



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 06:57 PM JST

PDB ID : 5X1V  
Title : PKM2 in complex with compound 2  
Authors : Matsui, Y.; Hanzawa, H.  
Deposited on : 2017-01-27  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

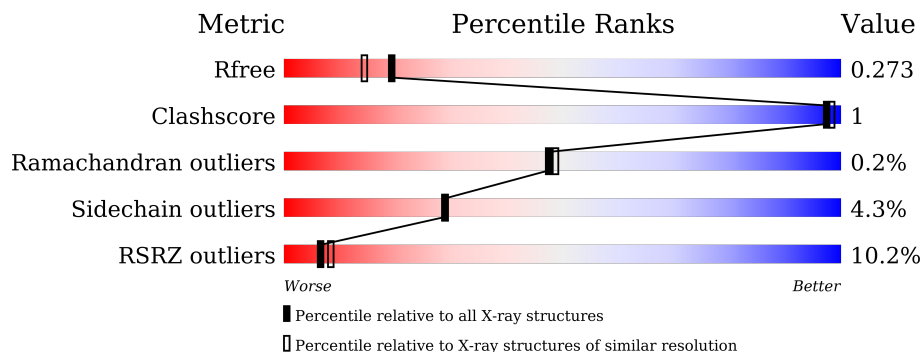
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	550	
1	B	550	
1	C	550	
1	D	550	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 16367 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	512	3919	2463	696	735	25	0	0	0
1	B	513	3935	2475	698	737	25	0	0	0
1	C	518	3965	2492	704	744	25	0	0	0
1	D	511	3919	2463	696	735	25	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

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

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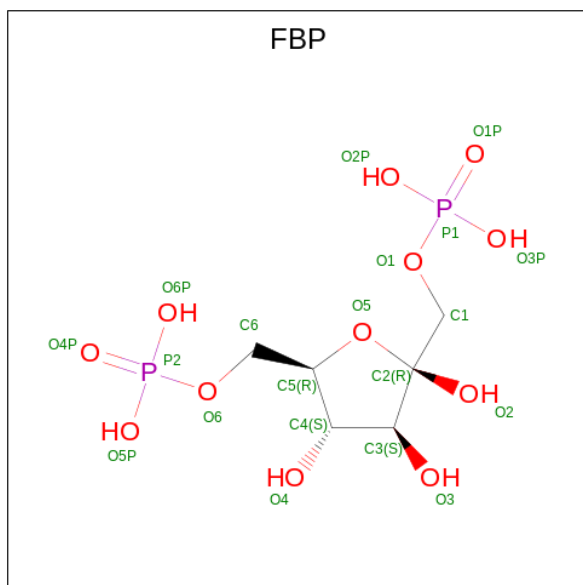
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag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

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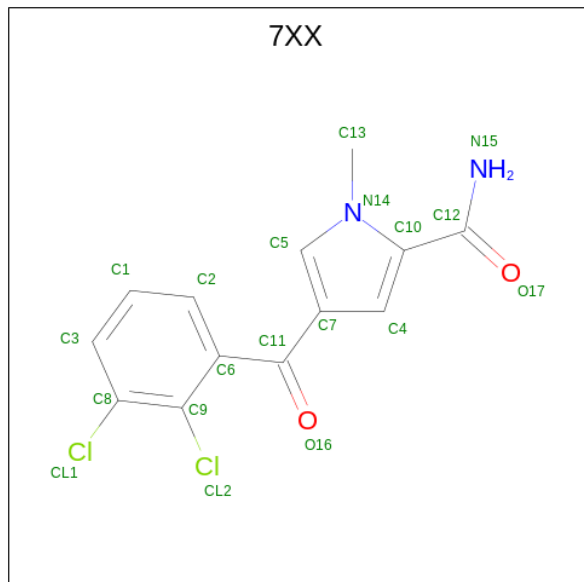
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618

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



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

- Molecule 3 is 4-[2,3-bis(chloranyl)phenyl]carbonyl-1-methyl-pyrrole-2-carboxamide (three-letter code: 7XX) (formula: C<sub>13</sub>H<sub>10</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
3	A	1	Total 19	C 13	Cl 2	N 2	O 2	0	0
3	B	1	Total 19	C 13	Cl 2	N 2	O 2	0	0
3	C	1	Total 19	C 13	Cl 2	N 2	O 2	0	0
3	D	1	Total 19	C 13	Cl 2	N 2	O 2	0	0

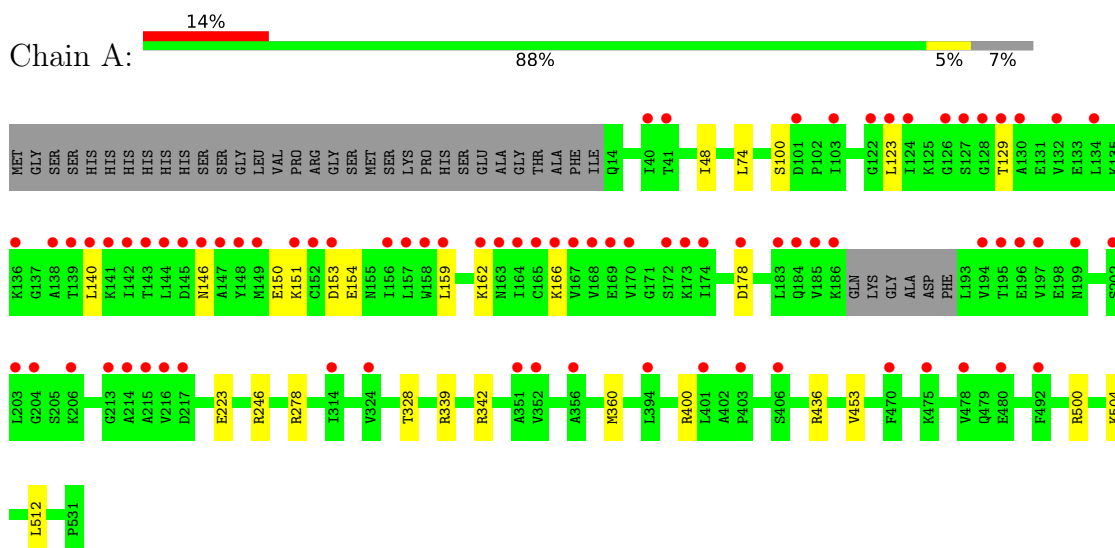
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total 94	O 94	0	0
4	B	120	Total 120	O 120	0	0
4	C	127	Total 127	O 127	0	0
4	D	132	Total 132	O 132	0	0

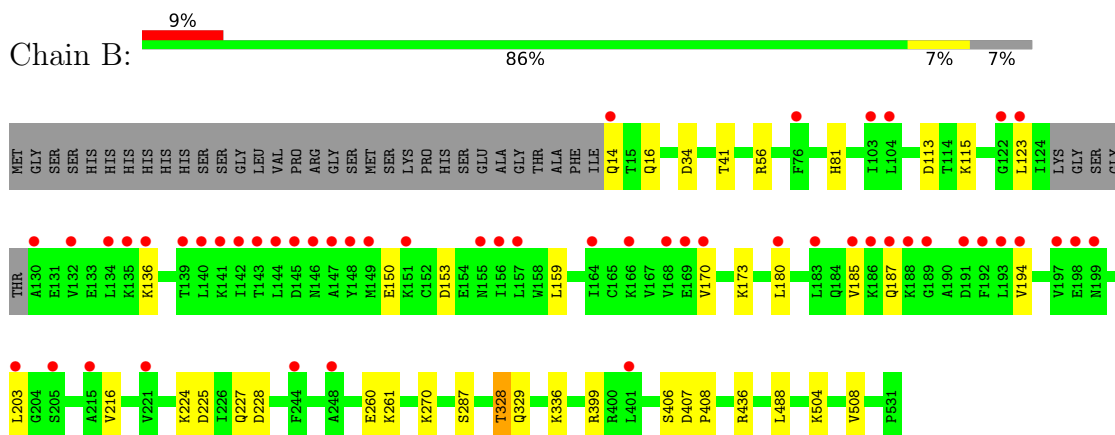
### 3 Residue-property plots

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.

