wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2026 – 01:24 PM EDT

PDB ID	:	14CL / pdb_000014cl
Title	:	Structure of liver pyruvate kinase in complex with TEPP-46
Authors	:	Lulla, A.; Rodriguez Rivero, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2026-04-28
Resolution	:	2.13 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

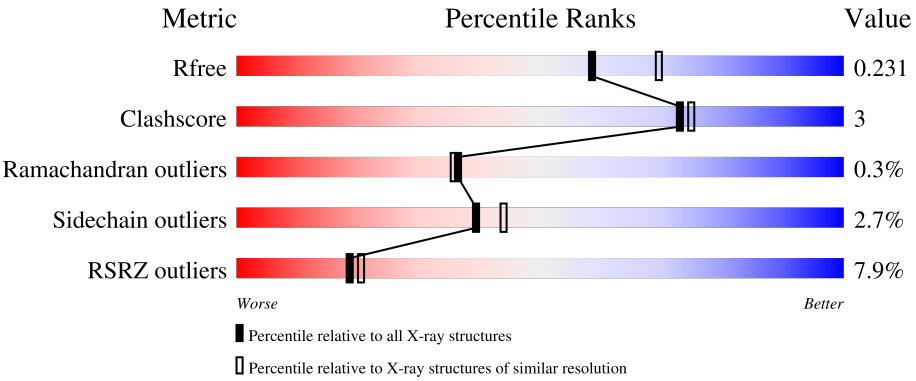
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.13 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 >=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	10% 83% 10% • 6%
1	B	447	19% 89% 8% •
1	C	447	6% 84% 10% • 5%
1	D	447	4% 87% 7% • 5%
1	E	447	8% 84% 10% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	447	6% 86% 10%
1	G	447	4% 83% 12%
1	H	447	3% 85% 9% 5%

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

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

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 27958 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 Isoform L-type of Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	13	0
			3249	2040	583	606	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	8	0
			3265	2056	584	606	19			
1	D	425	Total	C	N	O	S	0	8	0
			3261	2048	590	604	19			
1	E	423	Total	C	N	O	S	0	13	0
			3278	2061	588	609	20			
1	F	435	Total	C	N	O	S	0	8	0
			3341	2101	600	620	20			
1	G	427	Total	C	N	O	S	0	9	0
			3290	2070	588	613	19			
1	H	425	Total	C	N	O	S	0	9	0
			3269	2053	593	604	19			

There are 48 discrepancies between the modelled and reference sequences:

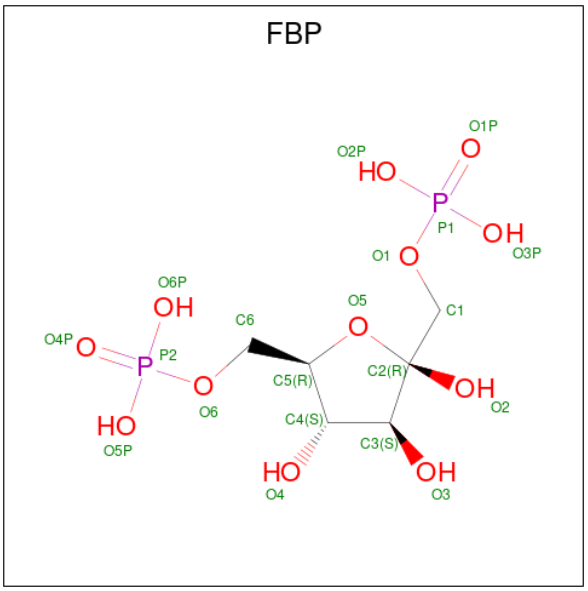
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30613
A	0	SER	-	expression tag	UNP P30613
A	12	ASP	SER	conflict	UNP P30613
A	130	GLY	-	linker	UNP P30613
A	131	SER	-	linker	UNP P30613
A	132	GLY	-	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
B	0	SER	-	expression tag	UNP P30613
B	12	ASP	SER	conflict	UNP P30613
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613

Continued on next page...

Continued from previous page...

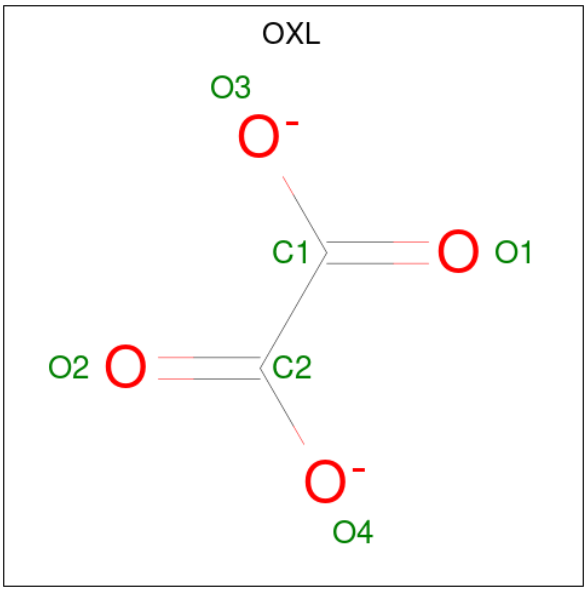
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	130	GLY	-	linker	UNP P30613
C	131	SER	-	linker	UNP P30613
C	132	GLY	-	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	12	ASP	SER	conflict	UNP P30613
D	130	GLY	-	linker	UNP P30613
D	131	SER	-	linker	UNP P30613
D	132	GLY	-	linker	UNP P30613
E	-1	GLY	-	expression tag	UNP P30613
E	0	SER	-	expression tag	UNP P30613
E	12	ASP	SER	conflict	UNP P30613
E	130	GLY	-	linker	UNP P30613
E	131	SER	-	linker	UNP P30613
E	132	GLY	-	linker	UNP P30613
F	-1	GLY	-	expression tag	UNP P30613
F	0	SER	-	expression tag	UNP P30613
F	12	ASP	SER	conflict	UNP P30613
F	130	GLY	-	linker	UNP P30613
F	131	SER	-	linker	UNP P30613
F	132	GLY	-	linker	UNP P30613
G	-1	GLY	-	expression tag	UNP P30613
G	0	SER	-	expression tag	UNP P30613
G	12	ASP	SER	conflict	UNP P30613
G	130	GLY	-	linker	UNP P30613
G	131	SER	-	linker	UNP P30613
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	130	GLY	-	linker	UNP P30613
H	131	SER	-	linker	UNP P30613
H	132	GLY	-	linker	UNP P30613

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



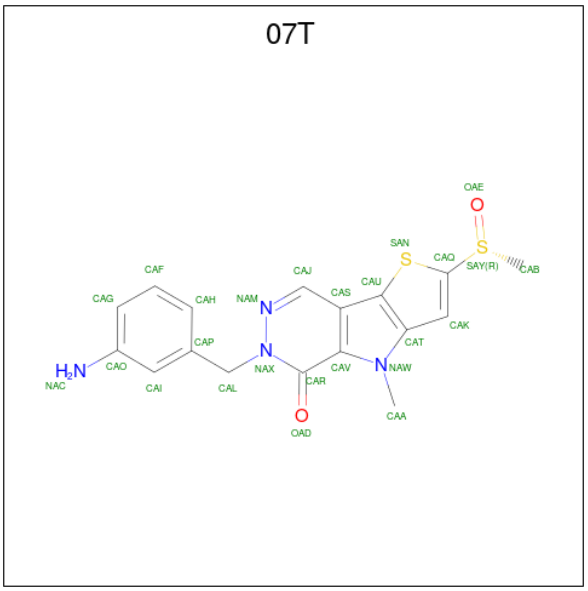
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 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 6-(3-aminobenzyl)-4-methyl-2-methylsulfinyl-4,6-dihydro-5H-thieno[2',3':4,5]pyrrolo[2,3-d]pyridazin-5-one (CCD ID: 07T) (formula: $C_{17}H_{16}N_4O_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 50 34 8 4 4	0	1
4	B	1	Total C N O S 50 34 8 4 4	0	1
4	E	1	Total C N O S 50 34 8 4 4	0	1
4	F	1	Total C N O S 50 34 8 4 4	0	1

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

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

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

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

- Molecule 7 is water.

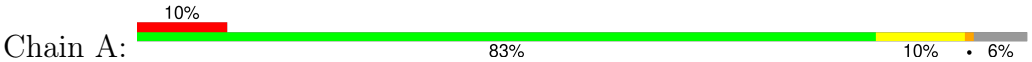
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	110	Total O 110 110	0	0
7	B	111	Total O 111 111	0	0
7	C	173	Total O 173 173	0	0
7	D	199	Total O 199 199	0	0
7	E	121	Total O 121 121	0	0
7	F	149	Total O 149 149	0	0
7	G	169	Total O 169 169	0	0
7	H	199	Total O 199 199	0	0

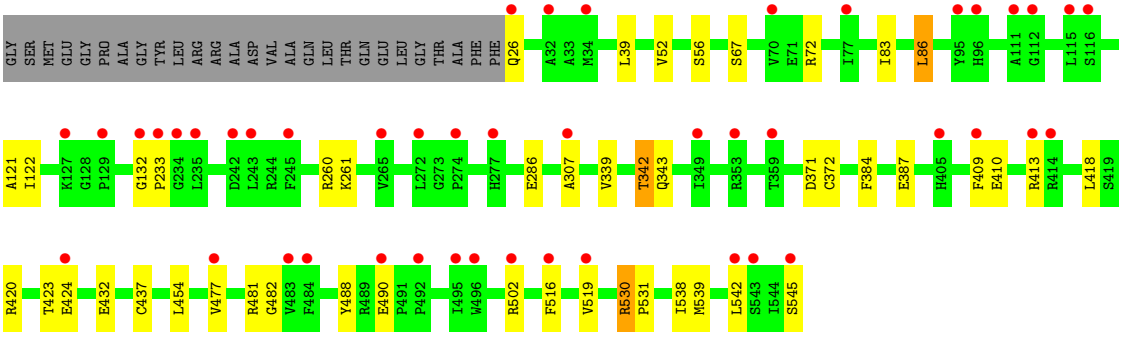
3 Residue-property plots (i)

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: Isoform L-type of Pyruvate kinase PKLR

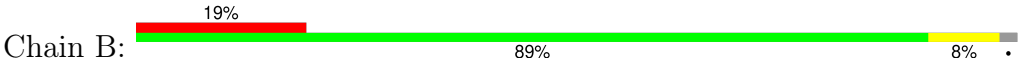
Chain A:

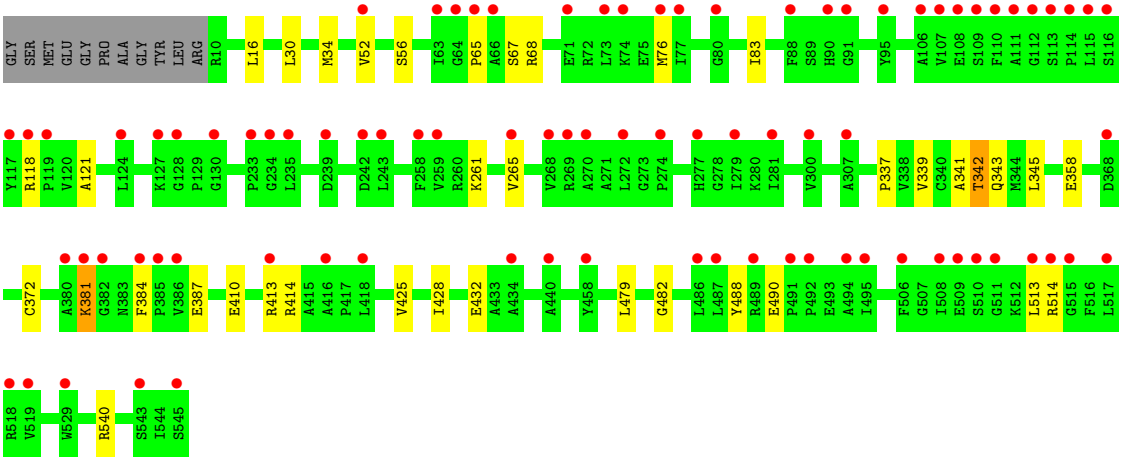




• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

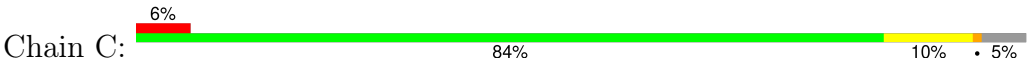
Chain B:

