wwPDB X-ray Structure Validation Summary Report (i)

Mar 7, 2022 – 05:04 PM EST

PDB ID	:	5SCB
Title	:	Structure of liver pyruvate kinase in complex with anthraquinone derivative 28
Authors	:	Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.
Deposited on	:	2021-12-01
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

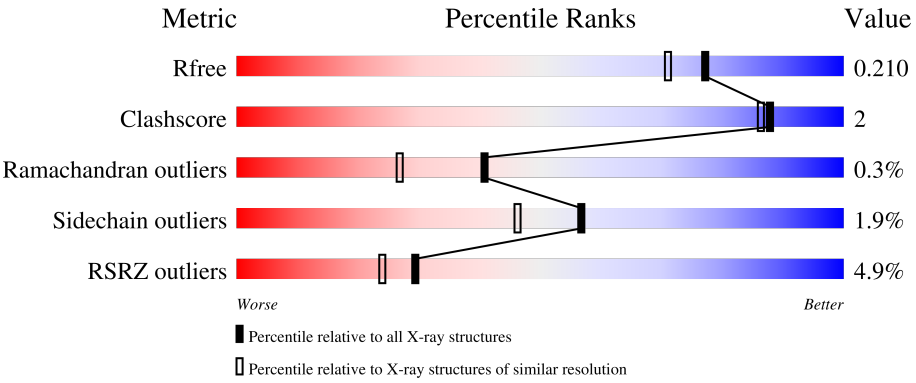
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5% 87% 7% 6%
1	B	447	8% 91% 7% •
1	C	447	4% 89% 6% 5%
1	D	447	4% 89% 5% • 5%
1	E	447	6% 89% 5% 6%

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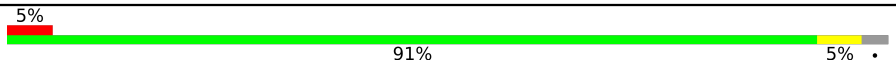
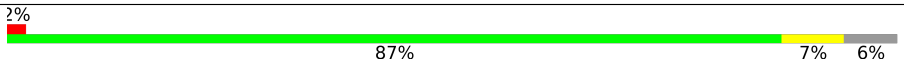
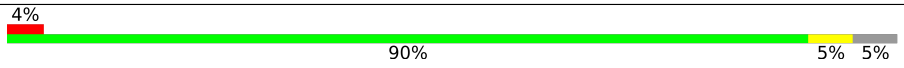
Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 29320 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
1	A	419	Total	C	N	O	S	0	13	0
			3242	2035	582	605	20			
1	B	436	Total	C	N	O	S	3	8	0
			3350	2104	604	622	20			
1	C	424	Total	C	N	O	S	0	7	0
			3260	2051	584	606	19			
1	D	425	Total	C	N	O	S	0	8	0
			3261	2048	590	604	19			
1	E	419	Total	C	N	O	S	0	13	0
			3257	2049	584	604	20			
1	F	432	Total	C	N	O	S	0	8	0
			3327	2094	597	616	20			
1	G	422	Total	C	N	O	S	0	9	0
			3257	2048	586	604	19			
1	H	425	Total	C	N	O	S	0	9	0
			3277	2057	597	604	19			

There are 48 discrepancies between the modelled and reference sequences:

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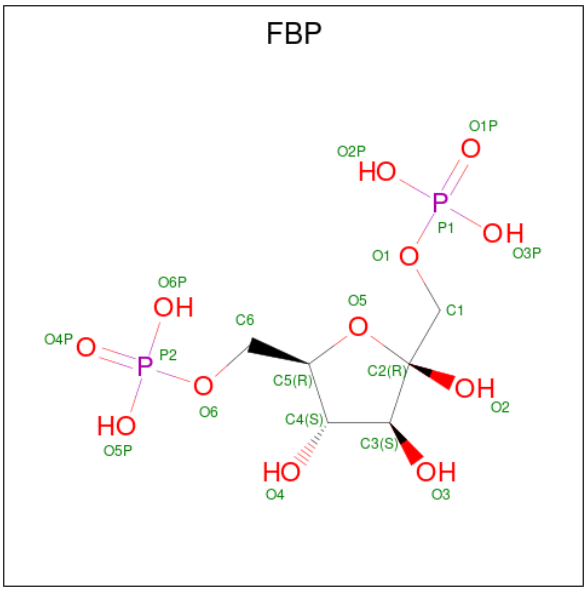
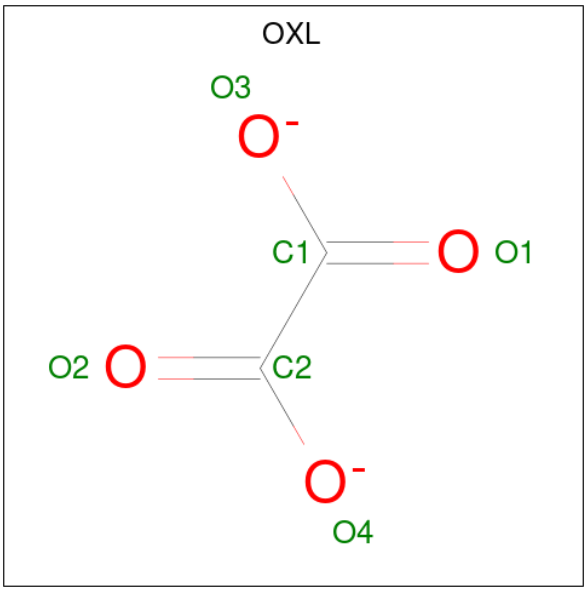
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	228	GLY	-	linker	UNP Q16716
C	229	SER	-	linker	UNP Q16716
C	230	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict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



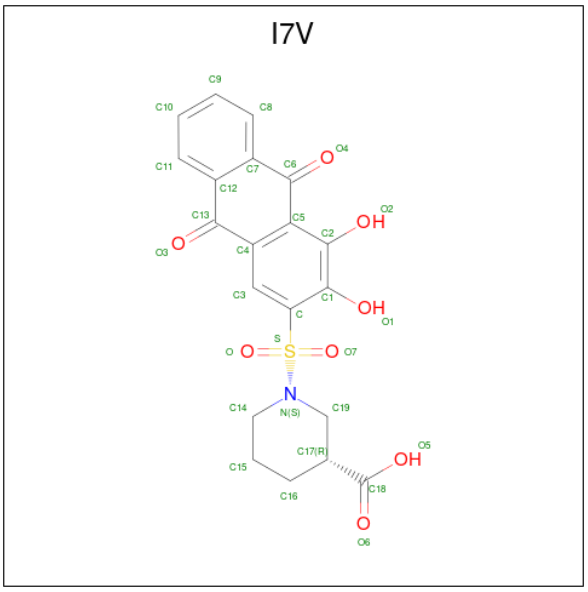
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2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

- Molecule 3 is OXALATE ION (three-letter code: 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 (3R)-1-(3,4-dihydroxy-9,10-dioxo-9,10-dihydroanthracene-2-sulfonyl)piperidine-3-carboxylic acid (three-letter code: I7V) (formula: $C_{20}H_{17}NO_8S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	17	0
			47	20	17	1	8	1		
4	B	1	Total	C	H	N	O	S	17	0
			47	20	17	1	8	1		
4	C	1	Total	C	H	N	O	S	17	0
			47	20	17	1	8	1		
4	E	1	Total	C	H	N	O	S	17	0
			47	20	17	1	8	1		
4	F	1	Total	C	H	N	O	S	17	0
			47	20	17	1	8	1		
4	G	1	Total	C	H	N	O	S	17	0
			47	20	17	1	8	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: 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		

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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 (three-letter code: 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	259	Total O 259 259	0	0
7	B	244	Total O 244 244	0	0
7	C	363	Total O 363 363	0	0
7	D	360	Total O 360 360	0	0
7	E	281	Total O 281 281	0	0
7	F	309	Total O 309 309	0	0
7	G	381	Total O 381 381	0	0

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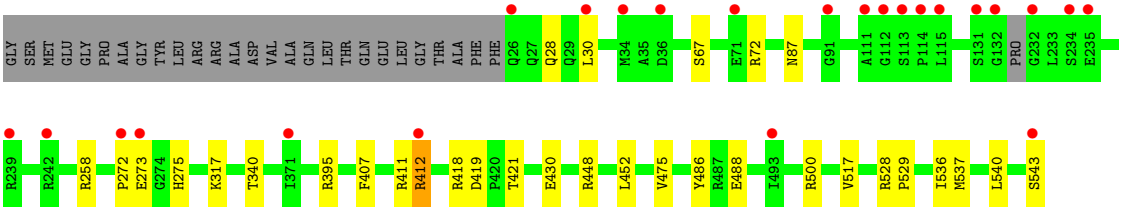
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	386	Total 386	O 386	0	0

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.

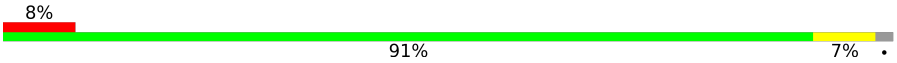
• Molecule 1: Pyruvate kinase

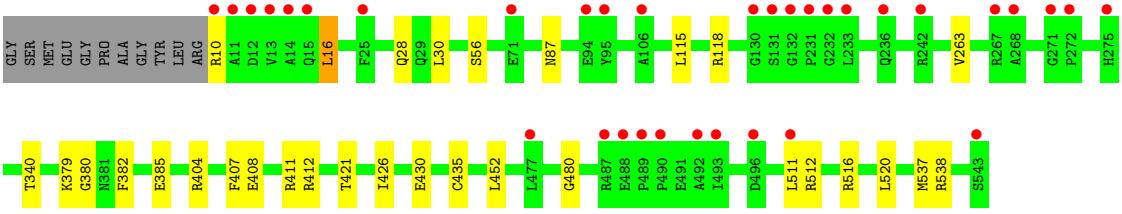
Chain A:



• Molecule 1: Pyruvate kinase

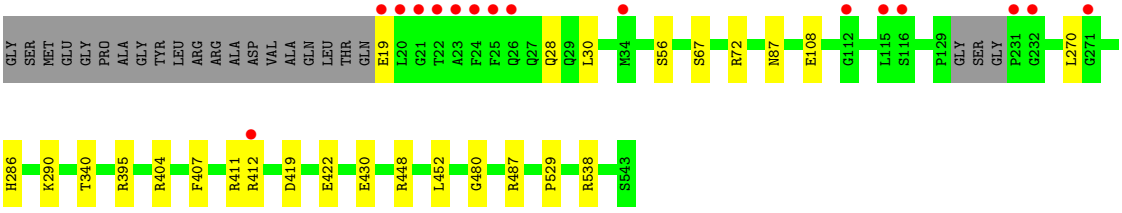
Chain B:





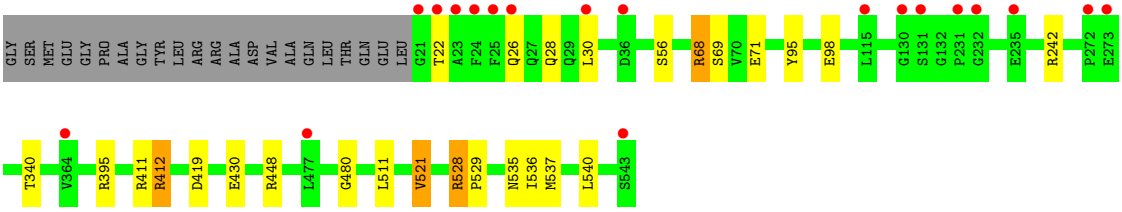
• Molecule 1: Pyruvate kinase

Chain C:



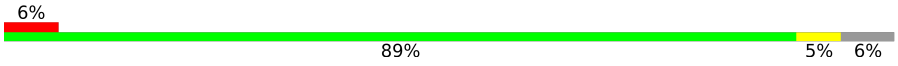
• Molecule 1: Pyruvate kinase

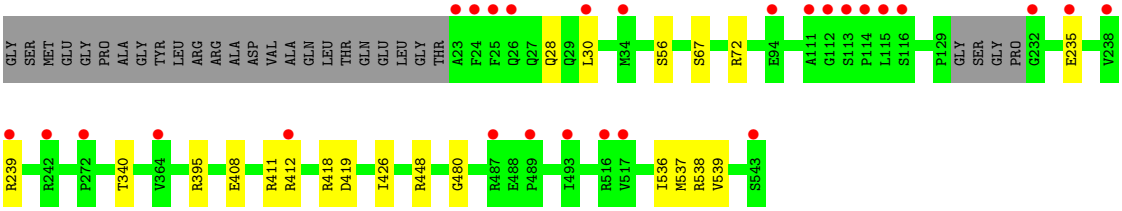
Chain D:



• Molecule 1: Pyruvate kinase

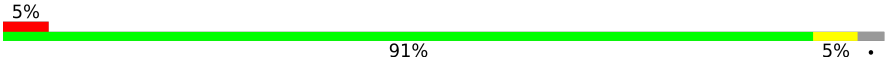
Chain E:

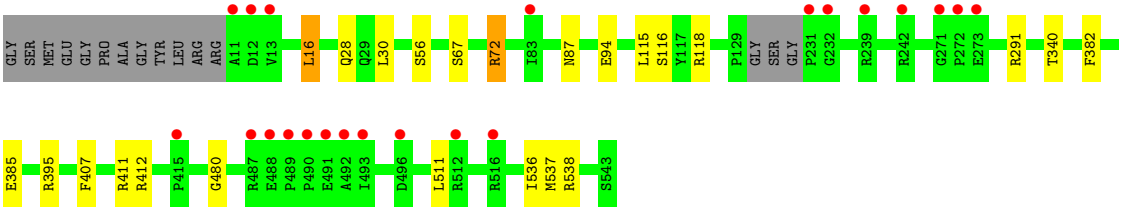




• Molecule 1: Pyruvate kinase

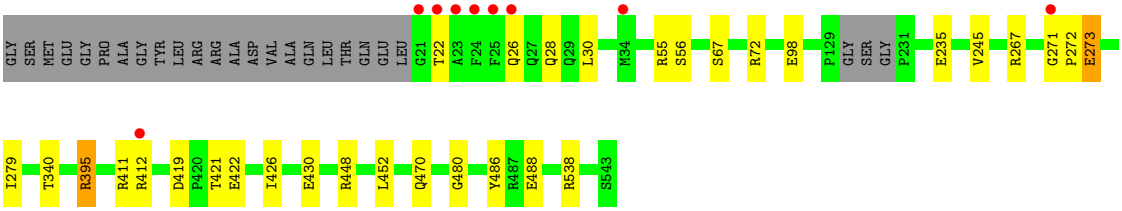
Chain F:





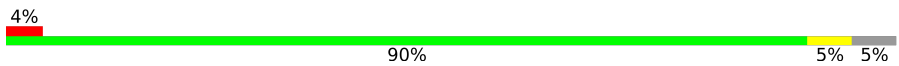
• Molecule 1: Pyruvate kinase

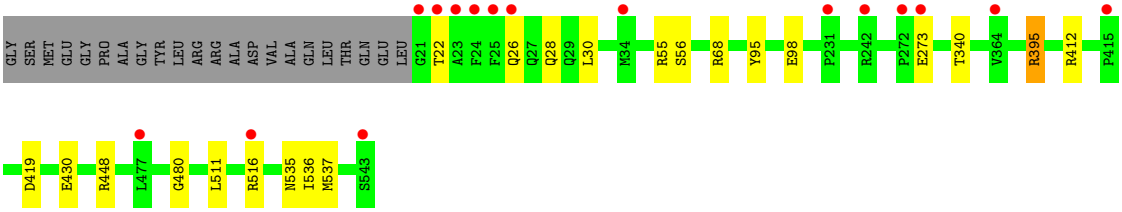
Chain G:



• Molecule 1: Pyruvate kinase

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	207.63Å 112.47Å 188.26Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	35.77 – 1.80 35.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	70.8 (35.77-1.80) 70.7 (35.77-1.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 1.79Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.193 , 0.219 0.185 , 0.210	Depositor DCC
R_{free} test set	14495 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29320	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.38 % 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 2.7603e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, MG, I7V, K, FBP

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	0.38	0/3332	0.54	0/4502
1	B	0.38	0/3429	0.53	0/4636
1	C	0.44	0/3335	0.56	0/4508
1	D	0.46	0/3341	0.57	0/4517
1	E	0.37	0/3350	0.52	0/4527
1	F	0.40	0/3405	0.53	0/4603
1	G	0.45	0/3335	0.55	0/4507
1	H	0.45	0/3357	0.55	0/4537
All	All	0.42	0/26884	0.54	0/36337

There are no bond length outliers.

