



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:53 AM UTC

PDB ID : 5SCA / pdb\_00005sca  
Title : Structure of liver pyruvate kinase in complex with anthraquinone derivative  
36  
Authors : Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.  
Deposited on : 2021-12-01  
Resolution : 1.92 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

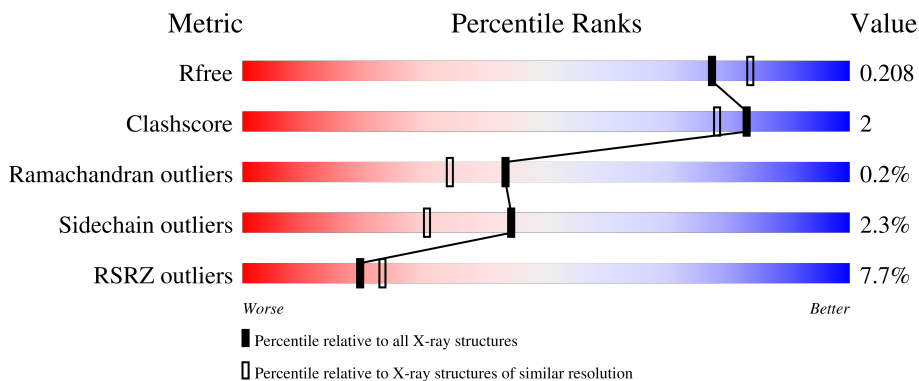
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	603	-	X	-	-
3	OXL	D	602	-	X	-	-
3	OXL	E	602	-	X	-	-
3	OXL	F	603	-	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 29195 atoms, of which 88 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	419	Total 3242	C 2035	N 582	O 605	S 20	0	13	0
1	B	436	Total 3350	C 2104	N 604	O 622	S 20	3	8	0
1	C	424	Total 3263	C 2053	N 584	O 607	S 19	0	8	0
1	D	425	Total 3261	C 2048	N 590	O 604	S 19	0	8	0
1	E	419	Total 3257	C 2049	N 584	O 604	S 20	0	13	0
1	F	432	Total 3322	C 2089	N 597	O 616	S 20	0	7	0
1	G	423	Total 3247	C 2042	N 583	O 603	S 19	0	7	0
1	H	425	Total 3277	C 2057	N 597	O 604	S 19	0	9	0

There are 48 discrepancies between the modelled and reference sequences:

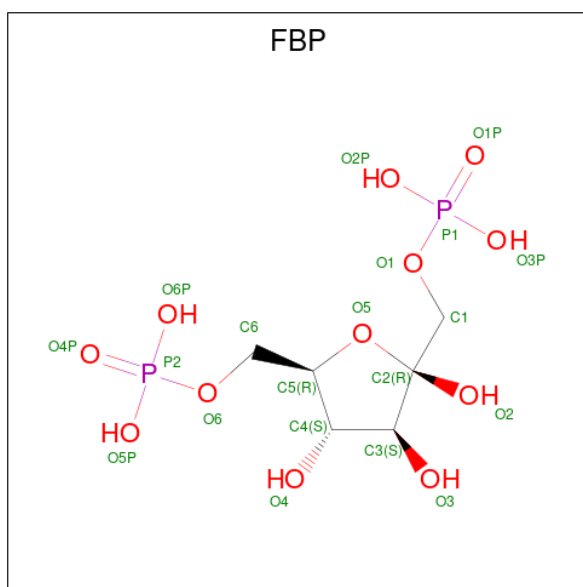
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	132	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression 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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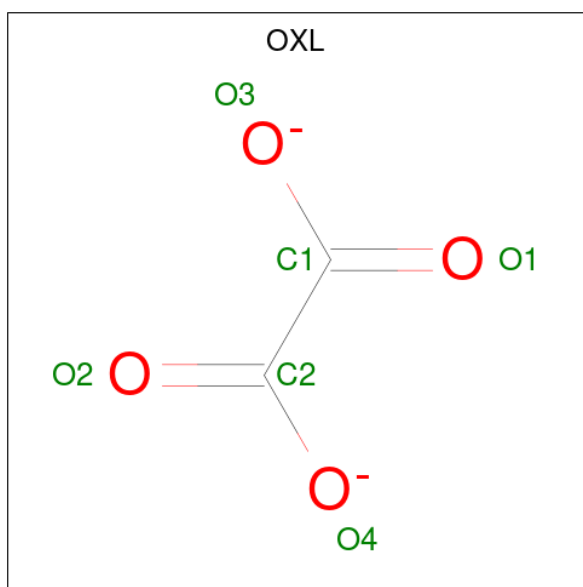
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	228	GLY	-	linker	UNP Q16716
C	229	SER	-	linker	UNP Q16716
C	230	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict	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:  $C_6H_{14}O_{12}P_2$ ).



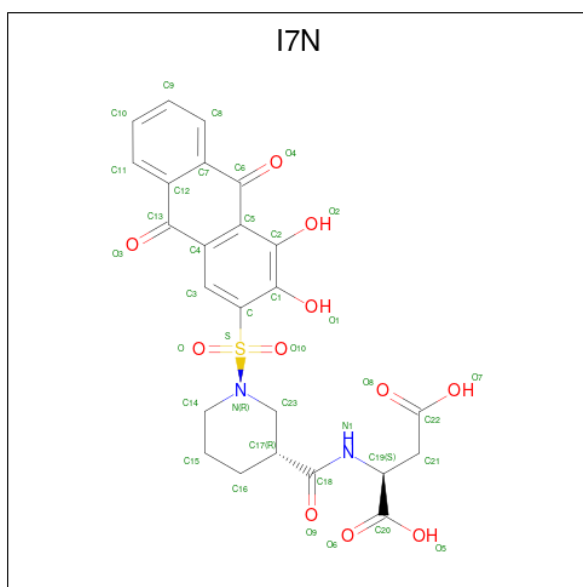
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	20	6	12	2	0	0
2	B	1	20	6	12	2	0	0
2	C	1	20	6	12	2	0	0
2	D	1	20	6	12	2	0	0
2	E	1	20	6	12	2	0	0
2	F	1	20	6	12	2	0	0
2	G	1	20	6	12	2	0	0
2	H	1	20	6	12	2	0	0

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



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

- Molecule 4 is N-[(3R)-1-(3,4-dihydroxy-9,10-dioxo-9,10-dihydroanthracene-2-sulfonyl)pyridine-3-carbonyl]-L-aspartic acid (CCD ID: I7N) (formula: C<sub>24</sub>H<sub>22</sub>N<sub>2</sub>O<sub>11</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	22	0
			60	24	22	2	11	1		
4	C	1	Total	C	H	N	O	S	22	0
			60	24	22	2	11	1		
4	E	1	Total	C	H	N	O	S	22	0
			60	24	22	2	11	1		
4	F	1	Total	C	H	N	O	S	22	0
			60	24	22	2	11	1		

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

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

- 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

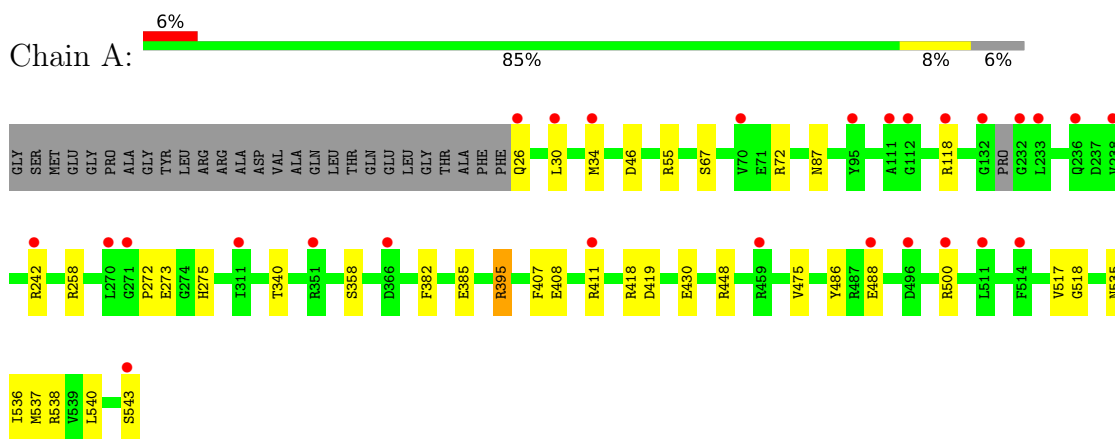
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	252	Total O 252 252	0	0
7	B	216	Total O 216 216	0	0
7	C	344	Total O 344 344	0	0
7	D	376	Total O 376 376	0	0
7	E	266	Total O 266 266	0	0
7	F	276	Total O 276 276	0	0
7	G	388	Total O 388 388	0	0
7	H	394	Total O 394 394	0	0

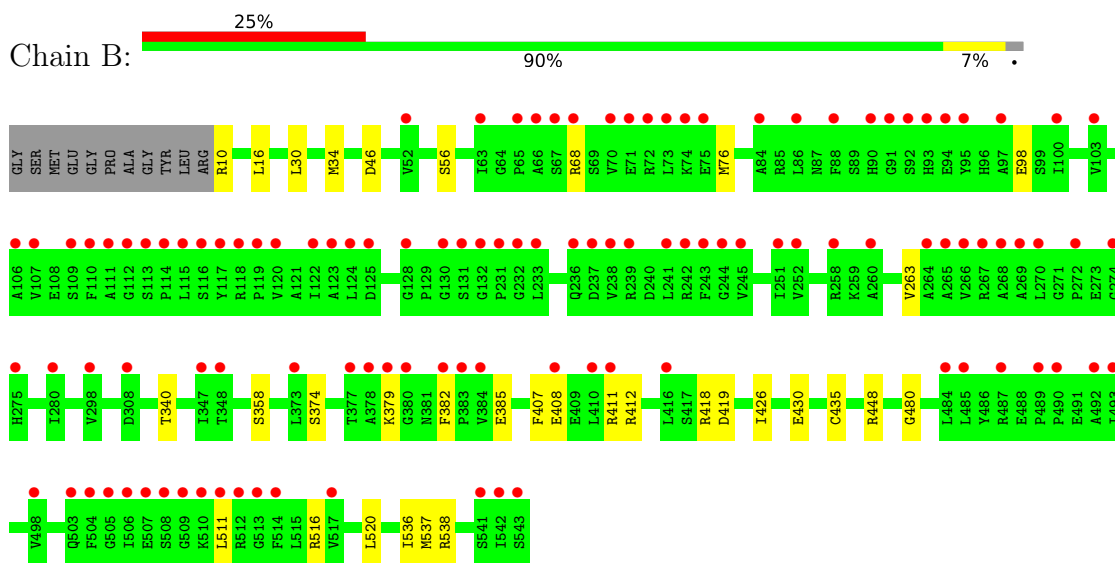
### 3 Residue-property plots [i](#)

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.