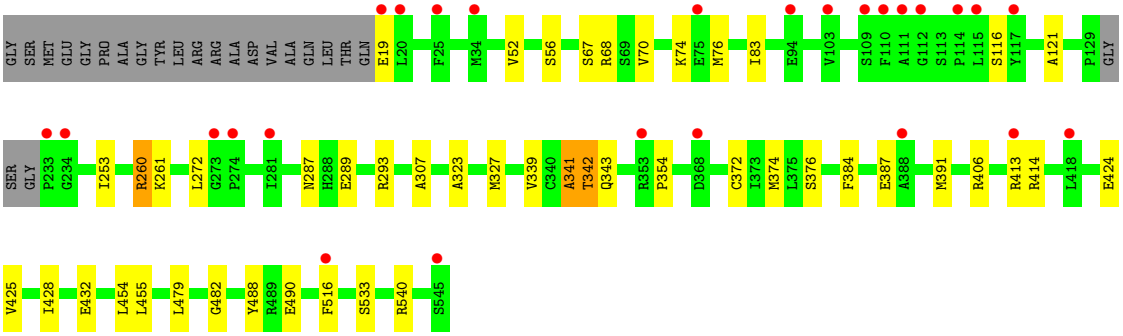




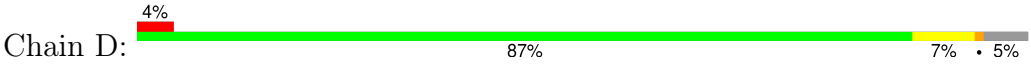
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

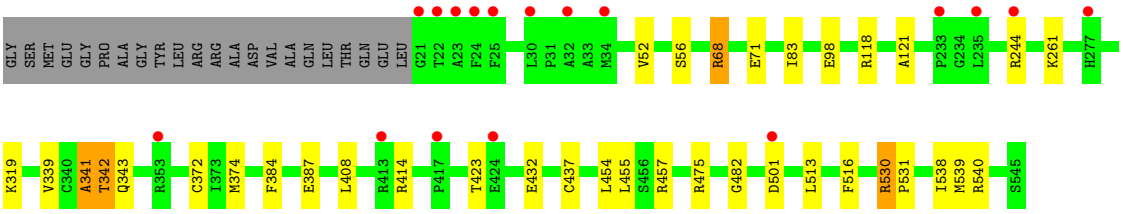
Chain C:



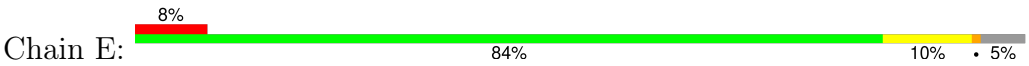


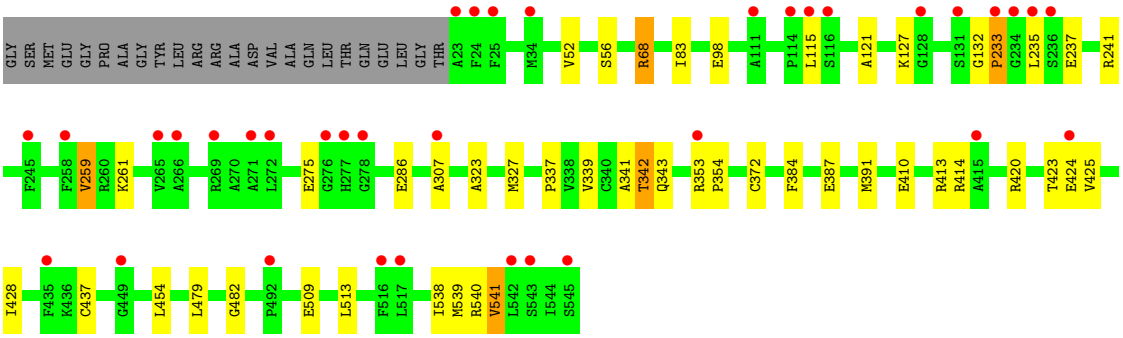
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR



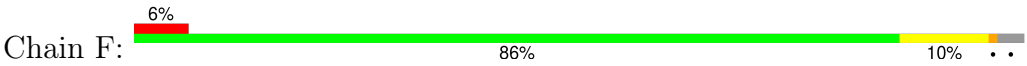


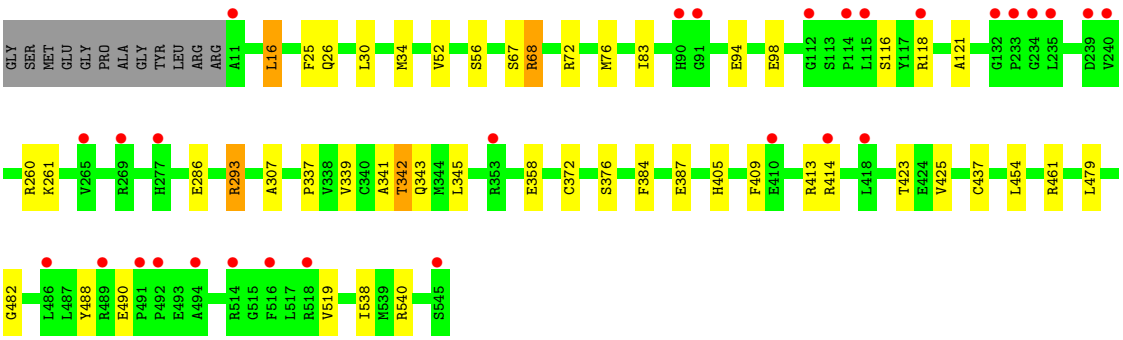
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR





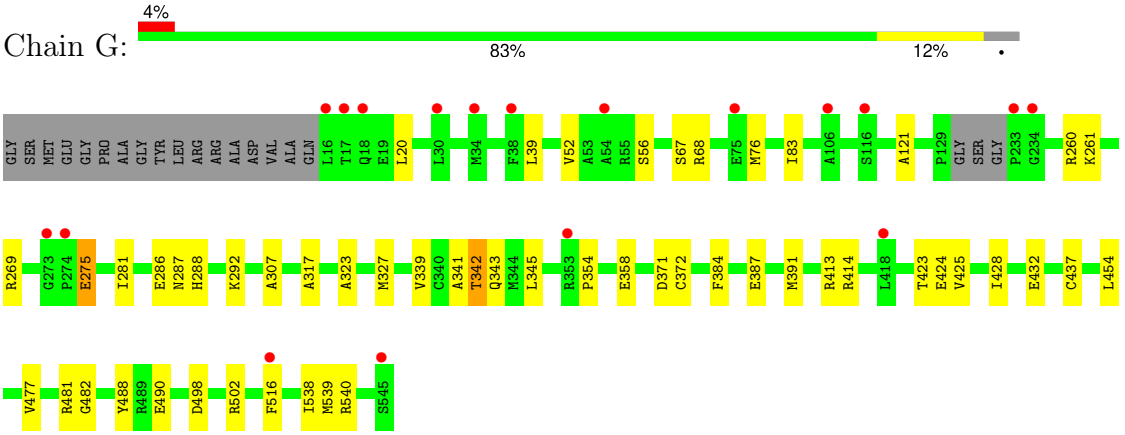
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR





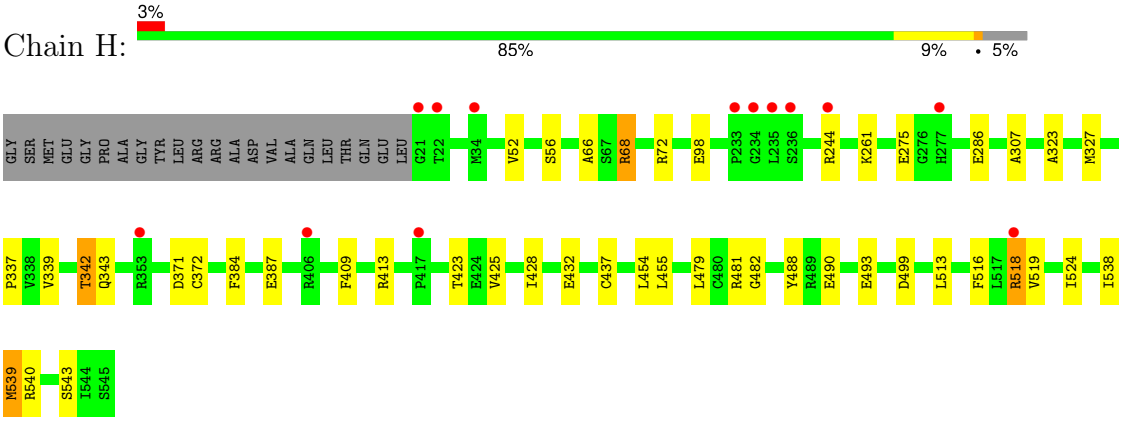
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain G:



• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

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	207.27Å 112.59Å 187.70Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	103.59 – 2.13 103.59 – 2.13	Depositor EDS
% Data completeness (in resolution range)	69.0 (103.59-2.13) 69.0 (103.59-2.13)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.215 , 0.248 0.203 , 0.231	Depositor DCC
R_{free} test set	8268 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27958	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 44.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5773e-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: FBP, OXL, K, MG, 07T

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	0.66	0/3341	1.01	1/4517 (0.0%)
1	B	0.67	0/3429	1.00	2/4636 (0.0%)
1	C	0.74	1/3343 (0.0%)	1.02	5/4519 (0.1%)
1	D	0.73	0/3341	1.02	5/4517 (0.1%)
1	E	0.66	0/3373	1.01	4/4560 (0.1%)
1	F	0.72	1/3420 (0.0%)	1.02	3/4625 (0.1%)
1	G	0.74	0/3371	1.02	4/4557 (0.1%)
1	H	0.75	0/3352	1.03	3/4531 (0.1%)
All	All	0.71	2/26970 (0.0%)	1.02	27/36462 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	376	SER	CA-C	7.71	1.56	1.52
1	F	376	SER	CA-C	5.00	1.54	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	259	VAL	N-CA-CB	7.51	118.72	110.53
1	G	516	PHE	CA-CB-CG	6.66	120.45	113.80
1	G	275	GLU	CB-CG-CD	6.32	123.34	112.60
1	H	516	PHE	CA-CB-CG	5.97	119.77	113.80
1	C	516	PHE	CA-CB-CG	5.94	119.74	113.80

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	3249	0	3323	25	0
1	B	3350	0	3417	20	1
1	C	3265	0	3331	24	0
1	D	3261	0	3321	21	0
1	E	3278	0	3342	23	0
1	F	3341	0	3410	25	0
1	G	3290	0	3356	31	0
1	H	3269	0	3334	26	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	50	0	32	1	0
4	B	50	0	32	1	0
4	E	50	0	32	1	0
4	F	50	0	32	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	110	0	0	0	0
7	B	111	0	0	0	0
7	C	173	0	0	0	0
7	D	199	0	0	2	0
7	E	121	0	0	0	0
7	F	149	0	0	1	0
7	G	169	0	0	0	0
7	H	199	0	0	0	0
All	All	27958	0	27042	170	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 3.

