	442/447 (99%)	434 (98%)	7 (2%)	1 (0%)	43	37
1	C	427/447 (96%)	420 (98%)	6 (1%)	1 (0%)	43	37
1	D	431/447 (96%)	427 (99%)	3 (1%)	1 (0%)	43	37
1	E	428/447 (96%)	424 (99%)	3 (1%)	1 (0%)	43	37
1	F	436/447 (98%)	432 (99%)	3 (1%)	1 (0%)	43	37
1	G	427/447 (96%)	419 (98%)	7 (2%)	1 (0%)	43	37
1	H	432/447 (97%)	426 (99%)	5 (1%)	1 (0%)	43	37
All	All	3450/3576 (96%)	3404 (99%)	38 (1%)	8 (0%)	43	37

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	E	340	THR

### 5.3.2 Protein sidechains [i](#)

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%)	333 (96%)	12 (4%)	32	18
1	B	353/352 (100%)	345 (98%)	8 (2%)	44	33
1	C	344/352 (98%)	334 (97%)	10 (3%)	37	24
1	D	344/352 (98%)	332 (96%)	12 (4%)	32	18
1	E	346/352 (98%)	340 (98%)	6 (2%)	53	44
1	F	351/352 (100%)	342 (97%)	9 (3%)	40	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	344/352 (98%)	338 (98%)	6 (2%)	53	44
1	H	345/352 (98%)	337 (98%)	8 (2%)	44	33
All	All	2772/2816 (98%)	2701 (97%)	71 (3%)	44	28

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	273	GLU
1	G	412	ARG
1	H	273	GLU
1	C	270[A]	LEU
1	C	258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	535	ASN
1	E	27	GLN
1	H	405	GLN
1	F	405	GLN
1	G	405	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 16 are monoatomic - leaving 22 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	I99	B	603	-	32,32,32	0.18	0	48,49,49	0.39	0
3	OXL	B	602	5	5,5,5	2.32	2 (40%)	6,6,6	1.34	1 (16%)
2	FBP	F	601	-	18,20,20	0.48	0	21,32,32	0.70	0
3	OXL	E	602	5	5,5,5	2.36	2 (40%)	6,6,6	1.43	2 (33%)
2	FBP	D	601	-	18,20,20	0.59	0	21,32,32	1.03	1 (4%)
3	OXL	D	602	5	5,5,5	2.09	2 (40%)	6,6,6	2.10	2 (33%)
3	OXL	C	602	5	5,5,5	1.81	2 (40%)	6,6,6	1.43	1 (16%)
2	FBP	B	601	-	18,20,20	0.74	0	21,32,32	0.93	2 (9%)
2	FBP	H	601	-	18,20,20	0.94	0	21,32,32	0.87	1 (4%)
3	OXL	H	602	5	5,5,5	1.79	2 (40%)	6,6,6	1.87	2 (33%)
4	I99	E	603	-	32,32,32	0.19	0	48,49,49	0.40	0
3	OXL	G	602	5	5,5,5	2.12	3 (60%)	6,6,6	2.68	3 (50%)
2	FBP	E	601	-	18,20,20	0.50	0	21,32,32	0.73	1 (4%)
2	FBP	C	601	-	18,20,20	0.68	0	21,32,32	0.79	0
2	FBP	G	601	-	18,20,20	0.67	1 (5%)	21,32,32	0.78	0
2	FBP	A	601	-	18,20,20	0.41	0	21,32,32	0.83	0
4	I99	C	603	-	32,32,32	0.29	0	48,49,49	0.50	0
4	I99	G	603	-	32,32,32	0.23	0	48,49,49	0.81	2 (4%)
4	I99	F	603	-	32,32,32	0.22	0	48,49,49	0.46	0
4	I99	A	603	-	32,32,32	0.19	0	48,49,49	0.40	0
3	OXL	A	602	5	5,5,5	1.93	2 (40%)	6,6,6	2.21	3 (50%)
3	OXL	F	602	5	5,5,5	2.88	4 (80%)	6,6,6	2.42	3 (50%)

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	I99	B	603	-	-	2/16/42/42	0/4/4/4
3	OXL	B	602	5	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	E	602	5	-	4/4/4/4	-
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	5	-	4/4/4/4	-
3	OXL	C	602	5	-	4/4/4/4	-
2	FBP	B	601	-	-	3/13/32/32	0/1/1/1
2	FBP	H	601	-	-	3/13/32/32	0/1/1/1
3	OXL	H	602	5	-	4/4/4/4	-
4	I99	E	603	-	-	2/16/42/42	0/4/4/4
3	OXL	G	602	5	-	4/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
4	I99	C	603	-	-	10/16/42/42	1/4/4/4
4	I99	G	603	-	-	7/16/42/42	1/4/4/4
4	I99	F	603	-	-	3/16/42/42	0/4/4/4
4	I99	A	603	-	-	2/16/42/42	0/4/4/4
3	OXL	A	602	5	-	4/4/4/4	-
3	OXL	F	602	5	-	4/4/4/4	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O1-C1	4.37	1.33	1.22
3	B	602	OXL	O2-C2	4.01	1.32	1.22
3	A	602	OXL	O2-C2	3.51	1.31	1.22
3	D	602	OXL	O2-C2	3.51	1.31	1.22
3	F	602	OXL	O2-C2	3.30	1.30	1.22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	OXL	O3-C1-C2	4.67	121.89	112.83
3	F	602	OXL	O4-C2-C1	4.17	120.92	112.83
3	A	602	OXL	O4-C2-C1	4.04	120.66	112.83
3	H	602	OXL	O4-C2-C1	3.98	120.55	112.83
2	D	601	FBP	O5P-P2-O6	3.56	115.94	106.67

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	I99	C18-C11-S-O5
4	A	603	I99	C18-C11-S-O4
4	B	603	I99	C18-C11-S-O5
4	B	603	I99	C18-C11-S-O4
4	C	603	I99	C18-C11-S-O5

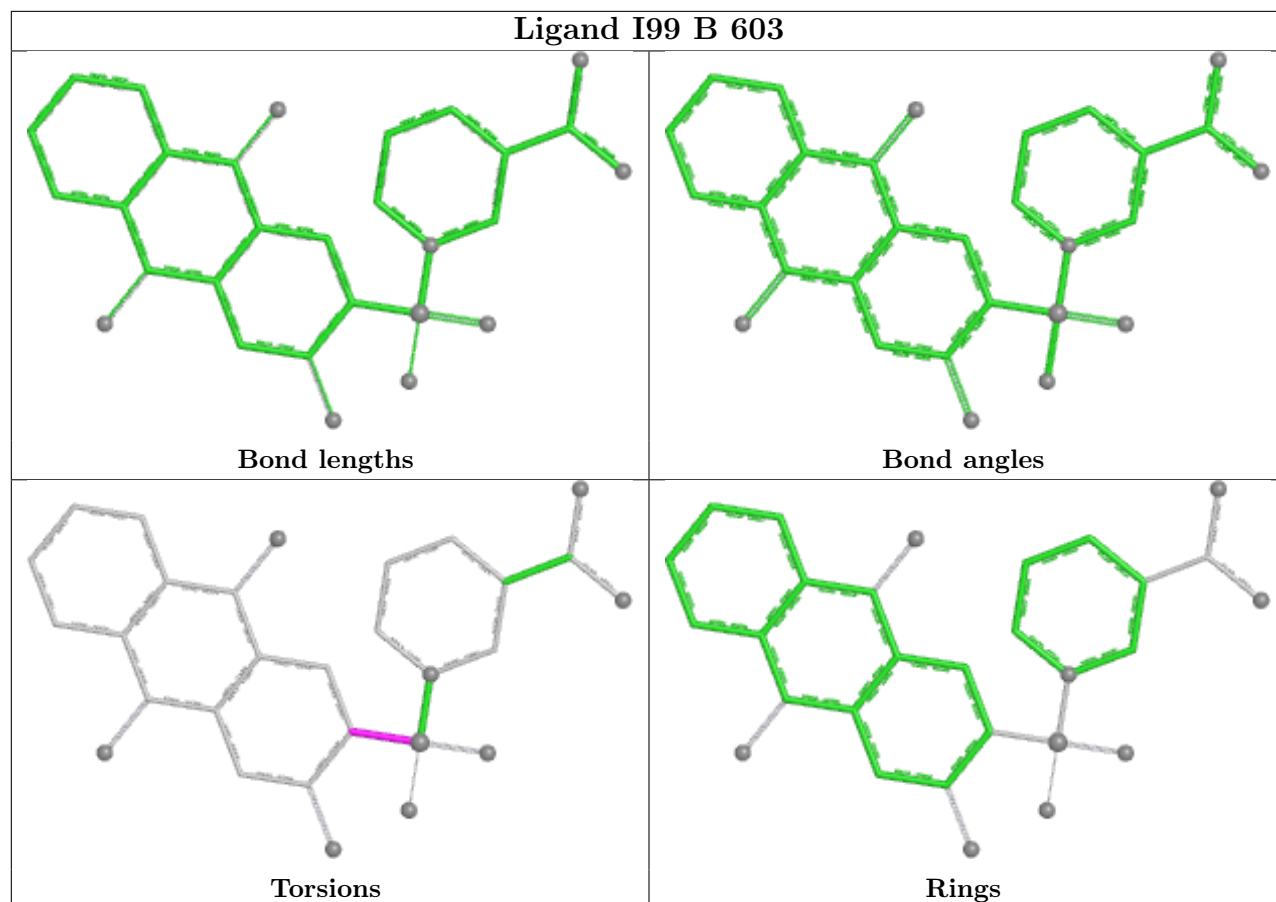
All (2) ring outliers are listed below:

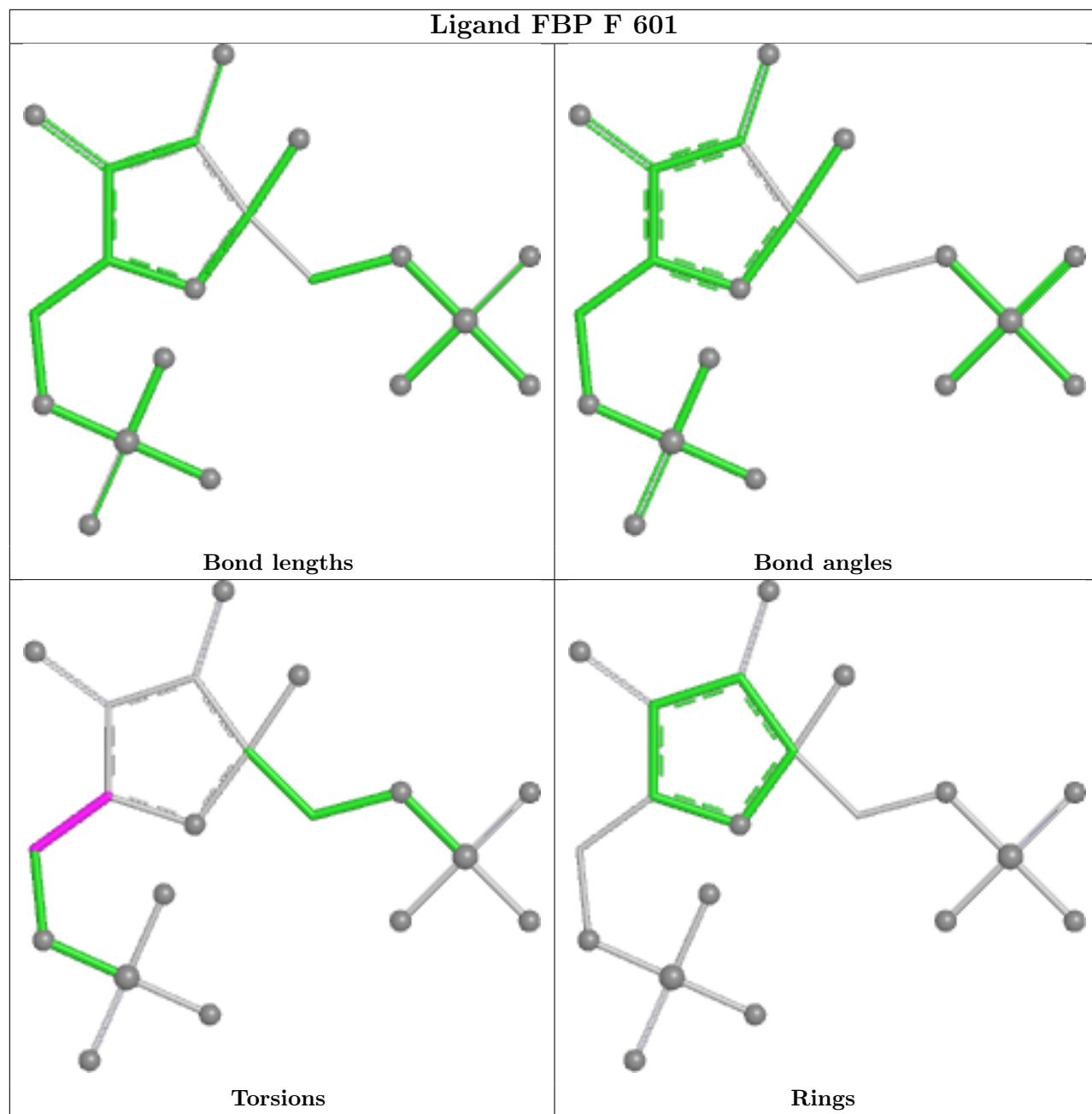
Mol	Chain	Res	Type	Atoms
4	G	603	I99	C12-C13-C15-C16-C17-N
4	C	603	I99	C12-C13-C15-C16-C17-N

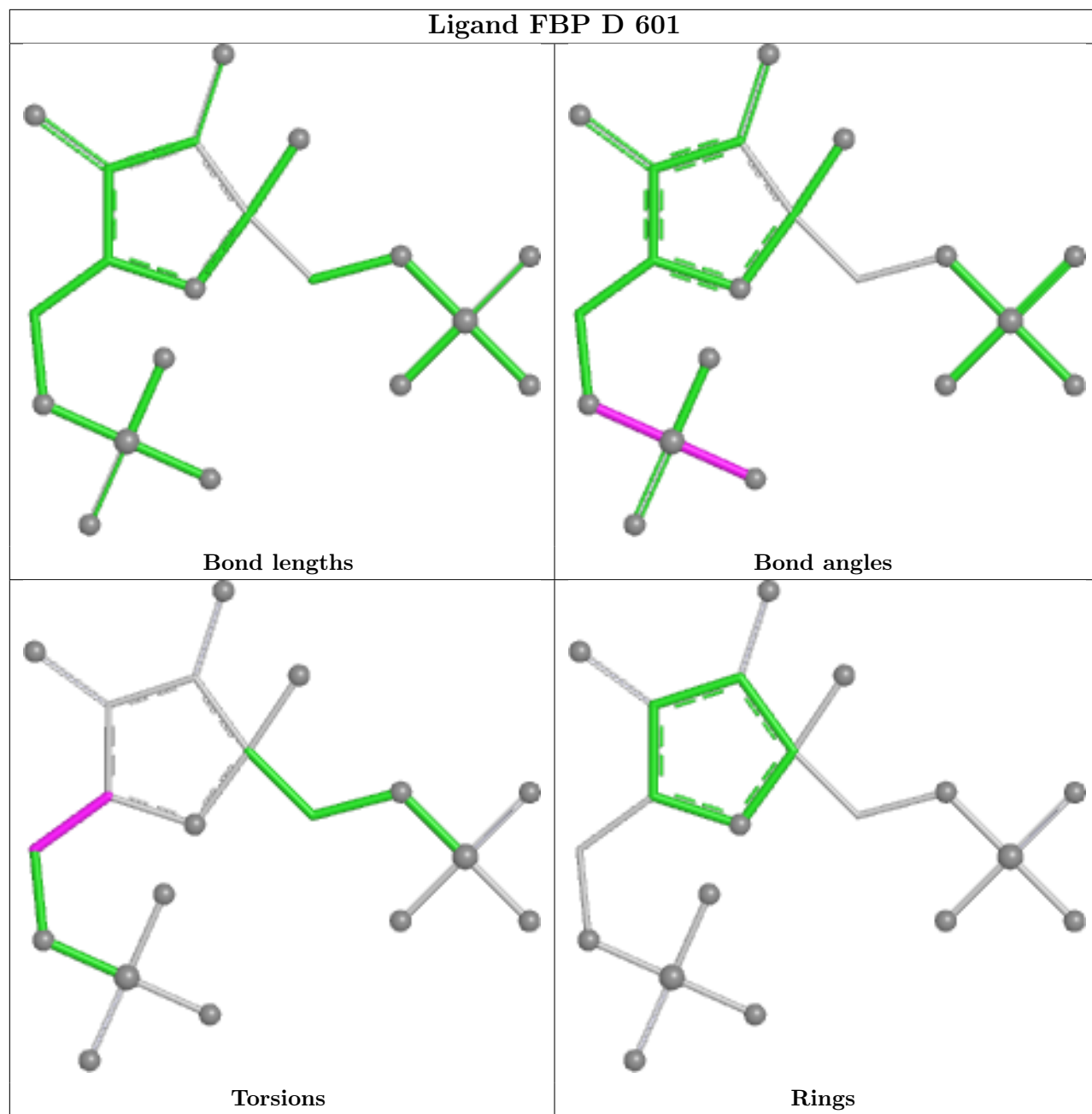
3 monomers are involved in 3 short contacts:

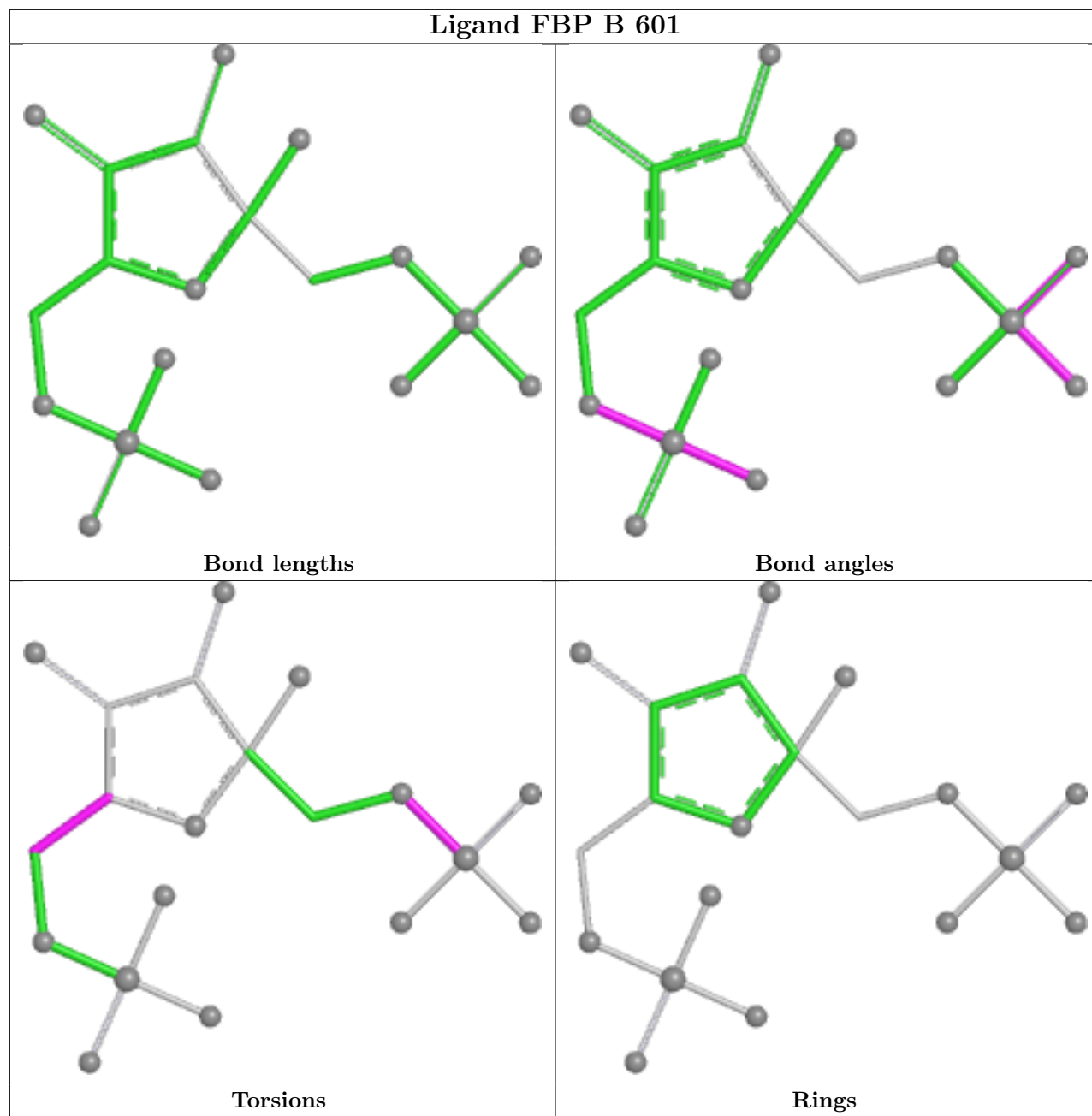
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	FBP	1	0
2	A	601	FBP	1	0
4	G	603	I99	1	0