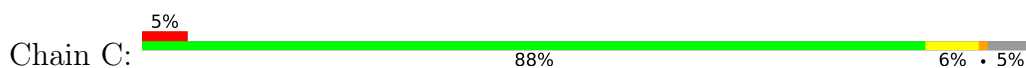
- Molecule 1: Pyruvate kinase

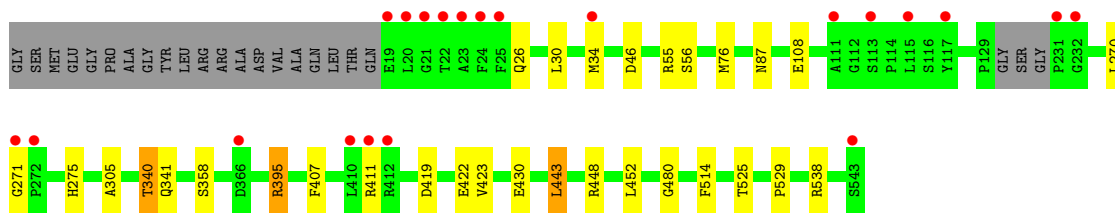


- Molecule 1: Pyruvate kinase

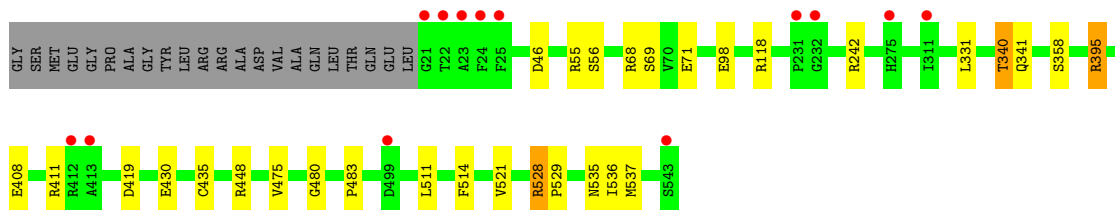
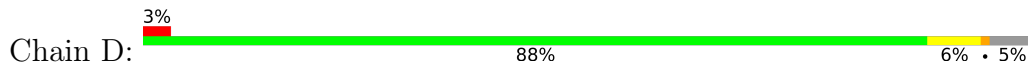


- Molecule 1: Pyruvate kinase

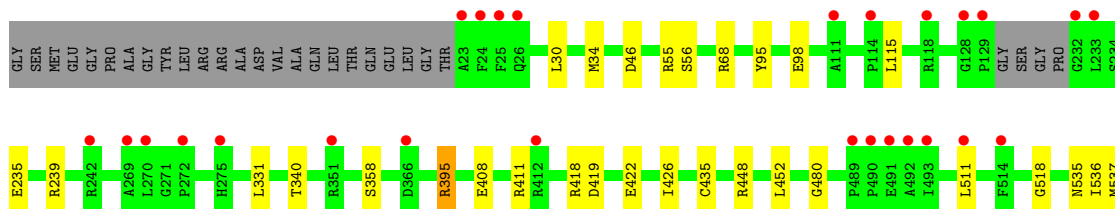
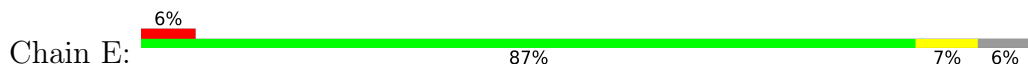




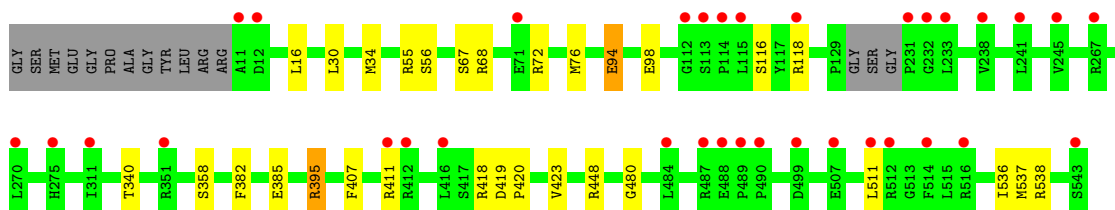
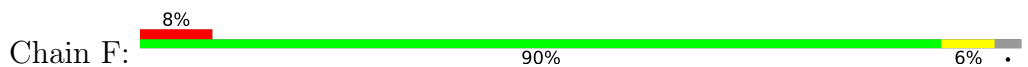
• Molecule 1: Pyruvate kinase



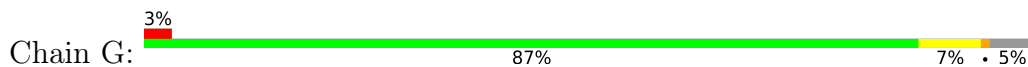
• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase

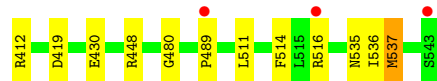
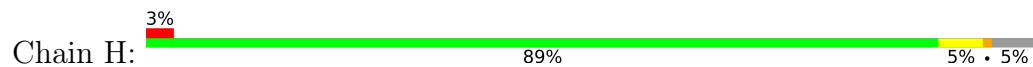


• Molecule 1: Pyruvate kinase





- Molecule 1: Pyruvate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.32Å 112.52Å 188.73Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	188.64 – 1.92 188.64 – 1.92	Depositor EDS
% Data completeness (in resolution range)	81.1 (188.64-1.92) 81.1 (188.64-1.92)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 1.92Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, $R_{free}$	0.192 , 0.216 0.185 , 0.208	Depositor DCC
$R_{free}$ test set	13593 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.001 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	29195	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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 30.86 % 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 1.2178e-03. 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: FBP, OXL, MG, I7N, 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	0.70	0/3332	0.96	3/4502 (0.1%)
1	B	0.70	2/3429 (0.1%)	0.97	1/4636 (0.0%)
1	C	0.76	0/3341	0.96	2/4516 (0.0%)
1	D	0.76	0/3341	0.98	2/4517 (0.0%)
1	E	0.69	0/3350	0.95	2/4527 (0.0%)
1	F	0.71	0/3397	0.96	0/4592
1	G	0.76	0/3322	0.97	3/4490 (0.1%)
1	H	0.79	1/3357 (0.0%)	0.96	3/4537 (0.1%)
All	All	0.73	3/26869 (0.0%)	0.96	16/36317 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374[A]	SER	CA-C	6.20	1.55	1.52
1	B	374[B]	SER	CA-C	6.20	1.55	1.52
1	H	489	PRO	CA-C	5.48	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	539	VAL	N-CA-CB	5.94	118.16	111.21
1	A	46	ASP	CA-CB-CG	5.90	118.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	46	ASP	CA-CB-CG	5.76	118.36	112.60
1	H	514	PHE	CA-CB-CG	5.76	119.56	113.80
1	G	514	PHE	CA-CB-CG	5.73	119.53	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	231	PRO	Peptide

## 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	3242	0	3315	21	0
1	B	3350	0	3417	17	0
1	C	3263	0	3325	23	0
1	D	3261	0	3321	19	0
1	E	3257	0	3323	19	0
1	F	3322	0	3388	20	0
1	G	3247	0	3304	22	0
1	H	3277	0	3341	15	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	1	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	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	6	0	0	0	0
4	A	38	22	0	1	0
4	C	38	22	0	1	0
4	E	38	22	0	1	0
4	F	38	22	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	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	252	0	0	1	0
7	B	216	0	0	0	1
7	C	344	0	0	2	0
7	D	376	0	0	0	0
7	E	266	0	0	0	1
7	F	276	0	0	0	0
7	G	388	0	0	0	0
7	H	394	0	0	1	0
All	All	29107	88	26814	127	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 2.

The worst 5 of 127 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:G:538:ARG:HG2	1:H:536:ILE:HG12	1.45	0.96
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.69	0.74
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.71	0.71
1:E:418[B]:ARG:HG3	1:F:16:LEU:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418[B]:ARG:HG3	1:B:16:LEU:HD11	1.74	0.69

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)
7:B:893:HOH:O	7:E:715:HOH:O[3_455]	2.14	0.06

## 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	428/447 (96%)	424 (99%)	3 (1%)	1 (0%)	43	34
1	B	442/447 (99%)	437 (99%)	4 (1%)	1 (0%)	43	34
1	C	428/447 (96%)	425 (99%)	2 (0%)	1 (0%)	43	34
1	D	431/447 (96%)	427 (99%)	3 (1%)	1 (0%)	43	34
1	E	428/447 (96%)	424 (99%)	3 (1%)	1 (0%)	43	34
1	F	435/447 (97%)	431 (99%)	3 (1%)	1 (0%)	43	34
1	G	426/447 (95%)	420 (99%)	5 (1%)	1 (0%)	43	34
1	H	432/447 (97%)	428 (99%)	3 (1%)	1 (0%)	43	34
All	All	3450/3576 (96%)	3416 (99%)	26 (1%)	8 (0%)	43	34

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

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Mol	Chain	Res	Type
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%)	335 (97%)	10 (3%)	37	21
1	B	353/352 (100%)	342 (97%)	11 (3%)	35	19
1	C	345/352 (98%)	337 (98%)	8 (2%)	44	30
1	D	344/352 (98%)	334 (97%)	10 (3%)	37	21
1	E	346/352 (98%)	338 (98%)	8 (2%)	44	30
1	F	350/352 (99%)	342 (98%)	8 (2%)	44	30
1	G	342/352 (97%)	332 (97%)	10 (3%)	37	21
1	H	345/352 (98%)	339 (98%)	6 (2%)	53	41
All	All	2770/2816 (98%)	2699 (97%)	71 (3%)	44	24

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

Mol	Chain	Res	Type
1	G	76[B]	MET
1	G	358	SER
1	H	68	ARG
1	C	270[A]	LEU
1	C	76[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	405	GLN
1	F	405	GLN
1	H	405	GLN
1	G	275	HIS

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Mol	Chain	Res	Type
1	C	275	HIS

### 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
4	I7N	F	602	6	41,41,41	0.34	0	60,62,62	0.67	1 (1%)
2	FBP	G	601	-	18,20,20	0.72	1 (5%)	21,32,32	0.76	0
3	OXL	C	603	5	5,5,5	1.87	2 (40%)	6,6,6	1.85	1 (16%)
3	OXL	E	602	5	5,5,5	2.33	2 (40%)	6,6,6	1.83	2 (33%)
2	FBP	F	601	-	18,20,20	0.52	0	21,32,32	0.53	0
4	I7N	A	603	-	41,41,41	0.31	0	60,62,62	0.56	1 (1%)
3	OXL	H	602	5	5,5,5	2.35	3 (60%)	6,6,6	1.84	1 (16%)
3	OXL	A	602	5	5,5,5	2.34	3 (60%)	6,6,6	2.13	3 (50%)
2	FBP	A	601	-	18,20,20	0.53	0	21,32,32	0.61	0
2	FBP	E	601	-	18,20,20	0.73	0	21,32,32	0.71	1 (4%)
2	FBP	H	601	-	18,20,20	0.97	1 (5%)	21,32,32	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FBP	C	601	-	18,20,20	0.98	2 (11%)	21,32,32	0.78	0
4	I7N	E	603	-	41,41,41	0.31	0	60,62,62	0.53	1 (1%)
3	OXL	B	602	5	5,5,5	2.37	2 (40%)	6,6,6	1.70	2 (33%)
3	OXL	D	602	5	5,5,5	2.43	3 (60%)	6,6,6	2.18	2 (33%)
3	OXL	F	603	5	5,5,5	3.10	4 (80%)	6,6,6	2.36	3 (50%)
2	FBP	B	601	-	18,20,20	0.79	1 (5%)	21,32,32	0.74	1 (4%)
4	I7N	C	602	-	41,41,41	0.30	0	60,62,62	0.79	2 (3%)
2	FBP	D	601	-	18,20,20	0.67	0	21,32,32	0.87	1 (4%)
3	OXL	G	602	5	5,5,5	2.20	2 (40%)	6,6,6	2.00	2 (33%)

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	I7N	F	602	6	-	6/28/54/54	0/4/4/4
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	C	603	5	-	4/4/4/4	-
3	OXL	E	602	5	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
4	I7N	A	603	-	-	7/28/54/54	0/4/4/4
3	OXL	H	602	5	-	4/4/4/4	-
3	OXL	A	602	5	-	4/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
4	I7N	E	603	-	-	11/28/54/54	0/4/4/4
3	OXL	B	602	5	-	4/4/4/4	-
3	OXL	D	602	5	-	4/4/4/4	-
3	OXL	F	603	5	-	4/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
4	I7N	C	602	-	-	14/28/54/54	1/4/4/4
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	G	602	5	-	4/4/4/4	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O1-C1	4.69	1.34	1.22
3	A	602	OXL	O2-C2	4.13	1.32	1.22
3	B	602	OXL	O2-C2	4.09	1.32	1.22
3	F	603	OXL	O2-C2	3.79	1.31	1.22
3	G	602	OXL	O3-C1	-3.52	1.21	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	I7N	C23-C17-C18	4.66	118.82	110.07
3	F	603	OXL	O4-C2-C1	4.11	120.80	112.83
3	H	602	OXL	O4-C2-C1	3.97	120.53	112.83
3	C	603	OXL	O3-C1-C2	3.91	120.42	112.83
3	A	602	OXL	O4-C2-C1	3.75	120.11	112.83