There are no bond angle outliers.

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	3242	0	3315	17	0
1	B	3350	0	3417	16	0
1	C	3260	0	3320	21	0
1	D	3261	0	3321	20	0
1	E	3257	0	3323	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3327	0	3399	13	0
1	G	3257	0	3320	22	0
1	H	3277	0	3341	12	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	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	30	17	0	1	0
4	B	30	17	0	1	0
4	C	30	17	0	1	0
4	E	30	17	0	0	0
4	F	30	17	0	1	0
4	G	30	17	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	259	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	244	0	0	1	0
7	C	363	0	0	2	0
7	D	360	0	0	0	0
7	E	281	0	0	0	0
7	F	309	0	0	0	0
7	G	381	0	0	2	1
7	H	386	0	0	0	0
All	All	29218	102	26836	109	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 109 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:A:500:ARG:HG2	7:A:894:HOH:O	1.64	0.96
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.70	0.74
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.70	0.73
1:H:68:ARG:NH2	1:H:95:TYR:O	2.23	0.72
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.72	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:A:894:HOH:O	7:G:844:HOH:O[3_455]	2.07	0.13

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%)	422 (99%)	5 (1%)	1 (0%)	47	33
1	B	442/447 (99%)	436 (99%)	5 (1%)	1 (0%)	47	33
1	C	427/447 (96%)	422 (99%)	4 (1%)	1 (0%)	47	33
1	D	431/447 (96%)	428 (99%)	2 (0%)	1 (0%)	47	33
1	E	428/447 (96%)	423 (99%)	4 (1%)	1 (0%)	47	33
1	F	436/447 (98%)	432 (99%)	3 (1%)	1 (0%)	47	33
1	G	427/447 (96%)	420 (98%)	5 (1%)	2 (0%)	29	15
1	H	432/447 (97%)	426 (99%)	5 (1%)	1 (0%)	47	33
All	All	3451/3576 (96%)	3409 (99%)	33 (1%)	9 (0%)	41	27

5 of 9 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%)	337 (98%)	8 (2%)	50	37
1	B	353/352 (100%)	341 (97%)	12 (3%)	37	22
1	C	344/352 (98%)	338 (98%)	6 (2%)	60	51
1	D	344/352 (98%)	334 (97%)	10 (3%)	42	29
1	E	346/352 (98%)	341 (99%)	5 (1%)	67	59
1	F	351/352 (100%)	343 (98%)	8 (2%)	50	37
1	G	344/352 (98%)	341 (99%)	3 (1%)	78	75
1	H	345/352 (98%)	339 (98%)	6 (2%)	60	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2772/2816 (98%)	2714 (98%)	58 (2%)	57 42

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	242[A]	ARG
1	H	511	LEU
1	D	537	MET
1	H	412	ARG
1	G	273	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	381	ASN
1	G	275	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	OXL	G	602	5	0,5,5	-	-	0,6,6	-	-
2	FBP	E	601	-	18,20,20	0.49	0	23,32,32	0.92	1 (4%)
3	OXL	D	602	5	0,5,5	-	-	0,6,6	-	-
3	OXL	C	603	5	0,5,5	-	-	0,6,6	-	-
4	I7V	G	603	-	30,33,33	0.35	0	44,51,51	0.44	0
2	FBP	F	601	-	18,20,20	0.43	0	23,32,32	0.64	0
3	OXL	H	602	5	0,5,5	-	-	0,6,6	-	-
4	I7V	F	602	-	30,33,33	0.26	0	44,51,51	0.38	0
3	OXL	E	602	5	0,5,5	-	-	0,6,6	-	-
2	FBP	G	601	-	18,20,20	0.58	0	23,32,32	0.82	1 (4%)
2	FBP	D	601	-	18,20,20	0.55	0	23,32,32	0.96	1 (4%)
2	FBP	A	601	-	18,20,20	0.54	0	23,32,32	0.75	0
3	OXL	A	602	5	0,5,5	-	-	0,6,6	-	-
4	I7V	E	603	-	30,33,33	0.27	0	44,51,51	0.42	0
4	I7V	B	603	-	30,33,33	0.34	0	44,51,51	0.37	0
3	OXL	F	603	5	0,5,5	-	-	0,6,6	-	-
4	I7V	A	603	-	30,33,33	0.28	0	44,51,51	0.32	0
2	FBP	C	601	-	18,20,20	0.56	0	23,32,32	0.74	1 (4%)
3	OXL	B	602	5	0,5,5	-	-	0,6,6	-	-
2	FBP	H	601	-	18,20,20	0.72	0	23,32,32	0.86	1 (4%)
4	I7V	C	602	-	30,33,33	0.33	0	44,51,51	0.68	2 (4%)
2	FBP	B	601	-	18,20,20	0.81	1 (5%)	23,32,32	0.98	2 (8%)

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
3	OXL	G	602	5	-	0/0/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	5	-	0/0/4/4	-
3	OXL	C	603	5	-	0/0/4/4	-
4	I7V	G	603	-	-	6/12/42/42	0/4/4/4
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	5	-	0/0/4/4	-
4	I7V	F	602	-	-	2/12/42/42	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	E	602	5	-	0/0/4/4	-
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	5	-	0/0/4/4	-
4	I7V	E	603	-	-	0/12/42/42	0/4/4/4
4	I7V	B	603	-	-	8/12/42/42	0/4/4/4
3	OXL	F	603	5	-	0/0/4/4	-
4	I7V	A	603	-	-	7/12/42/42	1/4/4/4
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	5	-	0/0/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
4	I7V	C	602	-	-	7/12/42/42	0/4/4/4
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FBP	P2-O5P	-2.03	1.47	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	FBP	O3P-P1-O2P	2.95	118.91	107.64
2	B	601	FBP	O5P-P2-O6	2.83	114.27	106.73
2	D	601	FBP	O5P-P2-O6	2.78	114.12	106.73
4	C	602	I7V	C14-N-C19	2.76	115.78	112.70
2	B	601	FBP	O3P-P1-O2P	2.50	117.20	107.64

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
4	A	603	I7V	C1-C-S-O7
4	A	603	I7V	C1-C-S-O

All (1) ring outliers are listed below:

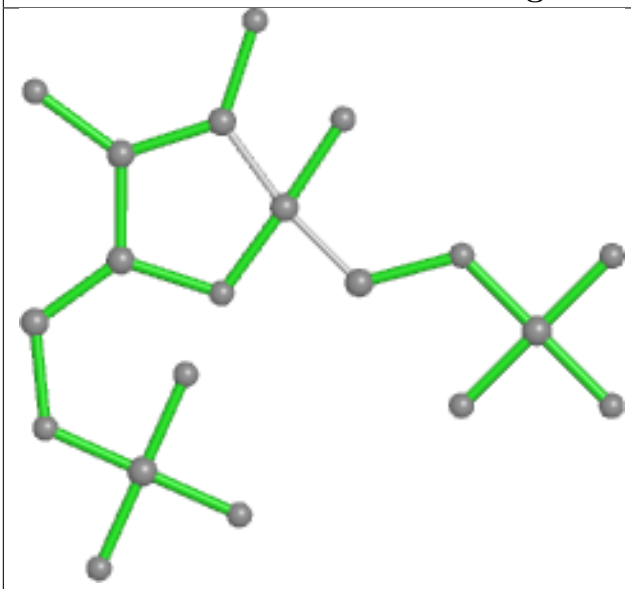
Mol	Chain	Res	Type	Atoms
4	A	603	I7V	C14-C15-C16-C17-C19-N

4 monomers are involved in 4 short contacts:

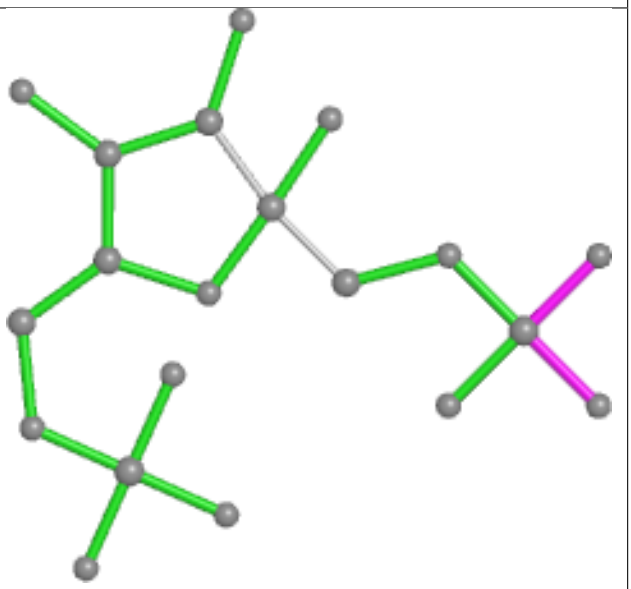
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	602	I7V	1	0
4	B	603	I7V	1	0
4	A	603	I7V	1	0
4	C	602	I7V	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

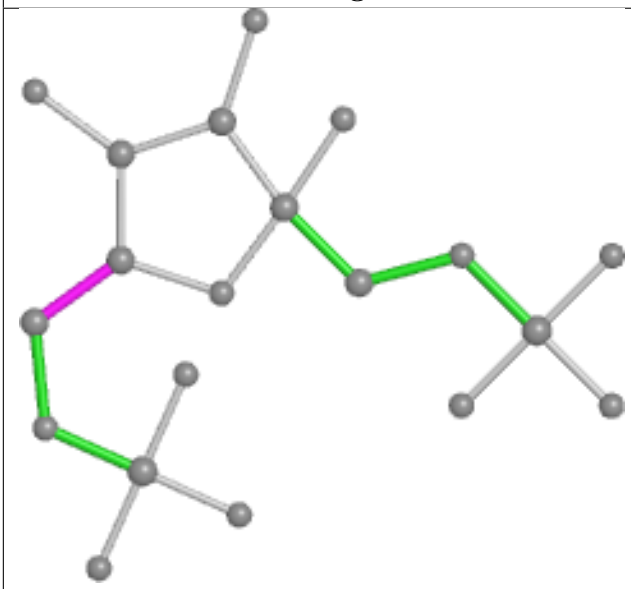
Ligand FBP E 601



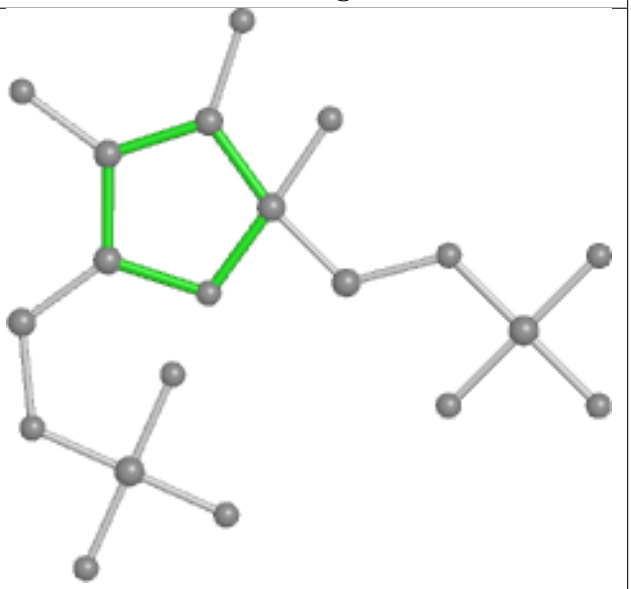
Bond lengths



Bond angles

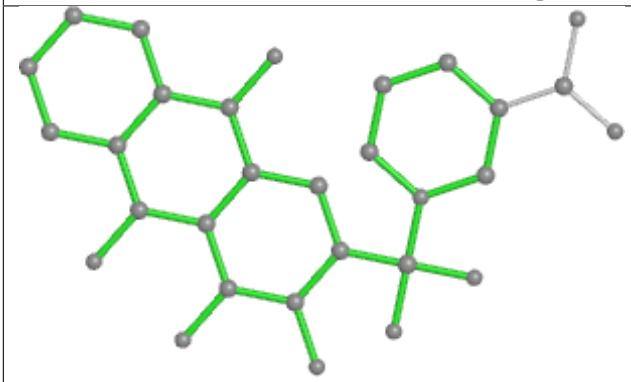


Torsions



Rings

Ligand I7V G 603



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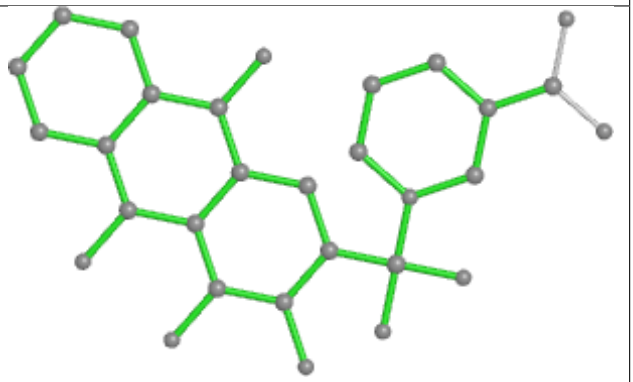