The worst 5 of 170 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ARG:HG3	1:C:428:ILE:HD11	1.58	0.83
1:G:540:ARG:HG2	1:H:538:ILE:HG12	1.62	0.79
1:A:420[A]:ARG:HD3	1:B:16:LEU:HD11	1.64	0.79
1:A:538:ILE:HG12	1:B:540:ARG:HG2	1.63	0.79
1:G:56:SER:HB2	1:G:482:GLY:HA2	1.66	0.77

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)
1:B:513:LEU:O	1:B:513:LEU:O[2_555]	2.16	0.04

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	431/447 (96%)	425 (99%)	5 (1%)	1 (0%)	43	44
1	B	442/447 (99%)	436 (99%)	5 (1%)	1 (0%)	43	44
1	C	428/447 (96%)	420 (98%)	7 (2%)	1 (0%)	43	44
1	D	431/447 (96%)	427 (99%)	3 (1%)	1 (0%)	43	44
1	E	434/447 (97%)	426 (98%)	6 (1%)	2 (0%)	24	22
1	F	441/447 (99%)	437 (99%)	3 (1%)	1 (0%)	43	44
1	G	432/447 (97%)	424 (98%)	7 (2%)	1 (0%)	43	44
1	H	432/447 (97%)	428 (99%)	3 (1%)	1 (0%)	43	44
All	All	3471/3576 (97%)	3423 (99%)	39 (1%)	9 (0%)	36	36

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	THR
1	B	342	THR
1	C	342	THR
1	D	342	THR
1	E	342	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	346/352 (98%)	334 (96%)	12 (4%)	32	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	353/352 (100%)	345 (98%)	8 (2%)	44 50
1	C	345/352 (98%)	334 (97%)	11 (3%)	34 37
1	D	344/352 (98%)	334 (97%)	10 (3%)	37 41
1	E	348/352 (99%)	335 (96%)	13 (4%)	30 31
1	F	352/352 (100%)	343 (97%)	9 (3%)	40 45
1	G	349/352 (99%)	342 (98%)	7 (2%)	48 55
1	H	345/352 (98%)	335 (97%)	10 (3%)	37 41
All	All	2782/2816 (99%)	2702 (97%)	80 (3%)	39 41

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	68	ARG
1	H	68	ARG
1	F	261	LYS
1	G	68	ARG
1	H	275	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	90	HIS
1	F	90	HIS
1	E	90	HIS
1	C	90	HIS
1	F	15	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 40 ligands modelled in this entry, 16 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	07T	B	603[B]	-	26,28,28	1.37	2 (7%)	30,42,42	1.29	4 (13%)
3	OXL	G	602	5	5,5,5	2.47	2 (40%)	6,6,6	1.29	1 (16%)
3	OXL	H	602	5	5,5,5	1.97	2 (40%)	6,6,6	1.86	1 (16%)
2	FBP	G	601	-	18,20,20	0.56	0	21,32,32	0.57	0
4	07T	E	603[B]	-	26,28,28	1.34	2 (7%)	30,42,42	1.37	6 (20%)
4	07T	B	603[A]	-	26,28,28	1.22	4 (15%)	30,42,42	1.31	5 (16%)
4	07T	A	603[B]	-	26,28,28	1.26	4 (15%)	30,42,42	1.20	5 (16%)
2	FBP	B	601	-	18,20,20	0.54	0	21,32,32	0.94	1 (4%)
2	FBP	H	601	-	18,20,20	0.59	0	21,32,32	0.79	1 (4%)
3	OXL	B	602	5	5,5,5	2.25	2 (40%)	6,6,6	1.41	1 (16%)
2	FBP	F	601	-	18,20,20	0.33	0	21,32,32	0.59	0
3	OXL	D	602	5	5,5,5	2.09	2 (40%)	6,6,6	1.94	2 (33%)
3	OXL	A	602	5	5,5,5	1.89	2 (40%)	6,6,6	2.55	3 (50%)
4	07T	F	603[B]	-	26,28,28	1.39	4 (15%)	30,42,42	1.34	3 (10%)
3	OXL	C	602	5	5,5,5	2.23	3 (60%)	6,6,6	2.01	2 (33%)
4	07T	E	603[A]	-	26,28,28	1.11	1 (3%)	30,42,42	1.33	5 (16%)
2	FBP	D	601	-	18,20,20	0.56	0	21,32,32	0.89	1 (4%)
4	07T	A	603[A]	-	26,28,28	1.41	5 (19%)	30,42,42	1.23	2 (6%)
3	OXL	F	602	5	5,5,5	2.26	3 (60%)	6,6,6	2.57	3 (50%)
3	OXL	E	602	5	5,5,5	2.03	2 (40%)	6,6,6	1.73	2 (33%)
2	FBP	E	601	-	18,20,20	0.57	0	21,32,32	0.54	0
2	FBP	C	601	-	18,20,20	0.59	0	21,32,32	0.55	0
4	07T	F	603[A]	-	26,28,28	1.28	3 (11%)	30,42,42	1.45	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FBP	A	601	-	18,20,20	0.44	0	21,32,32	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	07T	B	603[B]	-	-	0/4/8/8	0/4/4/4
3	OXL	G	602	5	-	4/4/4/4	-
3	OXL	H	602	5	-	4/4/4/4	-
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
4	07T	E	603[B]	-	-	0/4/8/8	0/4/4/4
4	07T	B	603[A]	-	-	0/4/8/8	0/4/4/4
4	07T	A	603[B]	-	-	0/4/8/8	0/4/4/4
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	5	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	5	-	4/4/4/4	-
3	OXL	A	602	5	-	4/4/4/4	-
4	07T	F	603[B]	-	-	0/4/8/8	0/4/4/4
3	OXL	C	602	5	-	4/4/4/4	-
4	07T	E	603[A]	-	-	0/4/8/8	0/4/4/4
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
4	07T	A	603[A]	-	-	0/4/8/8	0/4/4/4
3	OXL	F	602	5	-	0/4/4/4	-
3	OXL	E	602	5	-	4/4/4/4	-
2	FBP	E	601	-	-	3/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
4	07T	F	603[A]	-	-	0/4/8/8	0/4/4/4
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXL	O2-C2	4.41	1.33	1.22
3	G	602	OXL	O2-C2	4.26	1.33	1.22
4	E	603[B]	07T	CAU-SAN	-4.25	1.65	1.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603[B]	07T	CAL-NAX	4.11	1.52	1.46
4	F	603[B]	07T	CAL-NAX	3.84	1.52	1.46

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	OXL	O4-C2-C1	4.55	121.66	112.83
3	A	602	OXL	O4-C2-C1	4.44	121.44	112.83
3	C	602	OXL	O4-C2-C1	4.14	120.87	112.83
3	H	602	OXL	O4-C2-C1	3.82	120.24	112.83
4	F	603[B]	07T	CAL-NAX-CAR	3.54	122.53	119.22

There are no chirality outliers.

5 of 45 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	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6

There are no ring outliers.

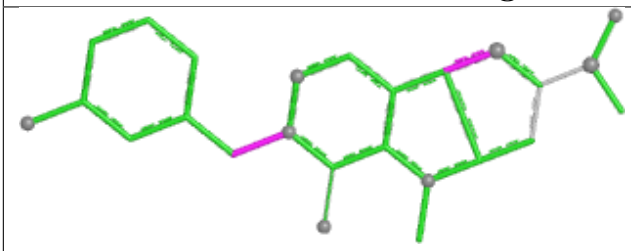
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603[B]	07T	1	0
4	A	603[B]	07T	1	0
3	C	602	OXL	1	0
4	E	603[A]	07T	1	0

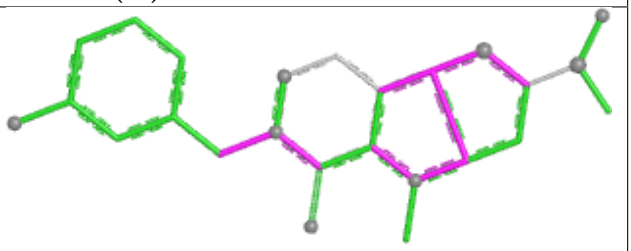
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

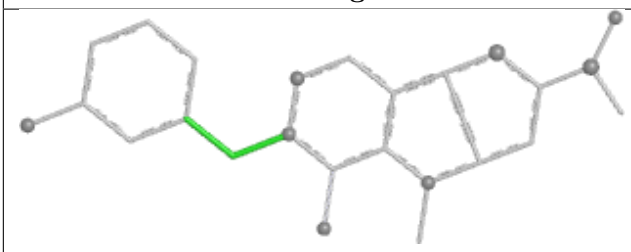
Ligand 07T B 603 (B)