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	I7N	C20-C19-C21-C22
4	A	603	I7N	C1-C-S-O10
4	A	603	I7N	C1-C-S-O
4	C	602	I7N	C23-N-S-C
4	C	602	I7N	C1-C-S-O10

All (1) ring outliers are listed below:

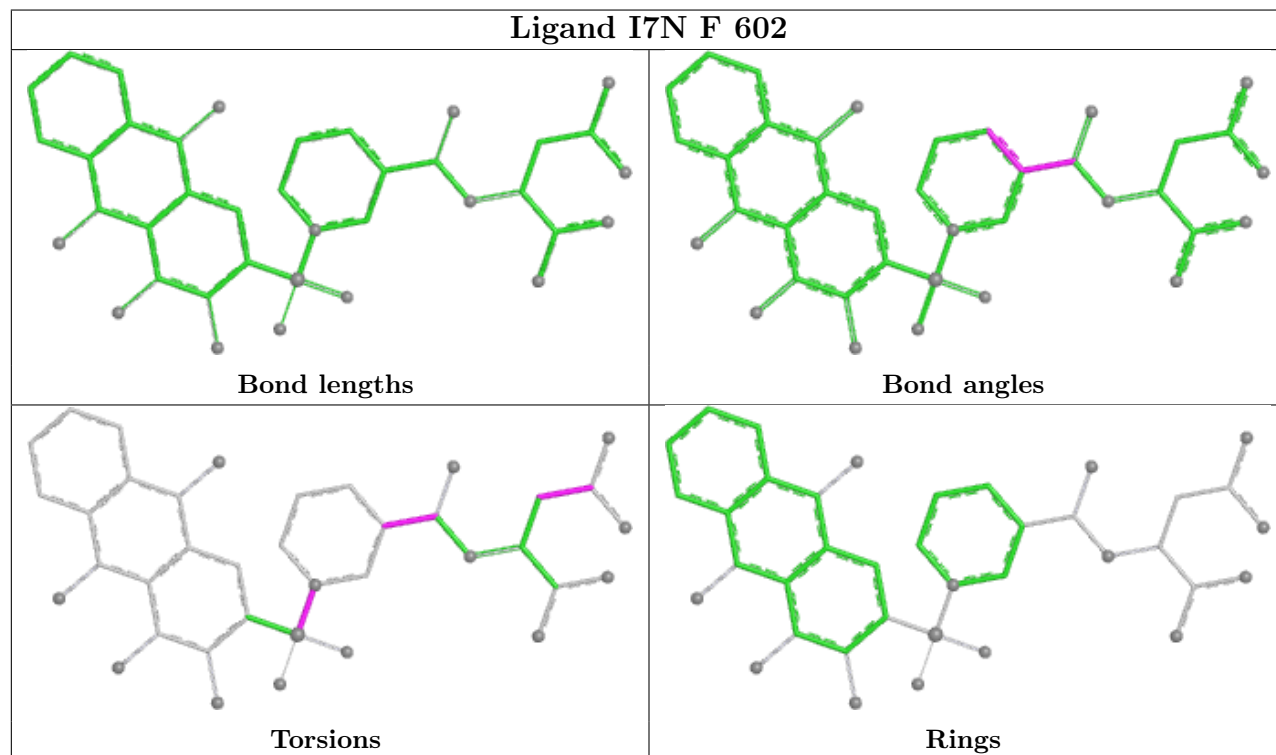
Mol	Chain	Res	Type	Atoms
4	C	602	I7N	C14-C15-C16-C17-C23-N

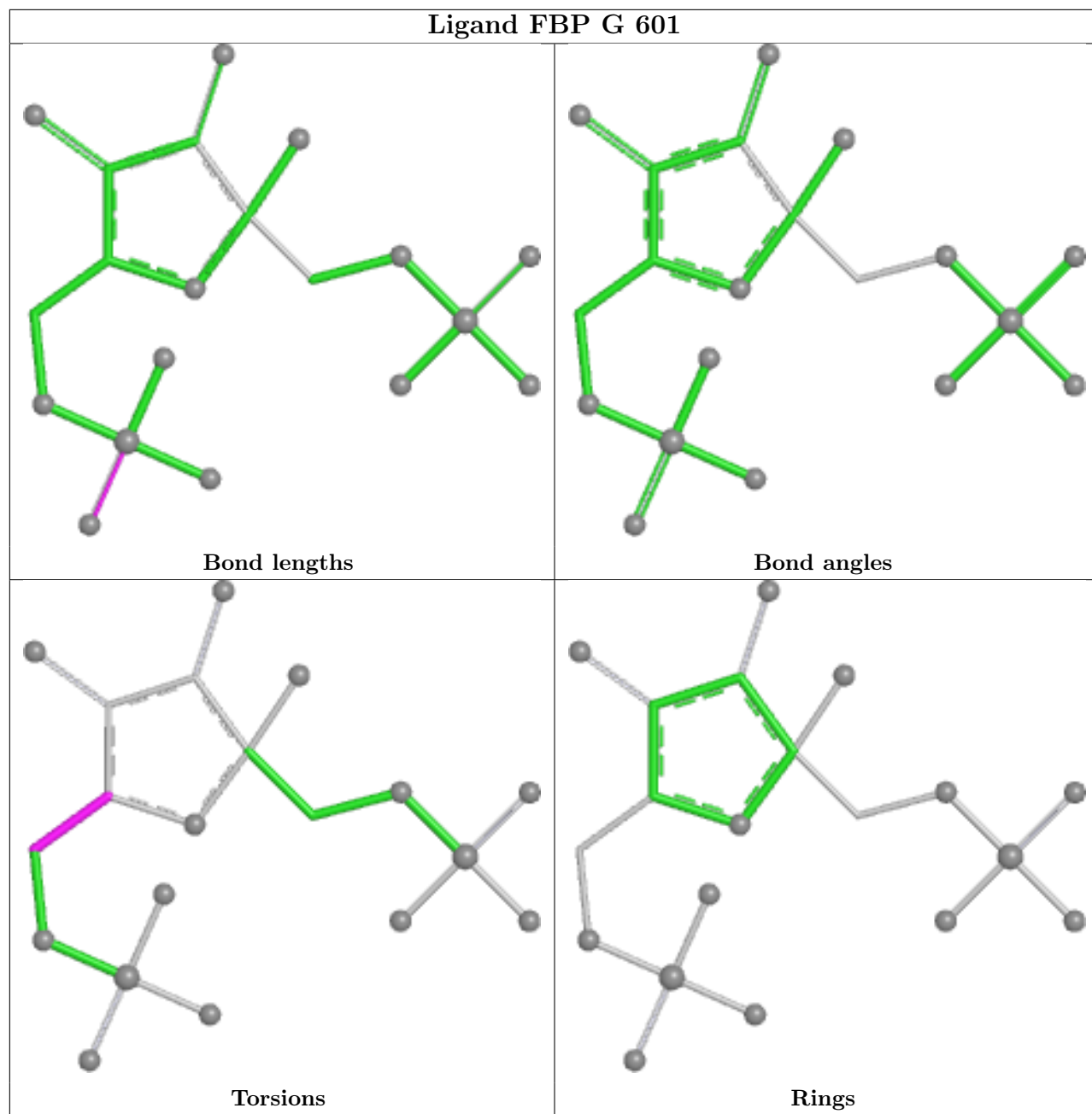
5 monomers are involved in 5 short contacts:

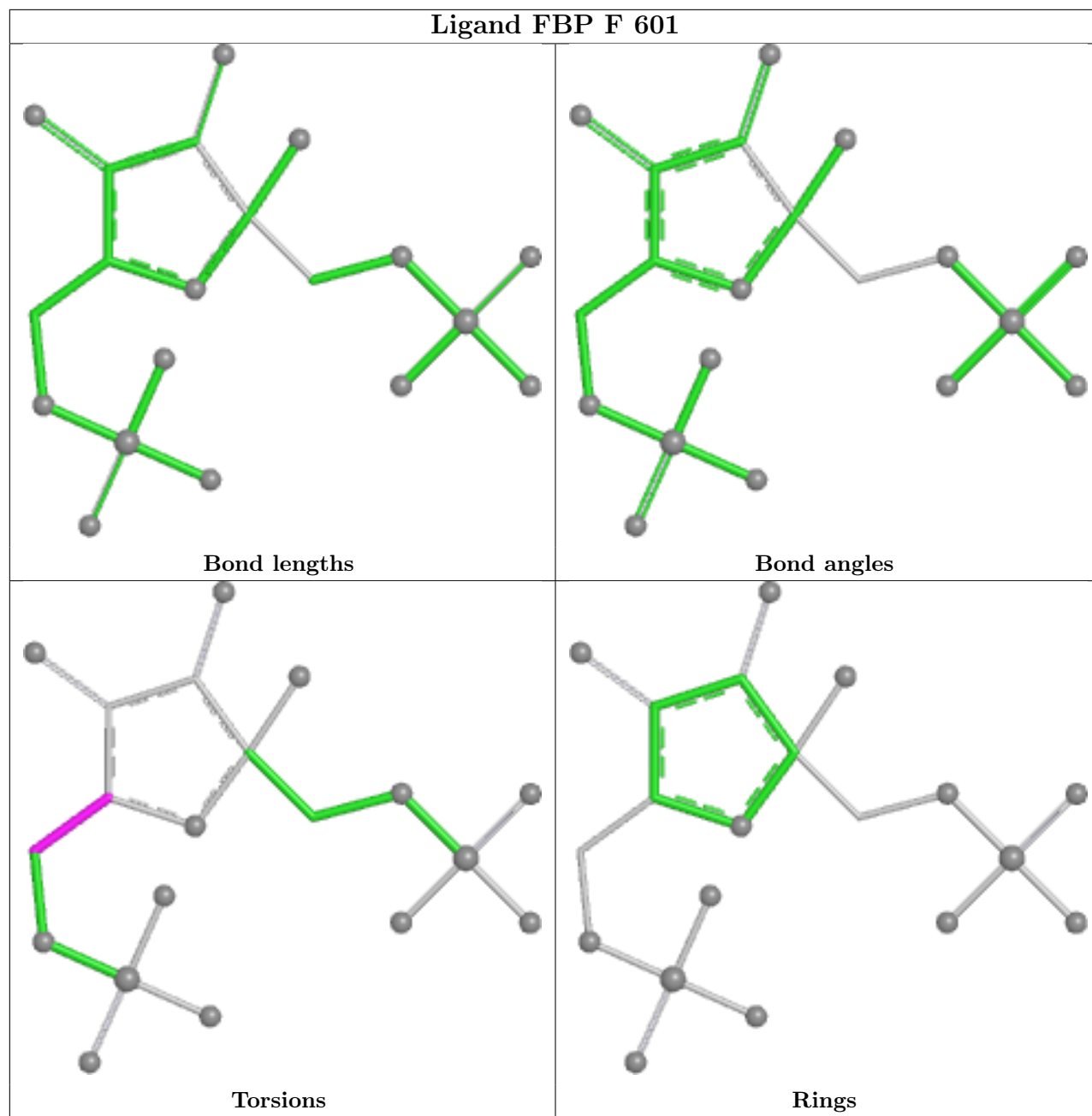
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	OXL	1	0
4	A	603	I7N	1	0
4	E	603	I7N	1	0
4	C	602	I7N	1	0
3	G	602	OXL	1	0