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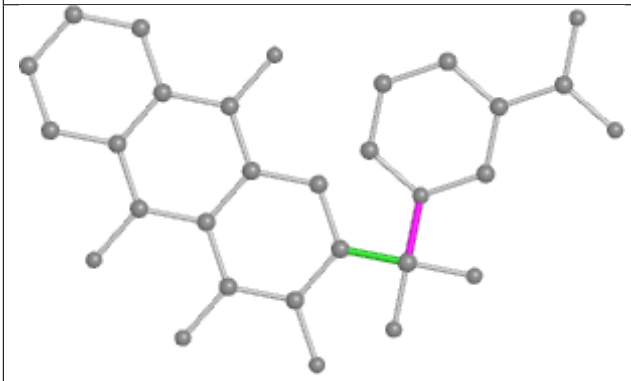

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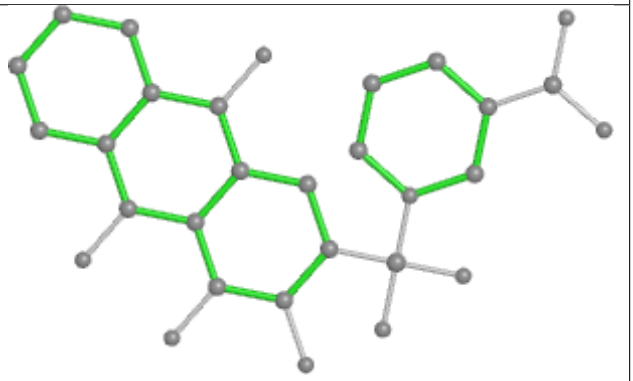
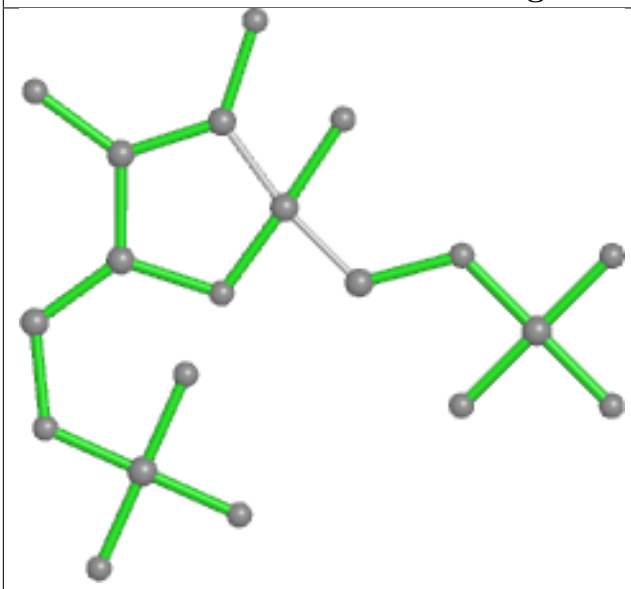


Rings

Ligand FBP F 601



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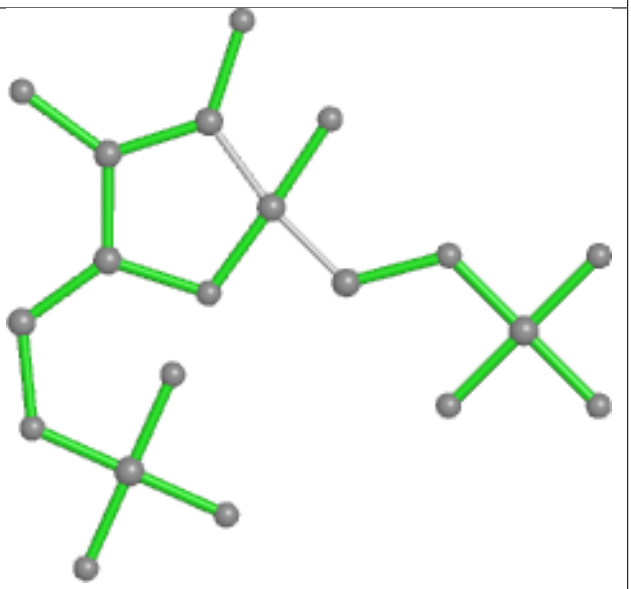
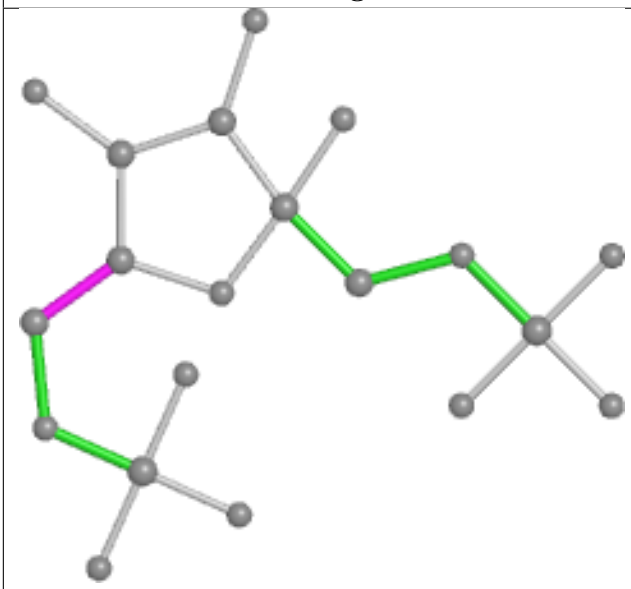


Bond angles



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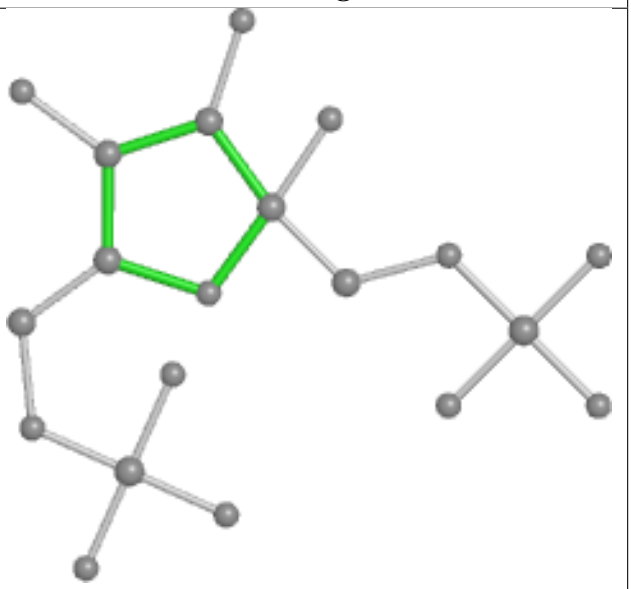
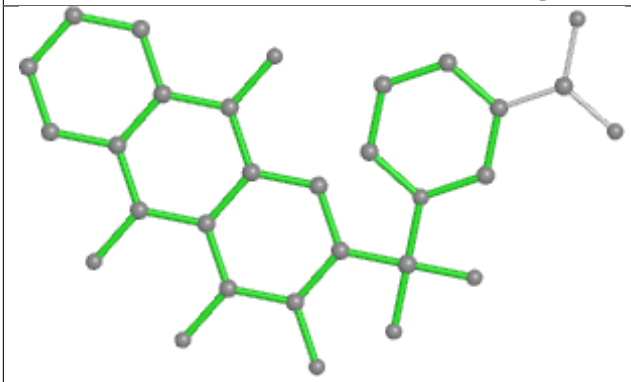


Rings

Ligand I7V F 602



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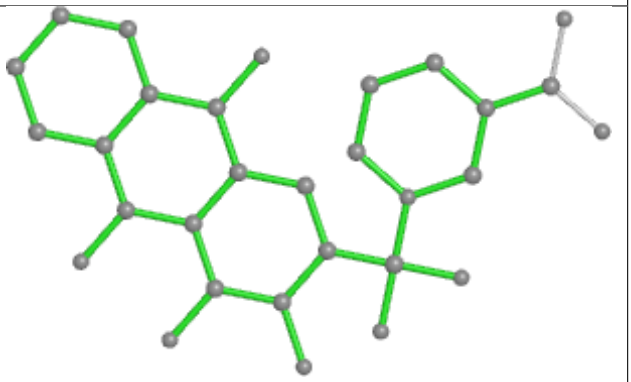
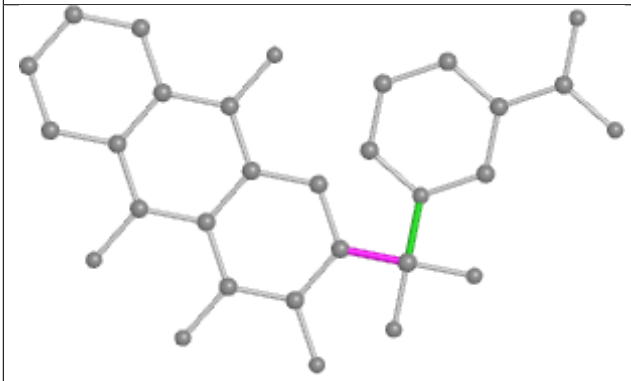


Bond angles



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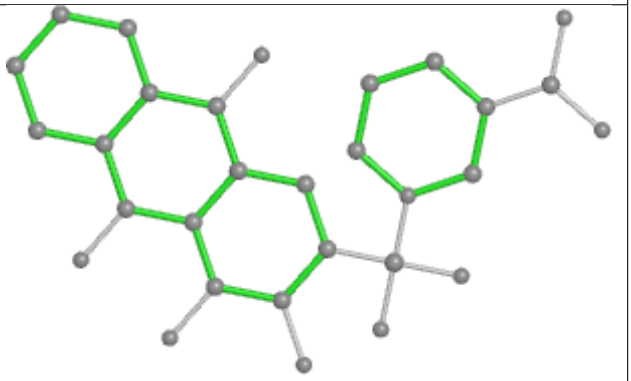
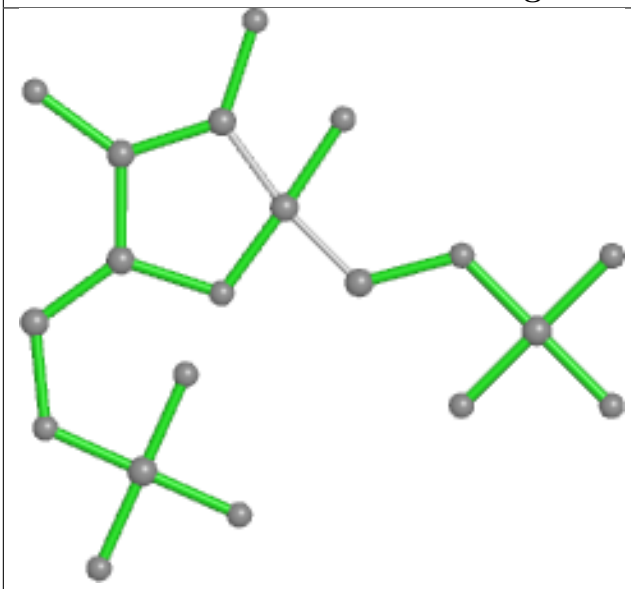


Rings

Ligand FBP G 601



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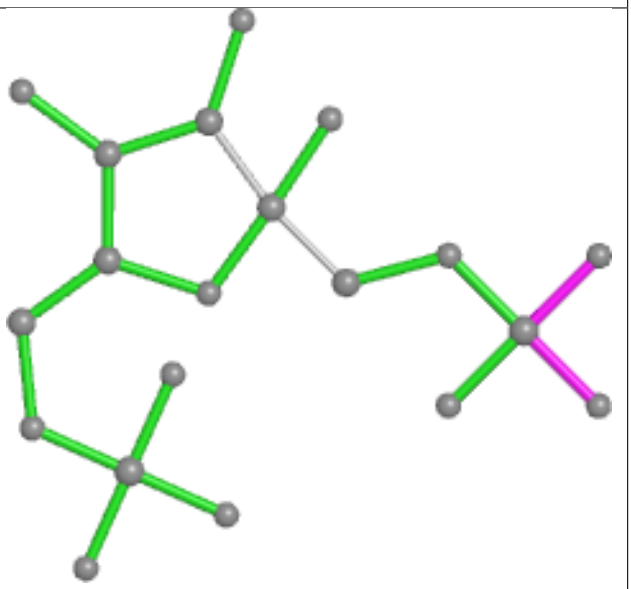
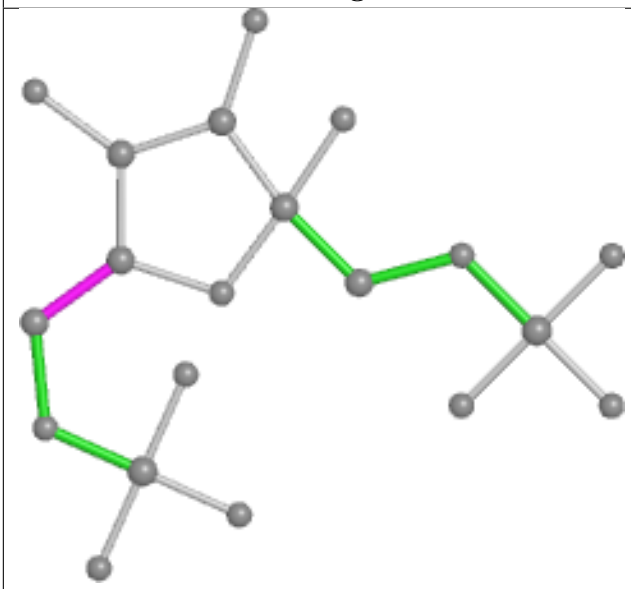


Bond angles



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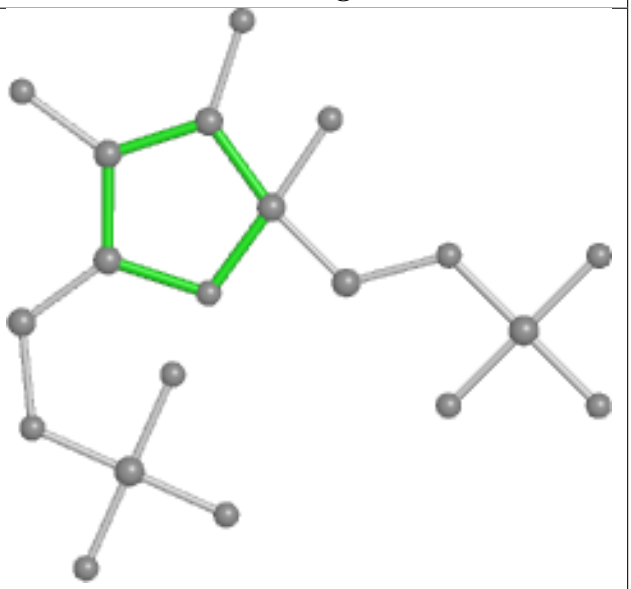
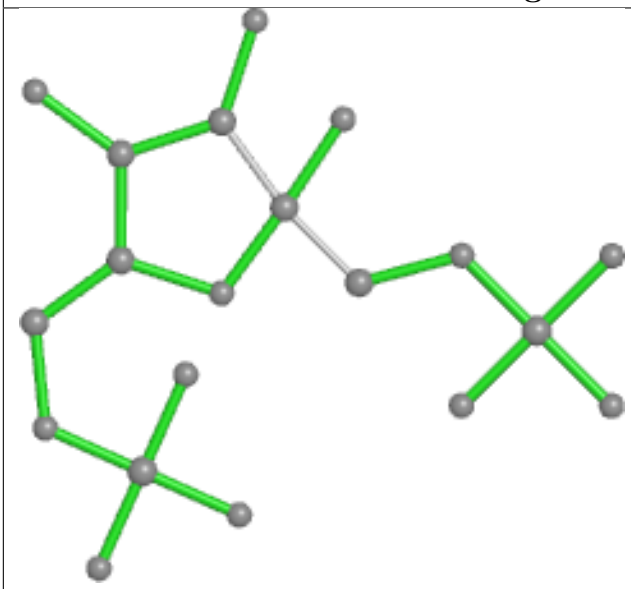