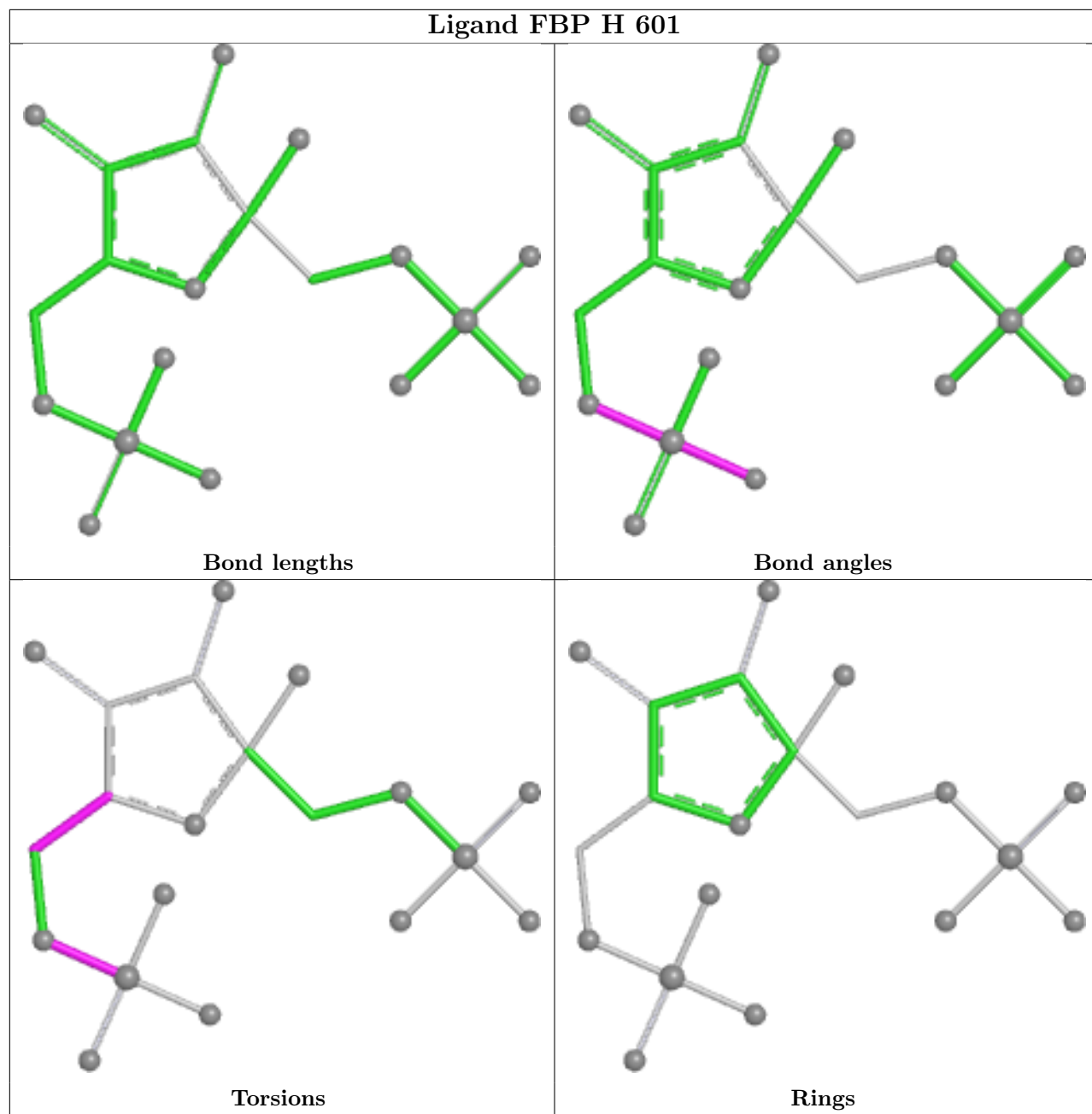
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