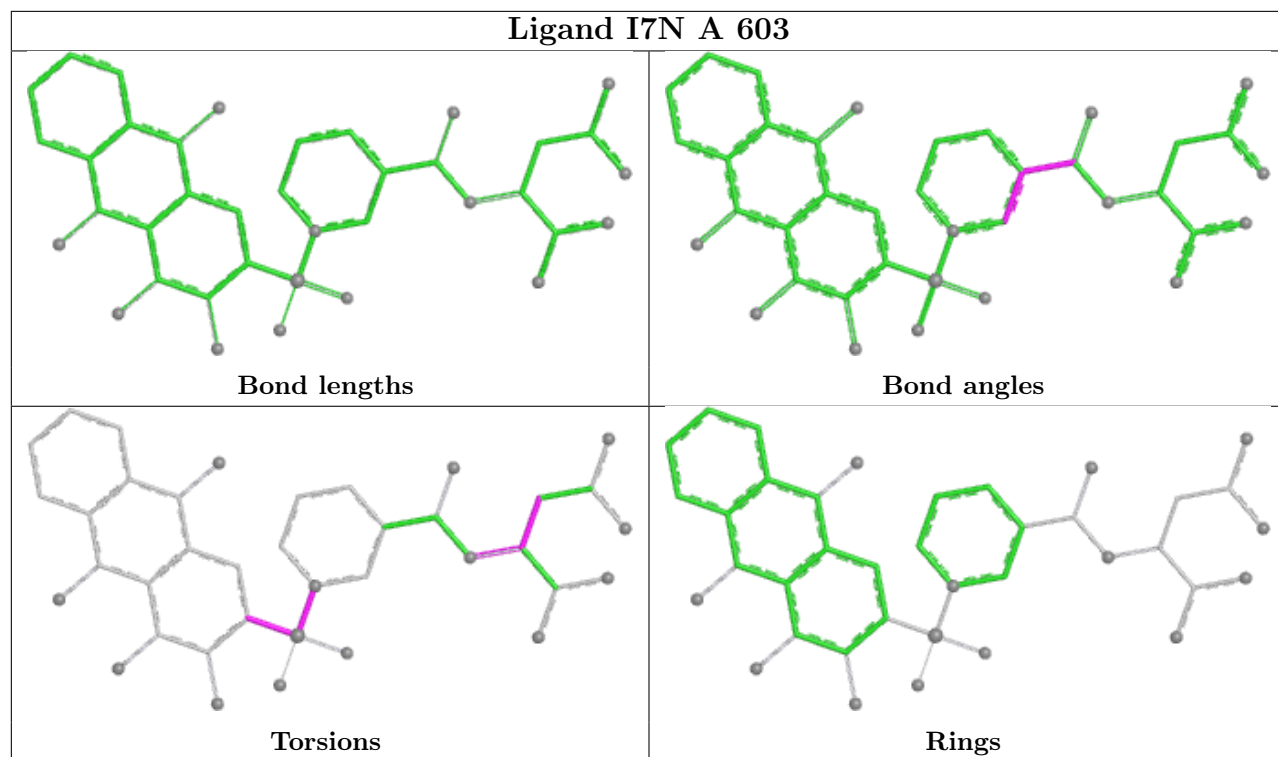
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

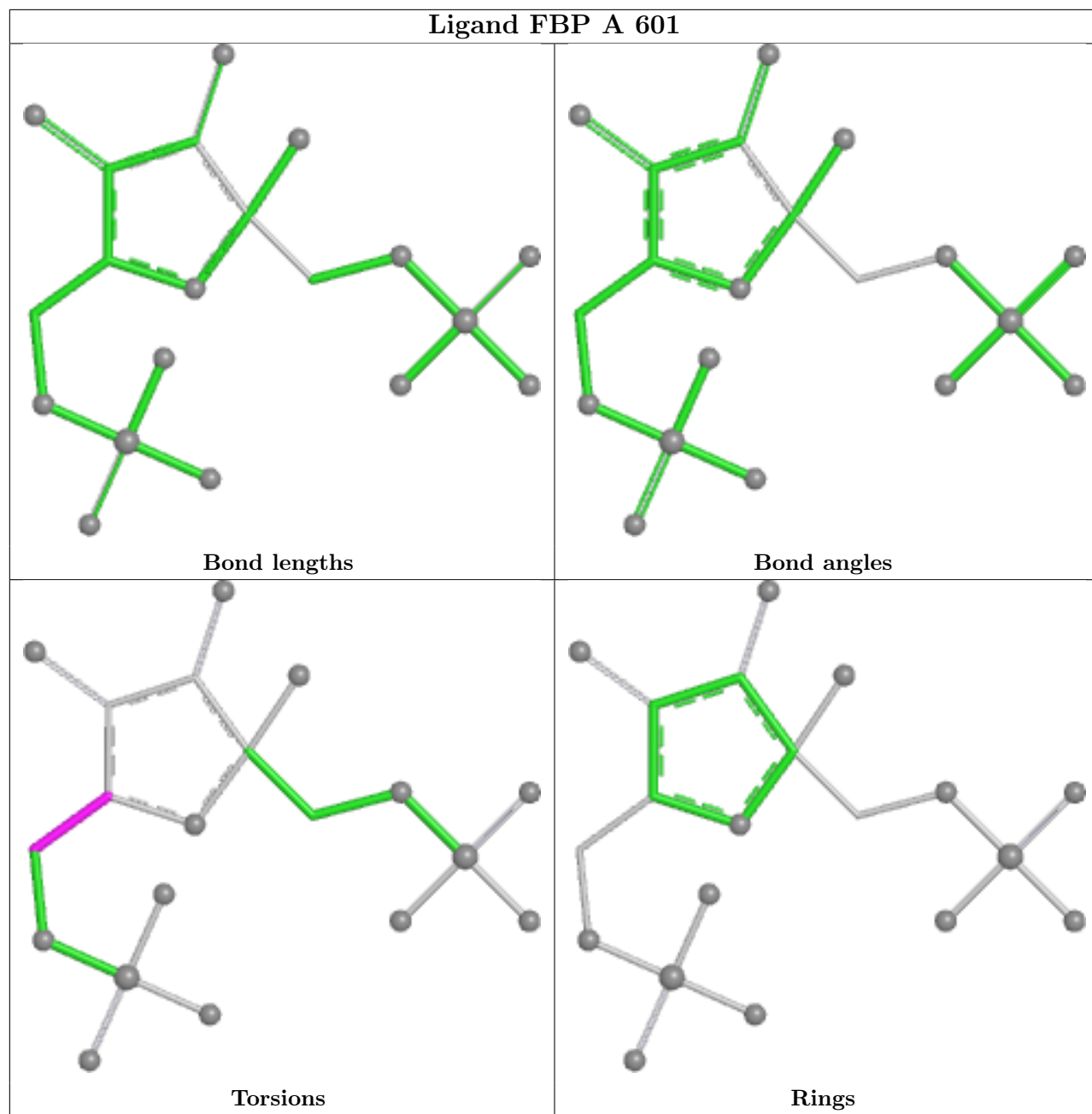
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