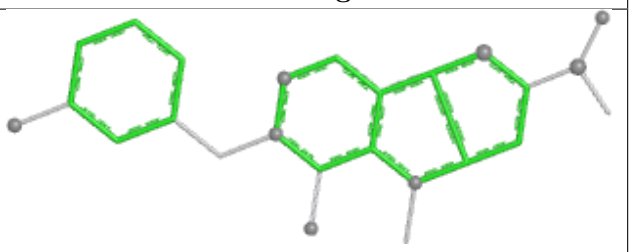
Bond lengths



Bond angles

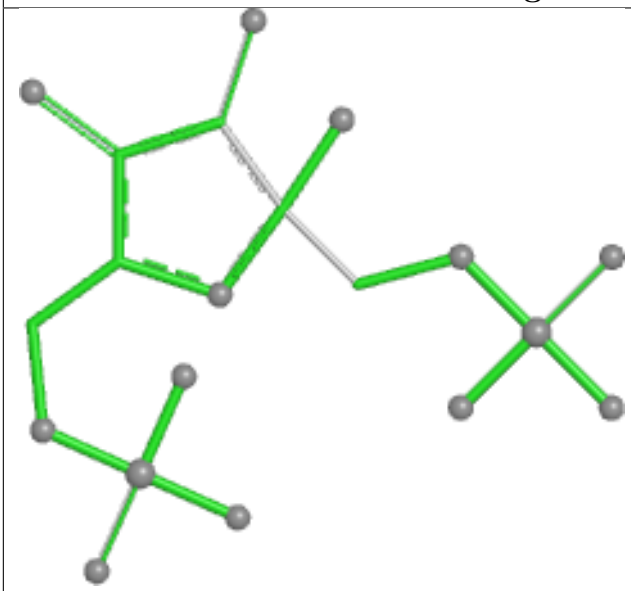


Torsions

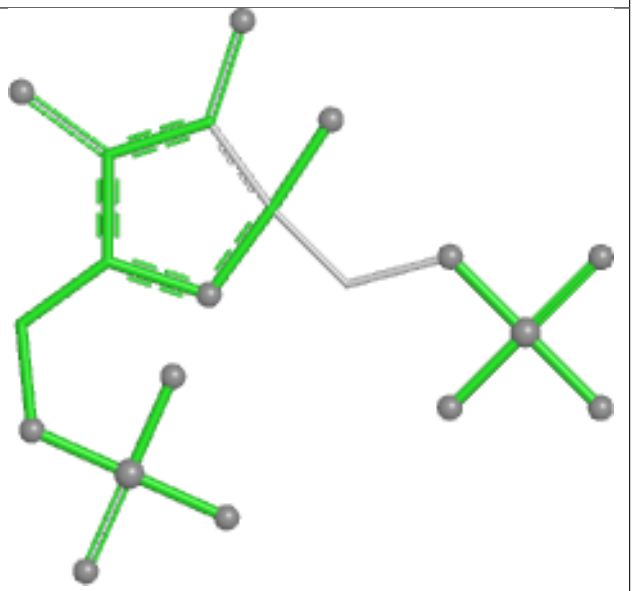


Rings

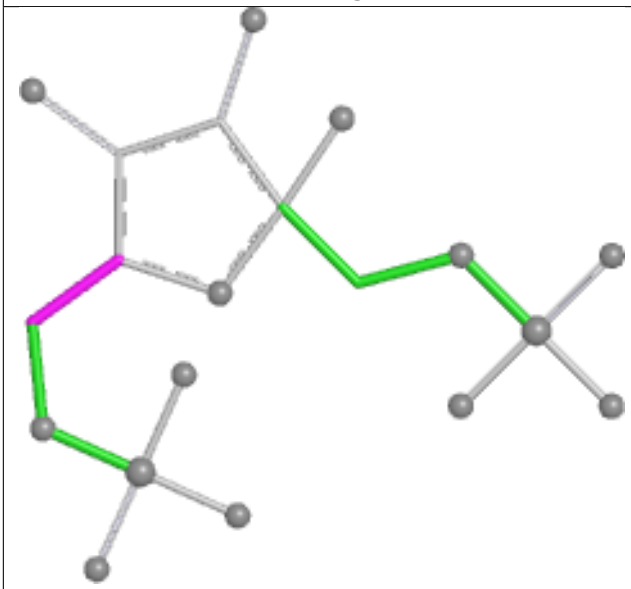
Ligand FBP G 601



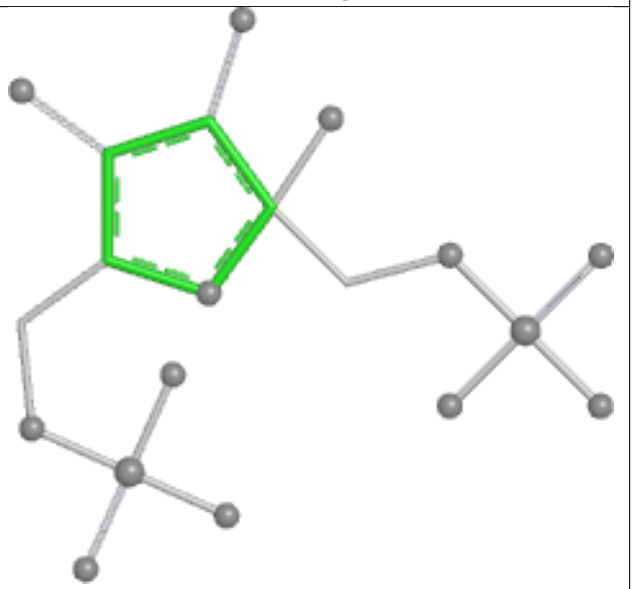
Bond lengths



Bond angles

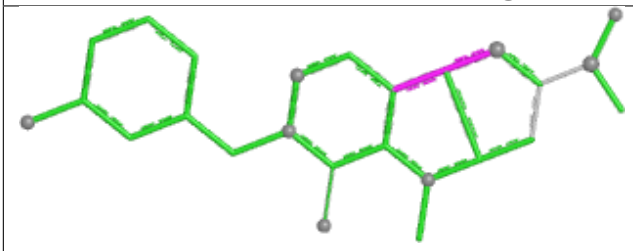


Torsions

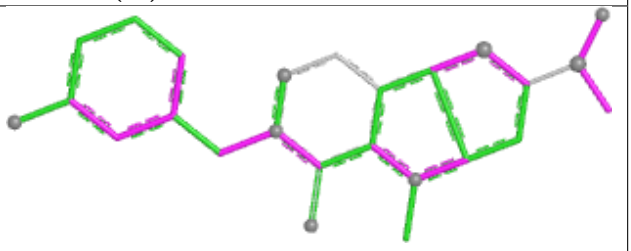


Rings

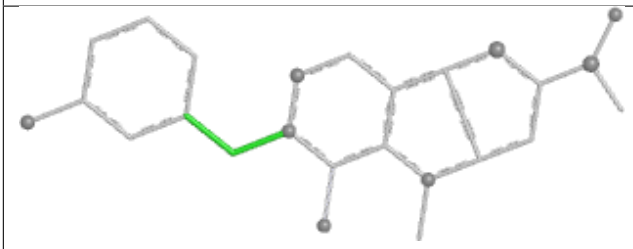
Ligand 07T E 603 (B)



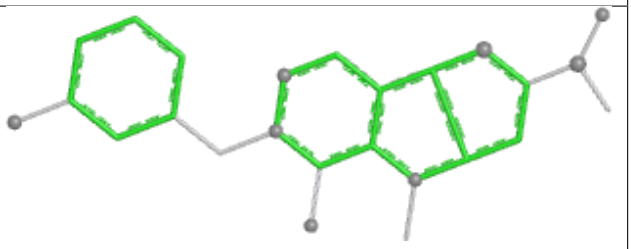
Bond lengths



Bond angles

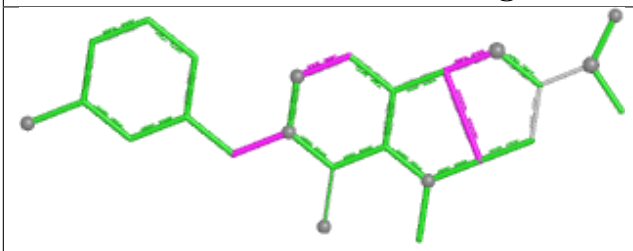


Torsions

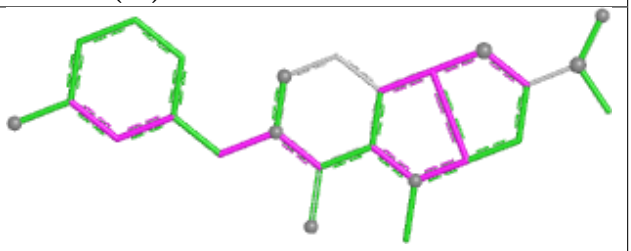


Rings

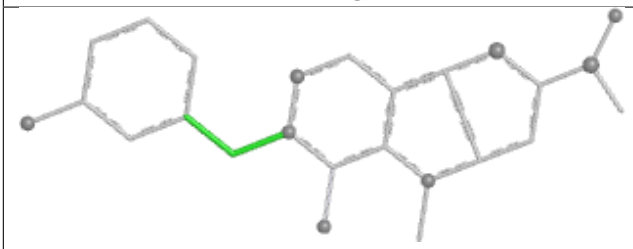
Ligand 07T B 603 (A)



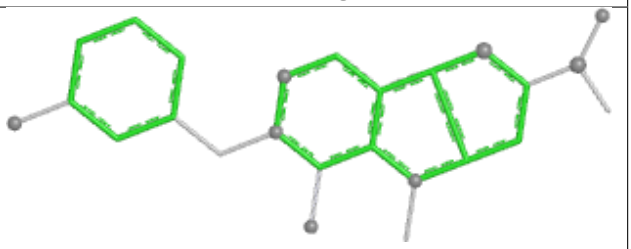
Bond lengths



Bond angles

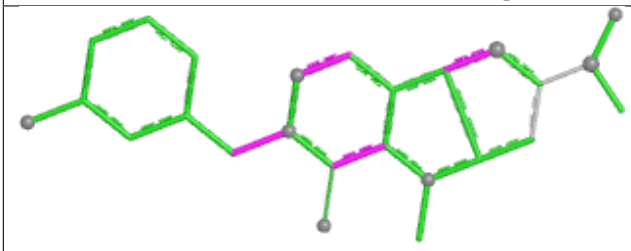


Torsions

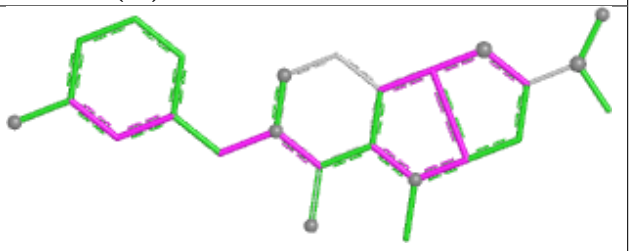


Rings

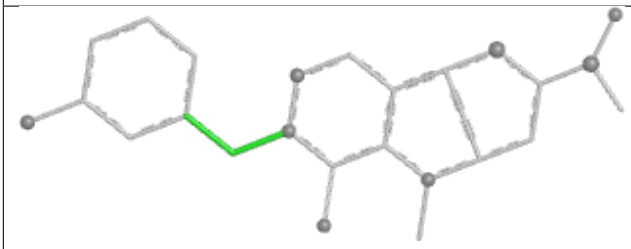
Ligand 07T A 603 (B)