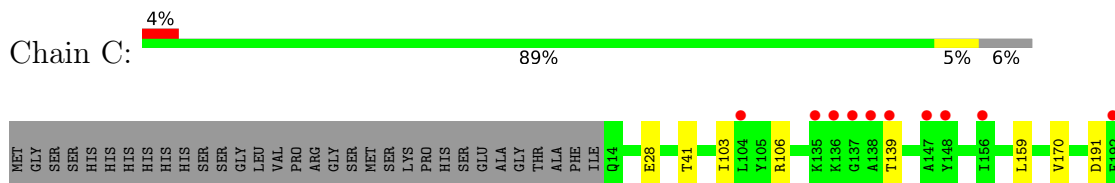
- Molecule 1: Pyruvate kinase PKM

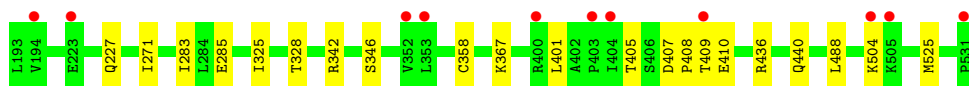


- Molecule 1: Pyruvate kinase PKM

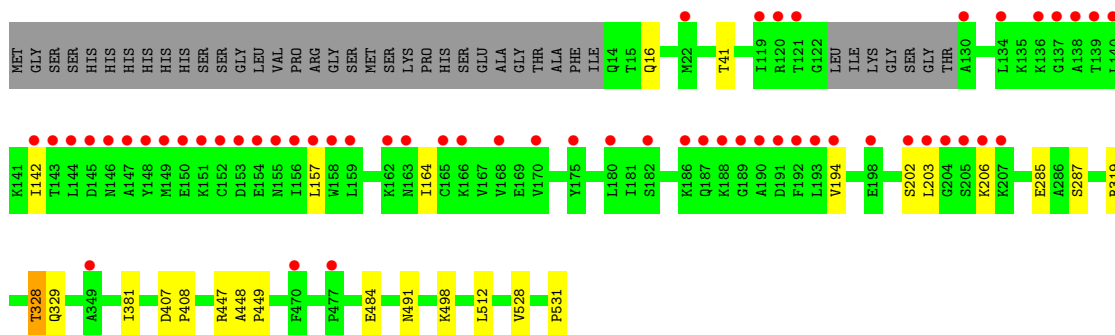
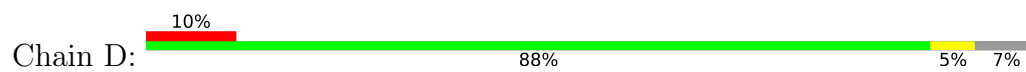


- Molecule 1: Pyruvate kinase PKM





● Molecule 1: Pyruvate kinase PKM





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.47Å 151.66Å 92.08Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 40.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.10) 98.0 (40.29-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.234 , 0.274 0.233 , 0.273	Depositor DCC
$R_{free}$ test set	12248 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtrriage
Anisotropy	0.448	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 7XX

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	0.48	0/3981	0.78	0/5376
1	B	0.54	0/3998	0.83	2/5399 (0.0%)
1	C	0.49	0/4029	0.80	0/5441
1	D	0.50	0/3982	0.79	1/5377 (0.0%)
All	All	0.50	0/15990	0.80	3/21593 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	381	ILE	CG1-CB-CG2	-5.54	99.22	111.40
1	B	225	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	34	ASP	CB-CG-OD2	5.41	123.17	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3919	0	4006	4	0
1	B	3935	0	4017	8	0
1	C	3965	0	4049	7	0
1	D	3919	0	3995	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	A	19	0	0	0	0
3	B	19	0	0	0	0
3	C	19	0	0	0	0
3	D	19	0	0	0	0
4	A	94	0	0	0	0
4	B	120	0	0	0	0
4	C	127	0	0	0	0
4	D	132	0	0	0	0
All	All	16367	0	16107	24	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 1.

All (24) 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:B:81:HIS:NE2	1:B:228:ASP:OD1	2.29	0.56
1:B:115:LYS:HD3	1:B:224:LYS:HE2	1.89	0.55
1:D:498:LYS:NZ	1:D:531:PRO:O	2.40	0.55
1:C:342:ARG:HG2	1:D:329:GLN:HE21	1.74	0.52
1:C:325:ILE:HG12	1:C:358:CYS:HB2	1.93	0.51
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.92	0.50
1:A:123:LEU:HD12	1:A:150:GLU:HG2	1.95	0.49
1:B:328:THR:HG22	1:B:329:GLN:HG3	1.96	0.47
1:B:123:LEU:HD13	1:B:150:GLU:HG2	1.97	0.46
1:A:48:ILE:HB	1:A:360:MET:HG3	2.00	0.44
1:C:28:GLU:OE1	1:D:319:ARG:NH2	2.52	0.43
1:B:113:ASP:OD1	1:B:270:LYS:NZ	2.49	0.42
1:D:157:LEU:HD13	1:D:203:LEU:HD21	2.01	0.42
1:A:342:ARG:HG2	1:B:329:GLN:HE21	1.84	0.42
1:B:407:ASP:HA	1:B:408:PRO:HD3	1.83	0.42
1:C:407:ASP:OD1	1:C:409:THR:OG1	2.28	0.42
1:D:407:ASP:HA	1:D:408:PRO:HD3	1.92	0.41
1:C:407:ASP:HA	1:C:408:PRO:HD3	1.88	0.41
1:A:153:ASP:HB2	1:A:154:GLU:H	1.68	0.41
1:B:187:GLN:HB3	1:B:194:VAL:HB	2.02	0.41
1:C:410:GLU:HG2	1:C:440:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:ALA:HA	1:D:449:PRO:HD2	1.88	0.40
1:D:16:GLN:O	1:D:447:ARG:NH2	2.52	0.40
1:C:271:ILE:HD11	1:C:283:ILE:HG21	2.03	0.40

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	508/550 (92%)	495 (97%)	12 (2%)	1 (0%)	47 49
1	B	509/550 (92%)	496 (97%)	12 (2%)	1 (0%)	47 49
1	C	516/550 (94%)	504 (98%)	11 (2%)	1 (0%)	47 49
1	D	507/550 (92%)	495 (98%)	11 (2%)	1 (0%)	47 49
All	All	2040/2200 (93%)	1990 (98%)	46 (2%)	4 (0%)	47 49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	C	328	THR
1	B	328	THR
1	D	328	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	422/452 (93%)	402 (95%)	20 (5%)	26	25
1	B	423/452 (94%)	399 (94%)	24 (6%)	20	18
1	C	426/452 (94%)	409 (96%)	17 (4%)	31	32
1	D	421/452 (93%)	409 (97%)	12 (3%)	42	46
All	All	1692/1808 (94%)	1619 (96%)	73 (4%)	29	29

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	100	SER
1	A	129	THR
1	A	140	LEU
1	A	146	ASN
1	A	151	LYS
1	A	159	LEU
1	A	162	LYS
1	A	166	LYS
1	A	178	ASP
1	A	223	GLU
1	A	246	ARG
1	A	278	ARG
1	A	339	ARG
1	A	400	ARG
1	A	436	ARG
1	A	453	VAL
1	A	500	ARG
1	A	504	LYS
1	A	512	LEU
1	B	14	GLN
1	B	16	GLN
1	B	41	THR
1	B	56	ARG
1	B	136	LYS
1	B	153	ASP
1	B	159	LEU
1	B	170	VAL
1	B	173	LYS
1	B	180	LEU
1	B	185	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	203	LEU
1	B	216	VAL
1	B	227	GLN
1	B	260	GLU
1	B	261	LYS
1	B	287	SER
1	B	336	LYS
1	B	399	ARG
1	B	406	SER
1	B	436	ARG
1	B	488	LEU
1	B	504	LYS
1	B	508	VAL
1	C	41	THR
1	C	103	ILE
1	C	106	ARG
1	C	139	THR
1	C	159	LEU
1	C	170	VAL
1	C	191	ASP
1	C	227	GLN
1	C	285	GLU
1	C	346	SER
1	C	367	LYS
1	C	401	LEU
1	C	405	THR
1	C	436	ARG
1	C	488	LEU
1	C	504	LYS
1	C	525	MET
1	D	41	THR
1	D	142	ILE
1	D	164	ILE
1	D	194	VAL
1	D	202	SER
1	D	206	LYS
1	D	285	GLU
1	D	287	SER
1	D	484	GLU
1	D	491	ASN
1	D	512	LEU
1	D	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	329	GLN
1	D	329	GLN
1	D	440	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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
2	FBP	D	601	-	18,20,20	0.83	1 (5%)	23,32,32	1.05	1 (4%)
3	7XX	D	602	-	18,20,20	1.07	2 (11%)	23,29,29	2.85	9 (39%)
2	FBP	A	601	-	18,20,20	0.68	0	23,32,32	1.00	2 (8%)
2	FBP	C	601	-	18,20,20	0.73	0	23,32,32	0.97	0
3	7XX	B	602	-	18,20,20	1.08	2 (11%)	23,29,29	3.19	11 (47%)
3	7XX	A	602	-	18,20,20	1.05	2 (11%)	23,29,29	3.28	11 (47%)
2	FBP	B	601	-	18,20,20	0.69	0	23,32,32	1.07	1 (4%)
3	7XX	C	602	-	18,20,20	1.06	2 (11%)	23,29,29	3.35	10 (43%)

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
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	7XX	D	602	-	-	0/4/12/12	0/2/2/2
2	FBP	A	601	-	-	3/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	7XX	B	602	-	-	0/4/12/12	0/2/2/2
3	7XX	A	602	-	-	0/4/12/12	0/2/2/2
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	7XX	C	602	-	-	0/4/12/12	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	7XX	C12-N15	2.71	1.38	1.33
3	B	602	7XX	C12-N15	2.49	1.37	1.33
3	D	602	7XX	C7-C11	-2.37	1.45	1.49
3	C	602	7XX	C7-C11	-2.36	1.45	1.49
3	A	602	7XX	C7-C11	-2.33	1.45	1.49
3	C	602	7XX	C12-N15	2.18	1.37	1.33
3	A	602	7XX	C12-N15	2.08	1.36	1.33
2	D	601	FBP	O2-C2	2.05	1.44	1.40
3	B	602	7XX	C7-C11	-2.03	1.46	1.49