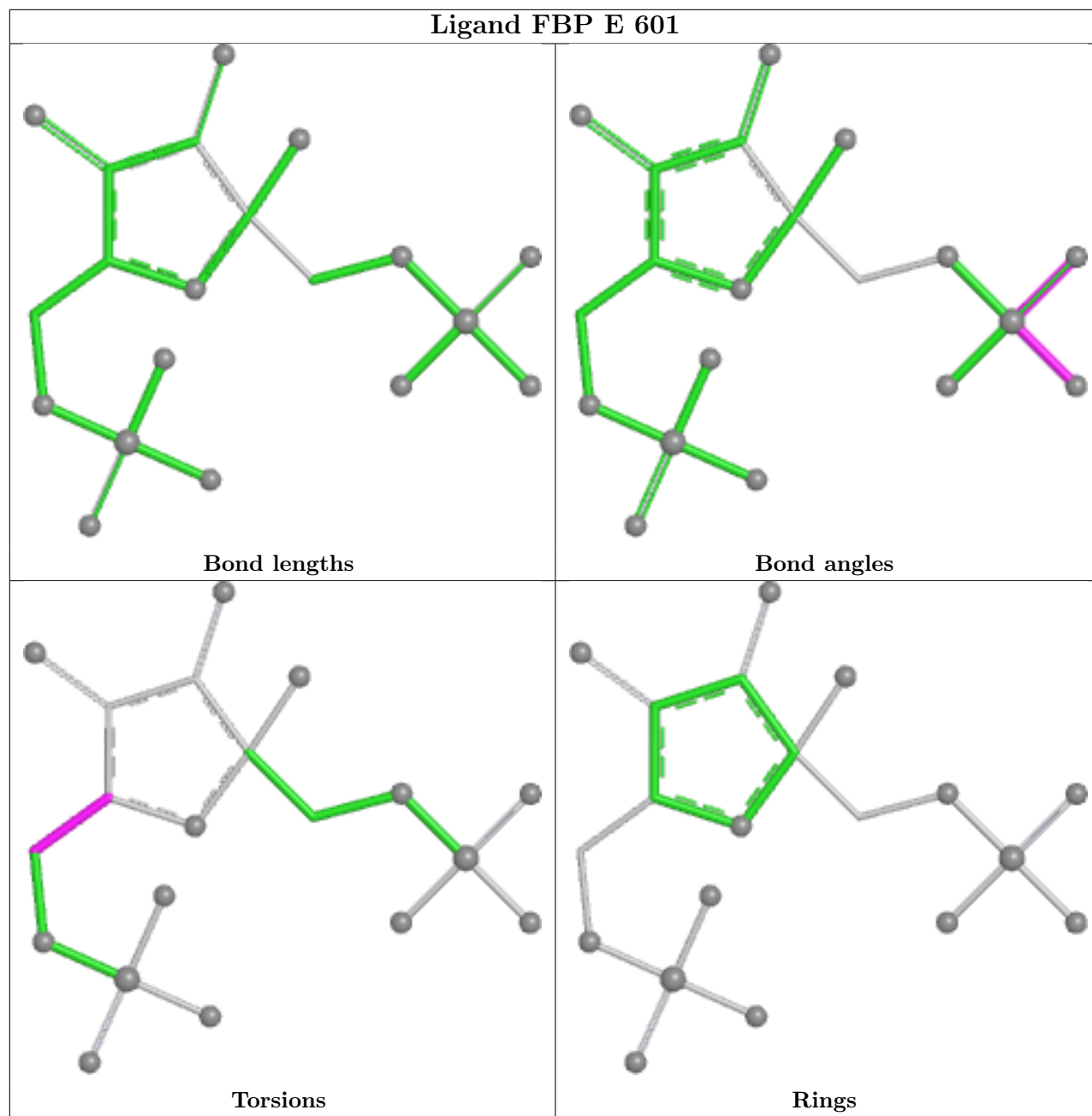


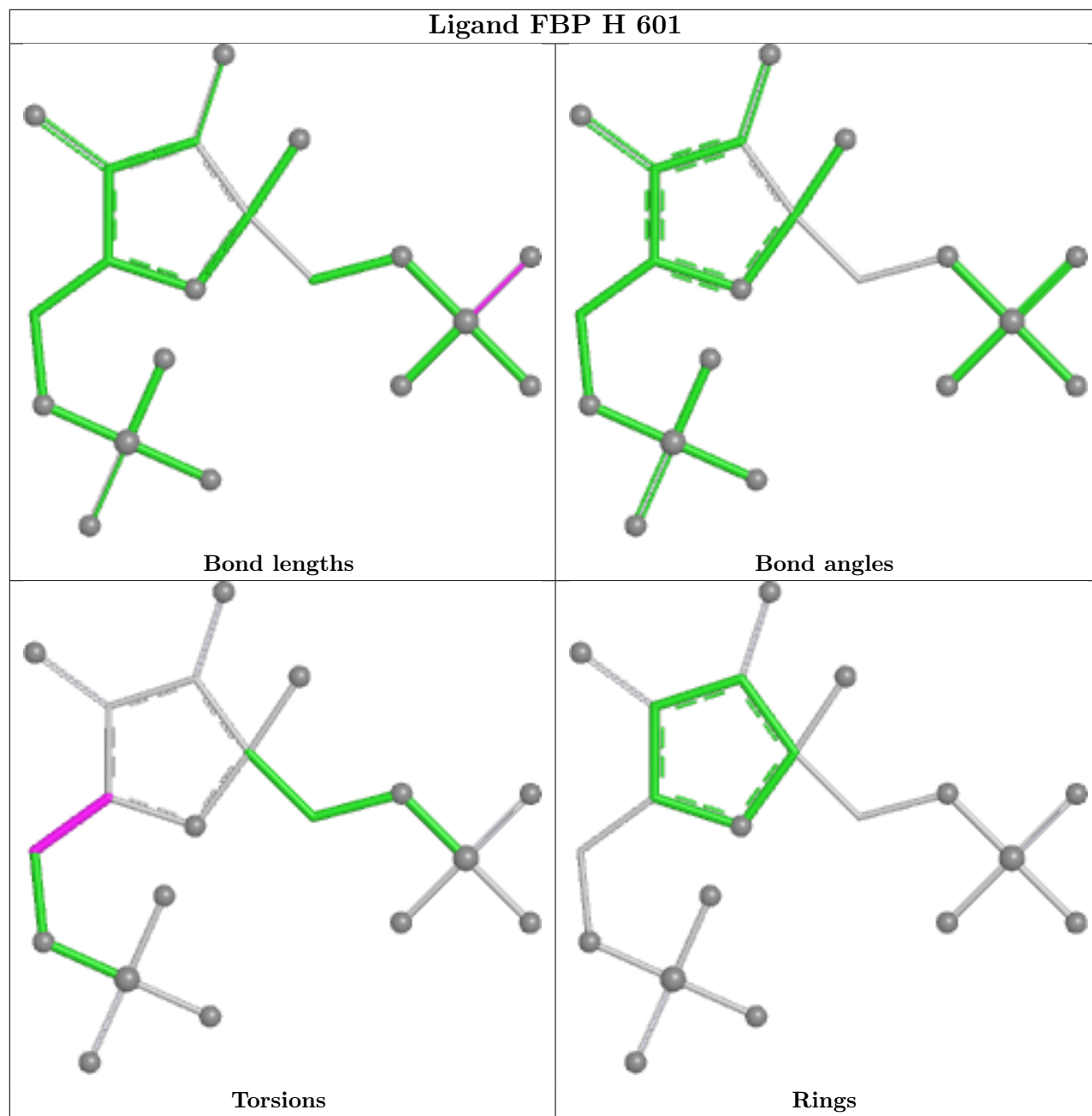


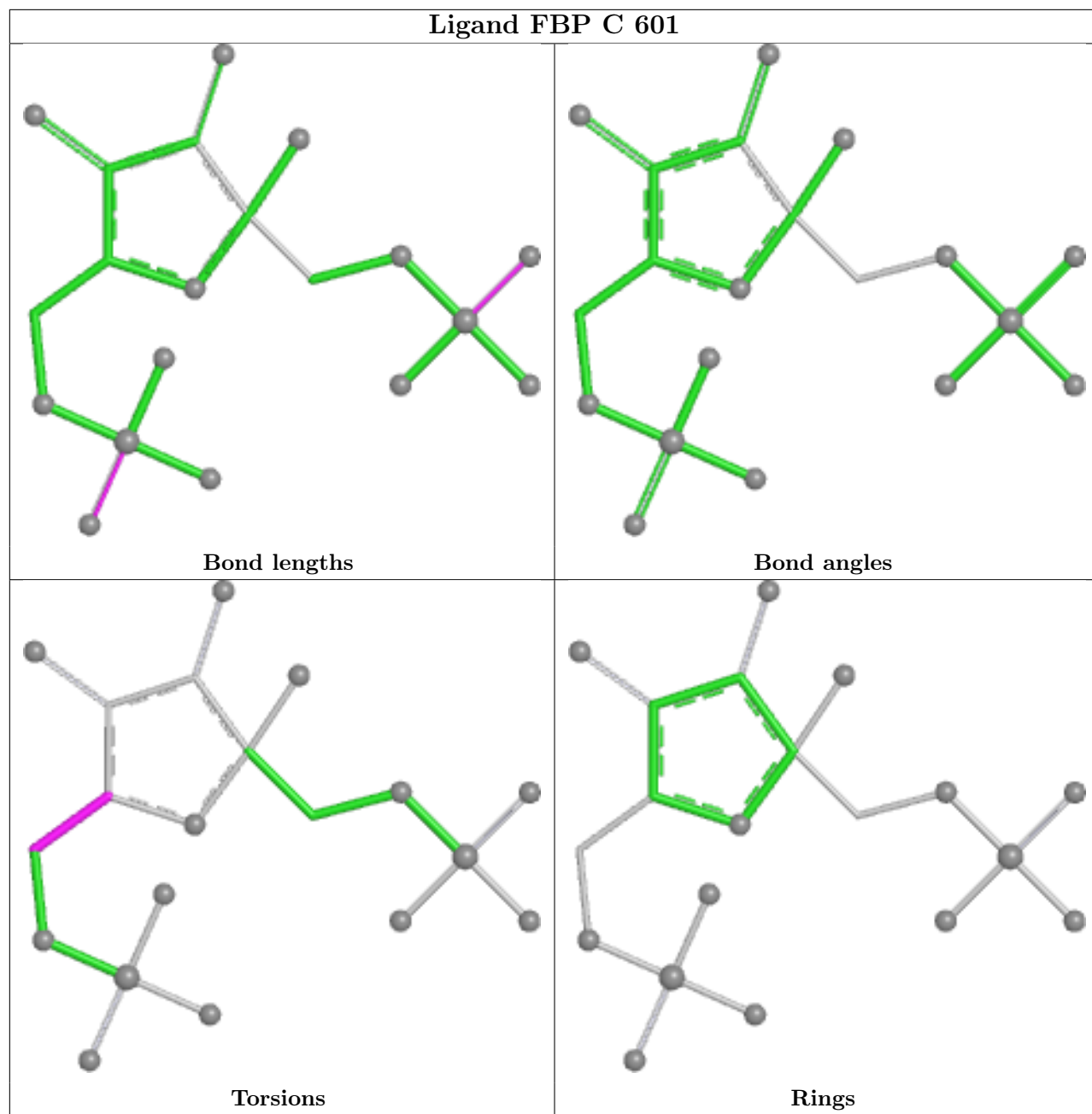


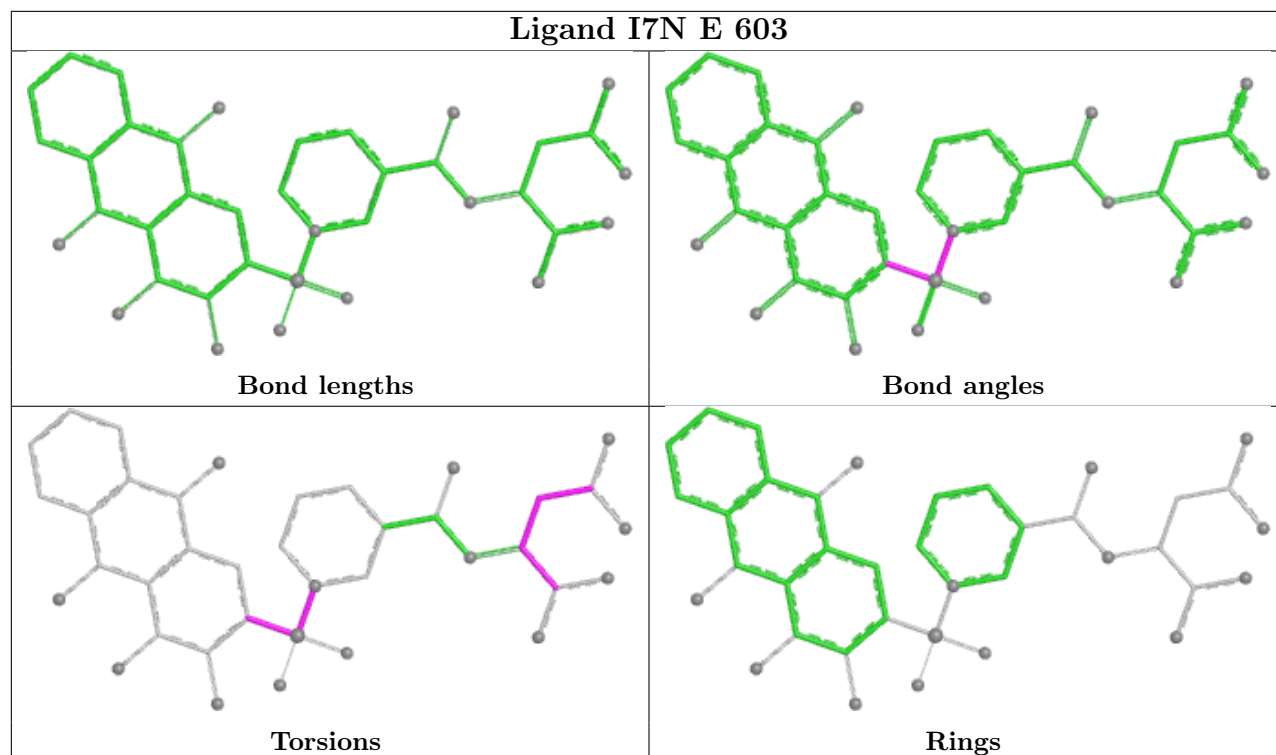


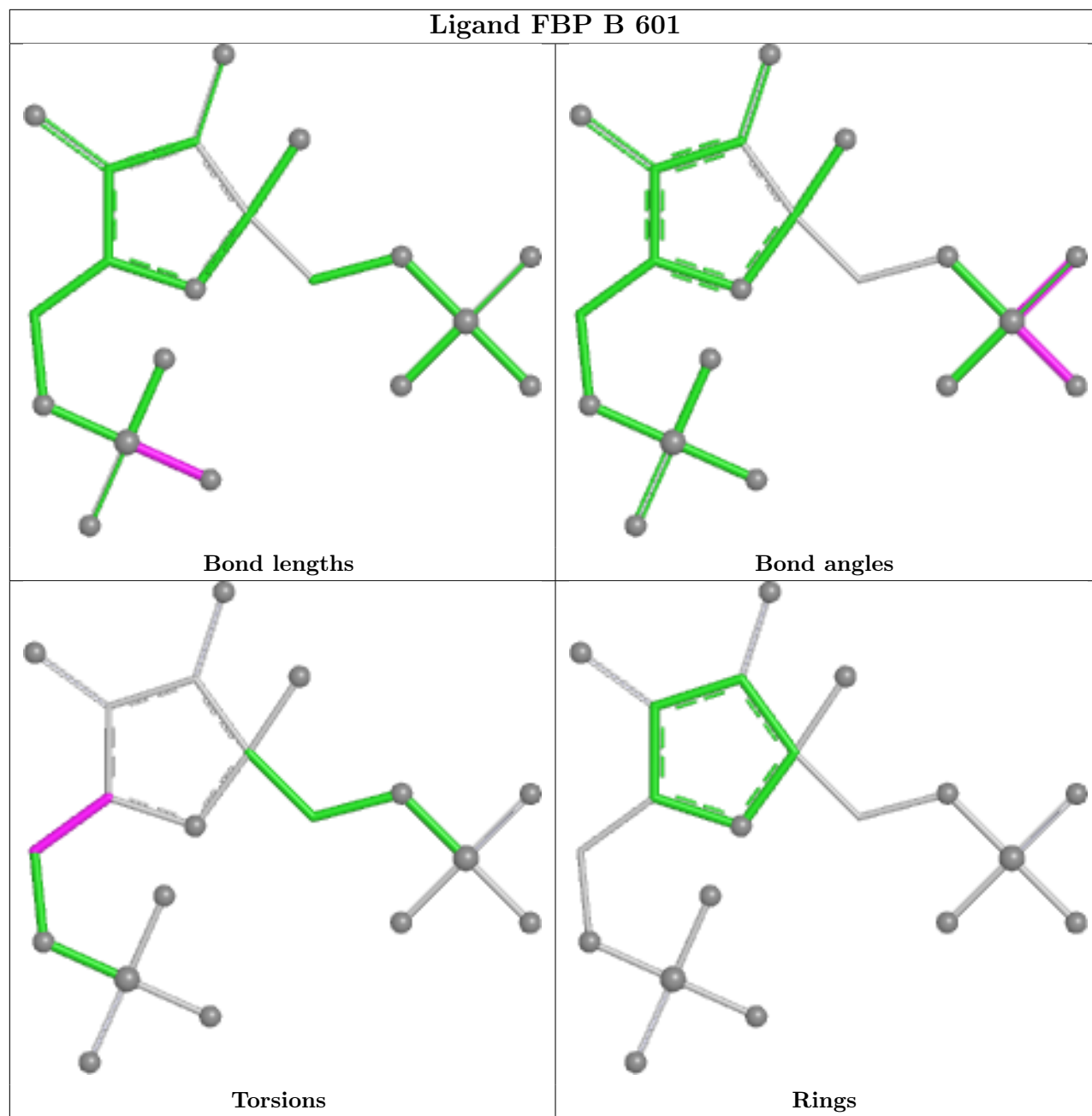


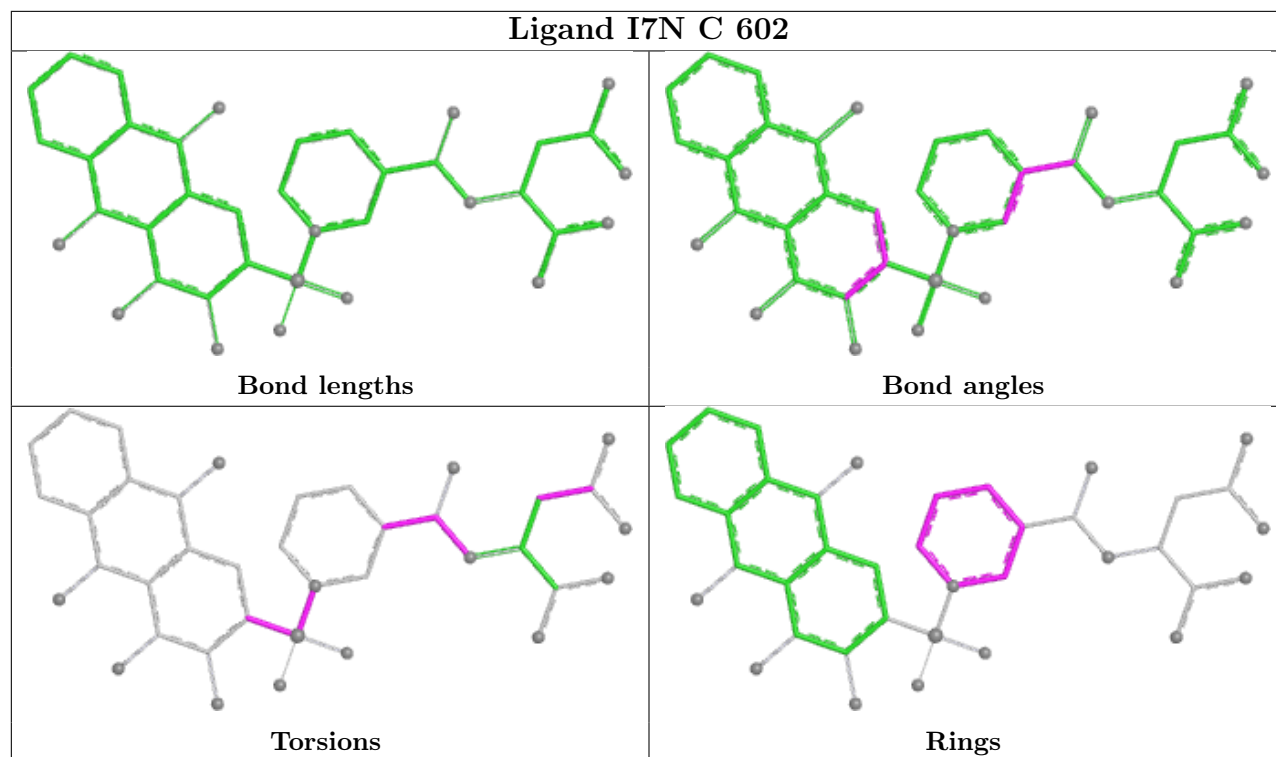


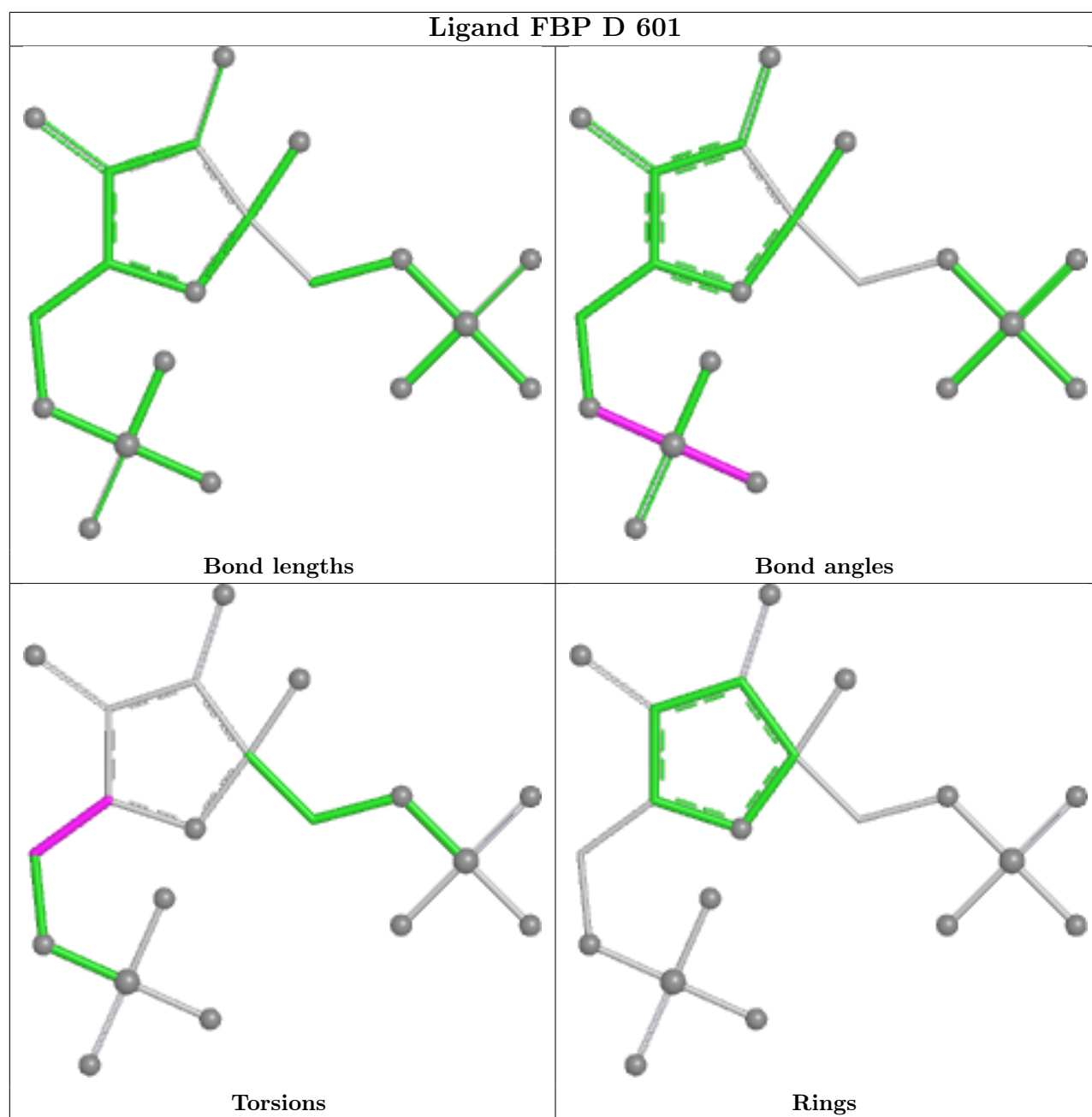












## 5.7 Other polymers [i](#)

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	419/447 (93%)	0.69	27 (6%) 25 29	21, 39, 61, 78	13 (3%)
1	B	436/447 (97%)	1.24	113 (25%) 1 2	20, 44, 75, 90	8 (1%)
1	C	424/447 (94%)	0.16	21 (4%) 34 38	20, 30, 51, 93	8 (1%)
1	D	425/447 (95%)	0.07	13 (3%) 51 56	14, 29, 51, 90	8 (1%)
1	E	419/447 (93%)	0.57	28 (6%) 24 28	20, 38, 62, 74	13 (3%)
1	F	432/447 (96%)	0.50	34 (7%) 18 22	20, 35, 59, 75	7 (1%)
1	G	423/447 (94%)	0.03	12 (2%) 55 61	16, 29, 44, 70	8 (1%)
1	H	425/447 (95%)	-0.06	14 (3%) 49 54	13, 27, 48, 70	9 (2%)
All	All	3403/3576 (95%)	0.40	262 (7%) 19 23	13, 34, 60, 93	74 (2%)

The worst 5 of 262 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	11.4
1	B	511	LEU	9.6
1	G	271	GLY	6.7
1	A	543	SER	6.7
1	F	115	LEU	5.9

### 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](#)

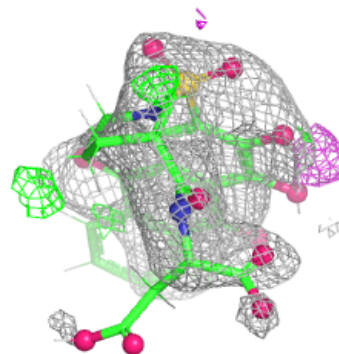
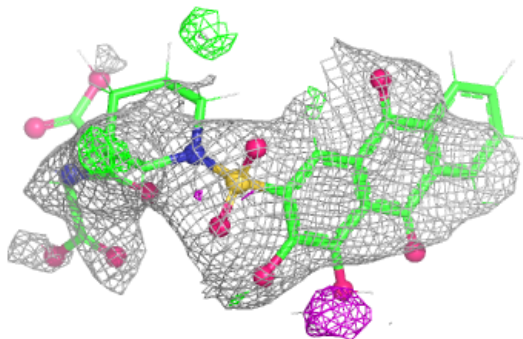
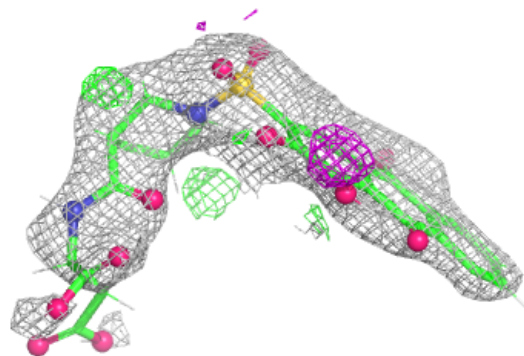
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	I7N	A	603	38/38	0.76	0.19	98,98,99,99	22
4	I7N	C	602	38/38	0.76	0.20	75,80,86,86	22