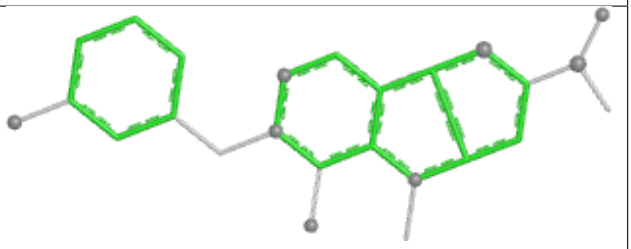
Bond lengths



Bond angles

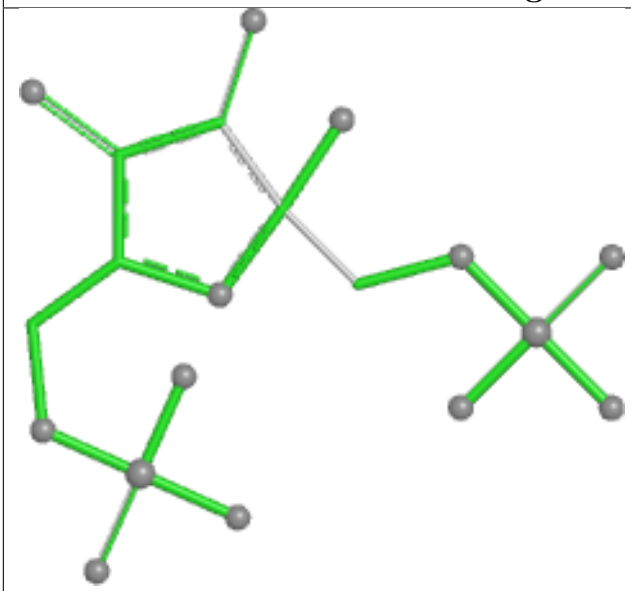


Torsions

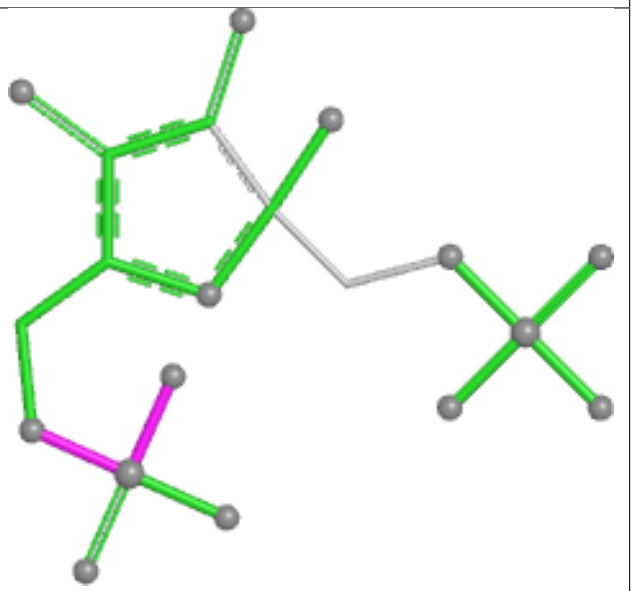


Rings

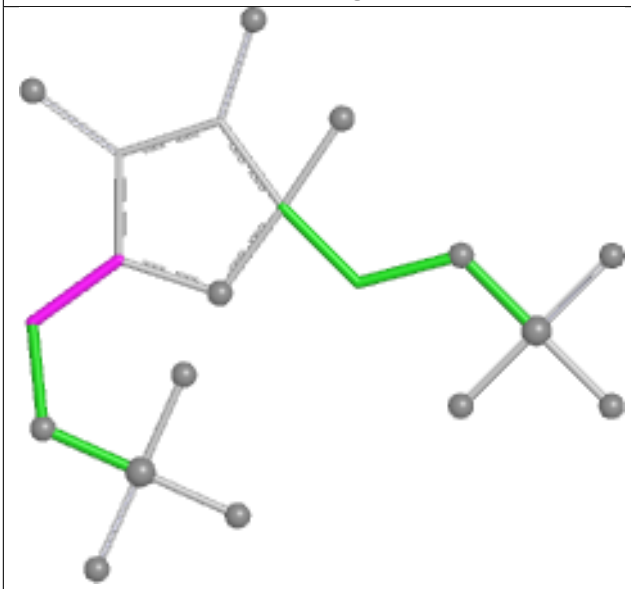
Ligand FBP B 601



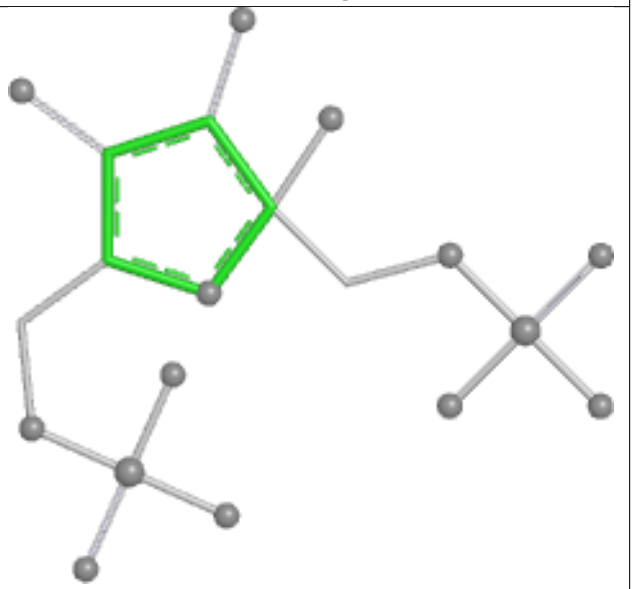
Bond lengths



Bond angles

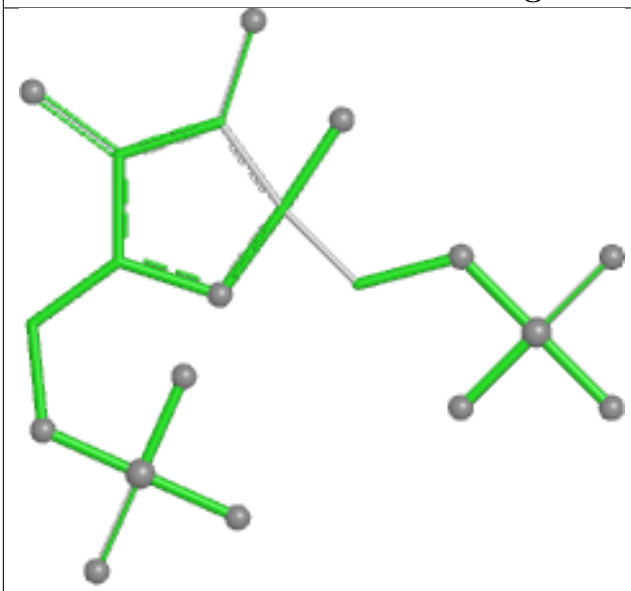


Torsions

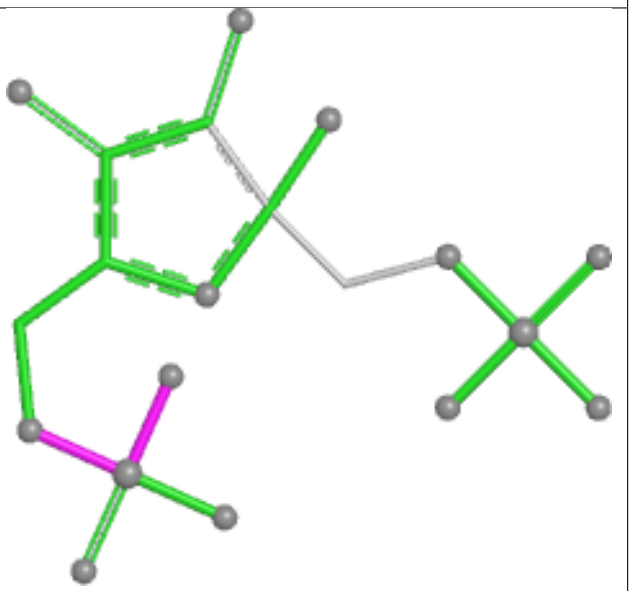


Rings

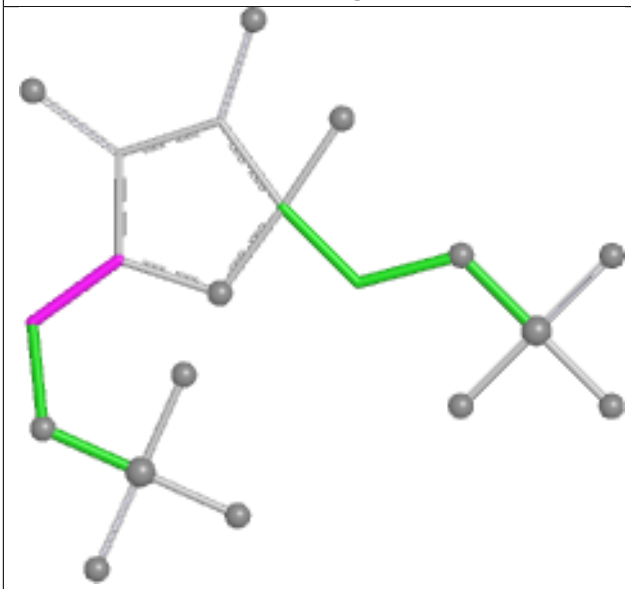
Ligand FBP H 601



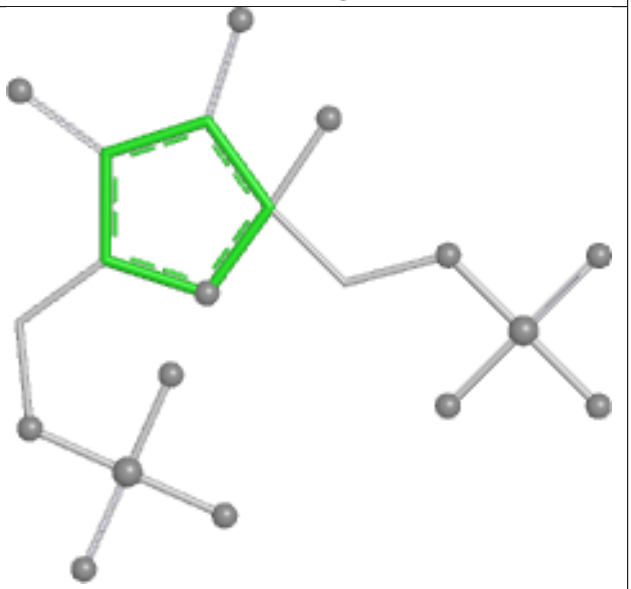
Bond lengths



Bond angles

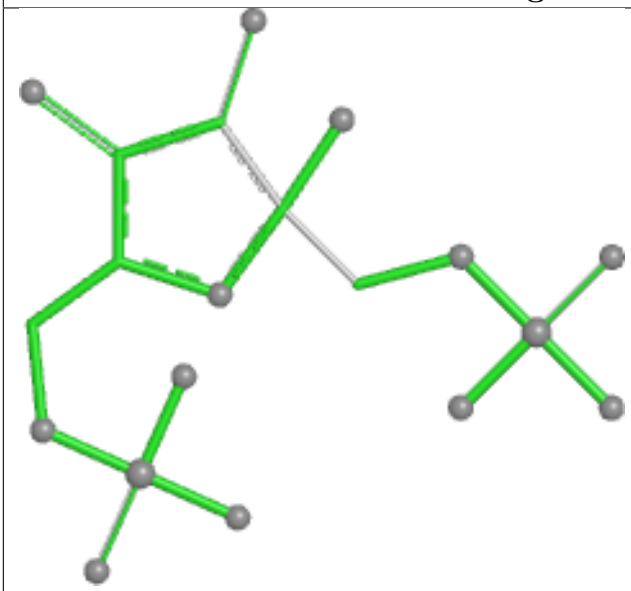


Torsions

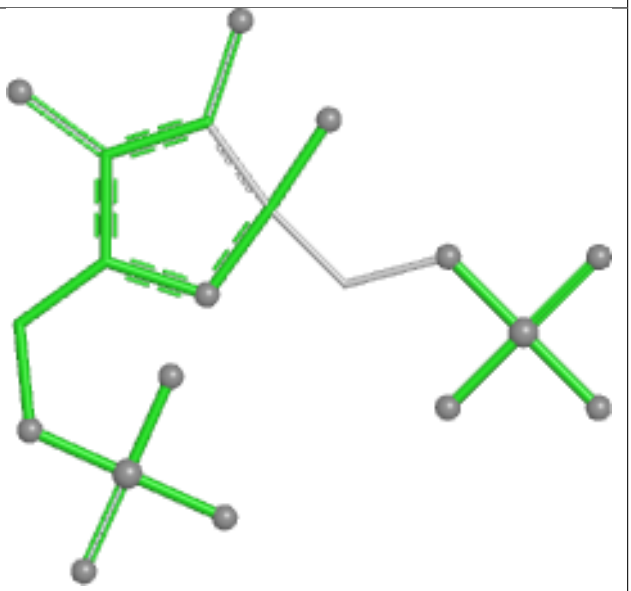


Rings

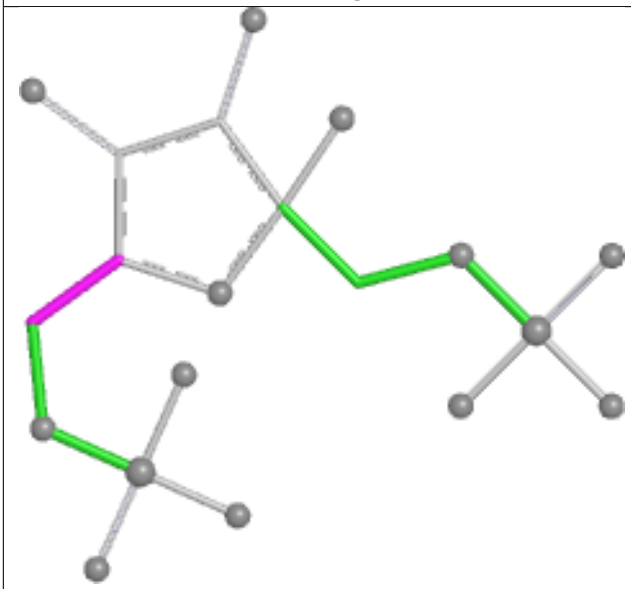
Ligand FBP F 601



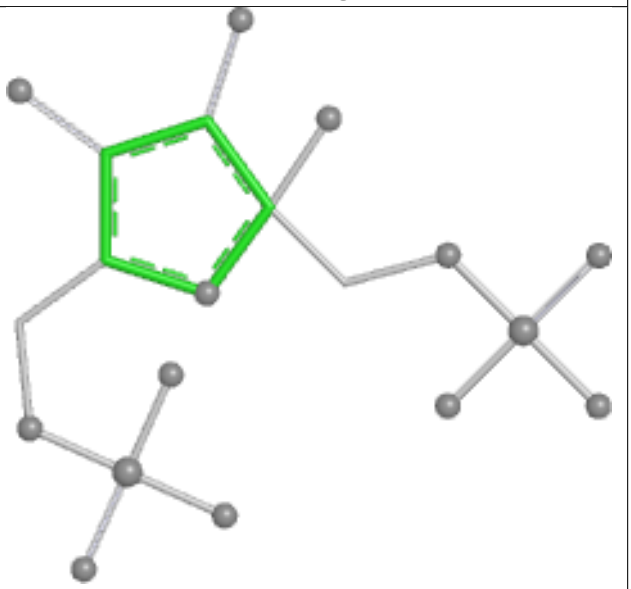
Bond lengths



Bond angles

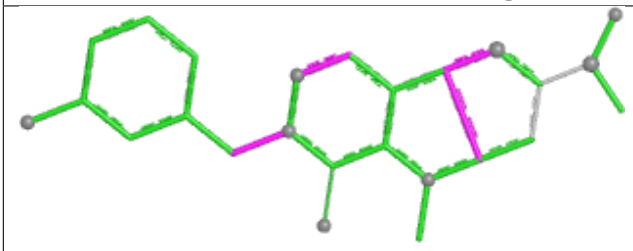


Torsions

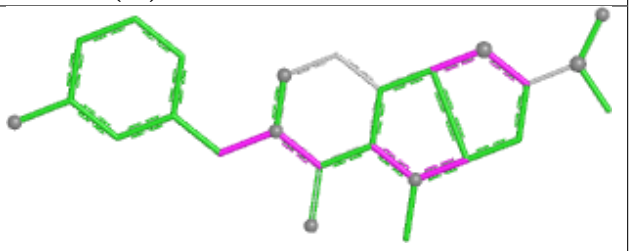


Rings

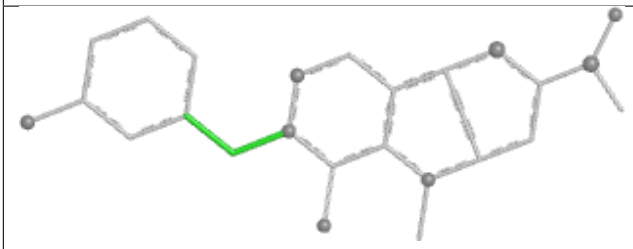
Ligand 07T F 603 (B)