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	7XX	O17-C12-C10	11.48	129.68	119.57
3	A	602	7XX	O17-C12-C10	10.69	128.99	119.57
3	B	602	7XX	O17-C12-C10	9.96	128.34	119.57
3	D	602	7XX	O17-C12-C10	9.05	127.54	119.57
3	A	602	7XX	C10-C12-N15	-5.61	110.40	116.30
3	C	602	7XX	C10-C12-N15	-5.40	110.62	116.30
3	B	602	7XX	C10-C12-N15	-5.16	110.87	116.30
3	C	602	7XX	C5-C7-C11	-4.71	120.78	127.78
3	A	602	7XX	C5-C7-C11	-4.62	120.92	127.78
3	D	602	7XX	C10-C12-N15	-4.46	111.61	116.30
3	D	602	7XX	C5-C7-C11	-4.31	121.37	127.78
3	B	602	7XX	C5-C7-C11	-4.20	121.53	127.78
3	C	602	7XX	C6-C11-C7	4.20	126.45	119.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	7XX	C6-C9-C8	-4.17	117.32	120.17
3	A	602	7XX	C6-C9-CL2	3.69	123.68	119.74
3	B	602	7XX	C6-C9-CL2	3.57	123.54	119.74
3	A	602	7XX	C6-C11-C7	3.52	125.33	119.53
3	B	602	7XX	C6-C11-C7	3.28	124.95	119.53
3	D	602	7XX	C6-C9-CL2	3.17	123.12	119.74
3	D	602	7XX	C6-C11-C7	3.13	124.69	119.53
3	B	602	7XX	C13-N14-C5	-3.05	119.17	124.90
3	A	602	7XX	C4-C7-C11	3.02	134.59	125.34
3	C	602	7XX	C13-N14-C5	-2.99	119.28	124.90
3	A	602	7XX	C13-N14-C5	-2.96	119.34	124.90
3	B	602	7XX	C4-C7-C11	2.89	134.18	125.34
3	B	602	7XX	O16-C11-C6	-2.89	114.77	119.82
3	B	602	7XX	C3-C8-C9	2.88	123.72	120.58
3	C	602	7XX	C4-C7-C11	2.85	134.05	125.34
3	D	602	7XX	C13-N14-C5	-2.81	119.62	124.90
3	D	602	7XX	C4-C7-C11	2.66	133.49	125.34
3	C	602	7XX	O16-C11-C6	-2.60	115.27	119.82
3	A	602	7XX	C3-C8-C9	2.51	123.32	120.58
3	C	602	7XX	C6-C9-CL2	2.51	122.41	119.74
2	A	601	FBP	O3P-P1-O2P	2.44	116.97	107.64
3	C	602	7XX	C6-C9-C8	-2.43	118.51	120.17
2	D	601	FBP	O6P-P2-O5P	2.42	116.90	107.64
3	D	602	7XX	C1-C2-C6	2.26	124.09	119.81
3	A	602	7XX	O16-C11-C6	-2.23	115.91	119.82
3	A	602	7XX	C6-C9-C8	-2.18	118.68	120.17
3	B	602	7XX	C1-C2-C6	2.13	123.84	119.81
2	A	601	FBP	O3P-P1-O1	-2.12	101.08	106.73
3	A	602	7XX	C1-C2-C6	2.10	123.79	119.81
3	D	602	7XX	O16-C11-C6	-2.03	116.27	119.82
3	C	602	7XX	O17-C12-N15	-2.03	119.70	122.58
2	B	601	FBP	O1-P1-O1P	-2.02	100.82	106.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6

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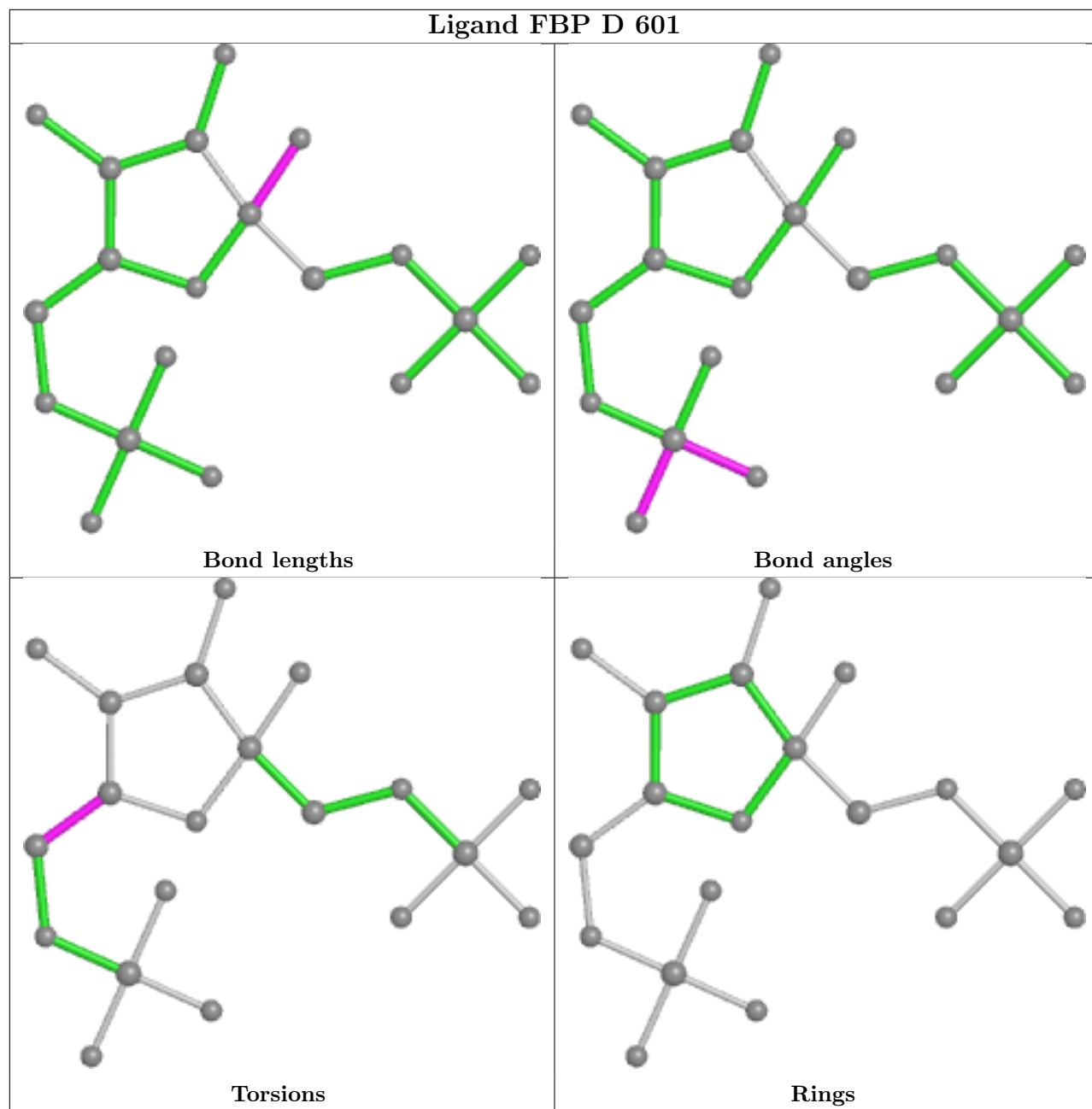
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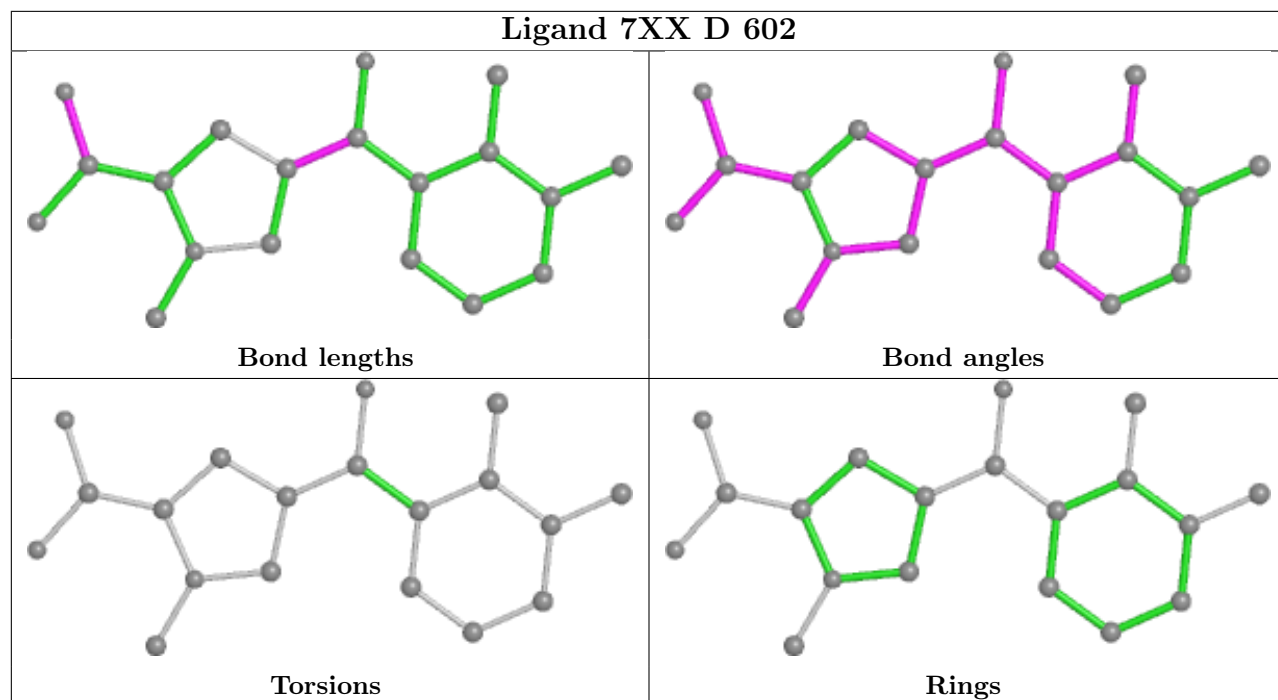
<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	A	601	FBP	C6-O6-P2-O4P