4	I7N	F	602	38/38	0.78	0.21	75,82,85,85	22
4	I7N	E	603	38/38	0.85	0.14	67,73,78,78	22
3	OXL	C	603	6/6	0.85	0.12	46,47,47,48	0
3	OXL	F	603	6/6	0.86	0.10	44,44,45,46	0
3	OXL	E	602	6/6	0.87	0.11	47,48,48,48	0
3	OXL	B	602	6/6	0.87	0.12	55,55,57,57	0
3	OXL	D	602	6/6	0.88	0.10	39,39,40,40	0
3	OXL	H	602	6/6	0.88	0.13	34,35,37,38	0
3	OXL	G	602	6/6	0.90	0.09	35,36,38,38	0
3	OXL	A	602	6/6	0.90	0.10	44,45,46,47	0
6	K	E	605	1/1	0.92	0.15	67,67,67,67	0
6	K	F	605	1/1	0.94	0.10	70,70,70,70	0
6	K	B	604	1/1	0.95	0.12	77,77,77,77	0
5	MG	A	604	1/1	0.95	0.06	50,50,50,50	0
6	K	A	605	1/1	0.95	0.10	64,64,64,64	0
2	FBP	B	601	20/20	0.96	0.07	36,37,40,40	0
6	K	C	605	1/1	0.96	0.14	50,50,50,50	0
5	MG	B	603	1/1	0.97	0.06	54,54,54,54	0
2	FBP	F	601	20/20	0.97	0.06	31,35,39,40	0
2	FBP	A	601	20/20	0.97	0.05	32,34,36,36	0
2	FBP	H	601	20/20	0.98	0.04	19,21,22,22	0
2	FBP	E	601	20/20	0.98	0.05	32,33,34,35	0
5	MG	F	604	1/1	0.99	0.05	37,37,37,37	0
5	MG	H	603	1/1	0.99	0.02	35,35,35,35	0
2	FBP	C	601	20/20	0.99	0.04	22,23,24,25	0
2	FBP	D	601	20/20	0.99	0.04	22,23,24,25	0
2	FBP	G	601	20/20	0.99	0.04	20,21,23,23	0
6	K	D	604	1/1	0.99	0.05	37,37,37,37	0
5	MG	D	603	1/1	0.99	0.02	33,33,33,33	0
5	MG	E	604	1/1	0.99	0.03	47,47,47,47	0
6	K	G	604	1/1	0.99	0.13	45,45,45,45	0
6	K	H	604	1/1	0.99	0.08	40,40,40,40	0
5	MG	G	603	1/1	1.00	0.03	34,34,34,34	0
5	MG	C	604	1/1	1.00	0.02	37,37,37,37	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.