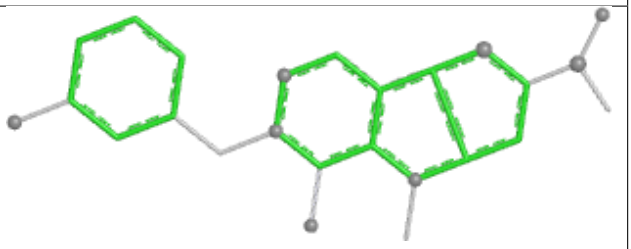
Bond lengths



Bond angles

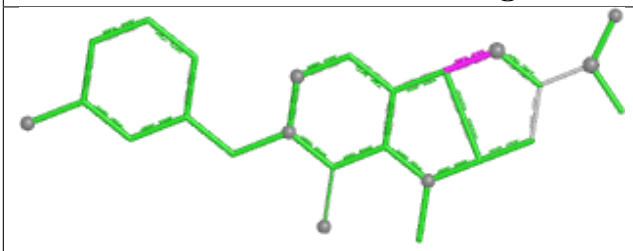


Torsions

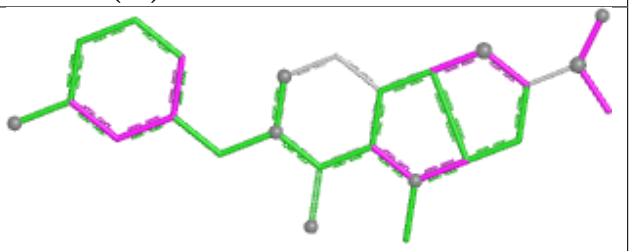


Rings

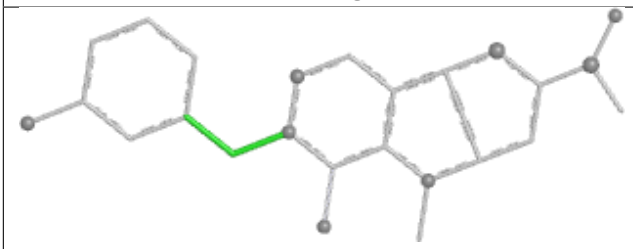
Ligand 07T E 603 (A)



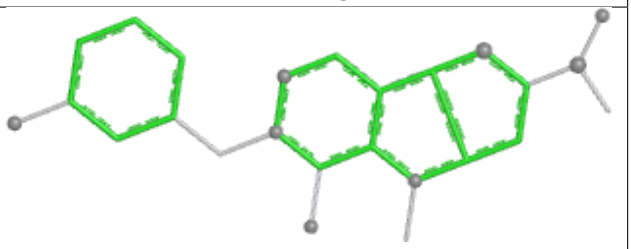
Bond lengths



Bond angles

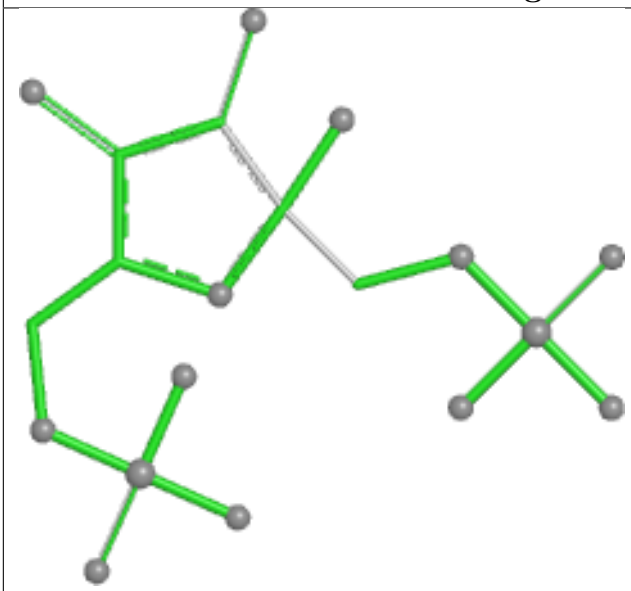


Torsions

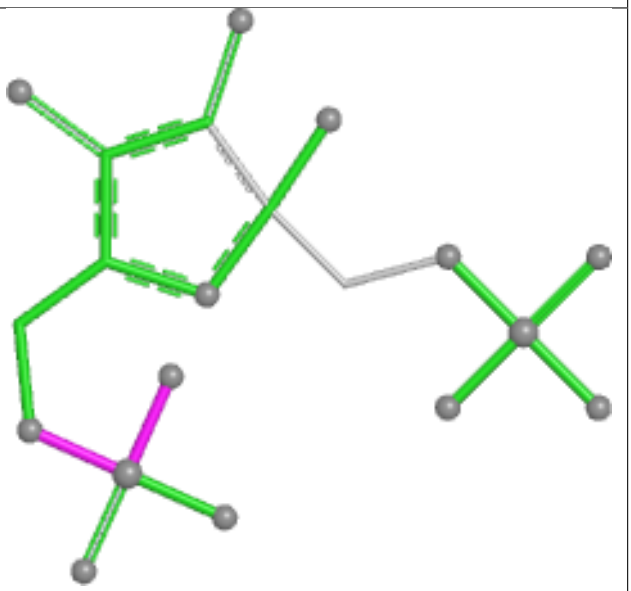


Rings

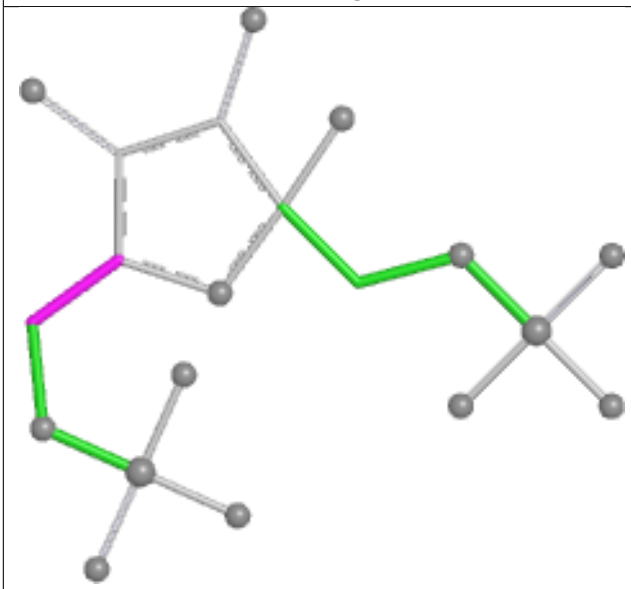
Ligand FBP D 601



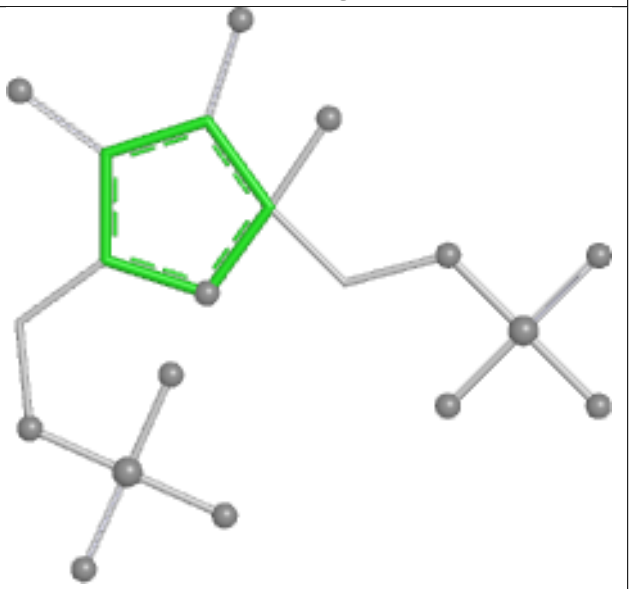
Bond lengths



Bond angles

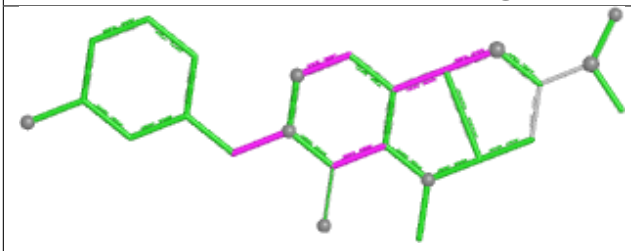


Torsions

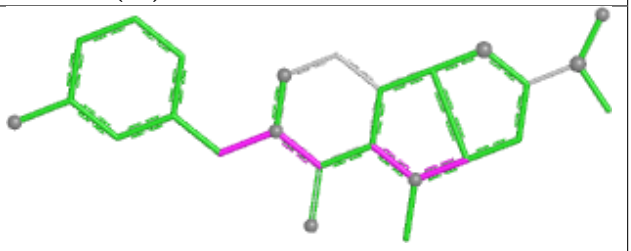


Rings

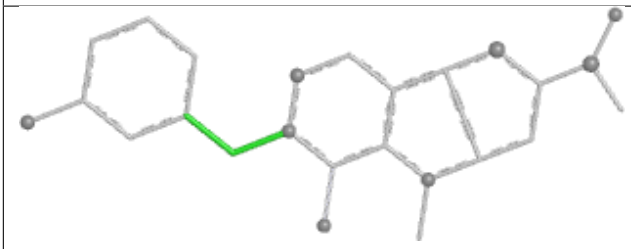
Ligand 07T A 603 (A)