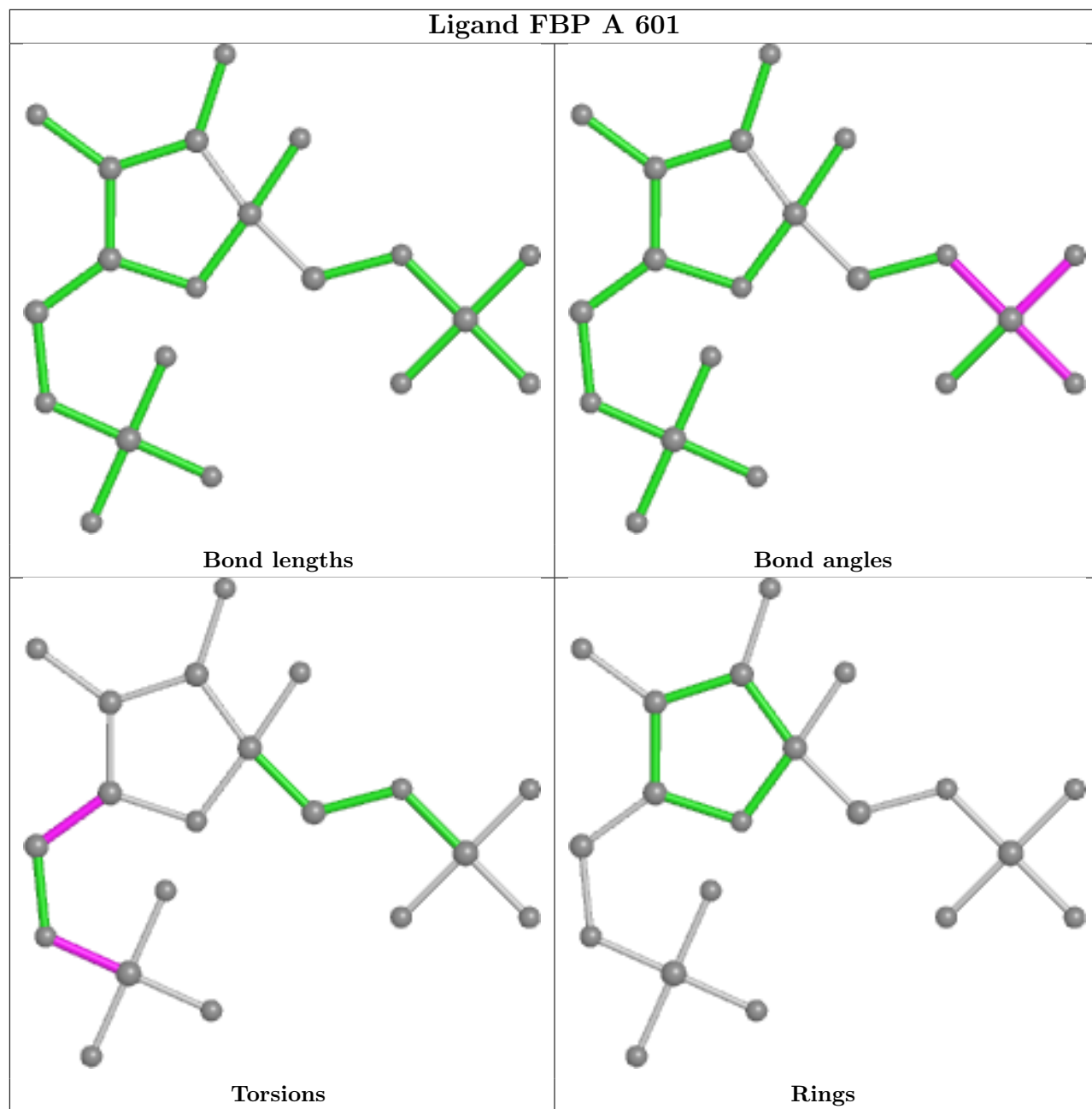
There are no ring outliers.

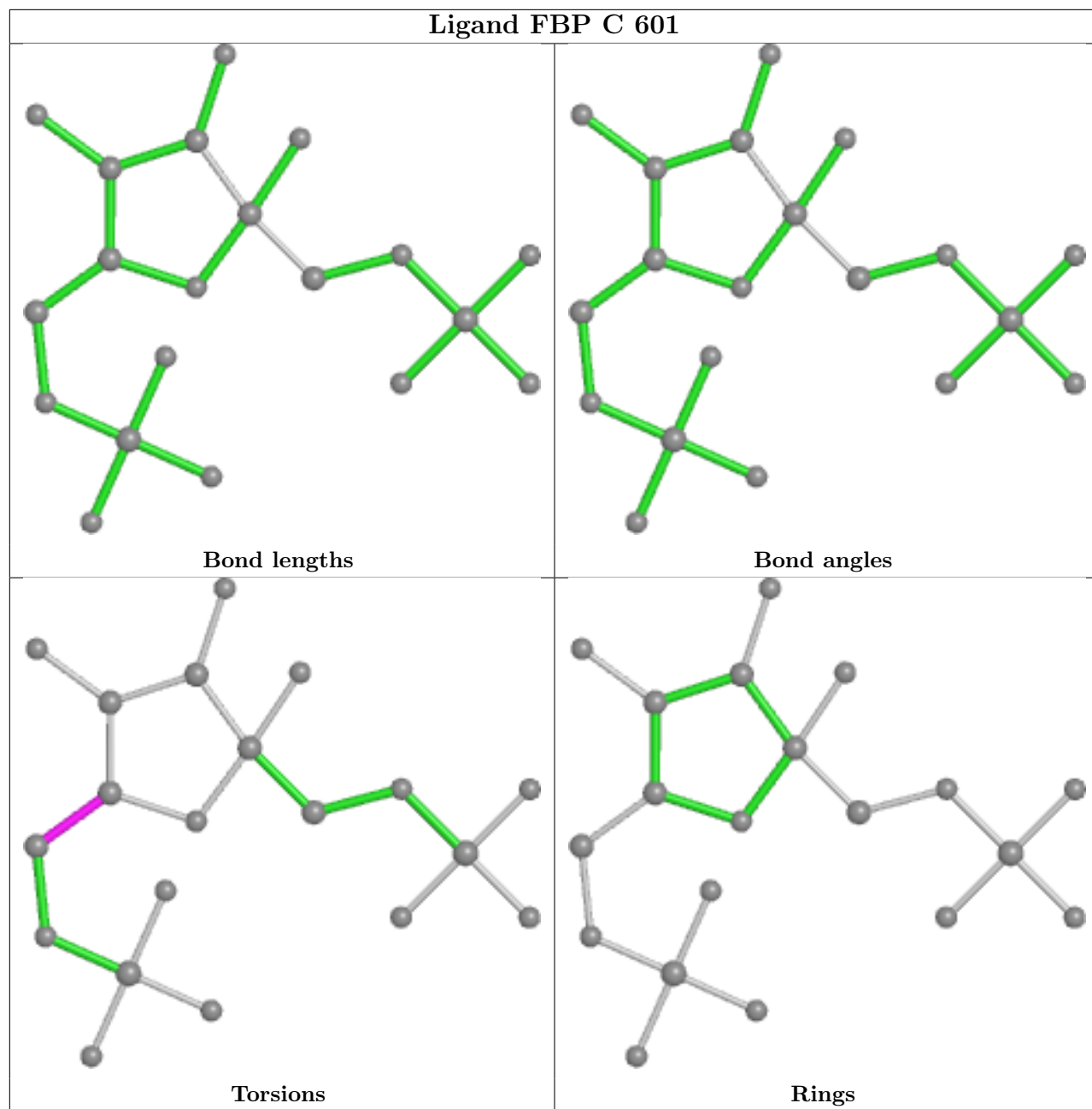
No monomer is involved in short contacts.