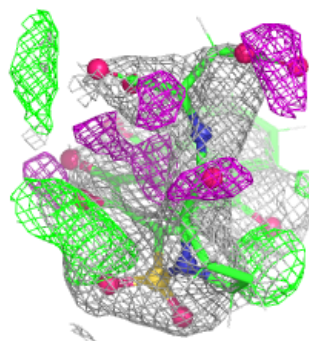
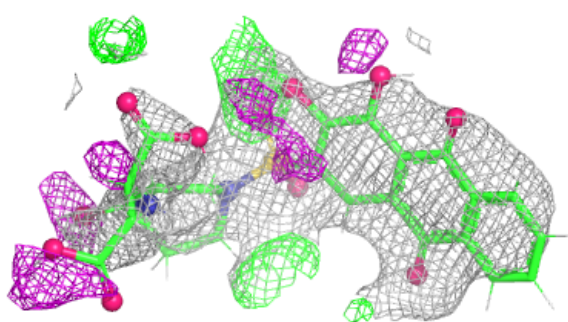
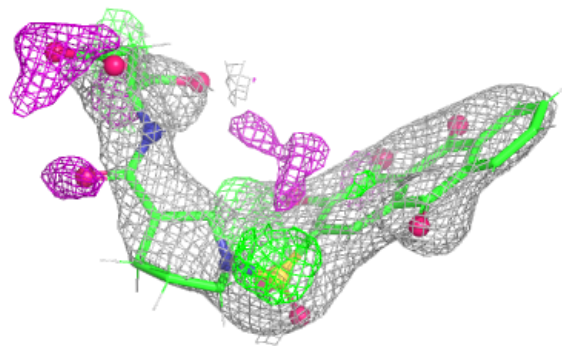
**Electron density around I7N A 603:**

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

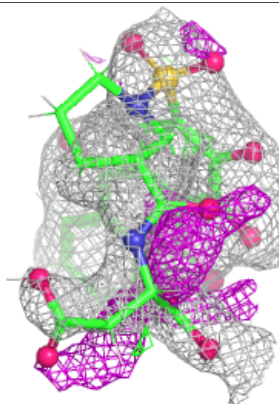
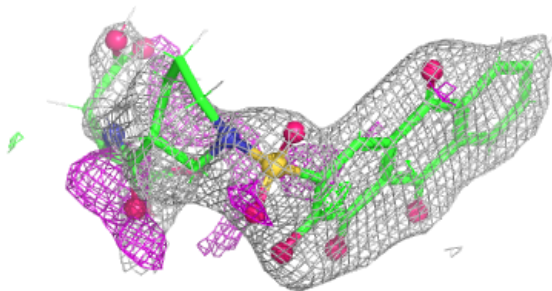
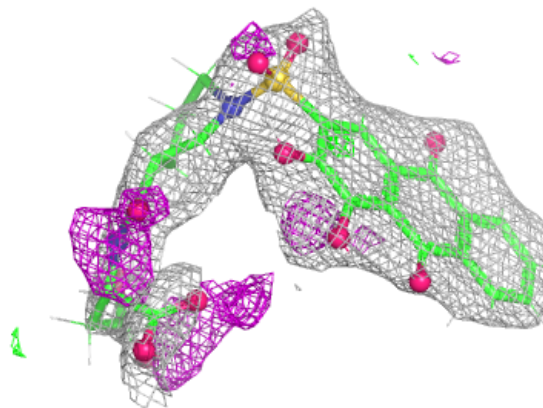


**Electron density around I7N C 602:**

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

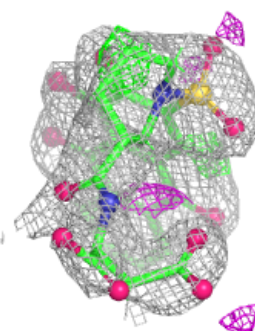
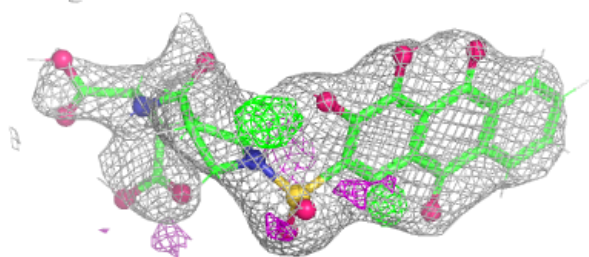
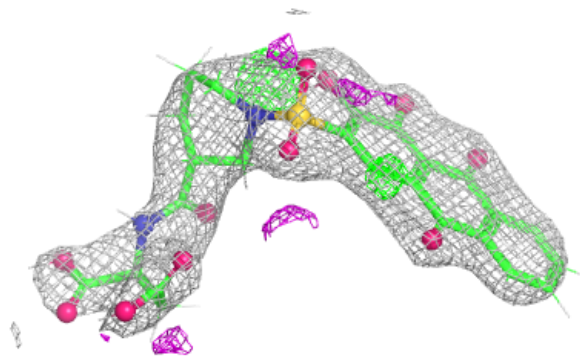
**Electron density around I7N F 602:**

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

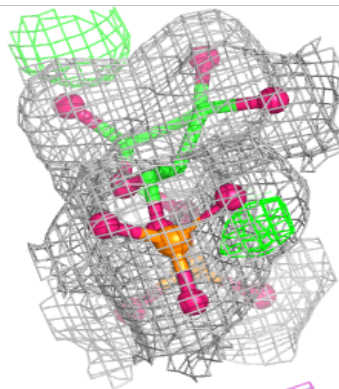
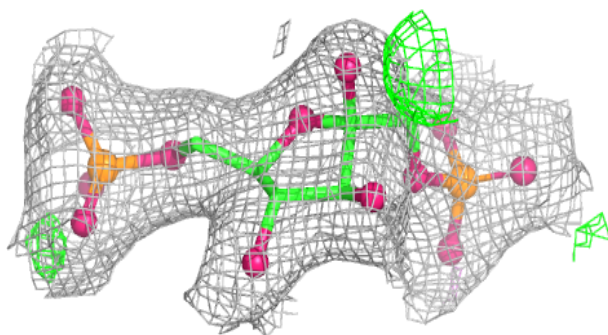
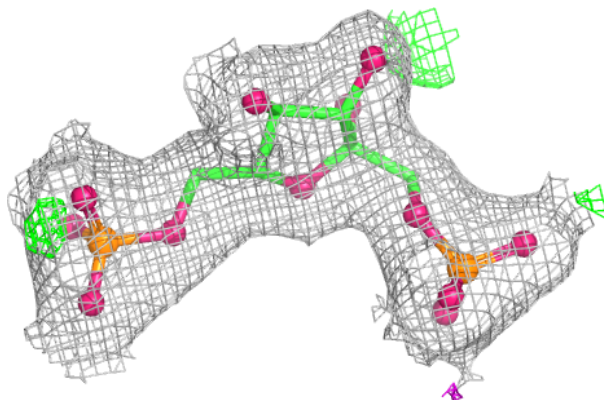


**Electron density around I7N E 603:**

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

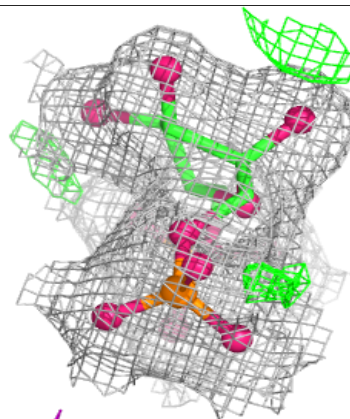
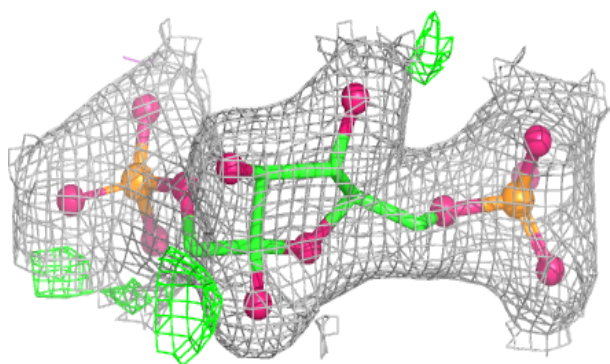
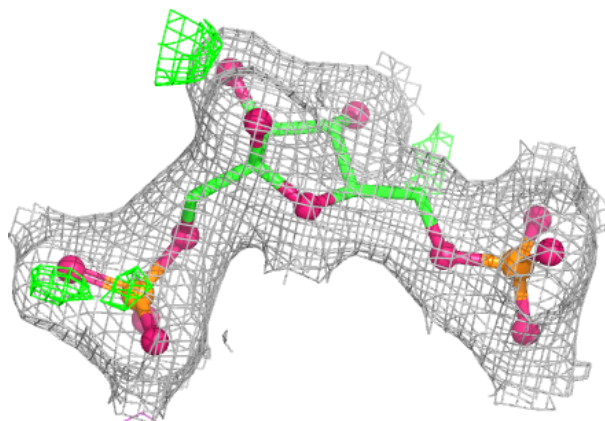
**Electron density around FBP B 601:**

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

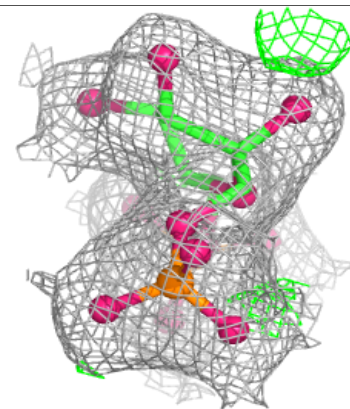
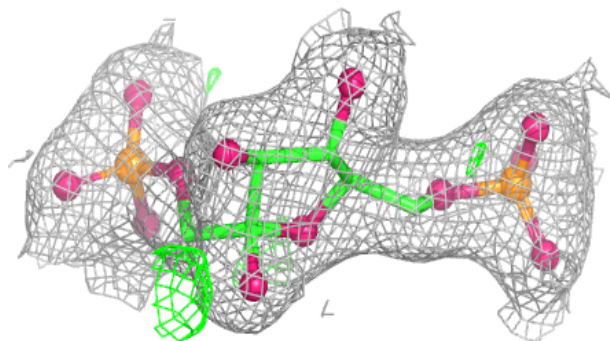
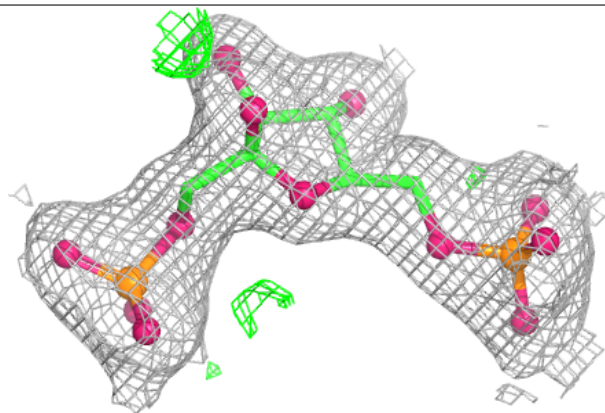