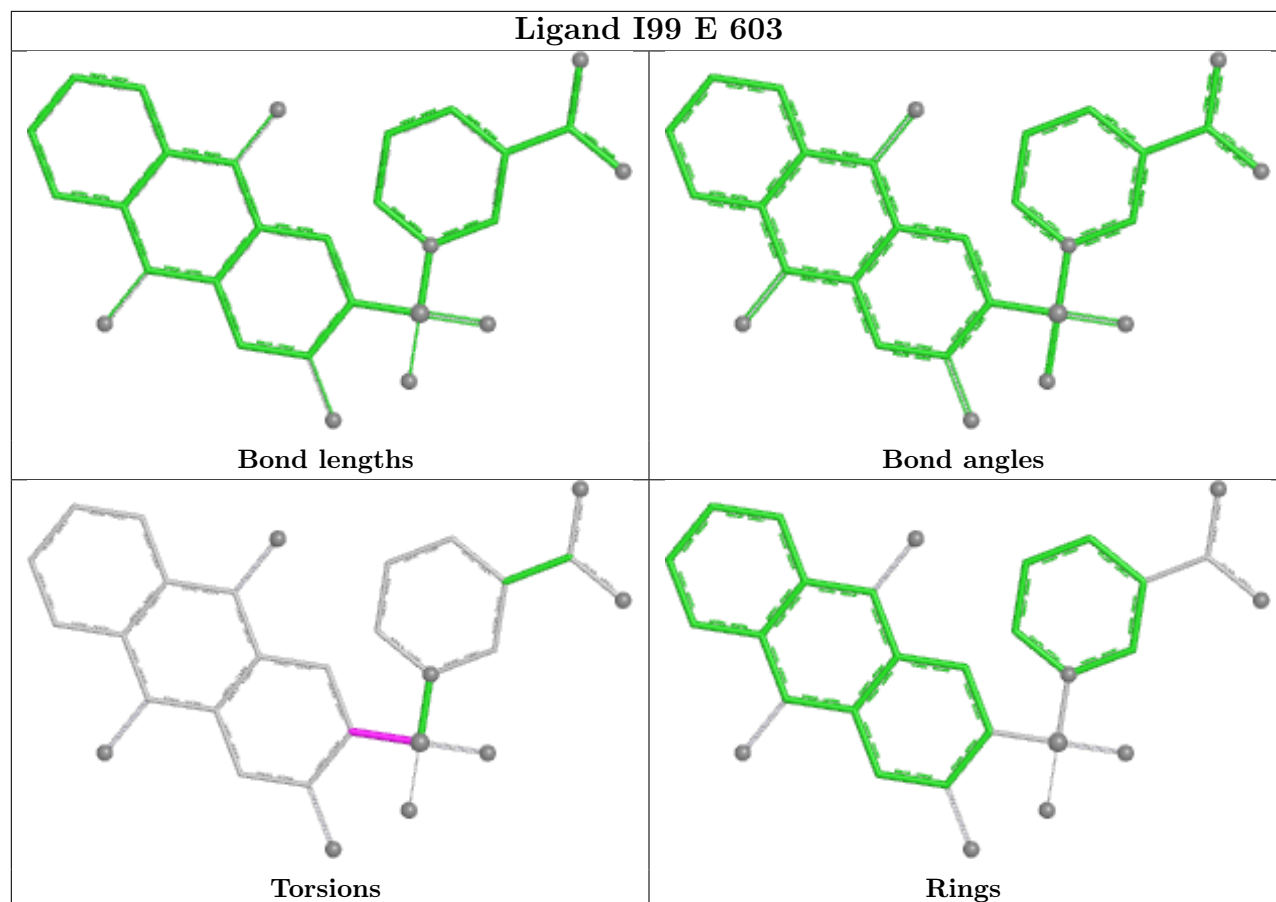


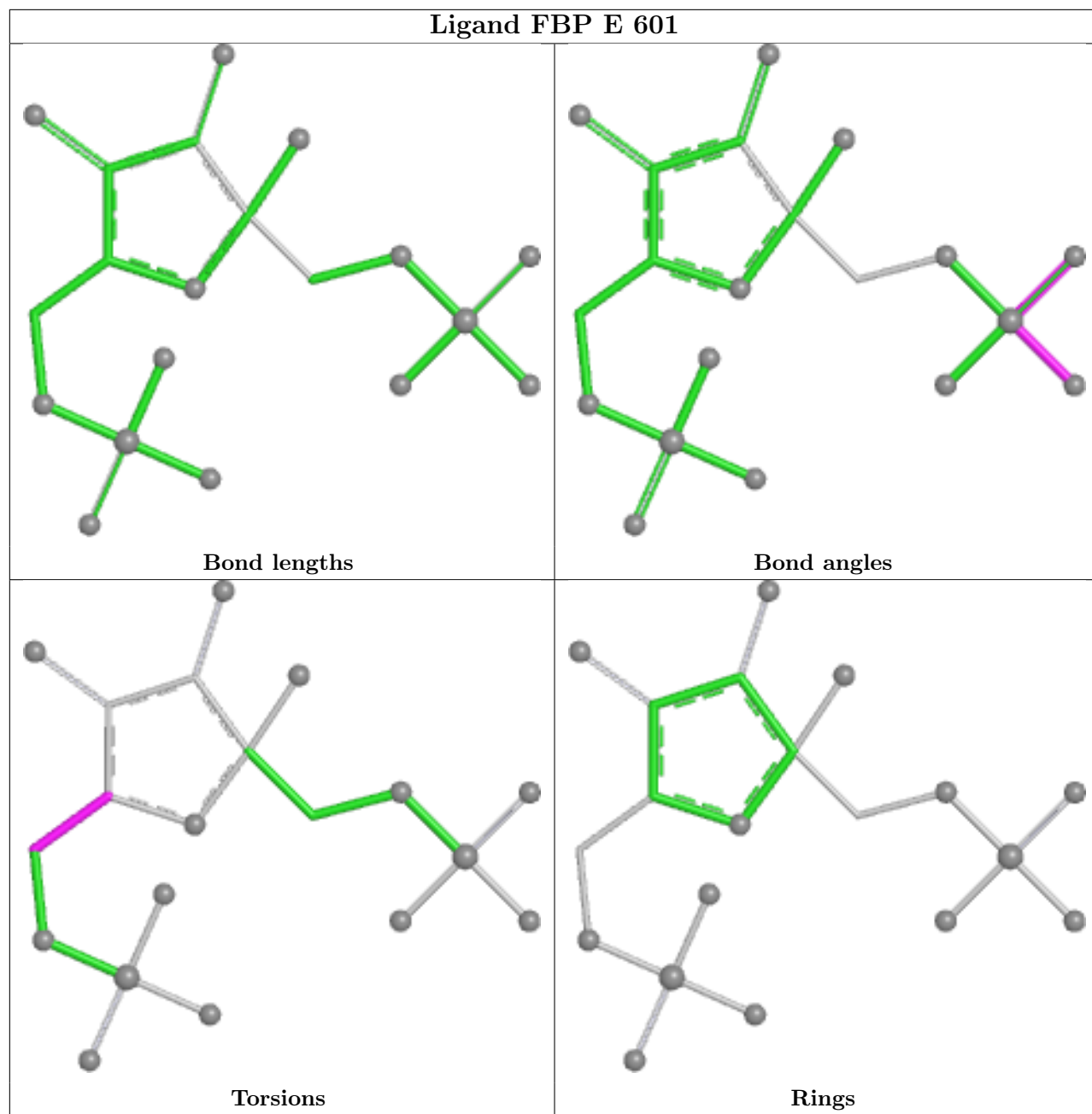


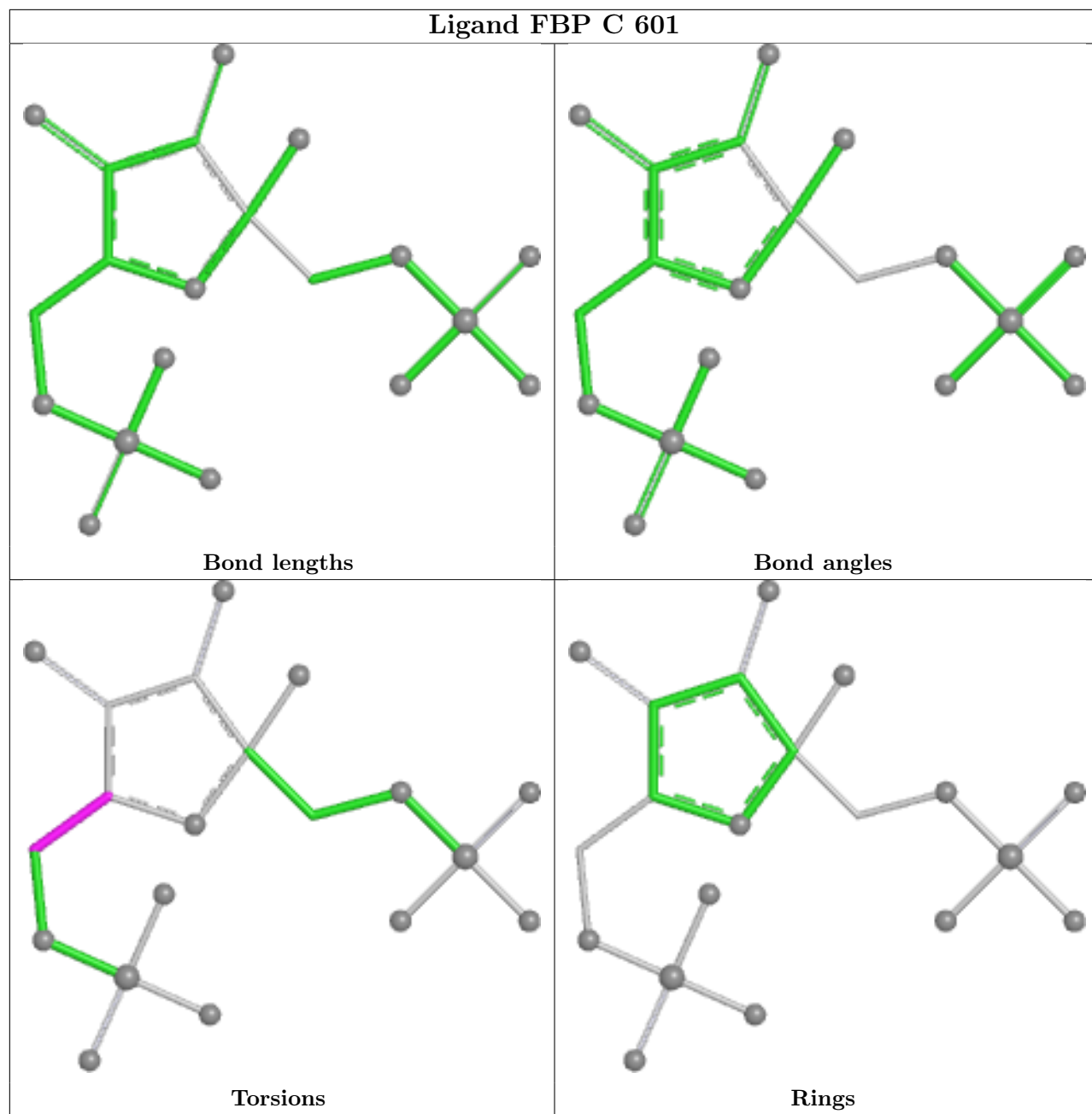


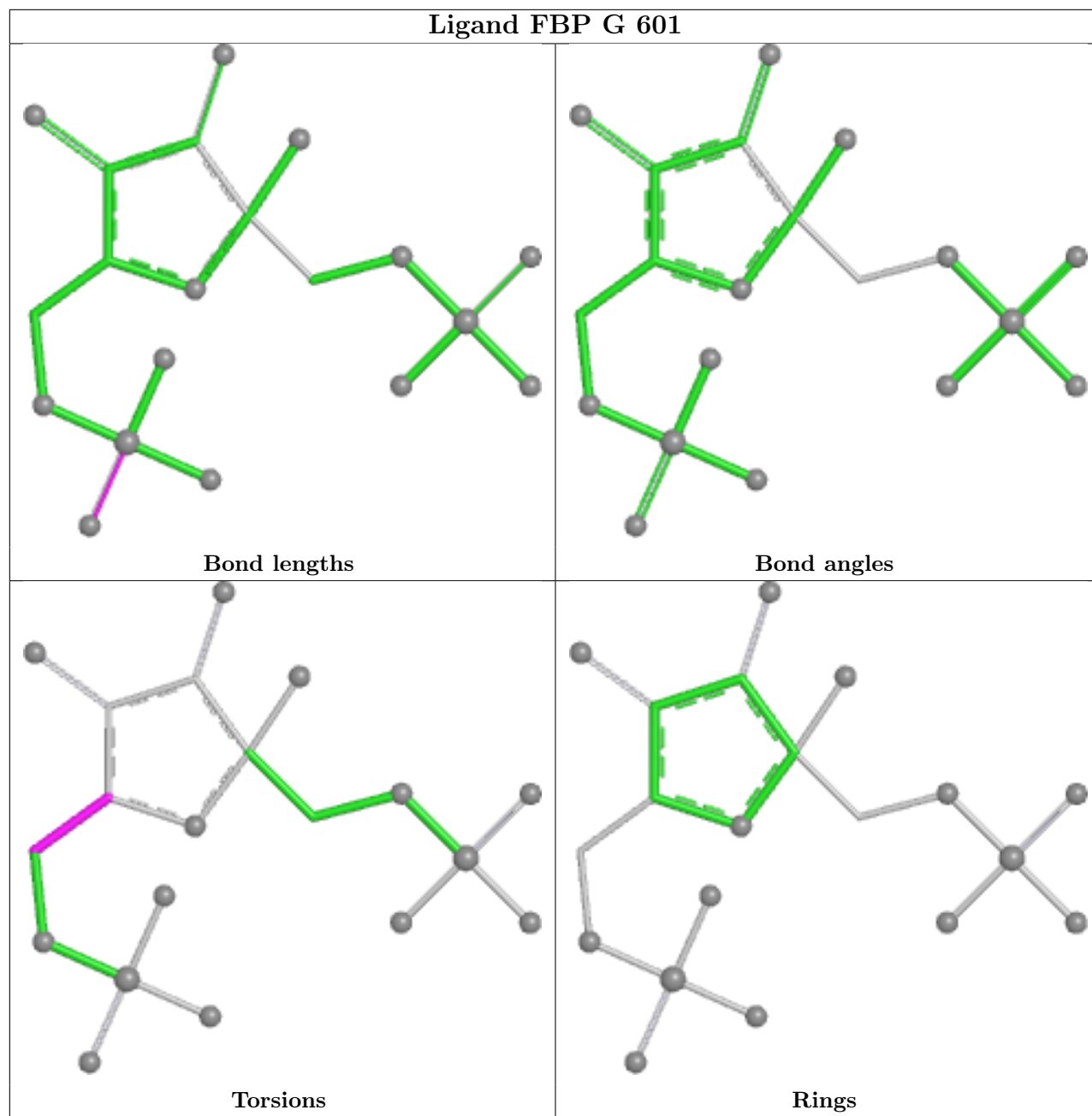


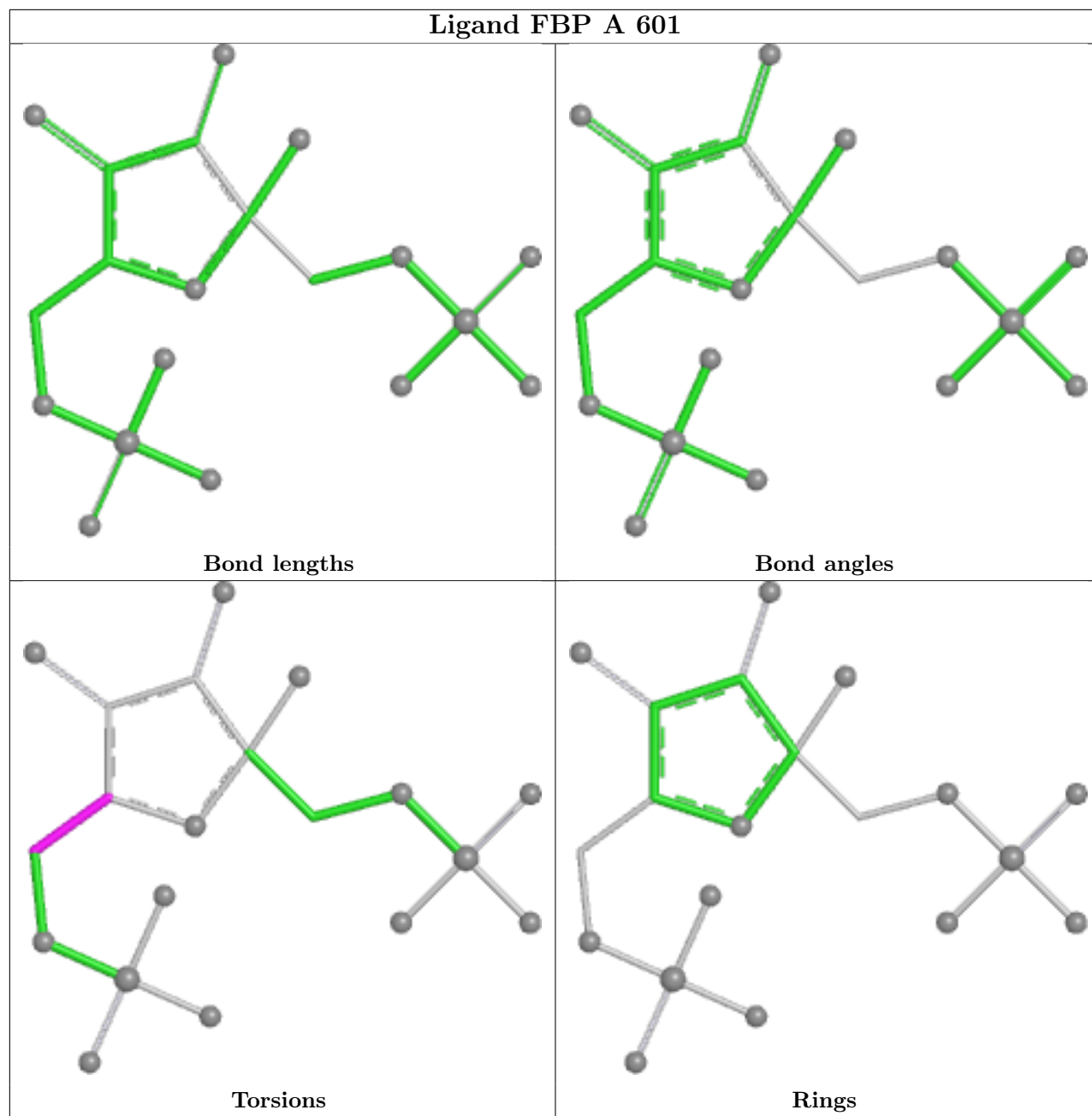


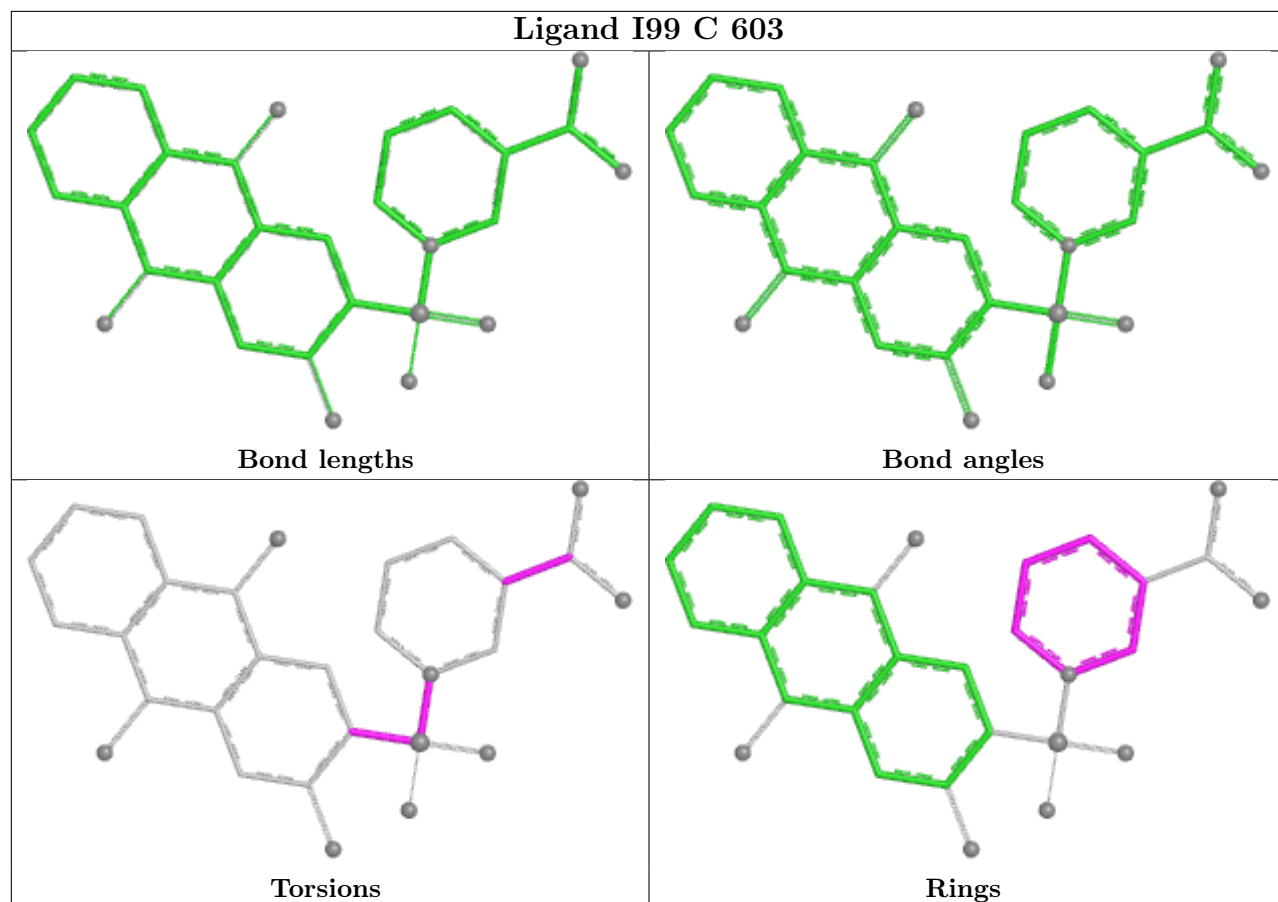


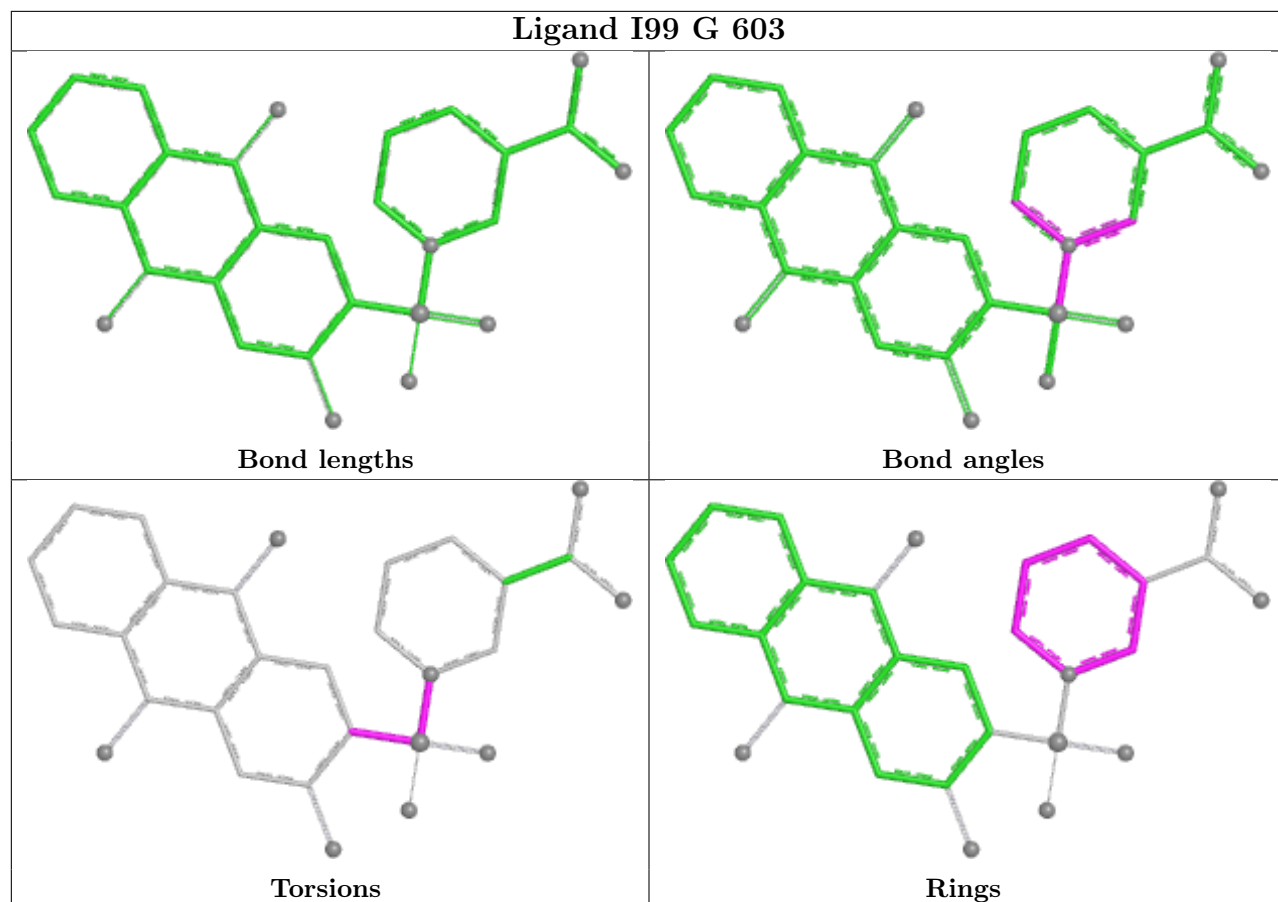


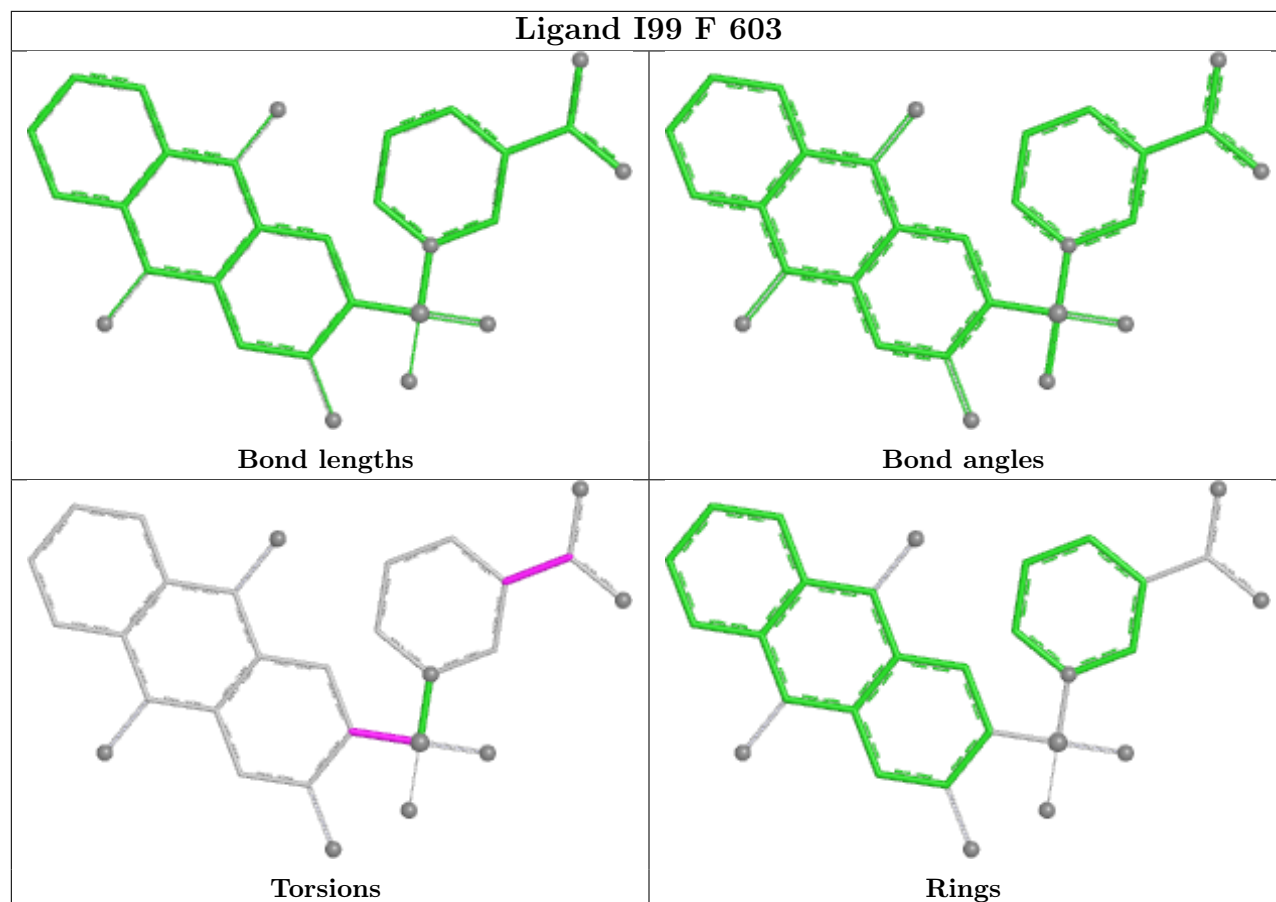


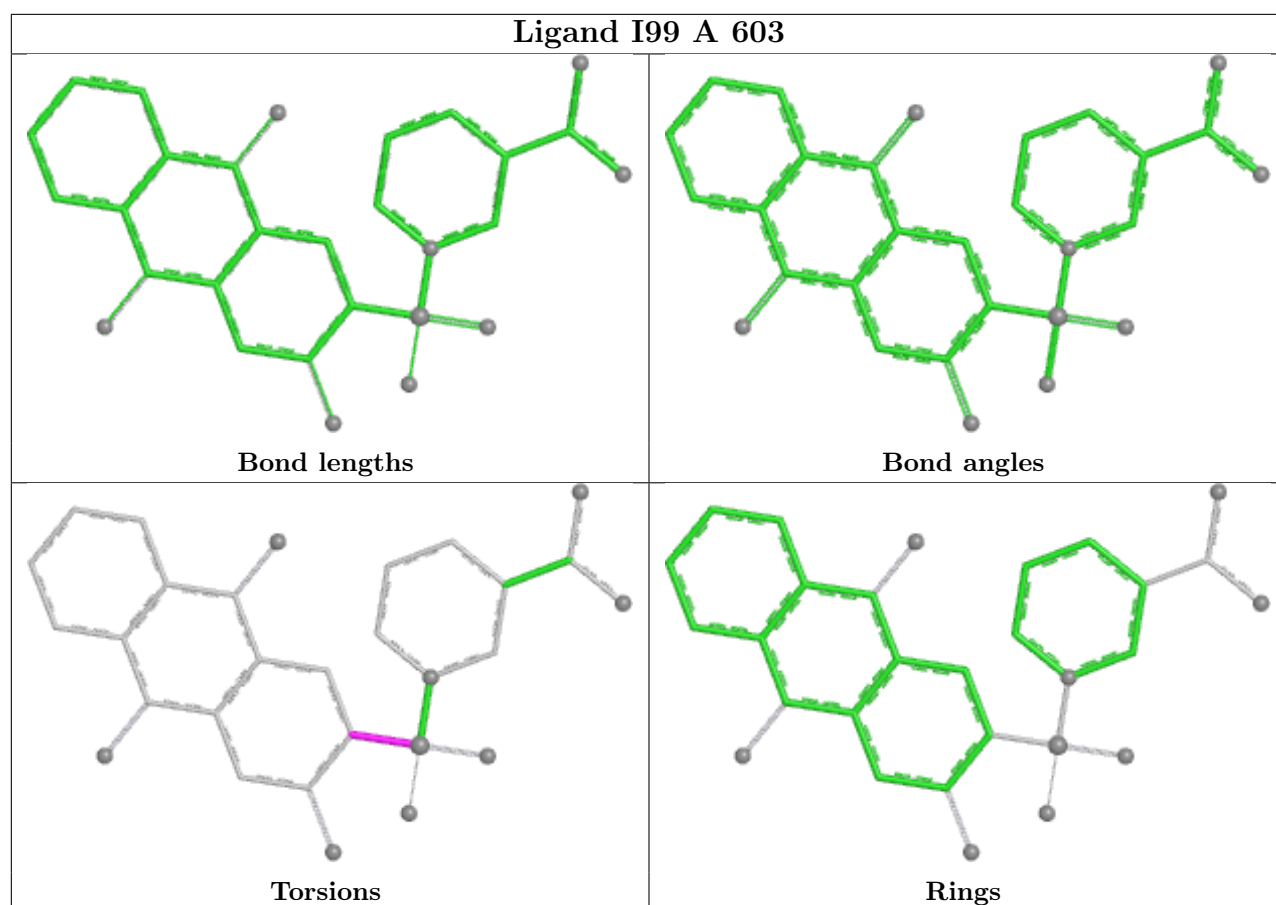












## 5.7 Other polymers [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	418/447 (93%)	1.13	65 (15%) 5 5	29, 53, 78, 93	13 (3%)
1	B	436/447 (97%)	1.57	155 (35%) 1 0	27, 54, 89, 100	8 (1%)
1	C	424/447 (94%)	0.38	22 (5%) 33 37	23, 40, 62, 114	7 (1%)
1	D	425/447 (95%)	0.16	12 (2%) 55 62	18, 35, 59, 110	8 (1%)
1	E	419/447 (93%)	1.08	70 (16%) 4 4	28, 52, 81, 95	13 (3%)
1	F	432/447 (96%)	0.71	45 (10%) 11 13	25, 45, 70, 87	8 (1%)
1	G	422/447 (94%)	0.29	20 (4%) 36 41	16, 37, 59, 106	10 (2%)
1	H	425/447 (95%)	0.04	15 (3%) 47 53	18, 34, 57, 100	9 (2%)
All	All	3401/3576 (95%)	0.67	404 (11%) 9 10	16, 44, 77, 114	76 (2%)