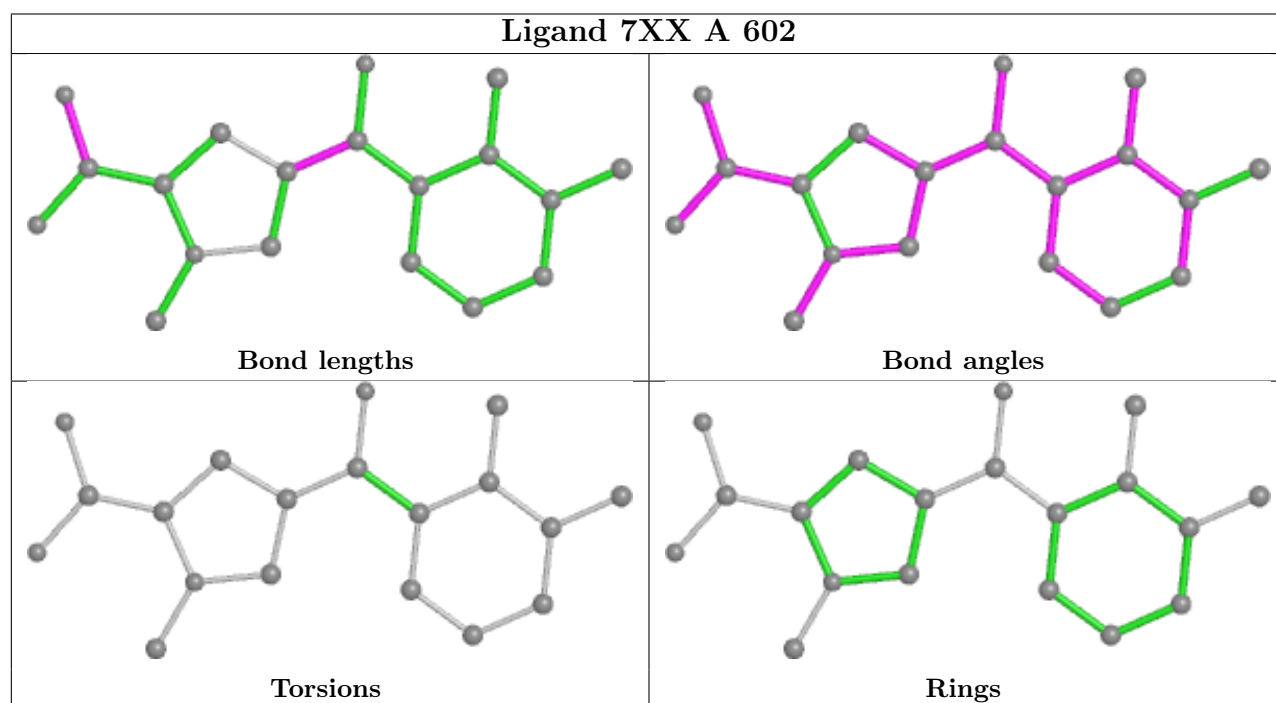
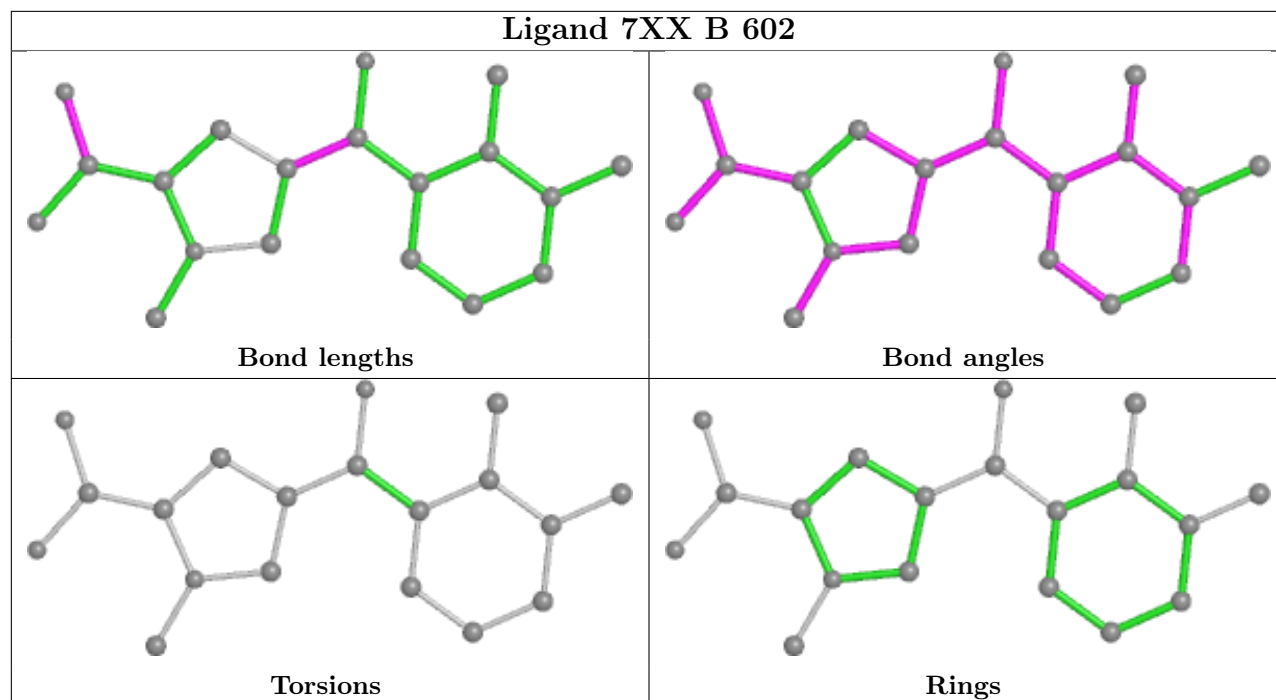
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