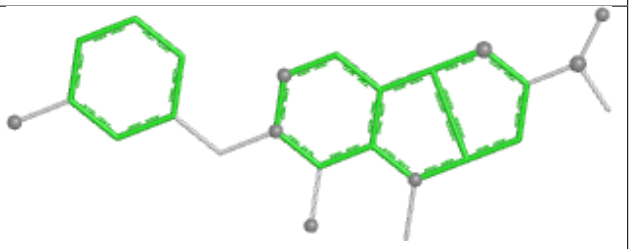
Bond lengths



Bond angles

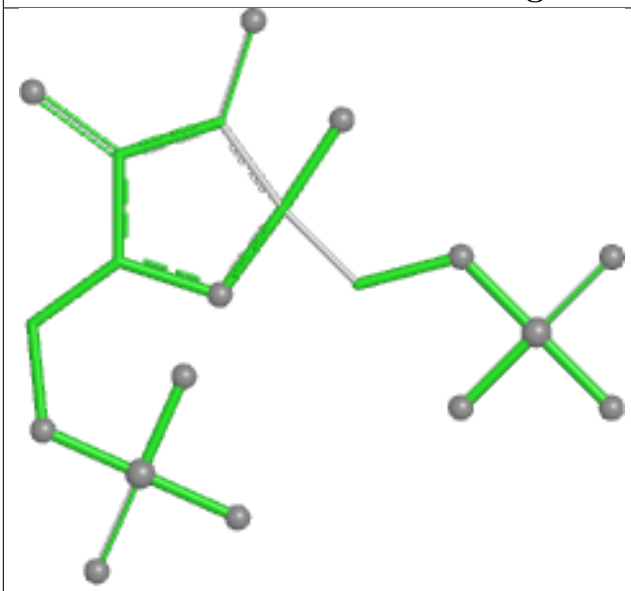


Torsions

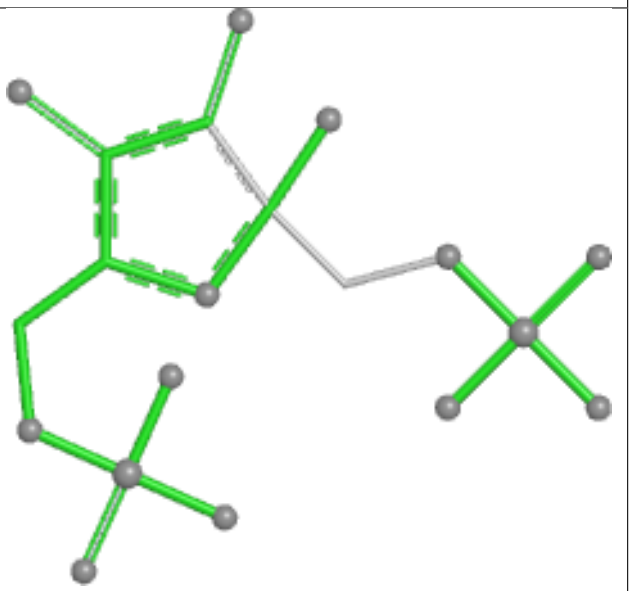


Rings

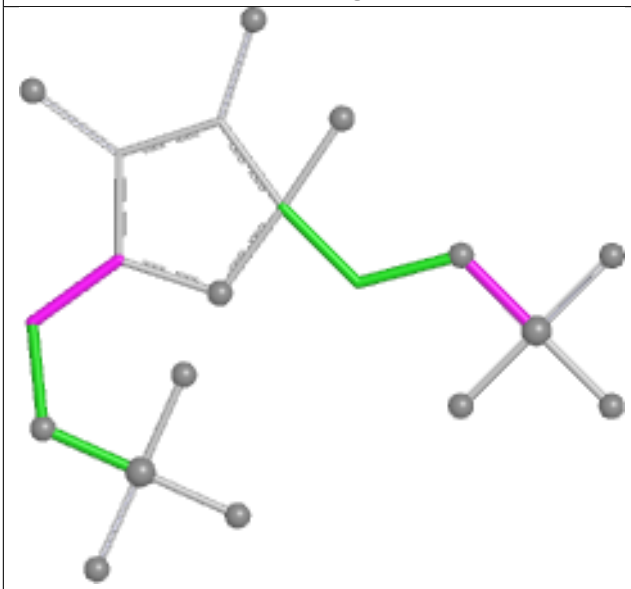
Ligand FBP E 601



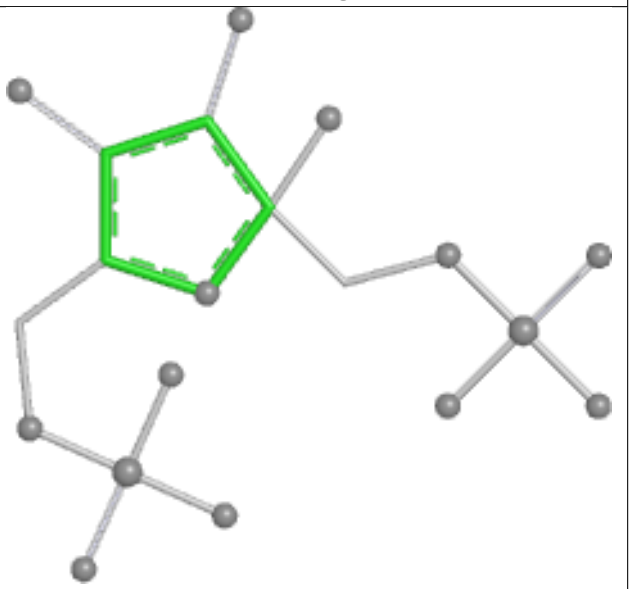
Bond lengths



Bond angles

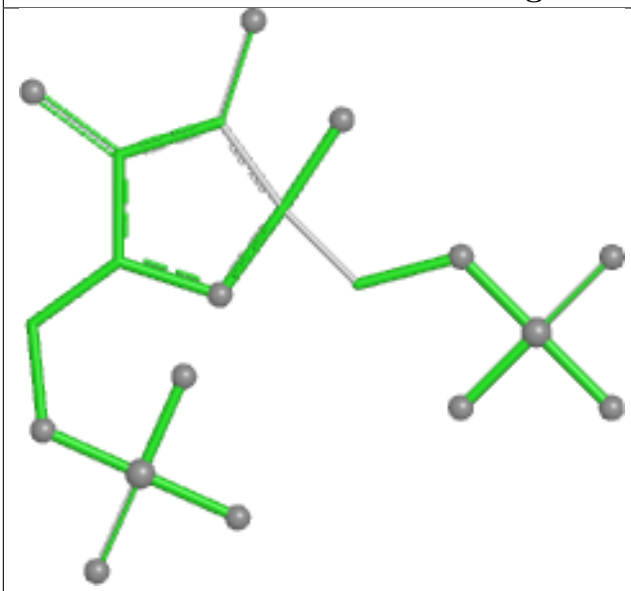


Torsions

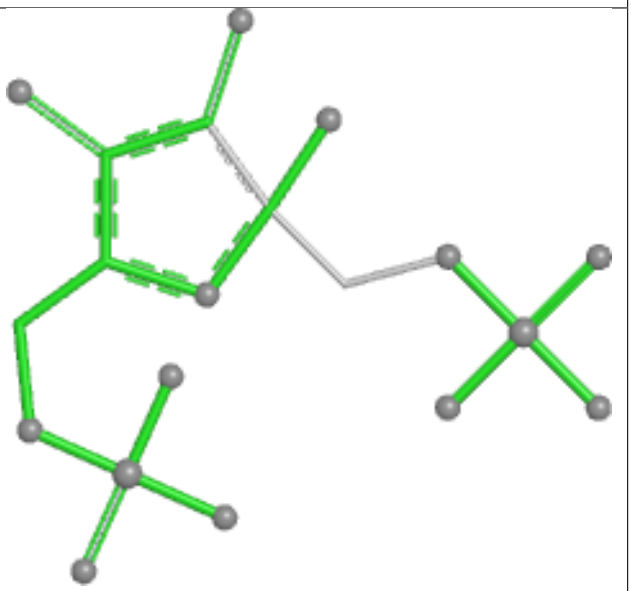


Rings

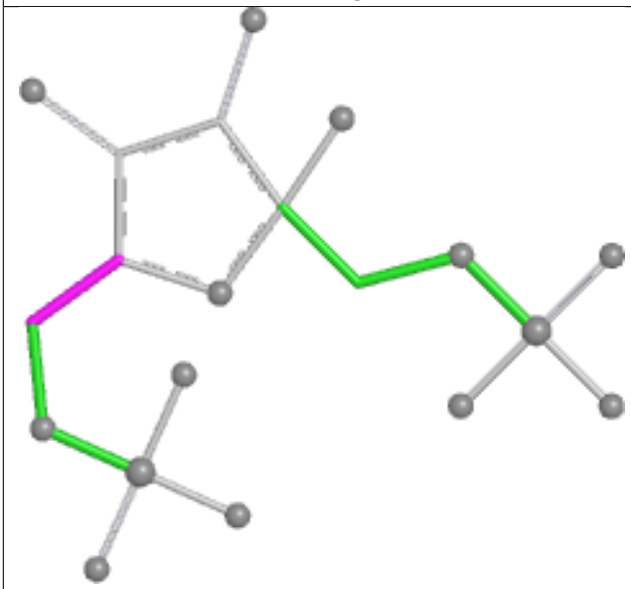
Ligand FBP C 601



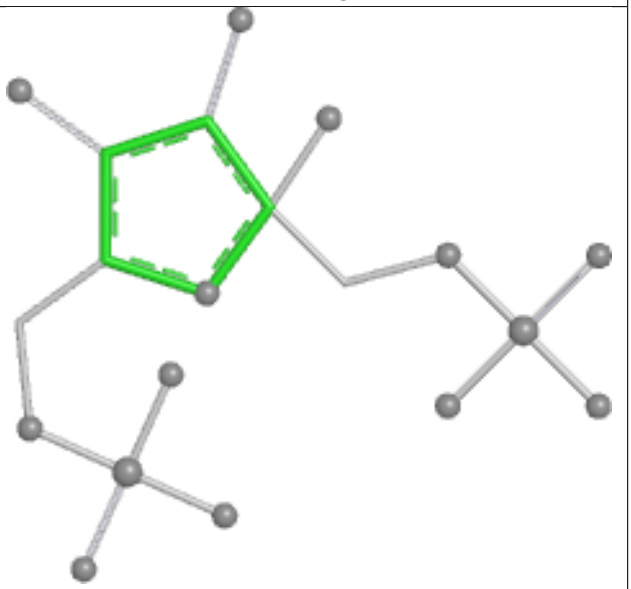
Bond lengths



Bond angles

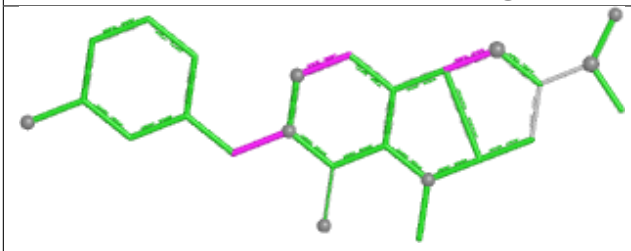


Torsions

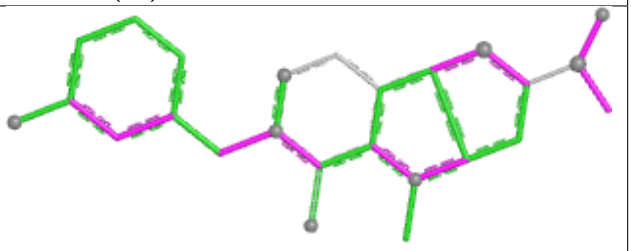


Rings

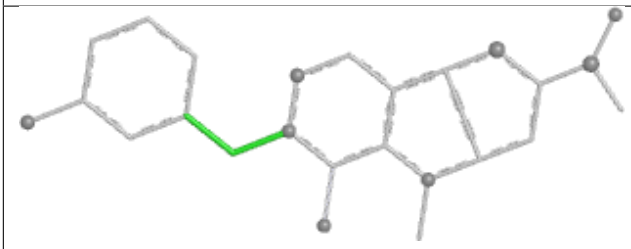
Ligand 07T F 603 (A)