The worst 5 of 404 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	LEU	6.7
1	G	271	GLY	6.2
1	D	25	PHE	6.1
1	E	25	PHE	6.0
1	E	275[A]	HIS	6.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

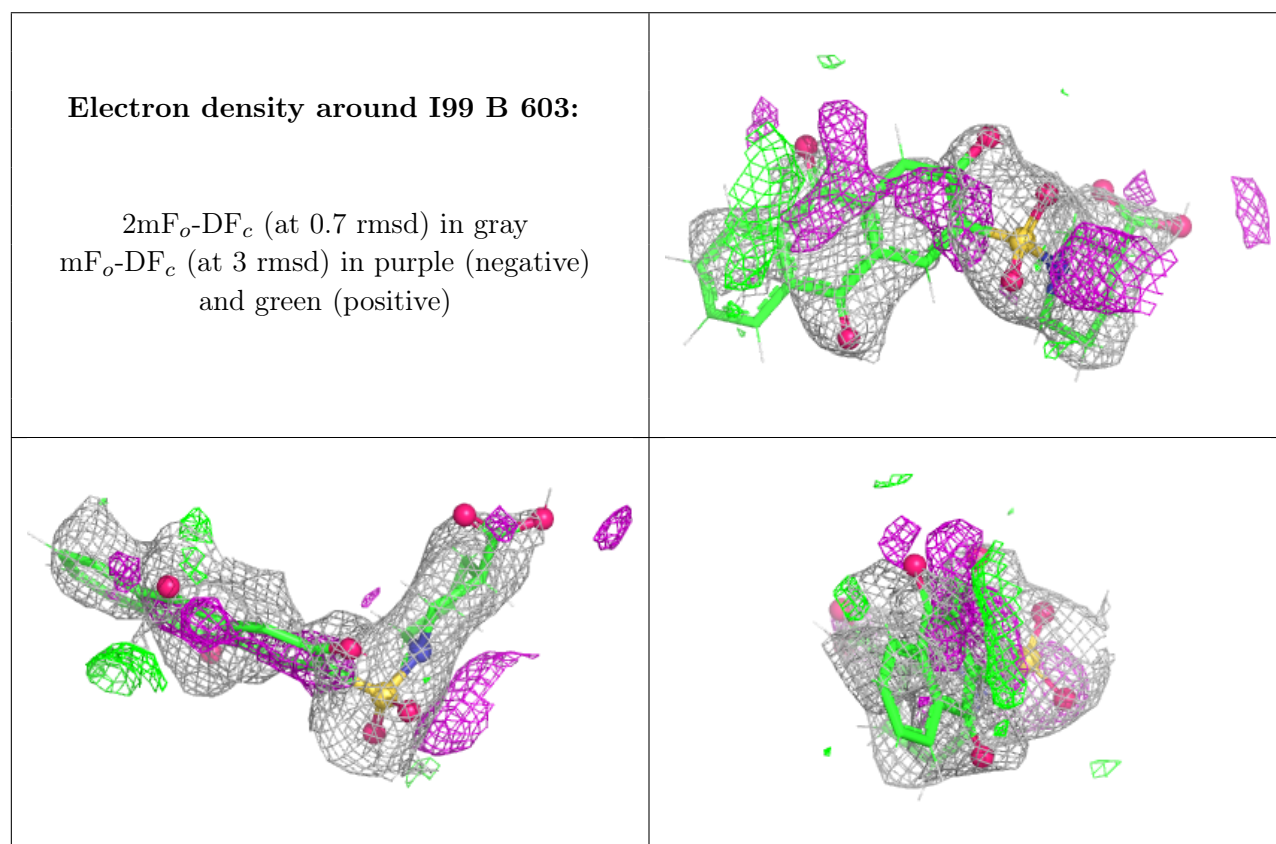
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	I99	B	603	29/29	0.80	0.20	81,85,87,87	17
4	I99	A	603	29/29	0.86	0.15	83,85,87,87	17
3	OXL	E	602	6/6	0.87	0.12	62,63,63,63	0
6	K	E	605	1/1	0.88	0.21	93,93,93,93	0
4	I99	G	603	29/29	0.89	0.16	61,65,67,67	17
4	I99	E	603	29/29	0.89	0.13	89,89,90,90	17
6	K	B	605	1/1	0.91	0.12	80,80,80,80	0
4	I99	F	603	29/29	0.92	0.11	59,60,63,63	17
5	MG	B	604	1/1	0.93	0.09	65,65,65,65	0
3	OXL	A	602	6/6	0.94	0.08	57,57,58,58	0
6	K	A	605	1/1	0.94	0.11	86,86,86,86	0
2	FBP	B	601	20/20	0.94	0.08	49,51,54,55	0
4	I99	C	603	29/29	0.94	0.09	57,58,62,63	17
6	K	F	605	1/1	0.94	0.11	80,80,80,80	0
6	K	G	605	1/1	0.94	0.17	60,60,60,60	0
3	OXL	B	602	6/6	0.95	0.07	46,47,47,47	0
2	FBP	E	601	20/20	0.95	0.08	46,47,48,49	0
3	OXL	G	602	6/6	0.95	0.07	40,41,41,42	0
2	FBP	F	601	20/20	0.95	0.08	44,47,52,52	0