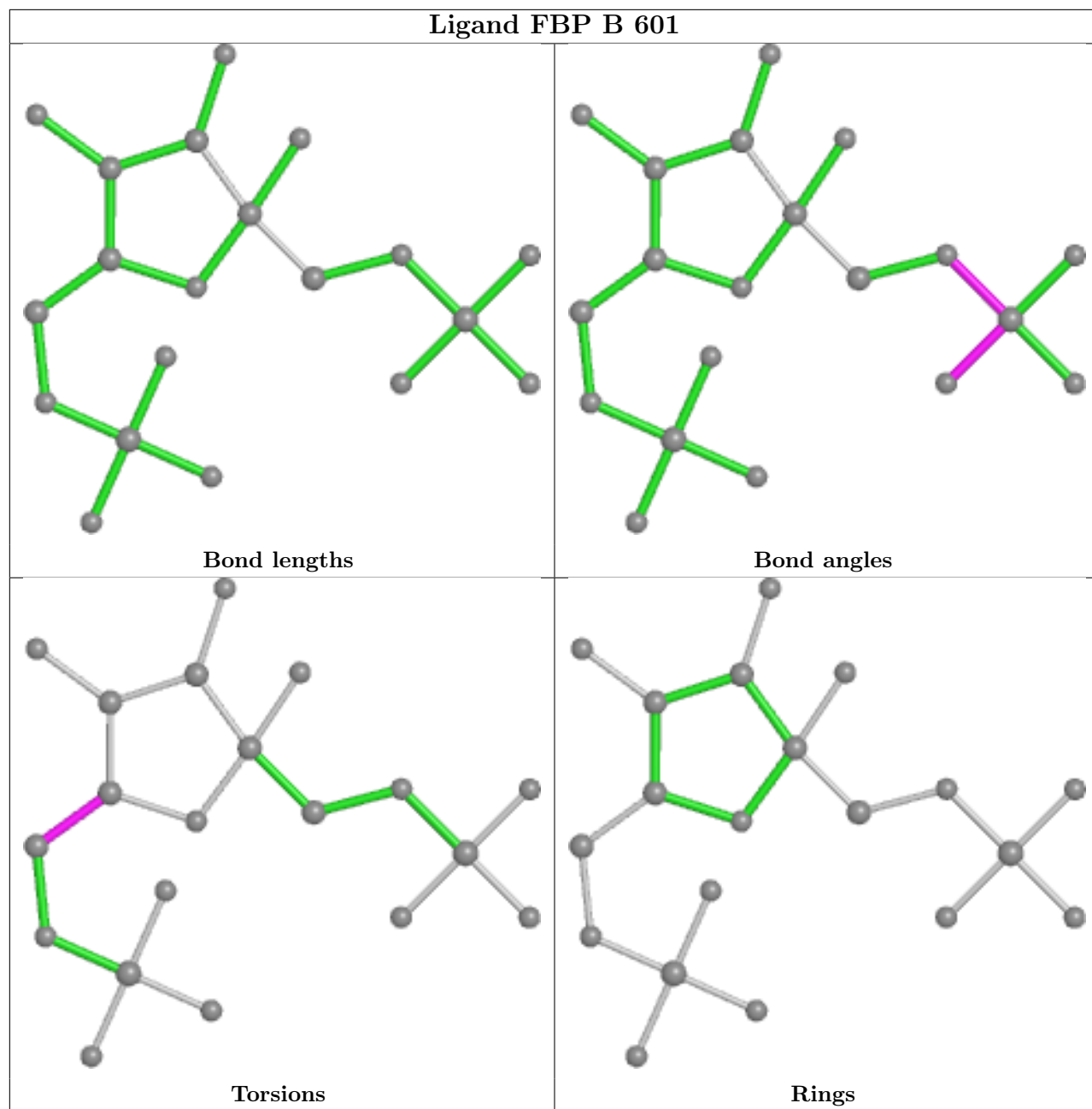




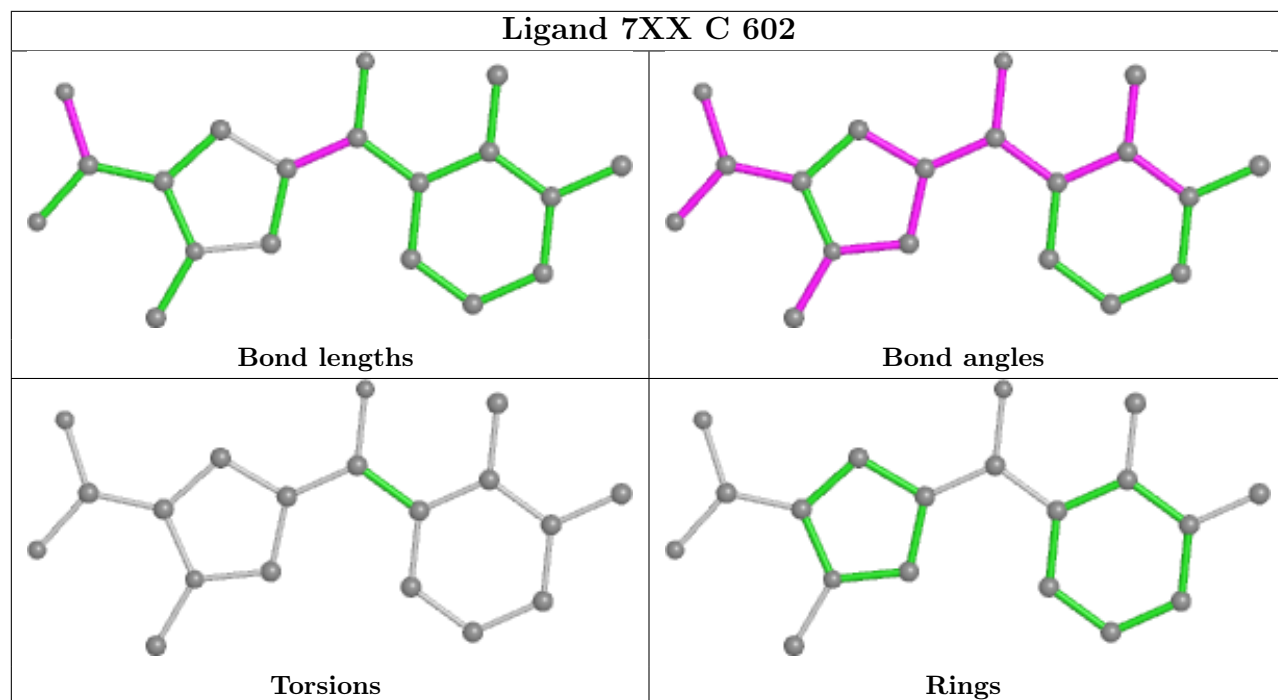












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	512/550 (93%)	0.97	79 (15%) <b>2</b> <b>2</b>	19, 42, 95, 108	0
1	B	513/550 (93%)	0.69	52 (10%) <b>7</b> <b>9</b>	22, 37, 82, 103	1 (0%)
1	C	518/550 (94%)	0.36	21 (4%) <b>37</b> <b>43</b>	23, 36, 55, 69	0
1	D	511/550 (92%)	0.70	57 (11%) <b>5</b> <b>6</b>	24, 36, 80, 97	0
All	All	2054/2200 (93%)	0.68	209 (10%) <b>6</b> <b>8</b>	19, 38, 81, 108	1 (0%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	LEU	9.5
1	D	155	ASN	7.8
1	A	144	LEU	7.7
1	A	126	GLY	7.6
1	A	213	GLY	7.4
1	A	170	VAL	7.3
1	A	148	TYR	7.2
1	B	147	ALA	7.1
1	D	192	PHE	6.9
1	B	156	ILE	6.7
1	A	159	LEU	6.6
1	B	148	TYR	6.5
1	D	148	TYR	6.2
1	A	151	LYS	6.2
1	A	152	CYS	5.9
1	D	190	ALA	5.9
1	B	142	ILE	5.8
1	B	140	LEU	5.7
1	B	143	THR	5.7
1	D	156	ILE	5.5
1	D	207	LYS	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	168	VAL	5.3
1	D	147	ALA	5.3
1	D	204	GLY	5.2
1	A	194	VAL	5.0
1	D	157	LEU	4.9
1	B	192	PHE	4.8
1	B	185	VAL	4.8
1	D	138	ALA	4.7
1	D	203	LEU	4.6
1	B	193	LEU	4.6
1	A	203	LEU	4.6
1	A	166	LYS	4.5
1	D	137	GLY	4.5
1	A	184	GLN	4.4
1	A	167	VAL	4.3
1	A	165	CYS	4.3
1	A	141	LYS	4.3
1	A	158	TRP	4.3
1	A	196	GLU	4.2
1	D	180	LEU	4.2
1	D	158	TRP	4.2
1	A	172	SER	4.2
1	D	168	VAL	4.1
1	A	164	ILE	4.1
1	B	170	VAL	4.1
1	A	139	THR	4.1
1	D	193	LEU	4.0
1	D	166	LYS	4.0
1	B	205	SER	3.9
1	A	204	GLY	3.9
1	B	144	LEU	3.9
1	D	149	MET	3.9
1	A	149	MET	3.9
1	A	185	VAL	3.9
1	B	168	VAL	3.9
1	D	142	ILE	3.8
1	A	183	LEU	3.8
1	A	138	ALA	3.8
1	A	403	PRO	3.7
1	D	151	LYS	3.7
1	B	139	THR	3.7
1	B	145	ASP	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	157	LEU	3.7
1	D	150	GLU	3.7
1	D	189	GLY	3.7
1	A	186	LYS	3.7
1	B	194	VAL	3.7
1	A	136	LYS	3.6
1	A	132	VAL	3.6
1	D	163	ASN	3.6
1	D	153	ASP	3.6
1	D	154	GLU	3.6
1	D	205	SER	3.6
1	A	215	ALA	3.6
1	A	351	ALA	3.5
1	B	132	VAL	3.5
1	A	156	ILE	3.5
1	B	151	LYS	3.5
1	A	122	GLY	3.5
1	D	121	THR	3.5
1	A	147	ALA	3.5
1	A	214	ALA	3.5
1	A	128	GLY	3.5
1	A	195	THR	3.4
1	A	169	GLU	3.4
1	A	123	LEU	3.4
1	D	143	THR	3.4
1	A	406	SER	3.4
1	B	183	LEU	3.3
1	A	324	VAL	3.3
1	A	401	LEU	3.3
1	A	470	PHE	3.2
1	D	139	THR	3.2
1	A	40	ILE	3.2
1	B	149	MET	3.2
1	A	146	ASN	3.2
1	B	122	GLY	3.2
1	B	197	VAL	3.2
1	D	170	VAL	3.2
1	B	130	ALA	3.1
1	A	145	ASP	3.1
1	B	123	LEU	3.0
1	D	194	VAL	3.0
1	D	140	LEU	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	165	CYS	3.0
1	A	217	ASP	3.0
1	C	135	LYS	3.0
1	A	153	ASP	3.0
1	B	157	LEU	3.0
1	B	188	LYS	3.0
1	A	143	THR	2.9
1	D	186	LYS	2.9
1	D	146	ASN	2.9
1	A	103	ILE	2.9
1	C	148	TYR	2.9
1	D	130	ALA	2.9
1	B	134	LEU	2.9
1	C	403	PRO	2.9
1	B	191	ASP	2.9
1	A	480	GLU	2.8
1	B	135	LYS	2.8
1	C	192	PHE	2.8
1	B	141	LYS	2.8
1	A	41	THR	2.8
1	D	144	LEU	2.8
1	D	134	LEU	2.8
1	D	119	ILE	2.7
1	D	145	ASP	2.7
1	D	198	GLU	2.7
1	A	129	THR	2.7
1	D	206	LYS	2.7
1	B	198	GLU	2.7
1	D	477	PRO	2.7
1	D	136	LYS	2.7
1	B	187	GLN	2.7
1	D	162	LYS	2.7
1	B	244	PHE	2.7
1	C	194	VAL	2.6
1	D	470	PHE	2.6
1	A	134	LEU	2.6
1	B	155	ASN	2.6
1	C	531	PRO	2.6
1	A	206	LYS	2.6
1	D	152	CYS	2.6
1	D	120	ARG	2.6
1	C	353	LEU	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	404	ILE	2.5
1	B	221	VAL	2.5
1	A	162	LYS	2.5
1	C	147	ALA	2.5
1	C	137	GLY	2.5
1	A	130	ALA	2.5
1	B	203	LEU	2.5
1	C	138	ALA	2.5
1	C	139	THR	2.5
1	A	197	VAL	2.4
1	C	223	GLU	2.4
1	B	136	LYS	2.4
1	B	199	ASN	2.4
1	A	127	SER	2.4
1	A	173	LYS	2.3
1	A	216	VAL	2.3
1	A	178	ASP	2.3
1	B	169	GLU	2.3
1	B	186	LYS	2.3
1	B	76	PHE	2.3
1	D	159	LEU	2.3
1	D	22	MET	2.3
1	A	394	LEU	2.3
1	D	188	LYS	2.3
1	A	356	ALA	2.3
1	A	475	LYS	2.3
1	B	166	LYS	2.3
1	B	146	ASN	2.3
1	D	182	SER	2.3
1	D	202	SER	2.3
1	B	164	ILE	2.3
1	A	478	VAL	2.2
1	D	349	ALA	2.2
1	B	14	GLN	2.2
1	A	174	ILE	2.2
1	A	314	ILE	2.2
1	B	104	LEU	2.2
1	B	401	LEU	2.2
1	A	202	SER	2.2
1	C	352	VAL	2.2
1	C	400	ARG	2.2
1	C	504	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	ILE	2.2
1	A	199	ASN	2.2
1	B	103	ILE	2.2
1	B	215	ALA	2.2
1	C	104	LEU	2.2
1	A	124	ILE	2.2
1	B	189	GLY	2.2
1	C	136	LYS	2.1
1	B	248	ALA	2.1
1	A	163	ASN	2.1
1	A	492	PHE	2.1
1	C	409	THR	2.1
1	D	187	GLN	2.1
1	C	156	ILE	2.0
1	A	352	VAL	2.0
1	A	101	ASP	2.0
1	C	505	LYS	2.0
1	D	175	TYR	2.0
1	B	180	LEU	2.0
1	D	191	ASP	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