Rings

Ligand FBP D 601



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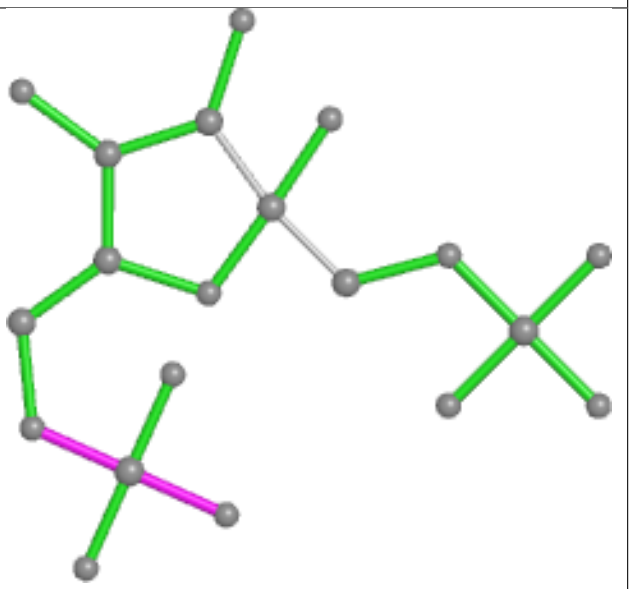
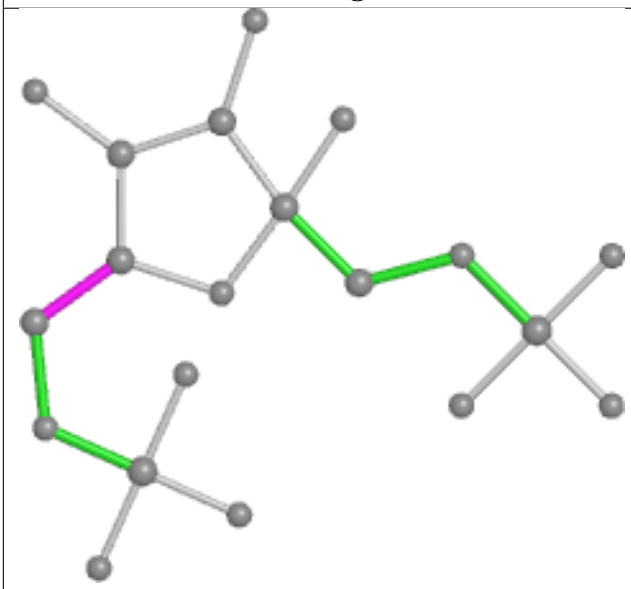


Bond angles



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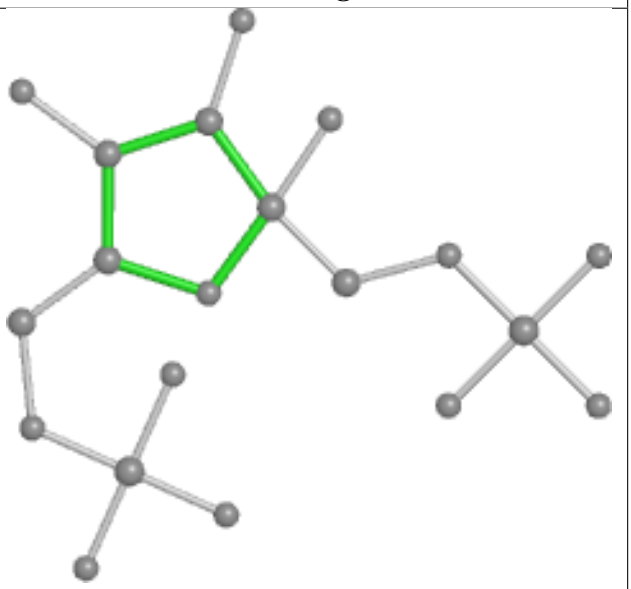
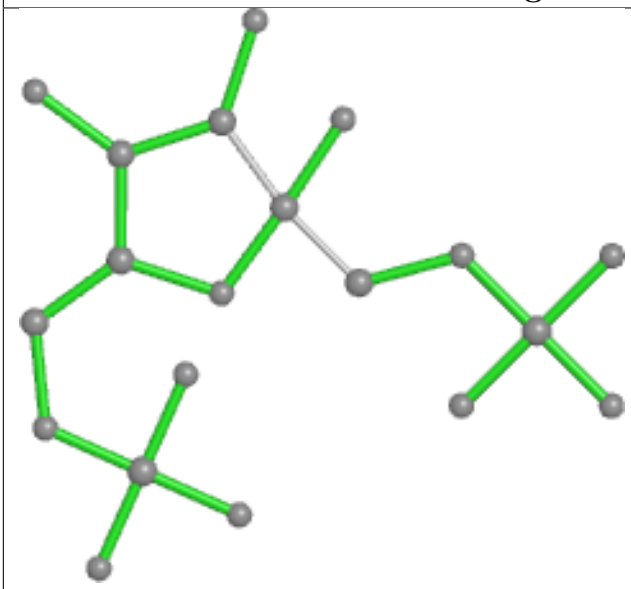
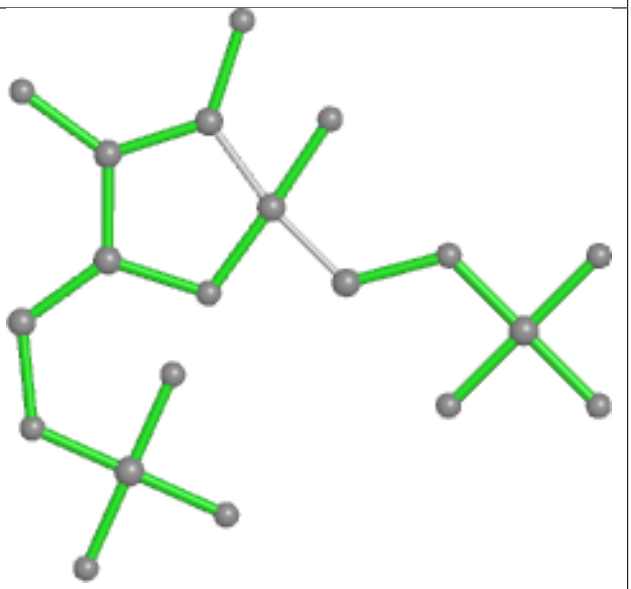