2	FBP	A	601	20/20	0.95	0.08	46,49,50,50	0
6	K	C	605	1/1	0.96	0.23	62,62,62,62	0
3	OXL	F	602	6/6	0.96	0.07	48,49,50,50	0
3	OXL	H	602	6/6	0.96	0.07	35,36,36,37	0
5	MG	A	604	1/1	0.96	0.06	62,62,62,62	0
3	OXL	C	602	6/6	0.97	0.06	44,45,45,45	0
3	OXL	D	602	6/6	0.97	0.06	38,39,39,40	0
2	FBP	D	601	20/20	0.98	0.04	27,29,30,32	0
6	K	D	604	1/1	0.98	0.13	51,51,51,51	0
5	MG	E	604	1/1	0.98	0.06	57,57,57,57	0
2	FBP	G	601	20/20	0.98	0.05	29,30,31,33	0
2	FBP	H	601	20/20	0.98	0.04	25,28,30,30	0
6	K	H	604	1/1	0.98	0.16	55,55,55,55	0
5	MG	G	604	1/1	0.99	0.06	38,38,38,38	0
5	MG	H	603	1/1	0.99	0.04	39,39,39,39	0
5	MG	C	604	1/1	0.99	0.04	46,46,46,46	0
5	MG	D	603	1/1	0.99	0.04	38,38,38,38	0
2	FBP	C	601	20/20	0.99	0.04	29,30,32,33	0

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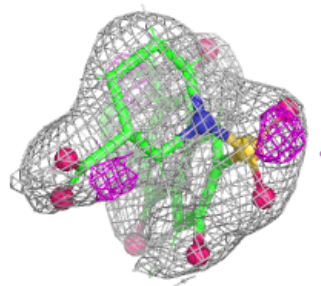
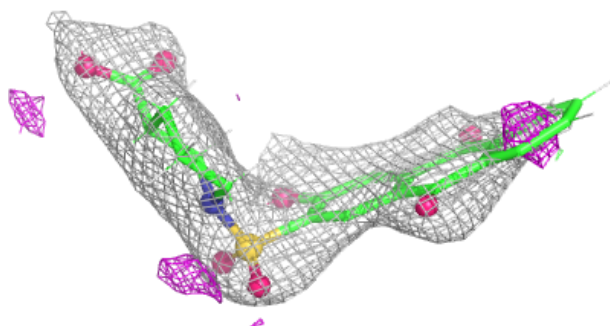
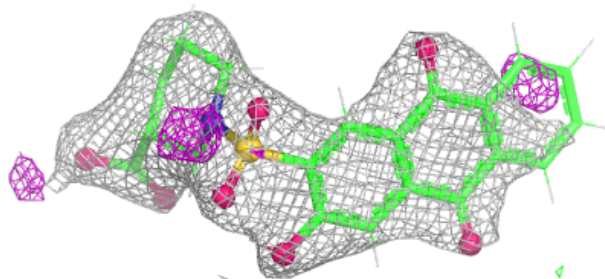
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	F	604	1/1	1.00	0.02	42,42,42,42	0

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.