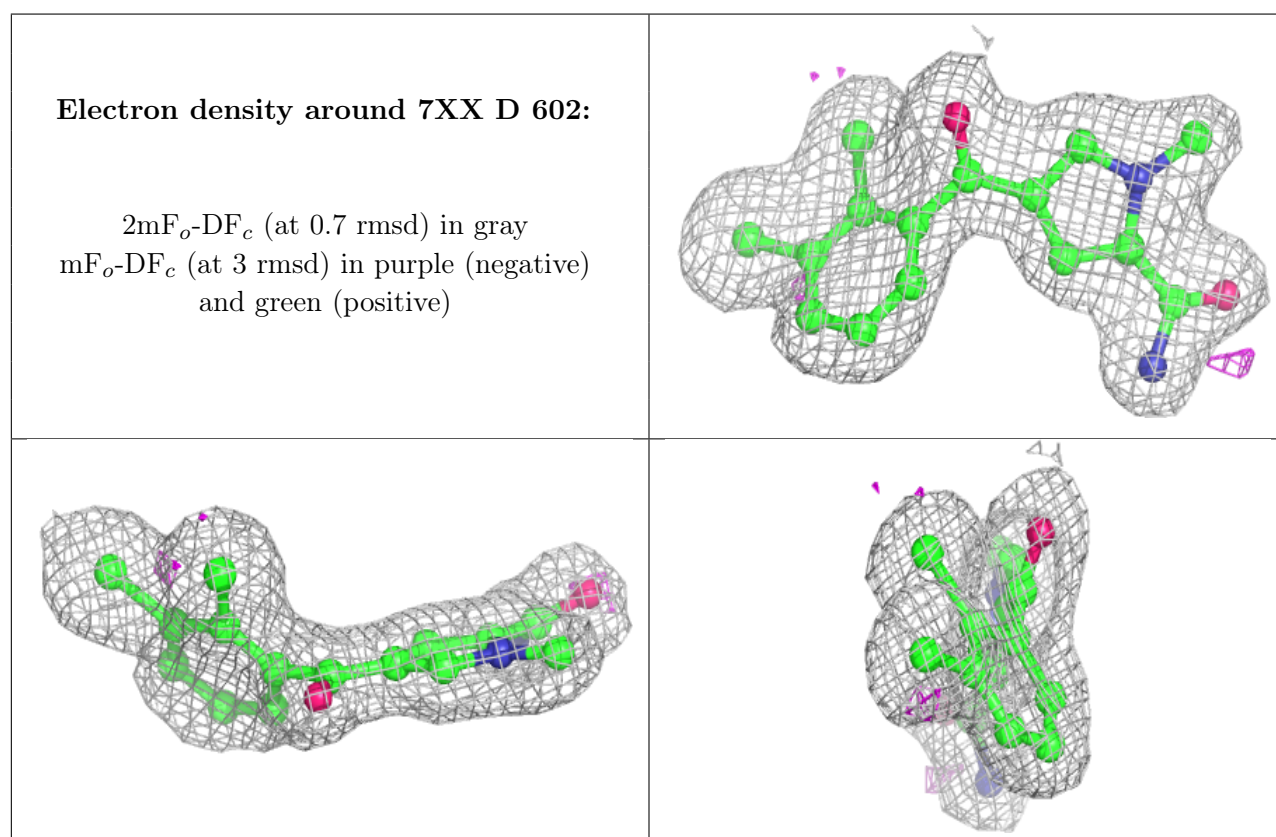
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	7XX	D	602	19/19	0.92	0.14	37,39,41,43	0
3	7XX	C	602	19/19	0.94	0.13	35,40,44,45	0
2	FBP	C	601	20/20	0.95	0.17	39,44,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FBP	A	601	20/20	0.95	0.12	41,46,52,53	0
2	FBP	B	601	20/20	0.95	0.14	33,39,44,45	0
3	7XX	A	602	19/19	0.96	0.16	37,41,48,52	0
3	7XX	B	602	19/19	0.96	0.13	35,38,39,40	0
2	FBP	D	601	20/20	0.97	0.14	31,32,39,40	0

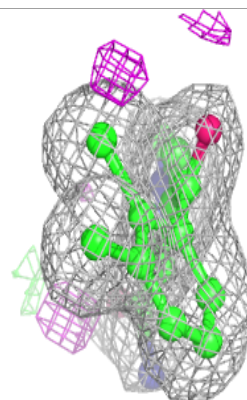
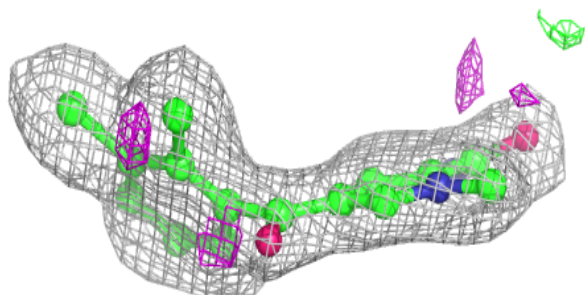
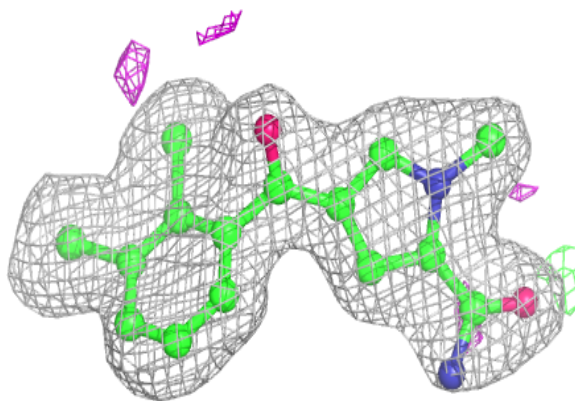
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



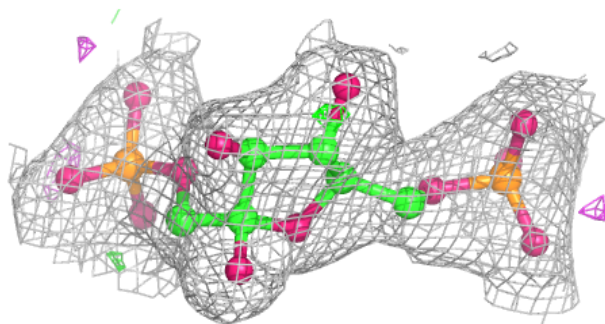
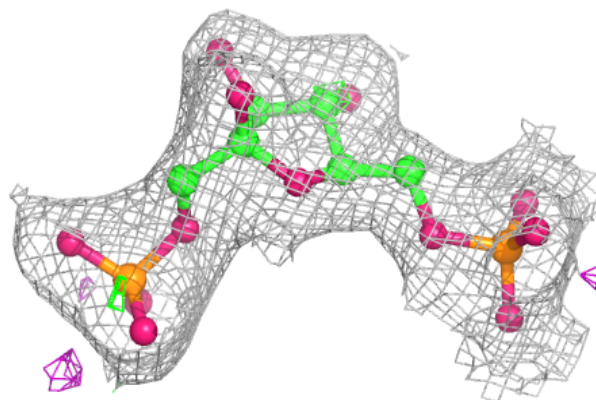


**Electron density around 7XX C 602:**

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

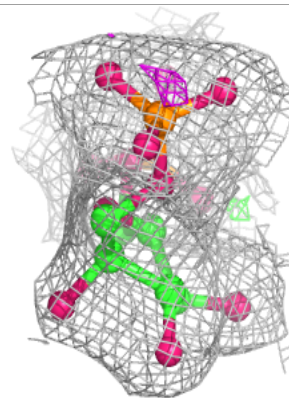
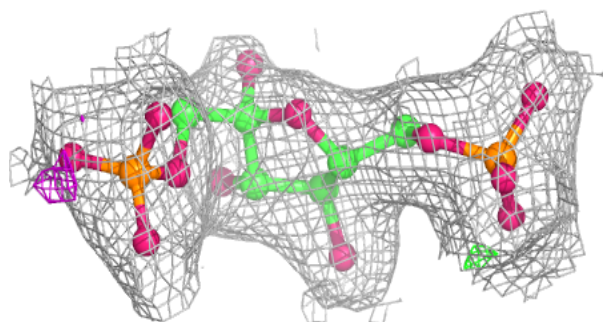
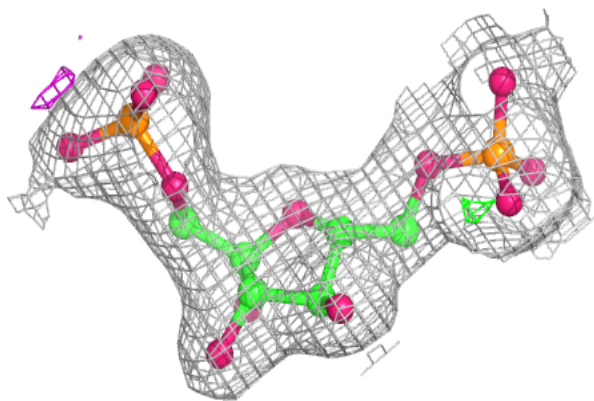
**Electron density around FBP C 601:**