Rings

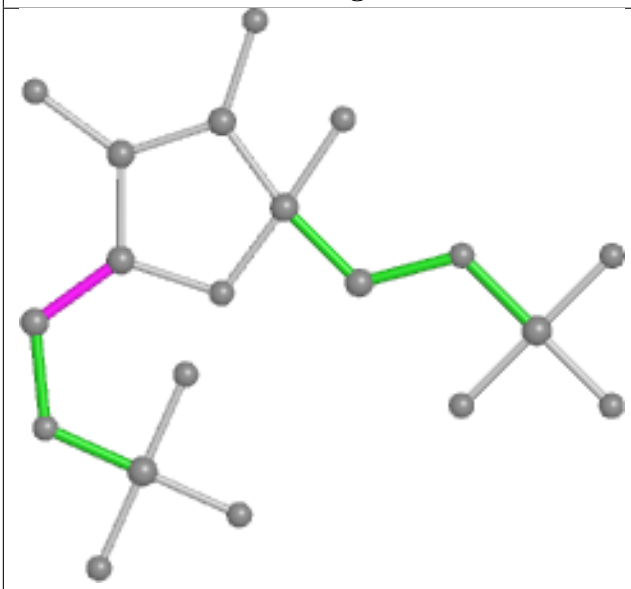
Ligand FBP A 601



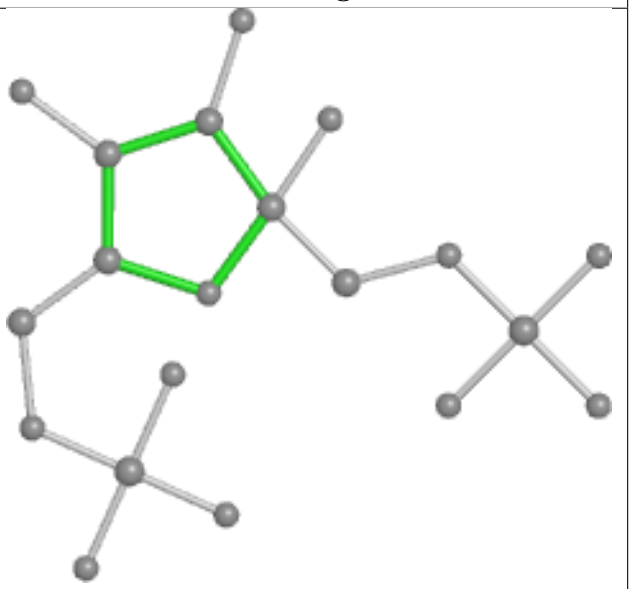
Bond lengths



Bond angles

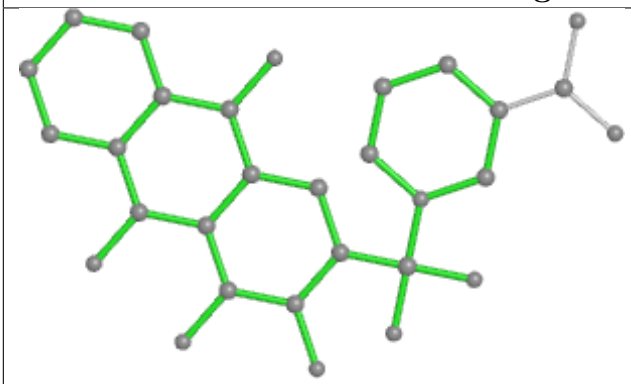


Torsions

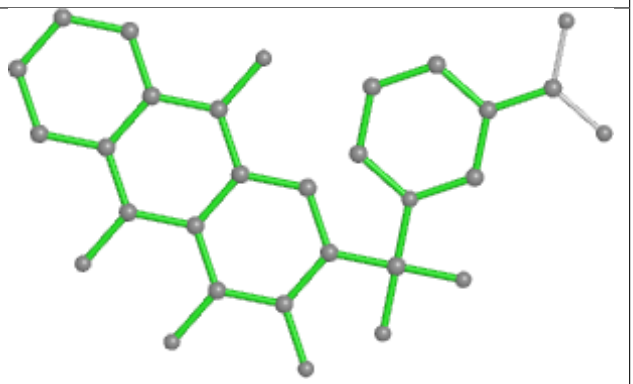


Rings

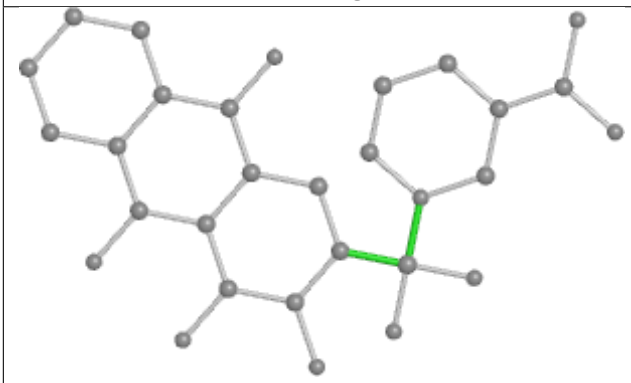
Ligand I7V E 603



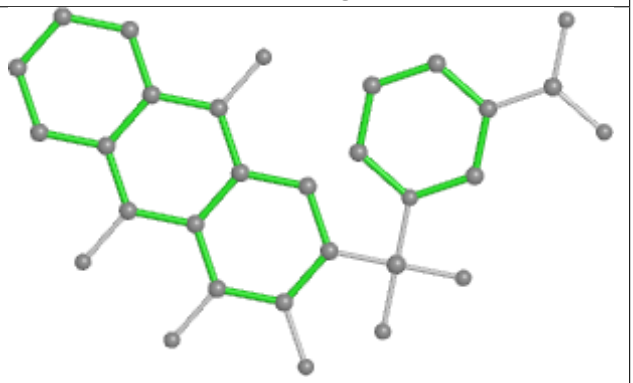
Bond lengths



Bond angles

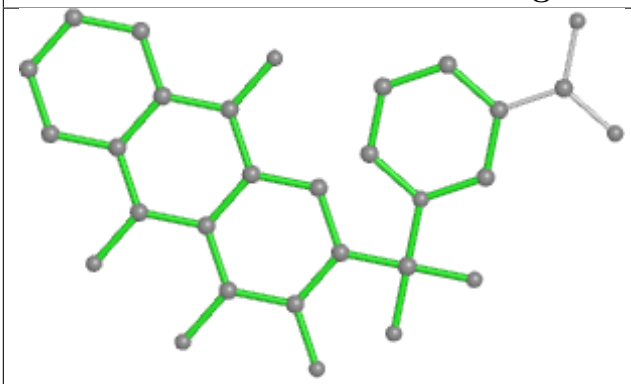


Torsions

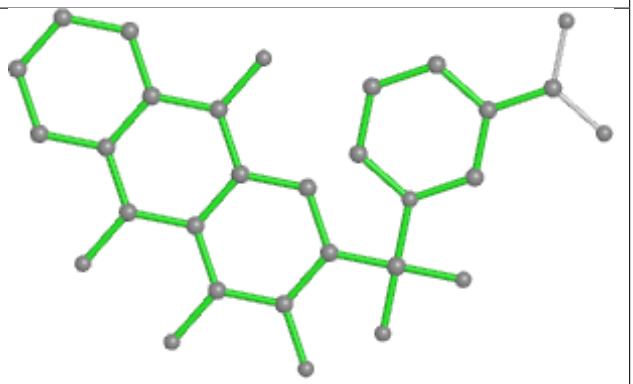


Rings

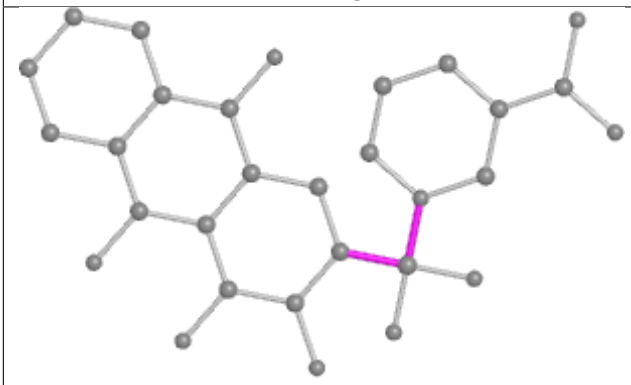
Ligand I7V B 603



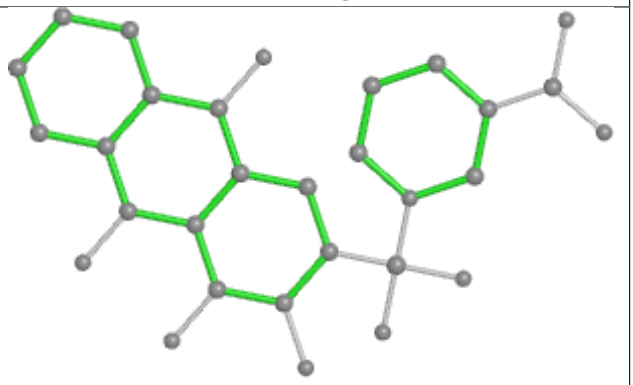
Bond lengths



Bond angles

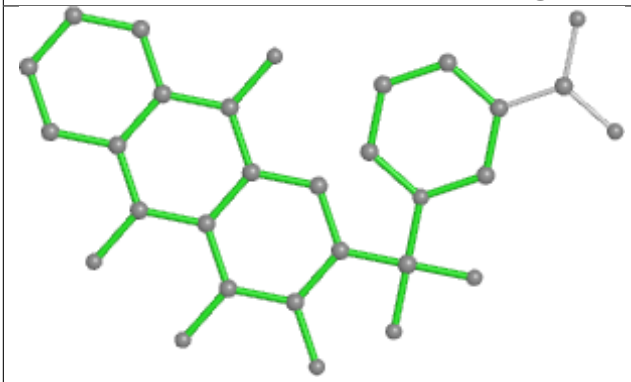


Torsions

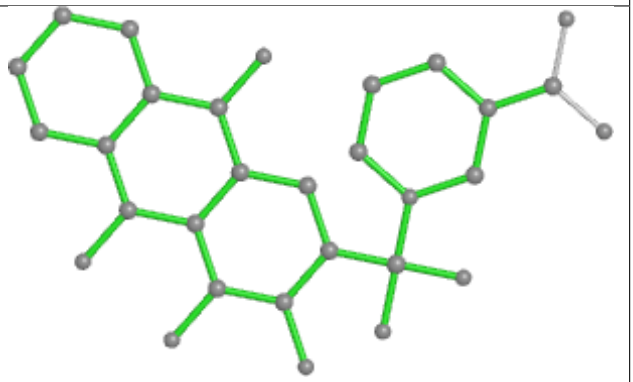


Rings

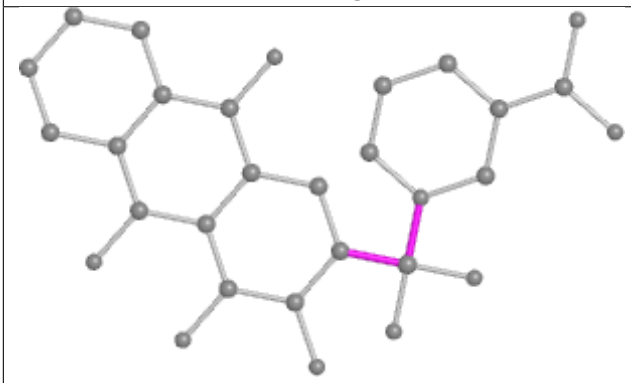
Ligand I7V A 603



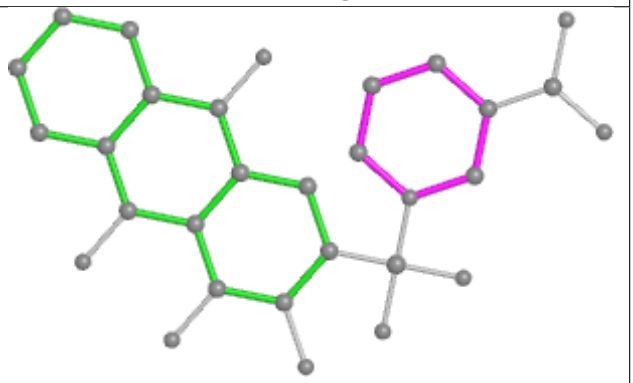
Bond lengths



Bond angles

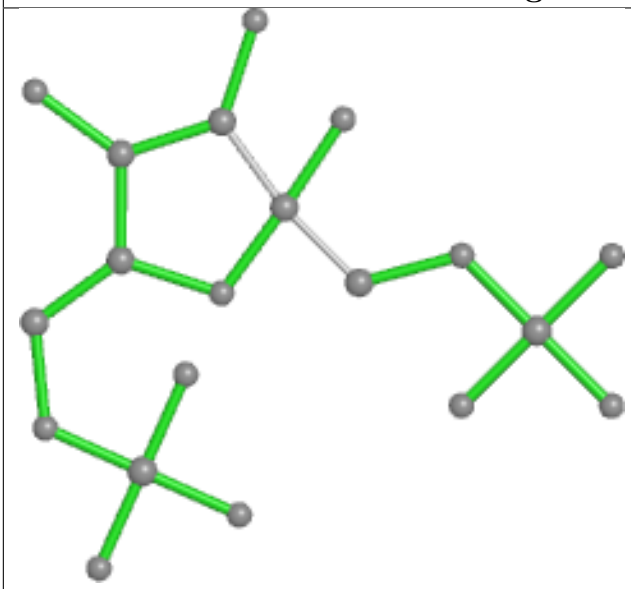


Torsions

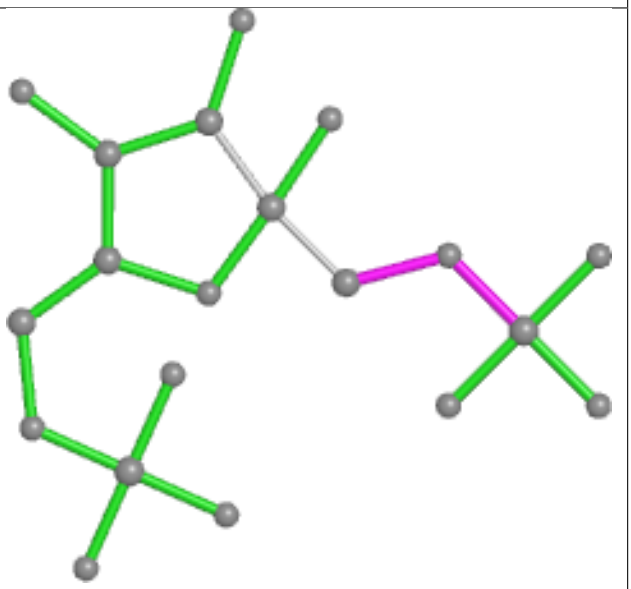


Rings

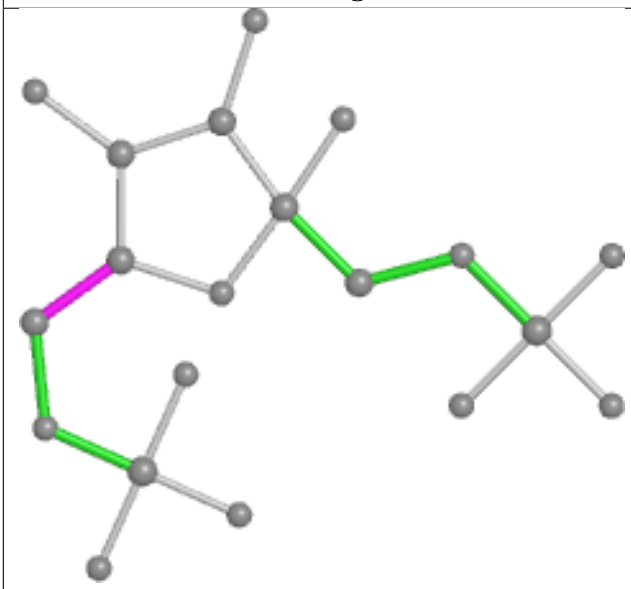
Ligand FBP C 601



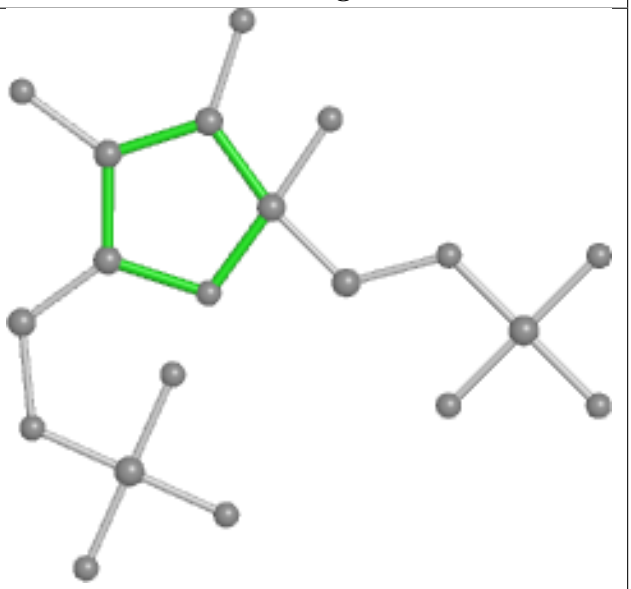
Bond lengths



Bond angles

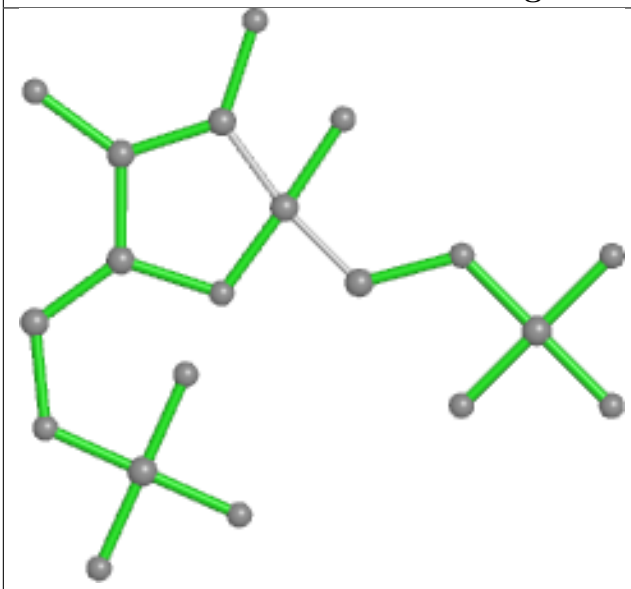


Torsions

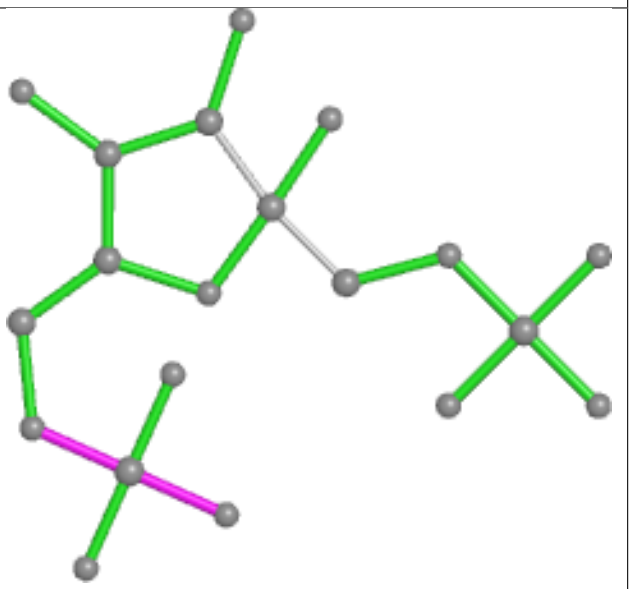


Rings

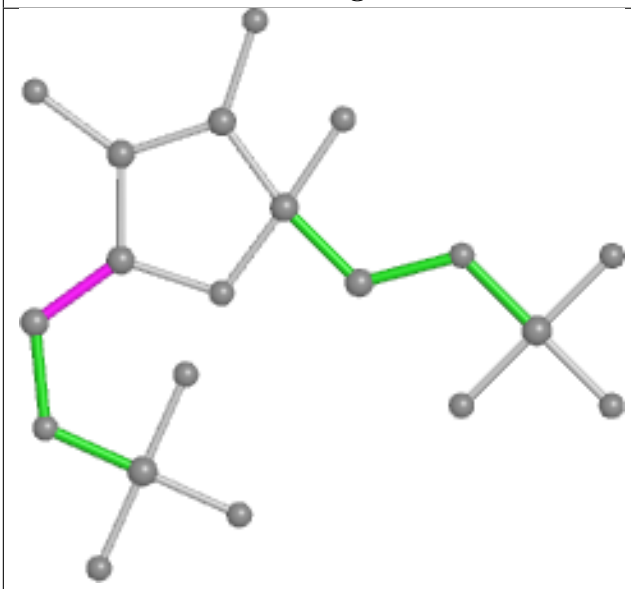
Ligand FBP H 601



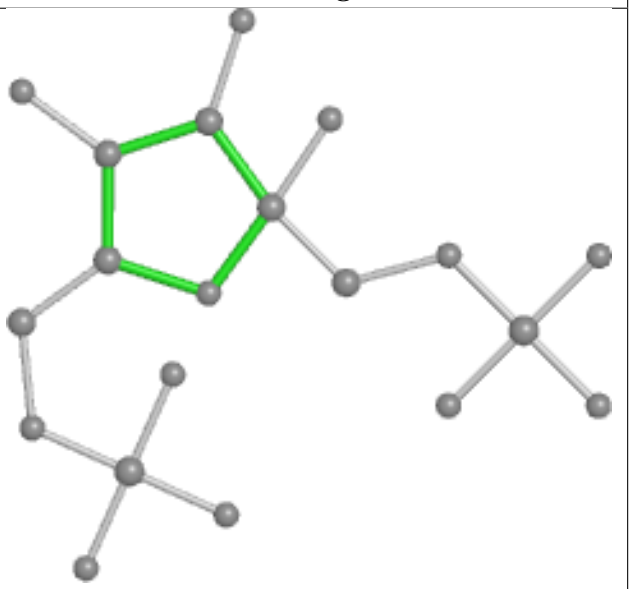
Bond lengths



Bond angles

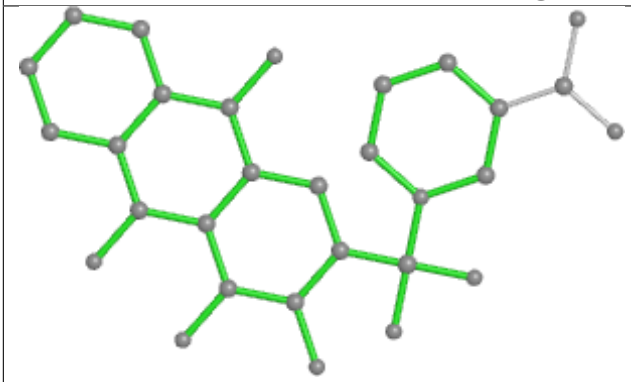


Torsions

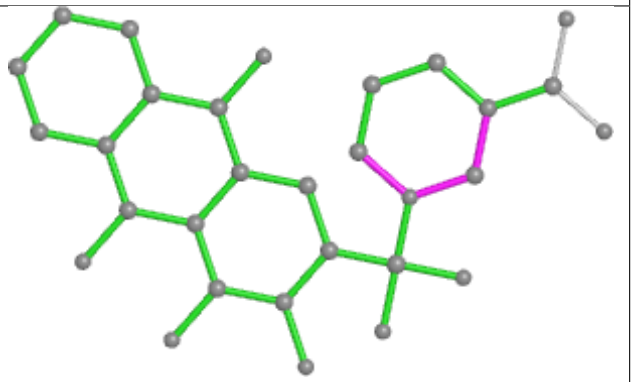


Rings

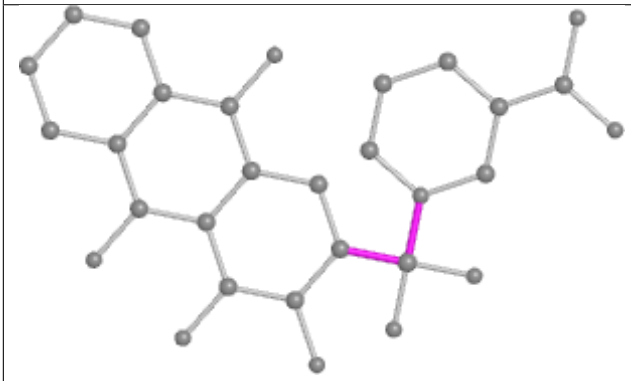
Ligand I7V C 602



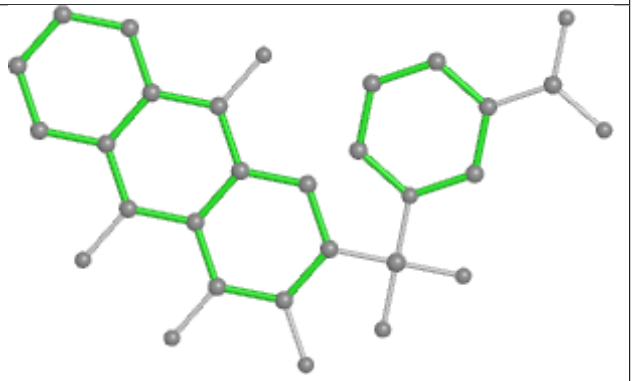
Bond lengths



Bond angles

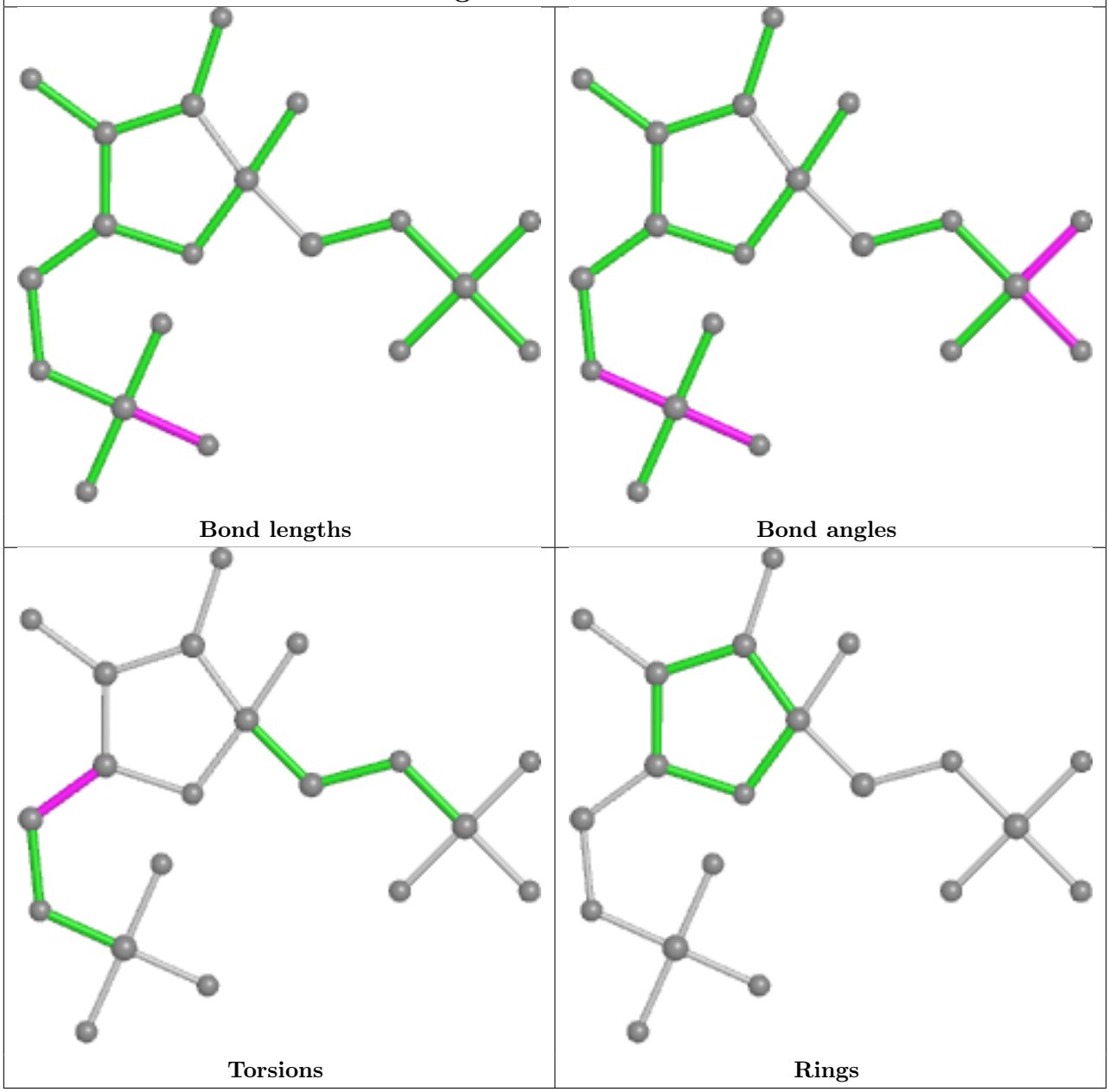


Torsions



Rings

Ligand FBP B 601



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	419/447 (93%)	0.19	24 (5%)	23	19	22, 36, 60, 73	0
1	B	436/447 (97%)	0.29	34 (7%)	13	10	20, 37, 62, 79	0
1	C	424/447 (94%)	-0.06	16 (3%)	40	35	15, 27, 50, 98	0
1	D	425/447 (95%)	0.08	19 (4%)	33	27	18, 26, 48, 93	0
1	E	419/447 (93%)	0.20	27 (6%)	19	15	21, 35, 60, 77	0
1	F	432/447 (96%)	0.06	22 (5%)	28	22	20, 32, 54, 74	0
1	G	422/447 (94%)	-0.18	9 (2%)	63	59	17, 25, 44, 78	1 (0%)
1	H	425/447 (95%)	-0.09	16 (3%)	40	35	16, 24, 47, 80	0
All	All	3402/3576 (95%)	0.06	167 (4%)	29	24	15, 31, 56, 98	1 (0%)

The worst 5 of 167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	PHE	14.1