**Electron density around FBP F 601:**

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

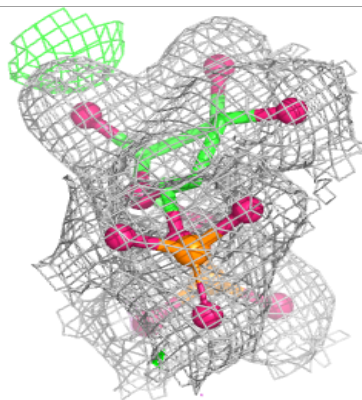
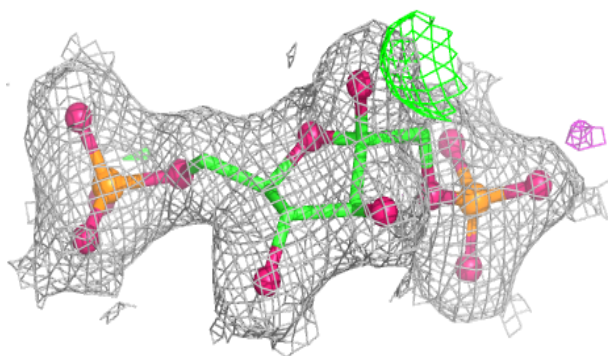
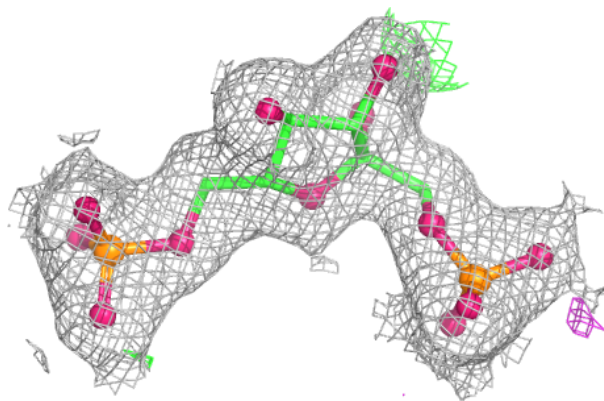
**Electron density around FBP A 601:**

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

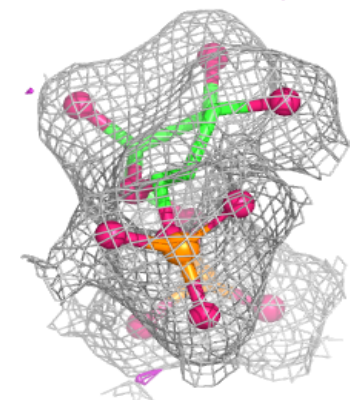
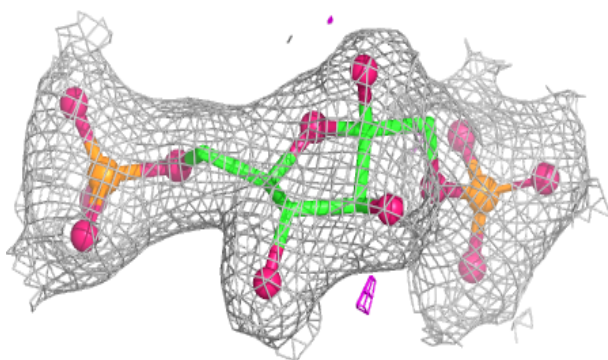
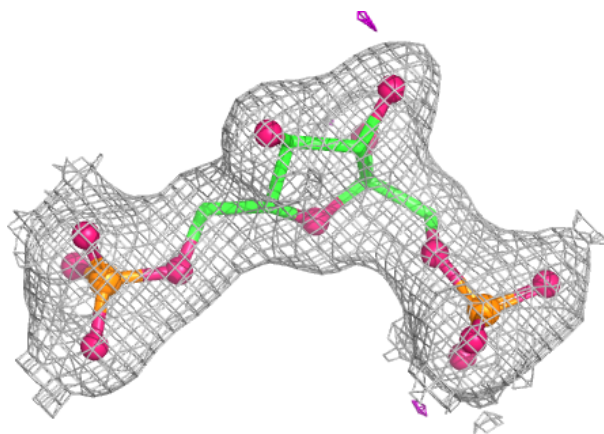


**Electron density around FBP H 601:**

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

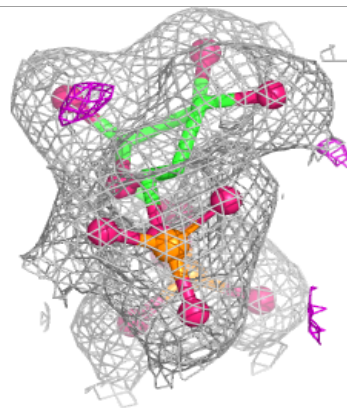
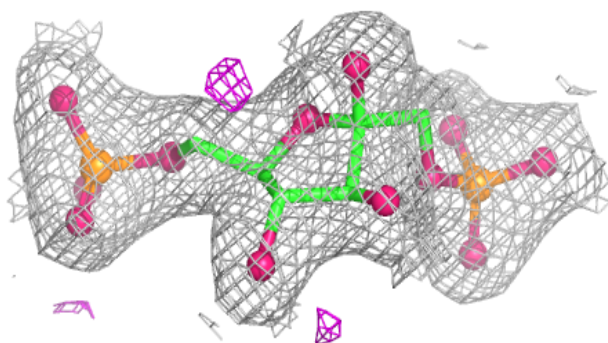
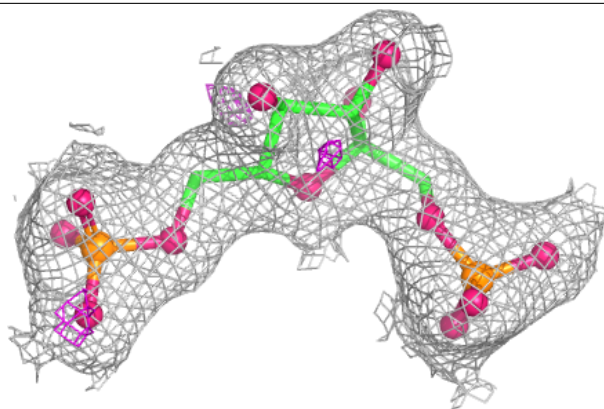
**Electron density around FBP E 601:**

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

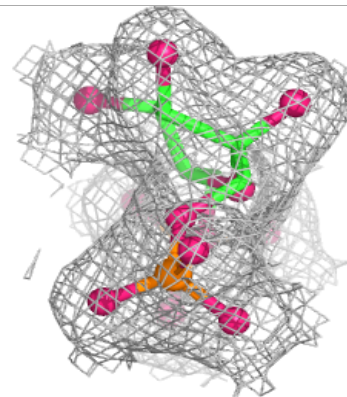
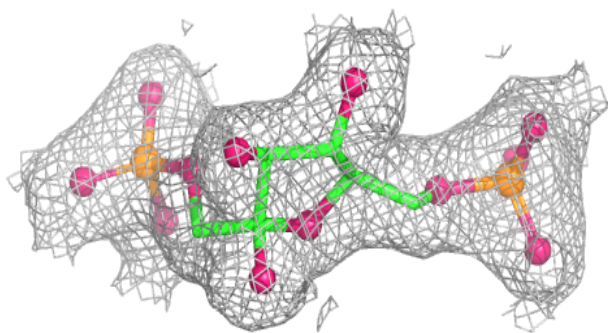
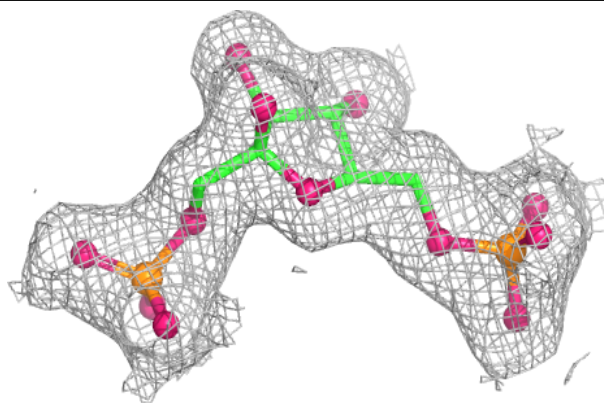


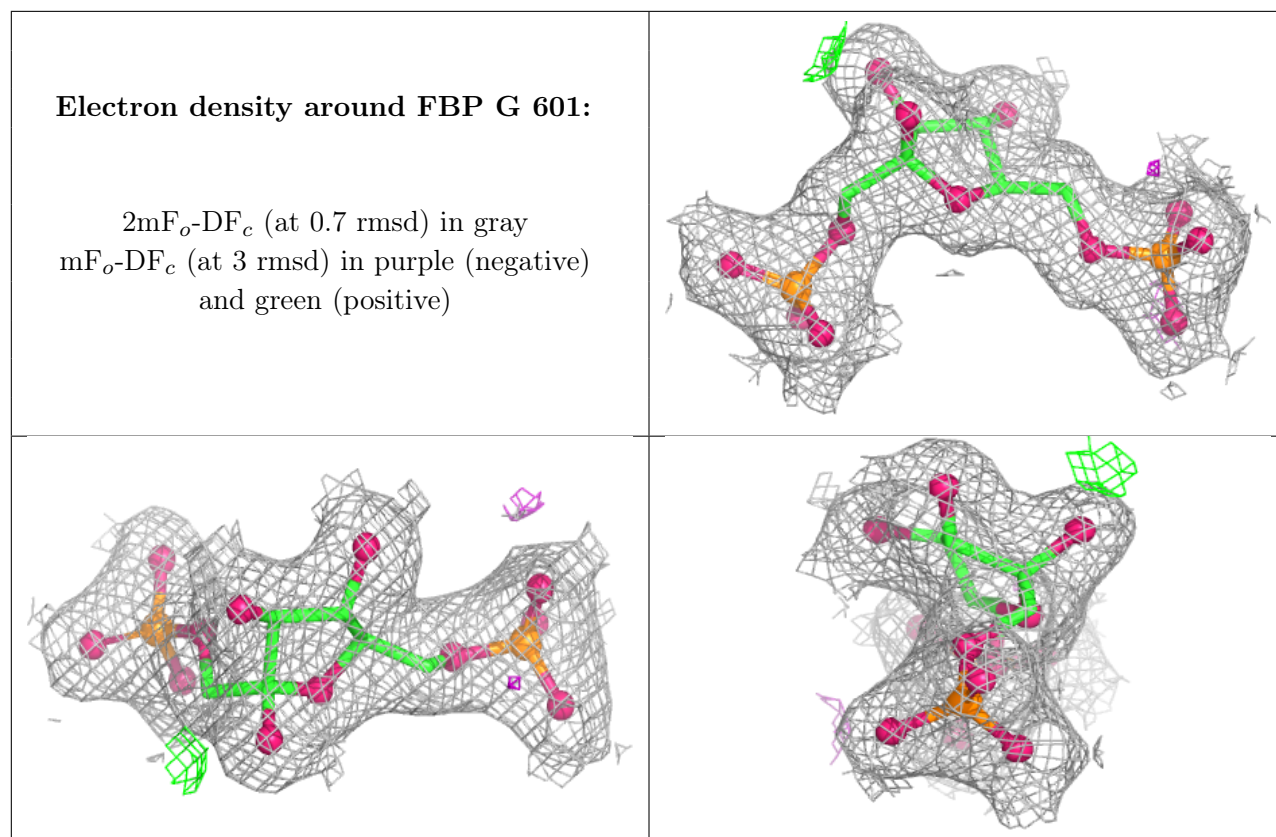
**Electron density around FBP C 601:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.