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

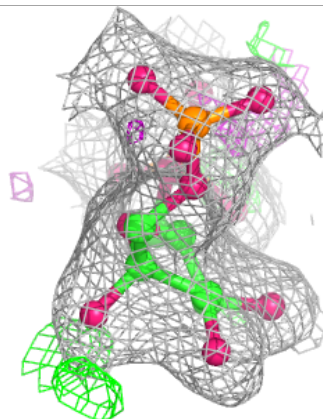
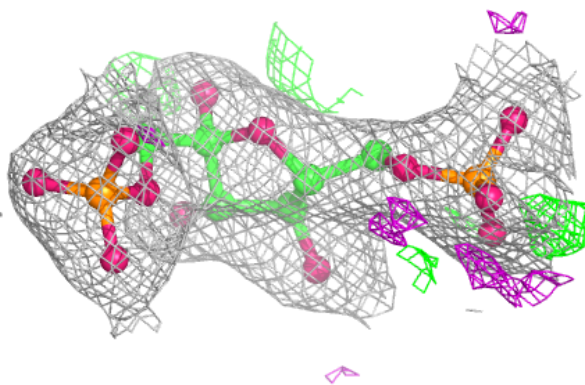
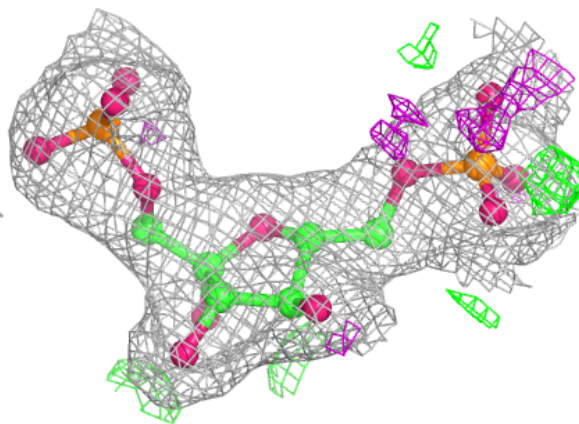


**Electron density around FBP A 601:**

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

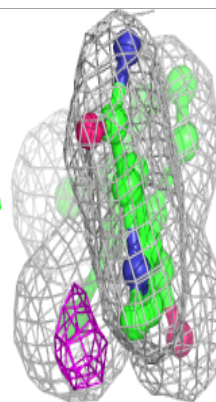
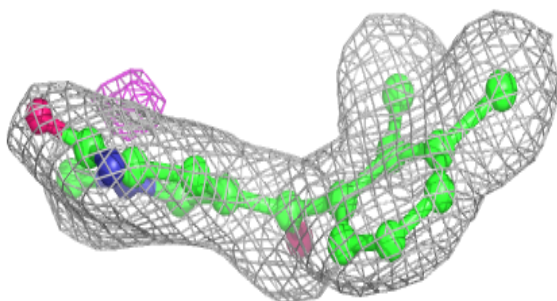
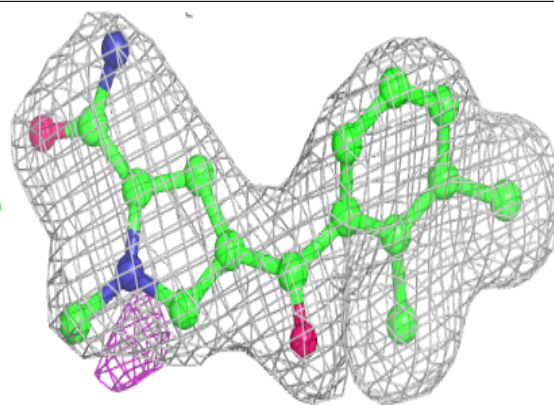
**Electron density around FBP B 601:**

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

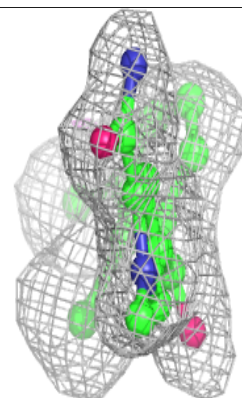
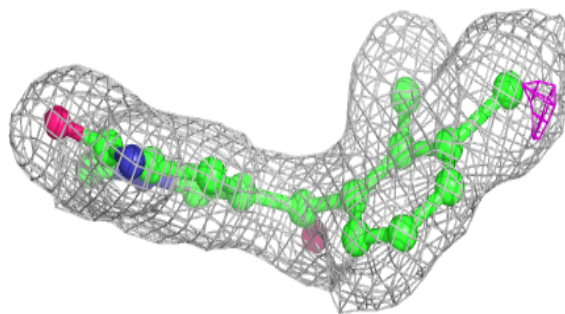
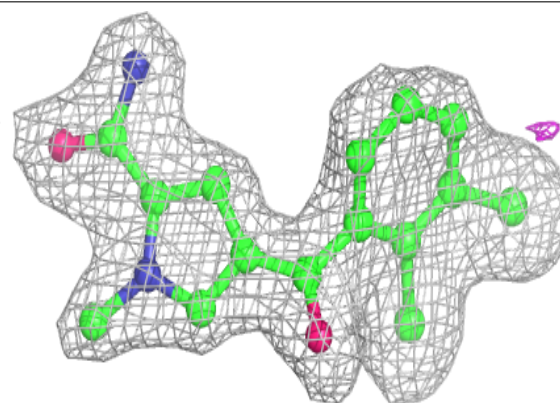


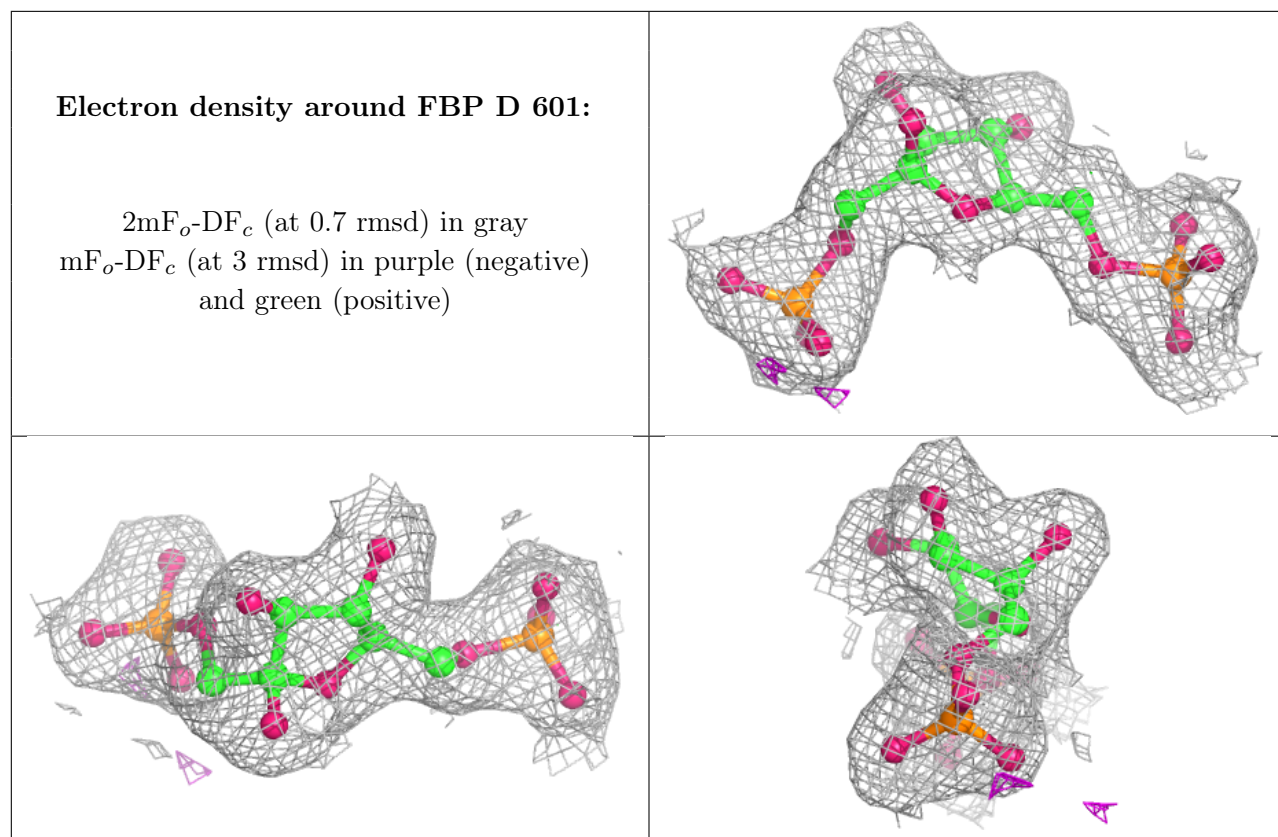
**Electron density around 7XX A 602:**

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

**Electron density around 7XX B 602:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.