1	D	25	PHE	13.5
1	H	21	GLY	12.0
1	D	22	THR	11.7
1	C	22	THR	11.1

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

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

6.3 Carbohydrates

There are no 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	I7V	A	603	30/30	0.79	0.23	95,95,96,96	17
4	I7V	B	603	30/30	0.86	0.20	79,81,82,82	17
4	I7V	C	602	30/30	0.86	0.22	63,65,66,66	17
4	I7V	E	603	30/30	0.87	0.19	56,56,62,63	17
4	I7V	F	602	30/30	0.87	0.19	64,65,66,66	17
3	OXL	E	602	6/6	0.89	0.13	40,41,41,41	0
6	K	A	605	1/1	0.89	0.06	69,69,69,69	0
6	K	B	605	1/1	0.89	0.07	61,61,61,61	0
5	MG	E	604	1/1	0.92	0.05	34,34,34,34	0
3	OXL	A	602	6/6	0.92	0.15	37,38,38,38	0
3	OXL	B	602	6/6	0.92	0.10	41,42,43,44	0
4	I7V	G	603	30/30	0.93	0.12	39,43,48,50	17
6	K	F	605	1/1	0.94	0.05	63,63,63,63	0
3	OXL	F	603	6/6	0.95	0.10	35,36,36,37	0
6	K	C	605	1/1	0.96	0.12	45,45,45,45	0
3	OXL	C	603	6/6	0.96	0.09	31,32,33,33	0
5	MG	B	604	1/1	0.97	0.06	43,43,43,43	0
2	FBP	B	601	20/20	0.97	0.07	30,31,36,36	0
2	FBP	A	601	20/20	0.97	0.07	29,30,31,32	0
3	OXL	G	602	6/6	0.97	0.06	26,28,28,28	0
3	OXL	H	602	6/6	0.97	0.07	26,27,28,29	0
3	OXL	D	602	6/6	0.97	0.09	25,26,26,27	0
2	FBP	E	601	20/20	0.98	0.07	28,29,31,31	0
2	FBP	F	601	20/20	0.98	0.06	27,31,36,36	0
6	K	E	605	1/1	0.98	0.14	61,61,61,61	0
5	MG	A	604	1/1	0.98	0.04	39,39,39,39	0
5	MG	F	604	1/1	0.99	0.02	32,32,32,32	0
5	MG	G	604	1/1	0.99	0.02	23,23,23,23	0
5	MG	H	603	1/1	0.99	0.02	26,26,26,26	0
2	FBP	D	601	20/20	0.99	0.07	19,21,23,24	0
2	FBP	G	601	20/20	0.99	0.06	17,19,20,21	0
2	FBP	H	601	20/20	0.99	0.06	17,18,21,22	0
6	K	D	604	1/1	0.99	0.03	34,34,34,34	0
5	MG	C	604	1/1	0.99	0.04	27,27,27,27	0
2	FBP	C	601	20/20	0.99	0.08	18,20,22,23	0
6	K	G	605	1/1	0.99	0.11	40,40,40,40	0
6	K	H	604	1/1	0.99	0.04	37,37,37,37	0

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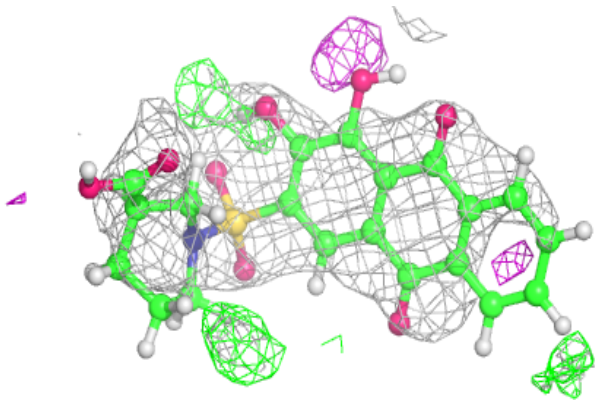
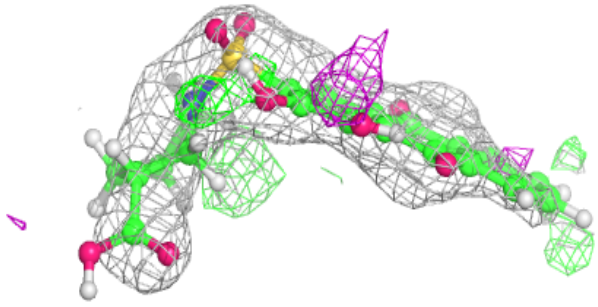
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	D	603	1/1	1.00	0.02	25,25,25,25	0

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 I7V A 603:

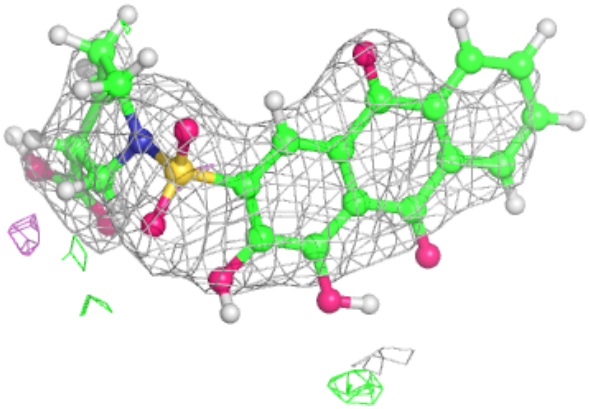
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

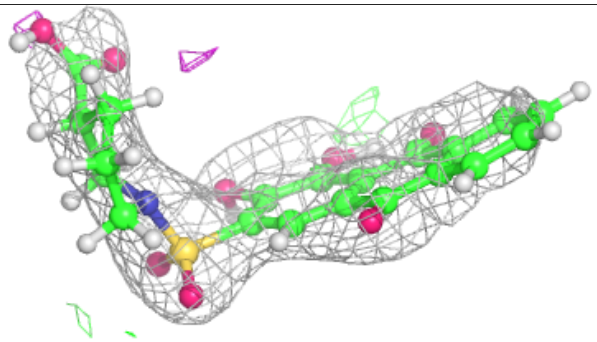


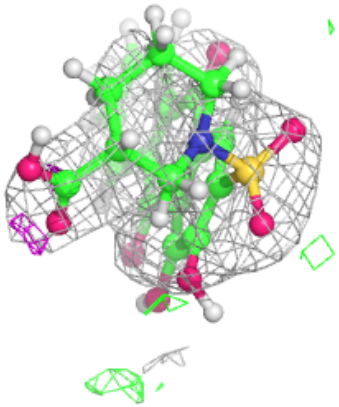


Electron density around I7V B 603:

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

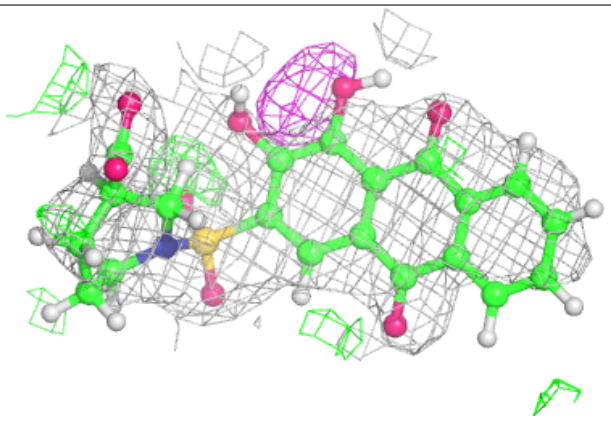


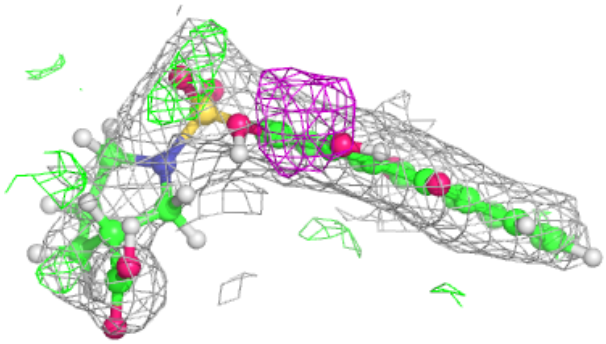


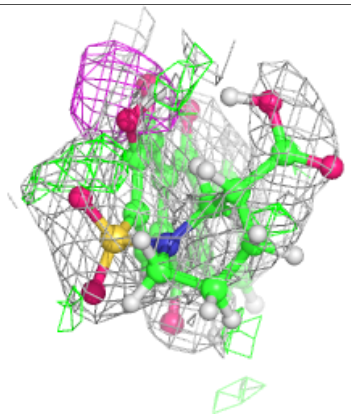


Electron density around I7V C 602:

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

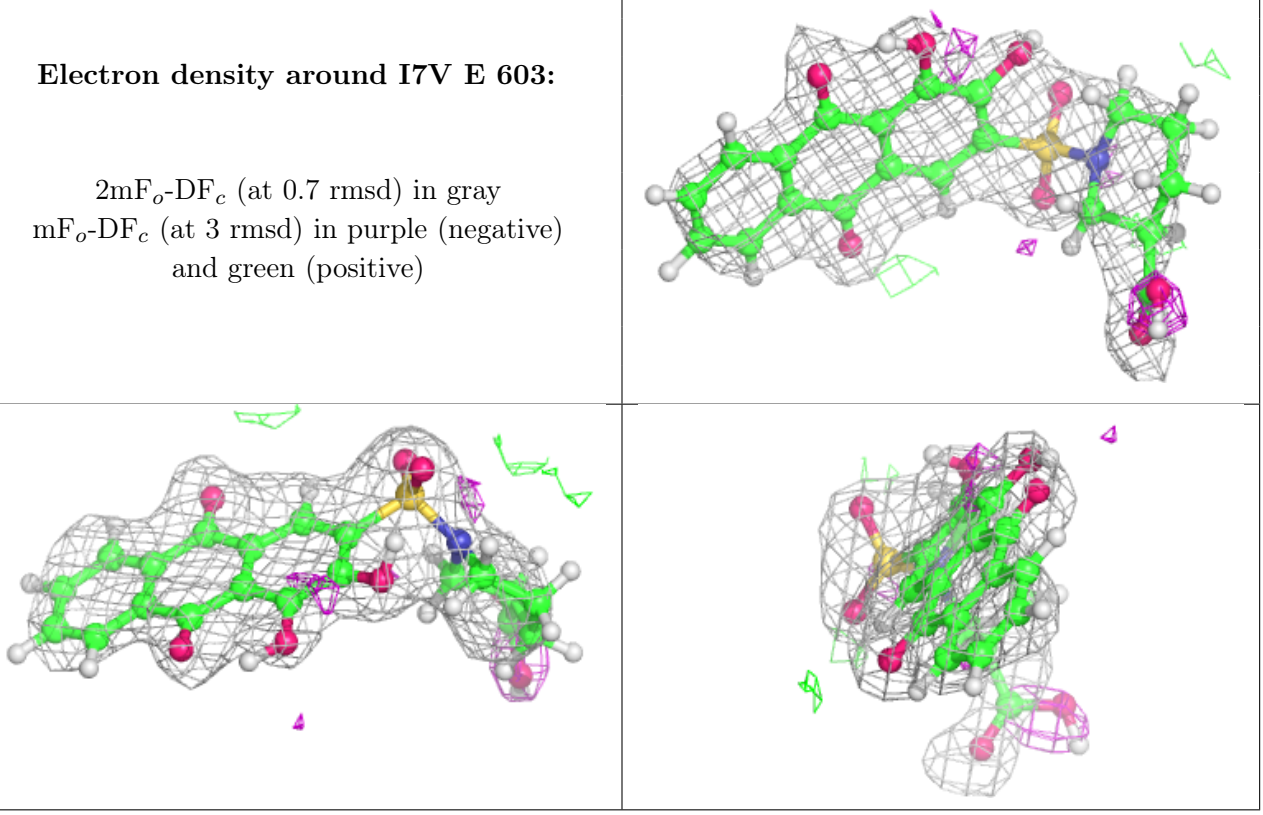






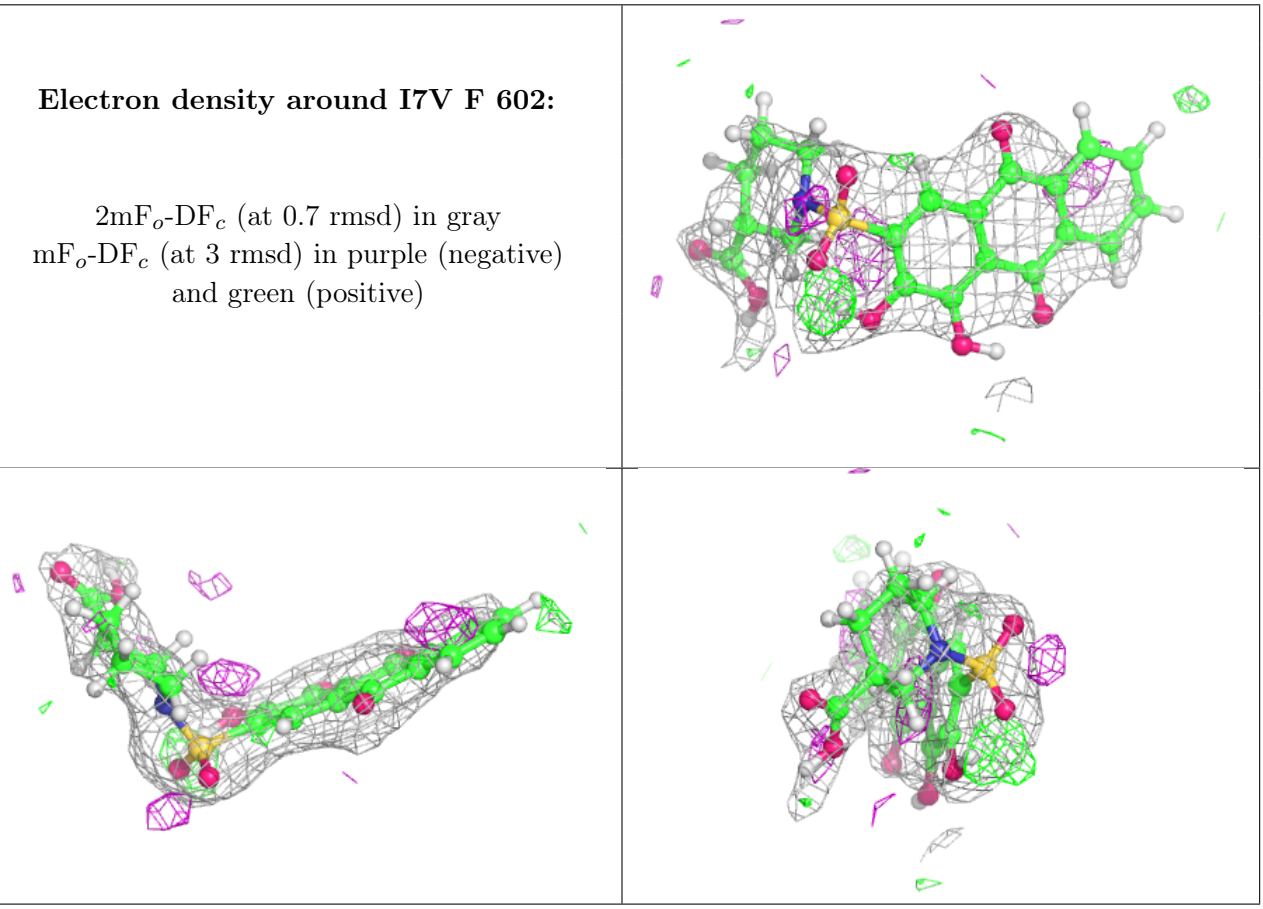
Electron density around I7V E 603:

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



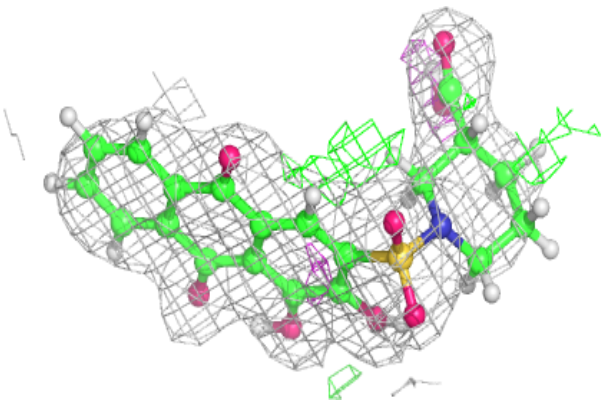
Electron density around I7V F 602:

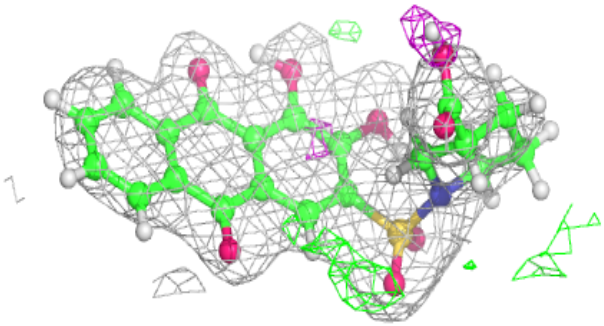
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

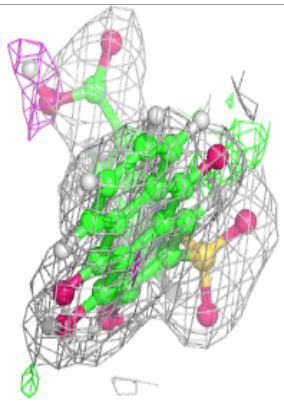


Electron density around I7V G 603:

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

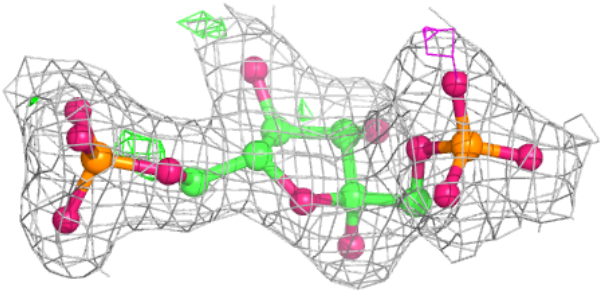


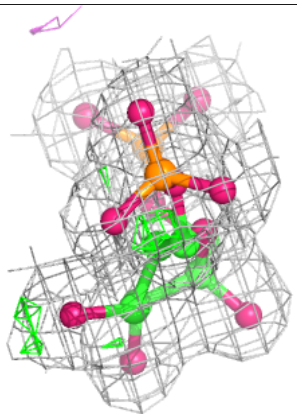




Electron density around FBP B 601:

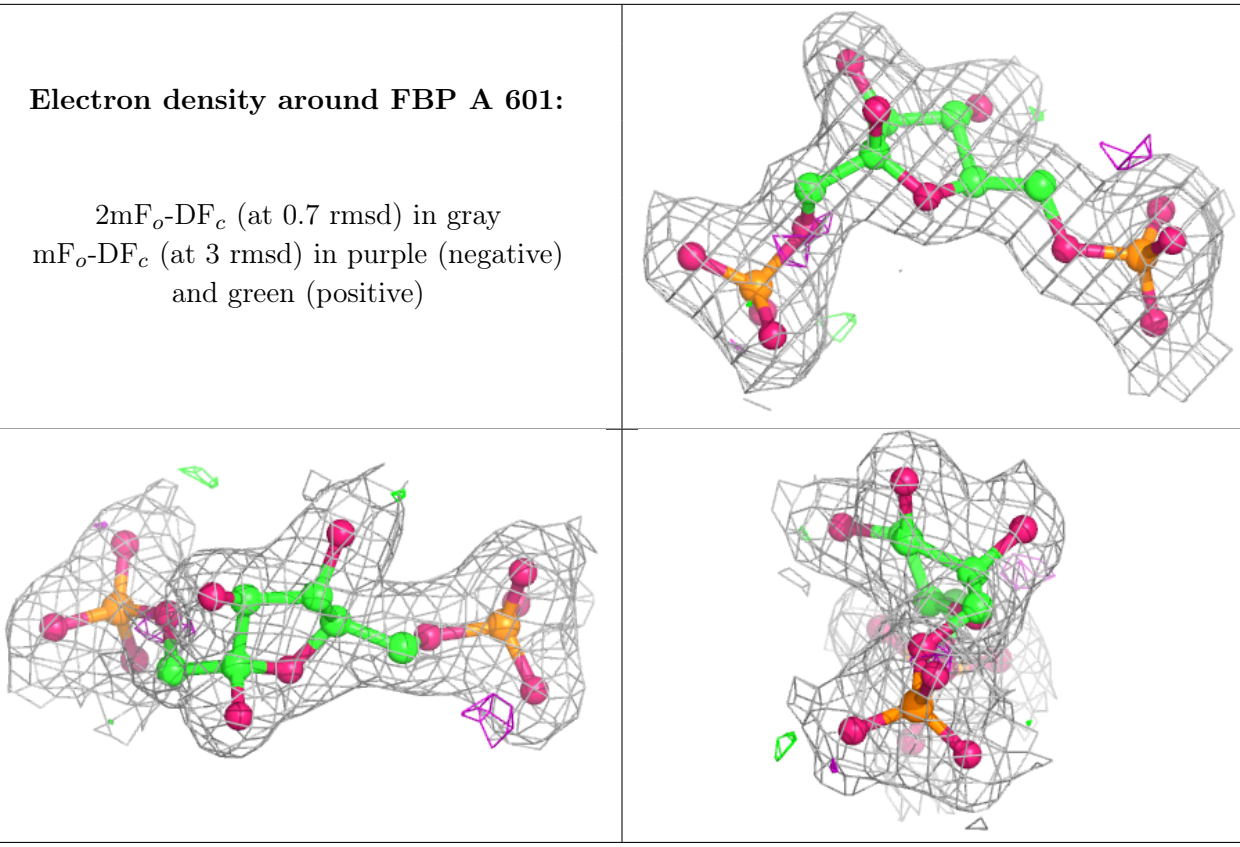
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