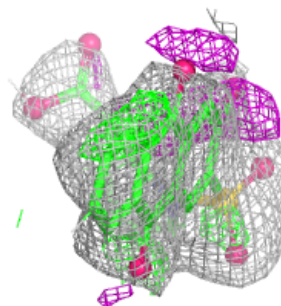
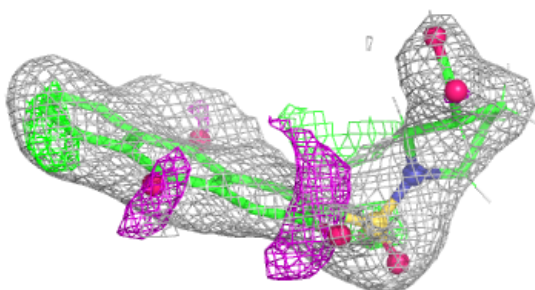
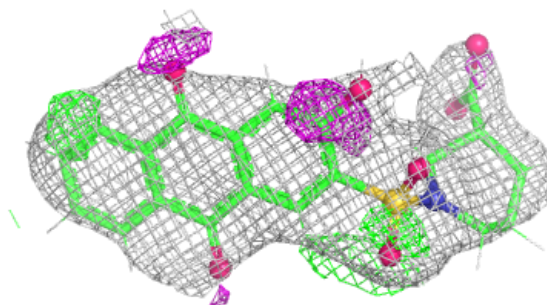


**Electron density around I99 A 603:**

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

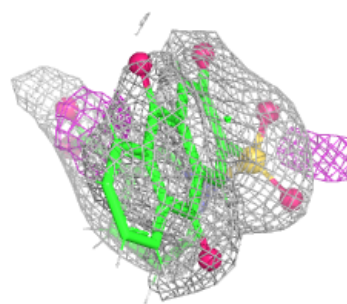
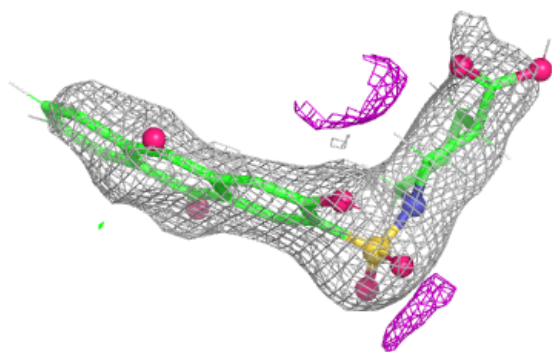
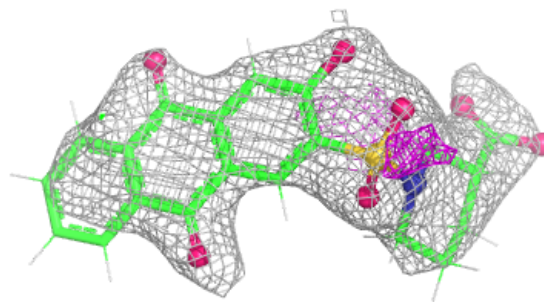
**Electron density around I99 G 603:**

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

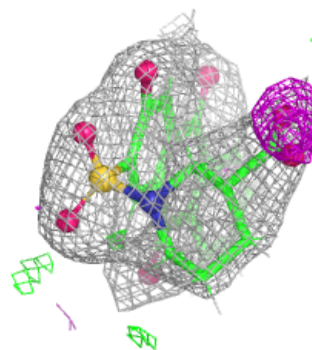
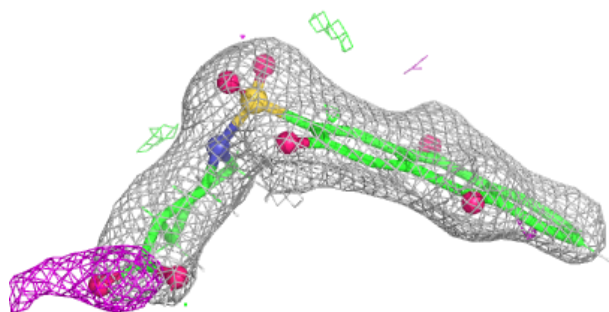
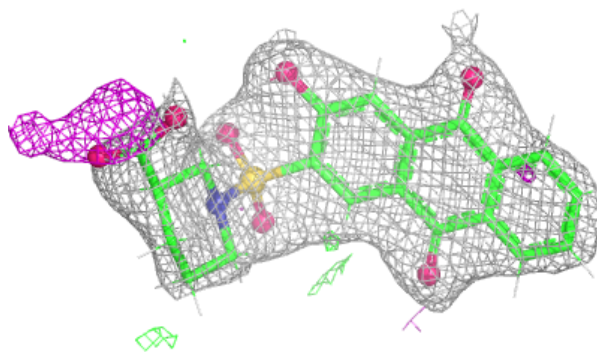


**Electron density around I99 E 603:**

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

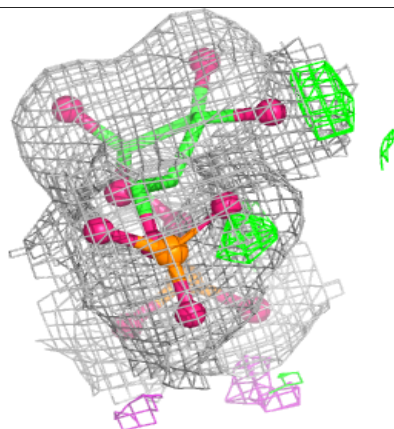
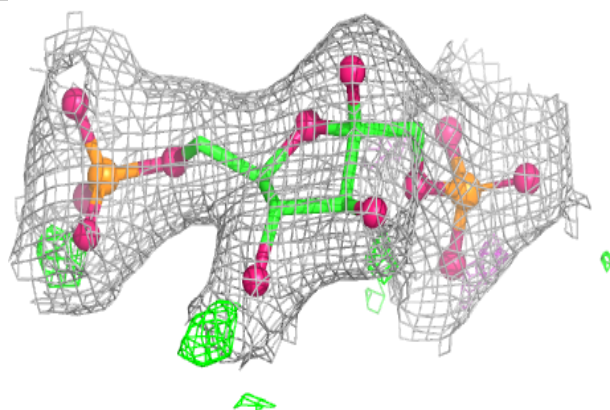
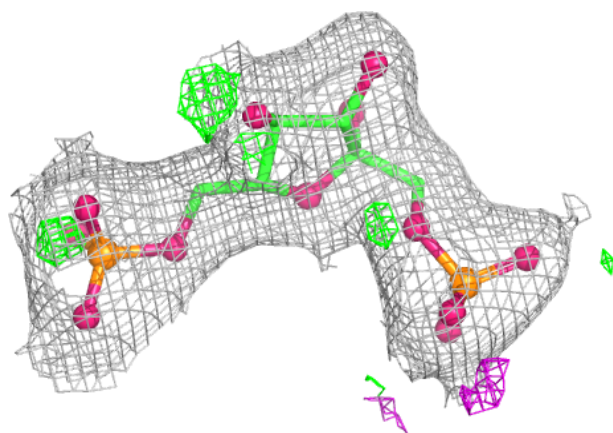
**Electron density around I99 F 603:**

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

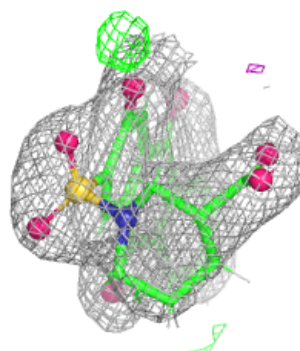
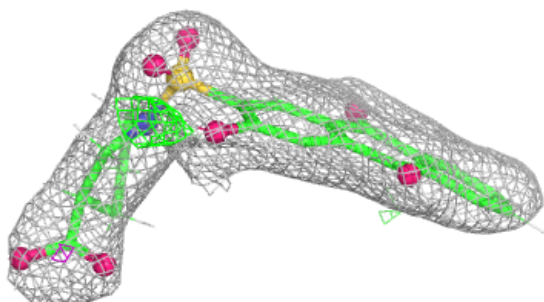
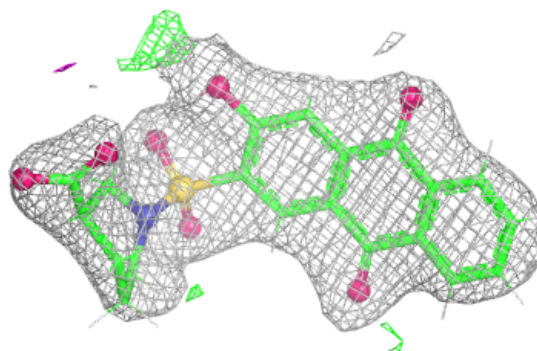


**Electron density around FBP B 601:**

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

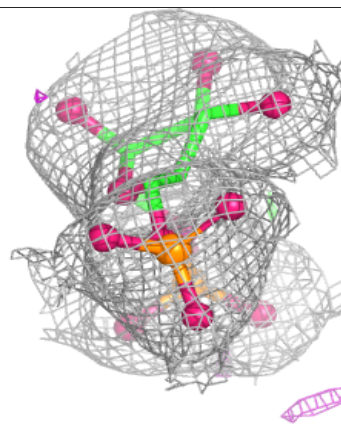
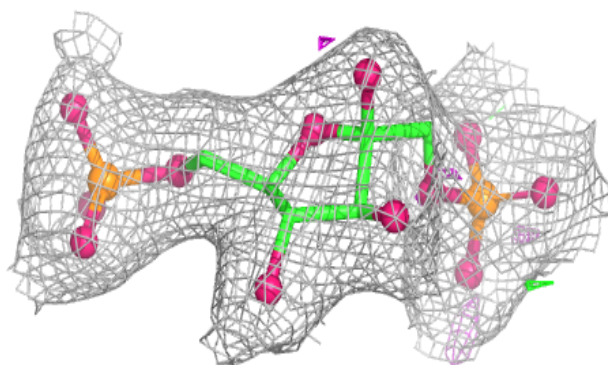
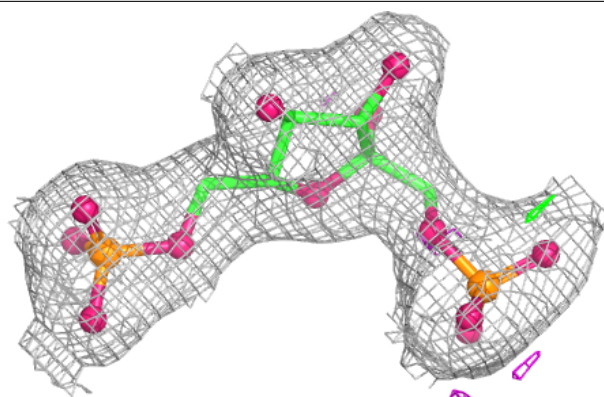
**Electron density around I99 C 603:**