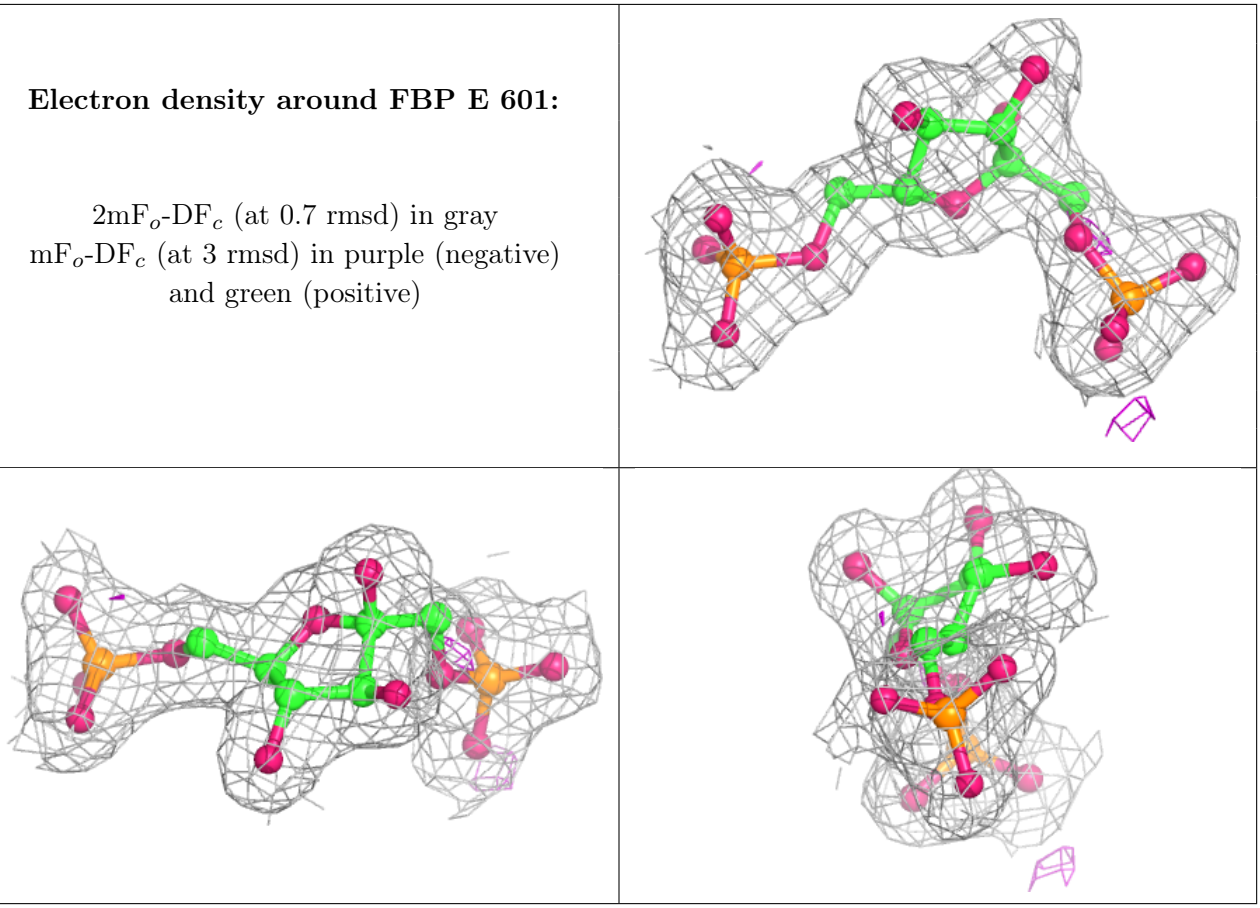
Electron density around FBP A 601:

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



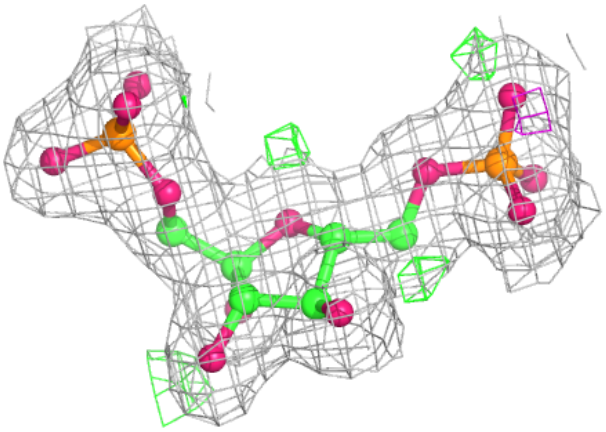
Electron density around FBP E 601:

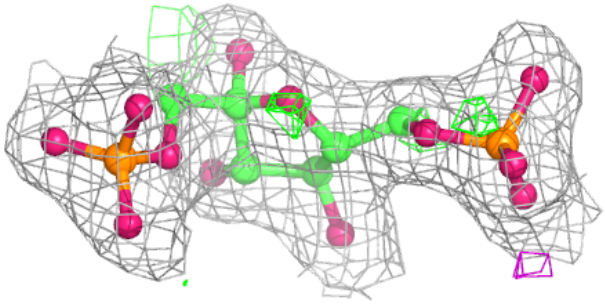
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

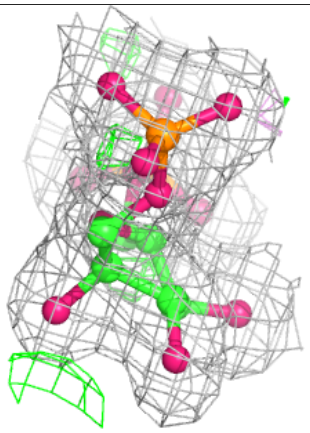


Electron density around FBP F 601:

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

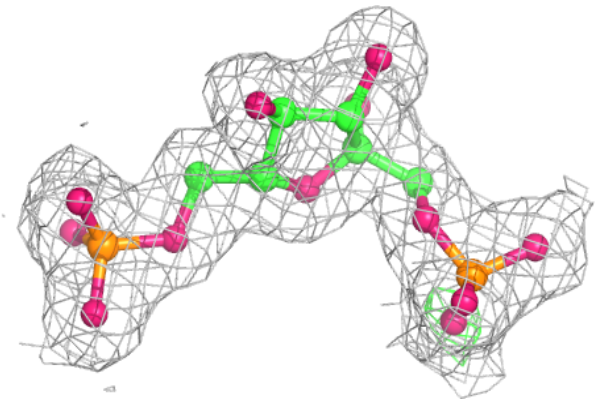


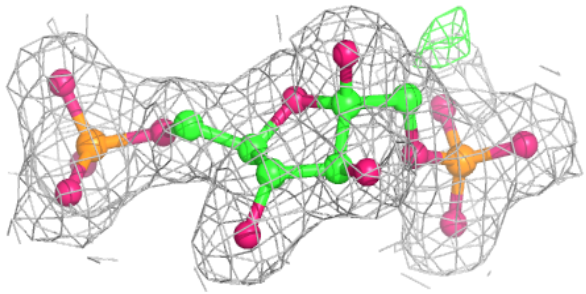


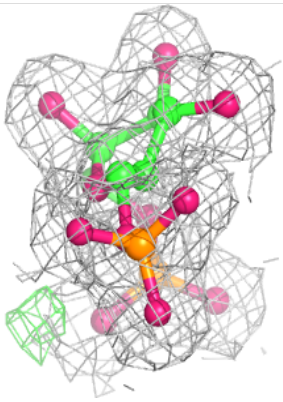


Electron density around FBP D 601:

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

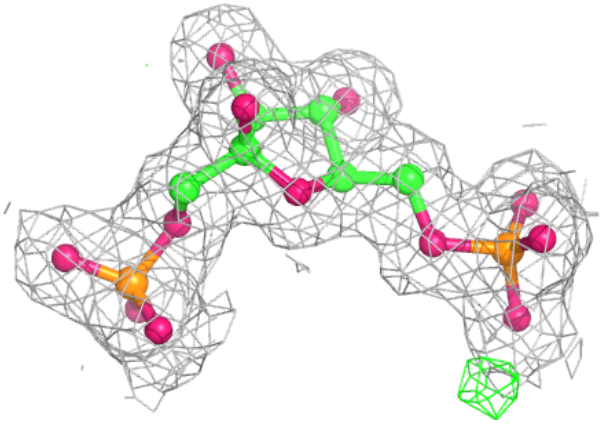


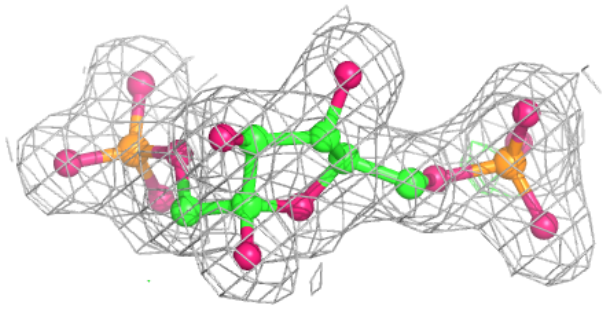


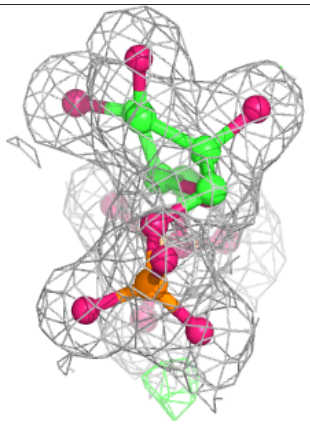


Electron density around FBP G 601:

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

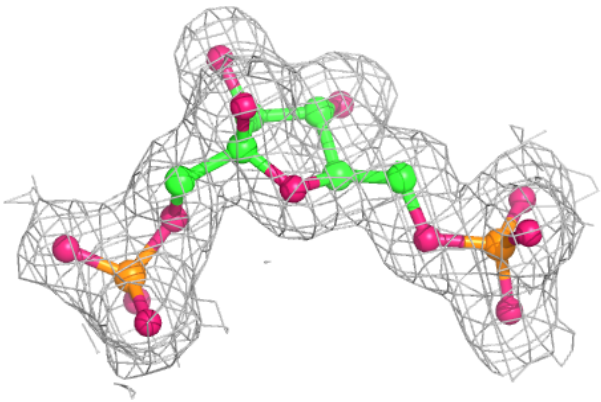


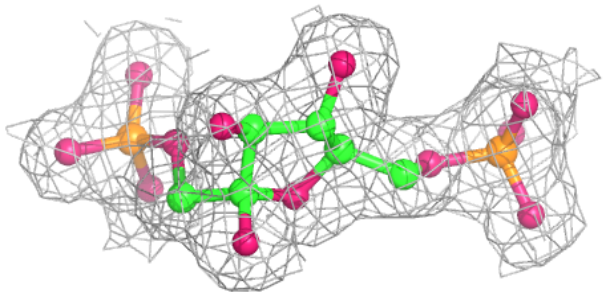


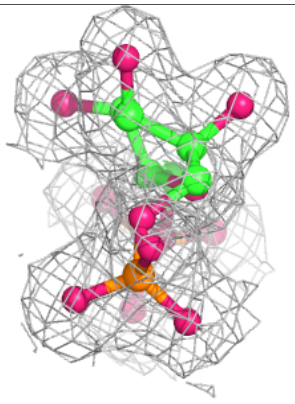


Electron density around FBP H 601:

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

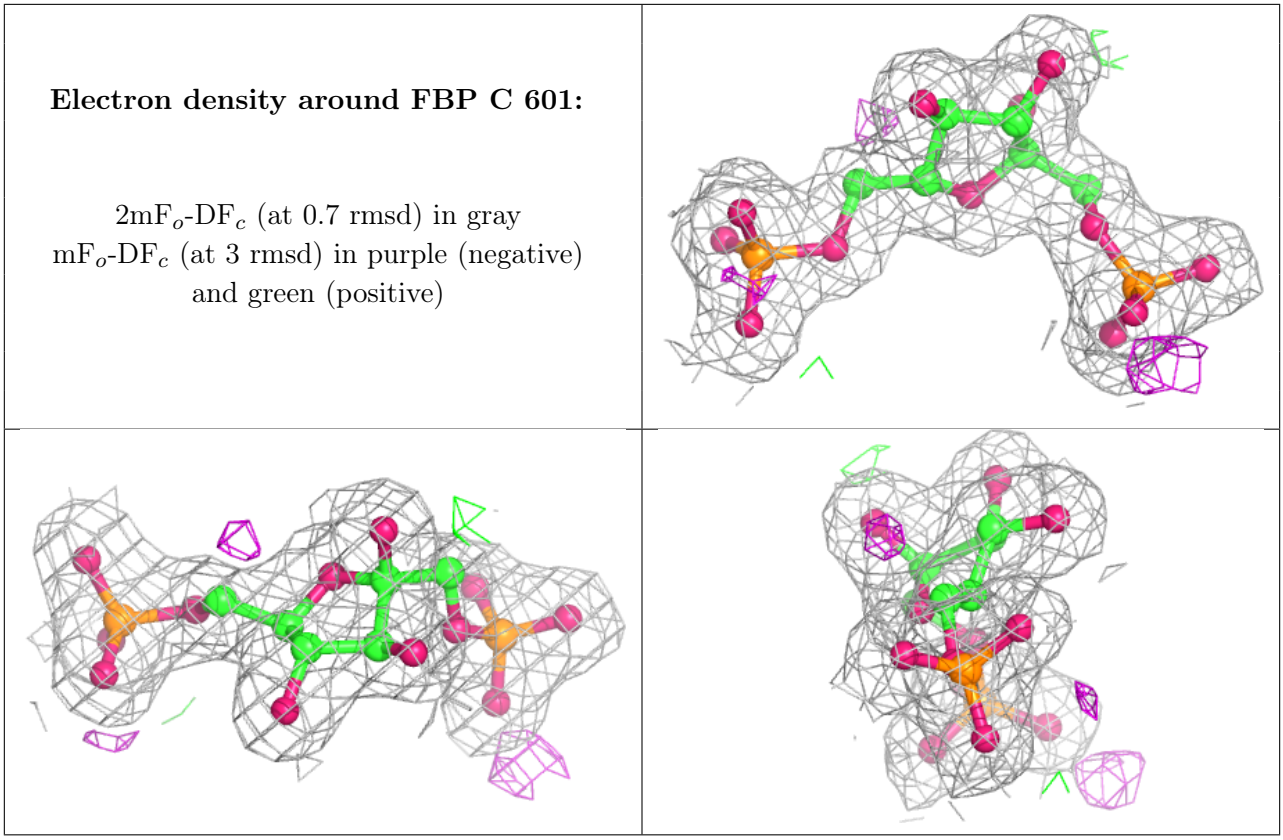






Electron density around FBP C 601:

$2mF_o$-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.