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



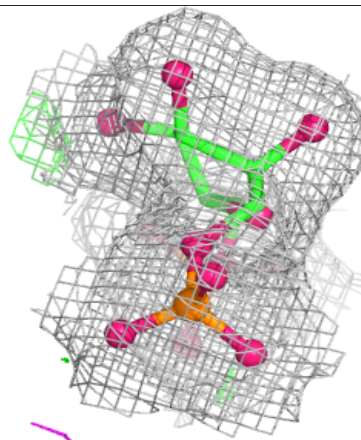
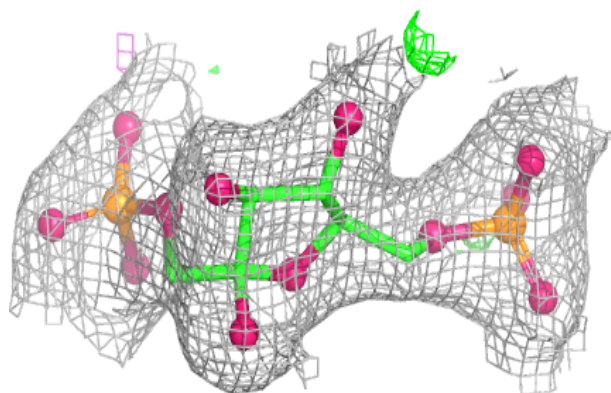
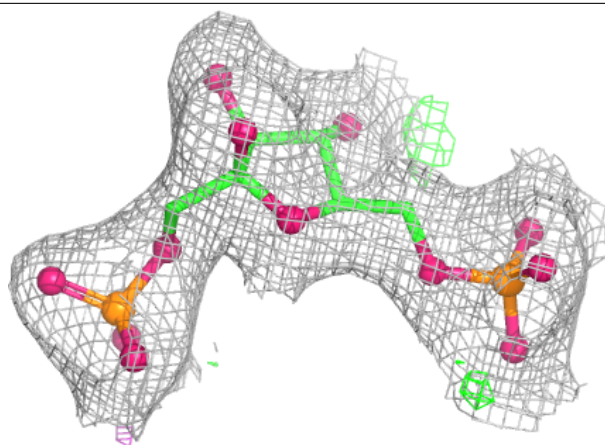
**Electron density around FBP E 601:**

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

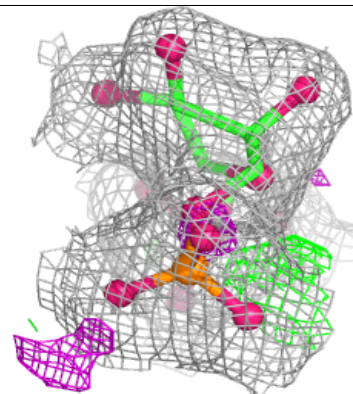
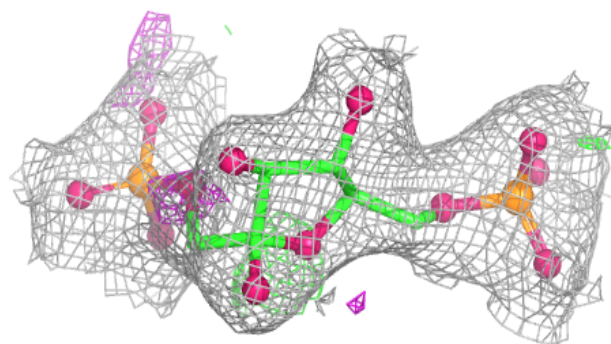
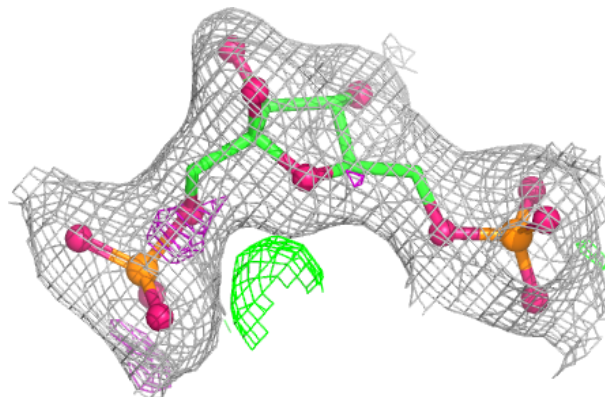


**Electron density around FBP F 601:**

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

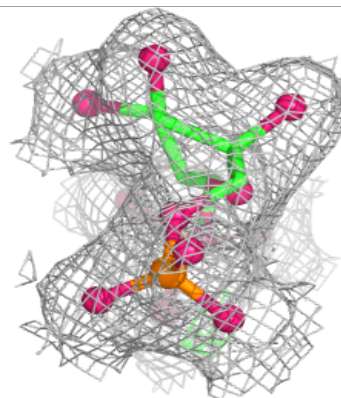
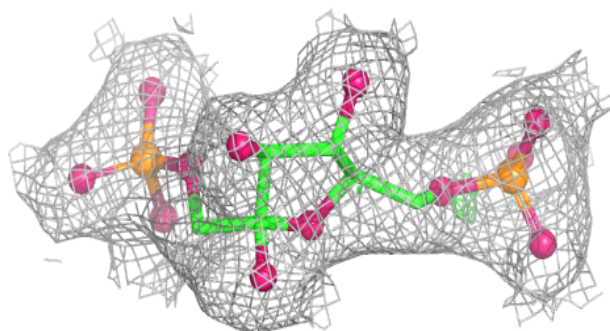
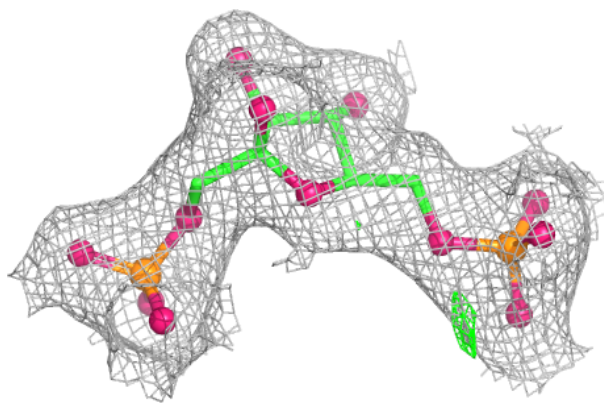
**Electron density around FBP A 601:**

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

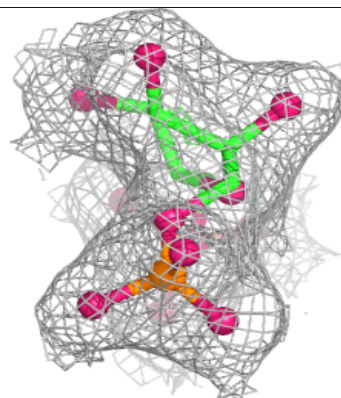
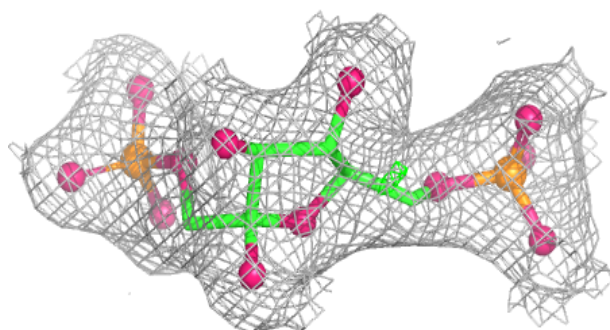
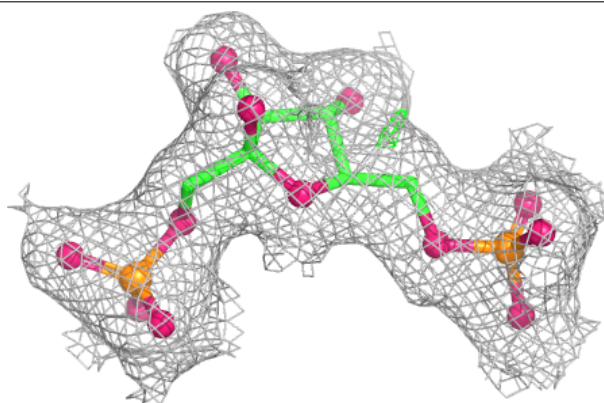


**Electron density around FBP D 601:**

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

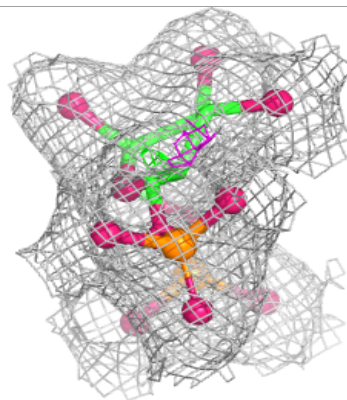
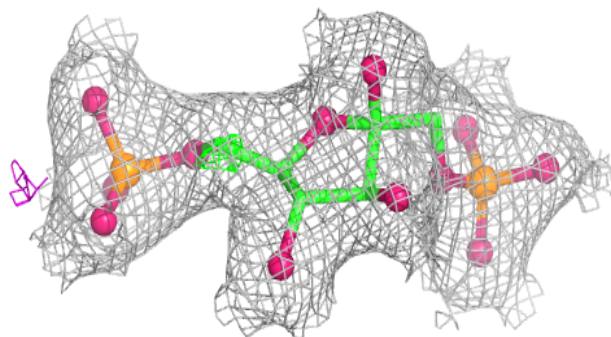
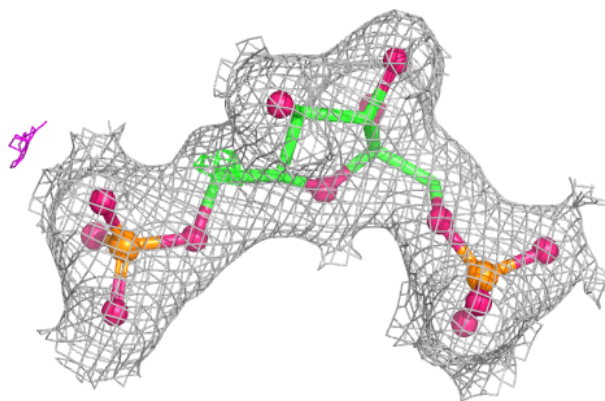
**Electron density around FBP G 601:**

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

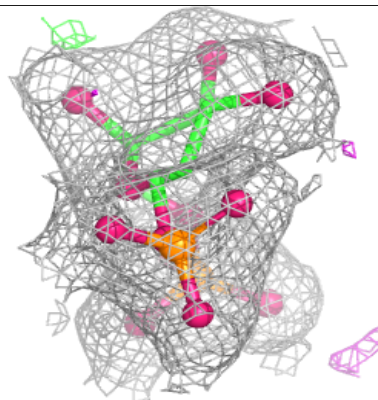
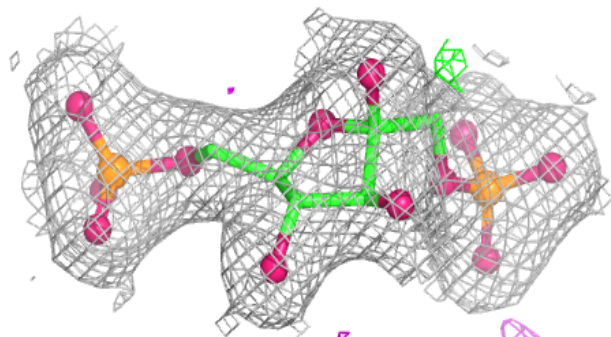
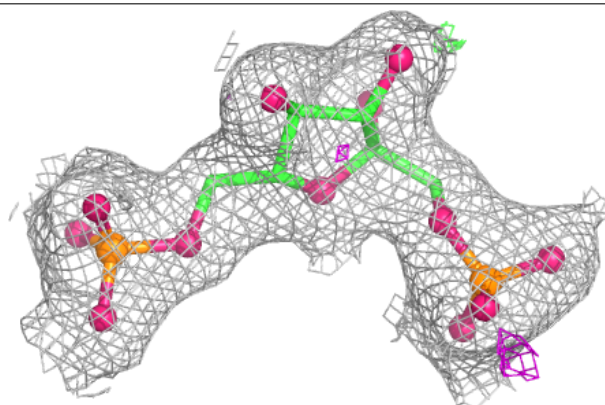


**Electron density around FBP H 601:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.