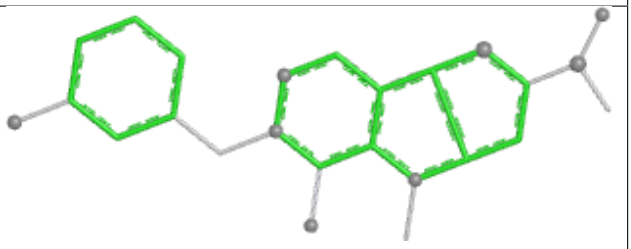
Bond lengths



Bond angles

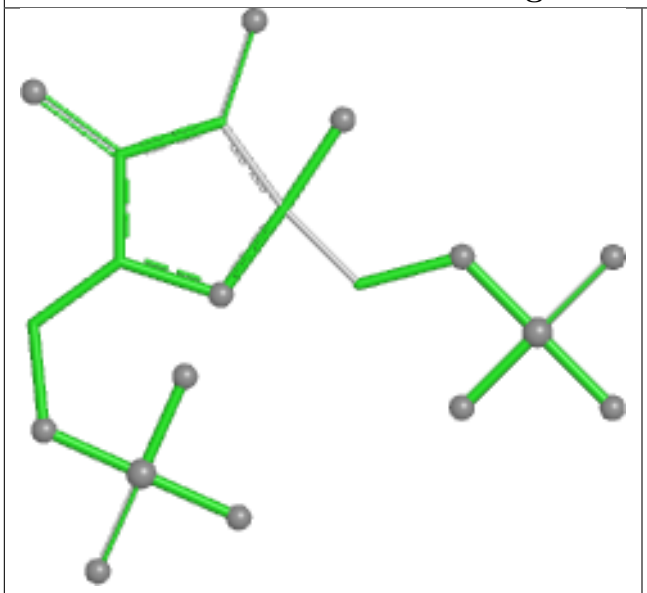


Torsions

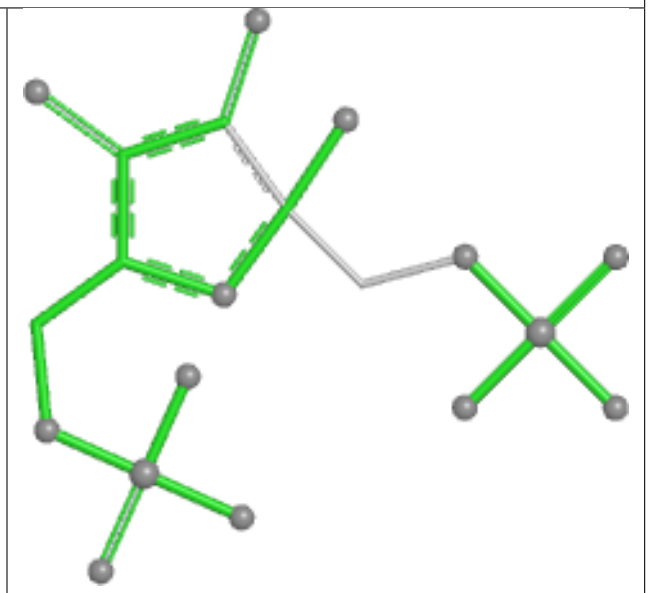


Rings

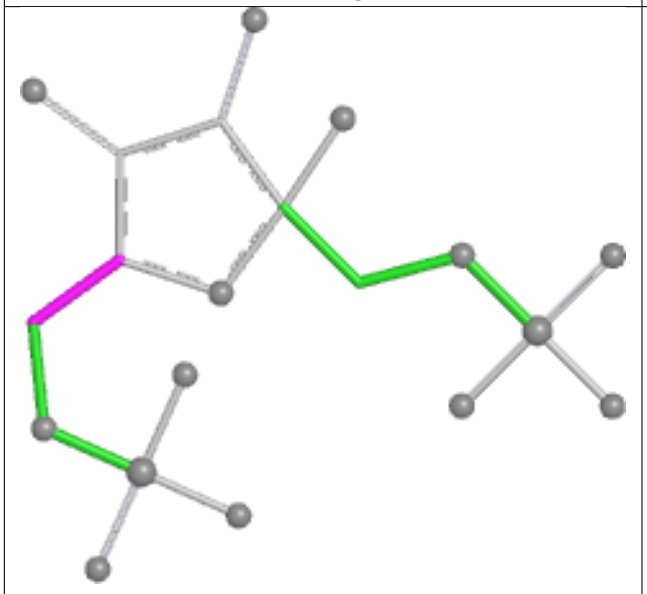
Ligand FBP A 601



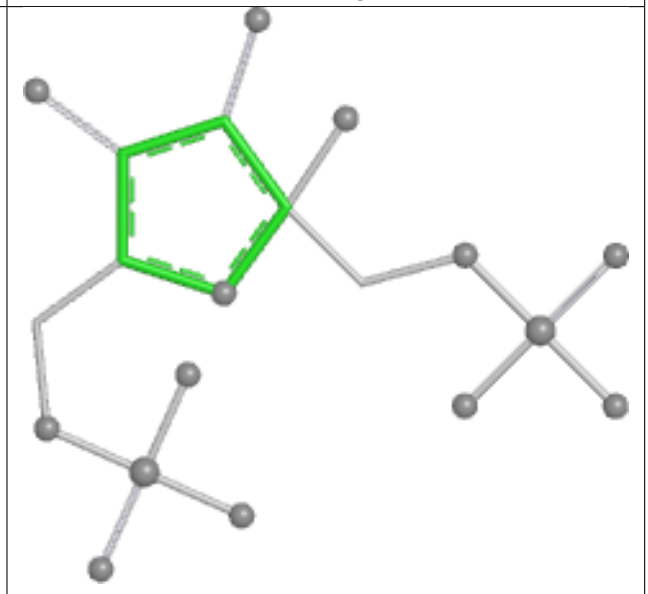
Bond lengths



Bond angles



Torsions



Rings

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	420/447 (93%)	0.99	46 (10%)	10	11	24, 49, 77, 97	13 (3%)
1	B	436/447 (97%)	1.20	86 (19%)	3	3	21, 49, 83, 93	8 (1%)
1	C	424/447 (94%)	0.56	26 (6%)	27	29	20, 40, 62, 82	8 (1%)
1	D	425/447 (95%)	0.35	17 (4%)	42	45	16, 35, 58, 86	8 (1%)
1	E	423/447 (94%)	0.89	36 (8%)	16	18	25, 47, 75, 93	13 (3%)
1	F	435/447 (97%)	0.70	29 (6%)	24	26	23, 42, 67, 80	8 (1%)
1	G	427/447 (95%)	0.45	18 (4%)	40	43	20, 37, 55, 87	10 (2%)
1	H	425/447 (95%)	0.23	13 (3%)	51	54	16, 34, 55, 71	9 (2%)
All	All	3415/3576 (95%)	0.67	271 (7%)	18	20	16, 42, 71, 97	77 (2%)

The worst 5 of 271 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	6.7
1	E	277[A]	HIS	6.1
1	H	21	GLY	6.0
1	B	513	LEU	5.8
1	D	21	GLY	5.4

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 oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
3	OXL	B	602	6/6	0.80	0.13	53,54,55,55	0
3	OXL	E	602	6/6	0.85	0.13	61,62,62,62	0
3	OXL	C	602	6/6	0.86	0.11	52,52,53,54	0
5	MG	A	604	1/1	0.86	0.17	52,52,52,52	0
3	OXL	F	602	6/6	0.87	0.11	49,50,51,51	0
4	07T	E	603[B]	25/25	0.88	0.12	39,41,43,43	25
4	07T	E	603[A]	25/25	0.88	0.12	26,30,34,35	25
5	MG	B	604	1/1	0.89	0.11	60,60,60,60	0
6	K	B	605	1/1	0.90	0.09	76,76,76,76	0
3	OXL	A	602	6/6	0.91	0.10	54,55,57,57	0
4	07T	A	603[A]	25/25	0.91	0.10	20,27,32,32	25
4	07T	F	603[A]	25/25	0.91	0.12	38,41,43,44	25
4	07T	F	603[B]	25/25	0.91	0.12	26,30,35,36	25
4	07T	A	603[B]	25/25	0.91	0.10	48,50,53,54	25
4	07T	B	603[A]	25/25	0.91	0.10	18,25,31,32	25
4	07T	B	603[B]	25/25	0.91	0.10	50,53,54,55	25
6	K	E	605	1/1	0.91	0.18	87,87,87,87	0
3	OXL	G	602	6/6	0.93	0.08	42,43,44,45	0
3	OXL	H	602	6/6	0.93	0.09	44,44,45,45	0
2	FBP	B	601	20/20	0.94	0.09	44,45,49,49	0
3	OXL	D	602	6/6	0.94	0.09	46,46,47,47	0
2	FBP	A	601	20/20	0.95	0.07	48,49,50,50	0
2	FBP	F	601	20/20	0.95	0.07	37,42,48,49	0
2	FBP	E	601	20/20	0.96	0.07	45,47,48,49	0
2	FBP	G	601	20/20	0.96	0.07	30,32,34,34	0
6	K	G	604	1/1	0.96	0.13	56,56,56,56	0
6	K	C	604	1/1	0.97	0.07	52,52,52,52	0
2	FBP	C	601	20/20	0.97	0.06	33,34,36,36	0
6	K	F	605	1/1	0.97	0.06	71,71,71,71	0
2	FBP	D	601	20/20	0.97	0.06	25,27,33,33	0
6	K	D	604	1/1	0.98	0.07	38,38,38,38	0
6	K	A	605	1/1	0.98	0.07	77,77,77,77	0
2	FBP	H	601	20/20	0.98	0.04	26,28,31,32	0
5	MG	C	603	1/1	0.98	0.04	44,44,44,44	0
6	K	H	604	1/1	0.98	0.07	41,41,41,41	0
5	MG	G	603	1/1	0.99	0.03	41,41,41,41	0
5	MG	H	603	1/1	0.99	0.04	41,41,41,41	0

Continued on next page...

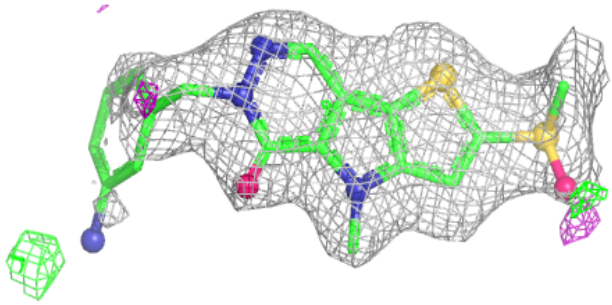
Continued from previous page...

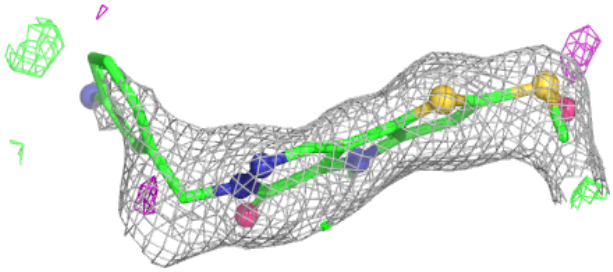
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	D	603	1/1	0.99	0.01	40,40,40,40	0
5	MG	E	604	1/1	0.99	0.02	45,45,45,45	0
5	MG	F	604	1/1	0.99	0.04	36,36,36,36	0

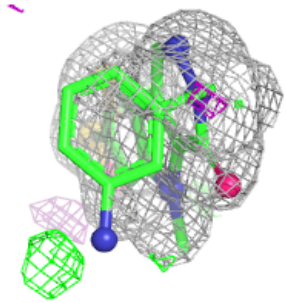
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 07T E 603 (B):

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

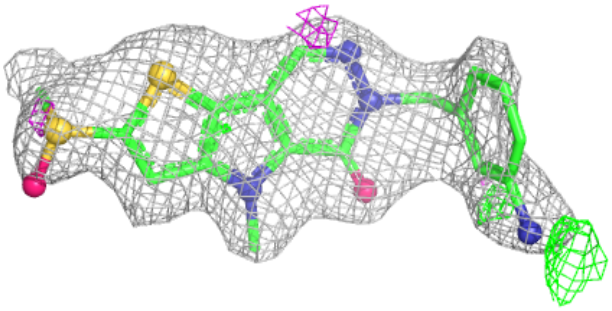


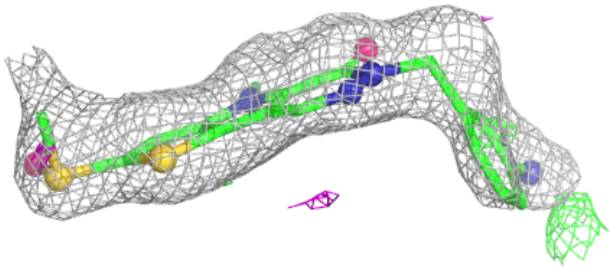


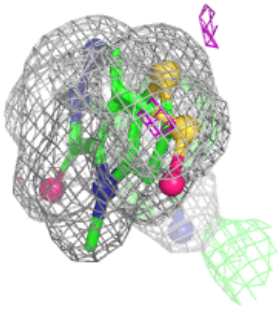


Electron density around 07T E 603 (A):

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

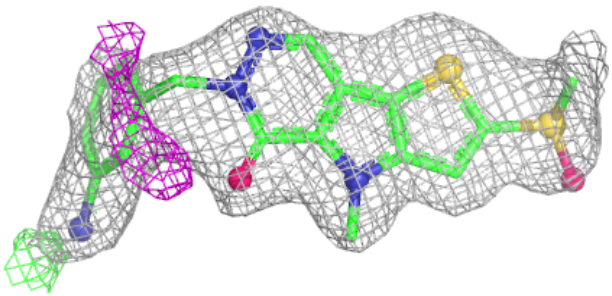


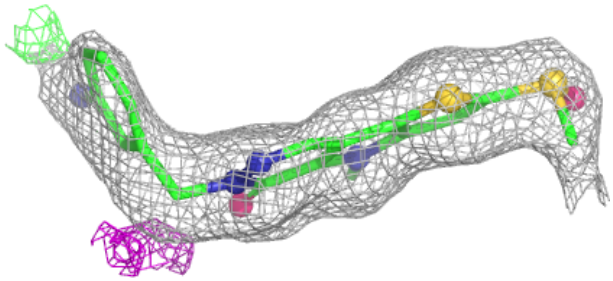


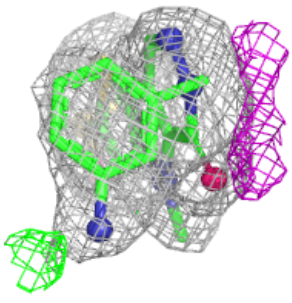


Electron density around 07T A 603 (A):

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

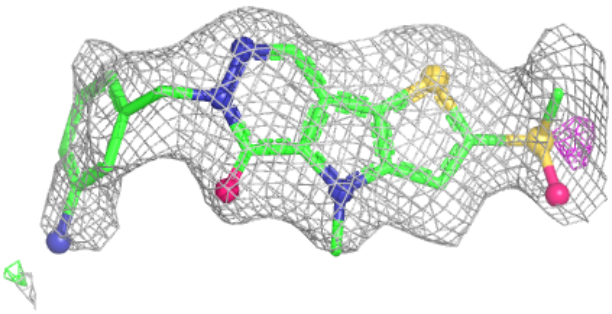


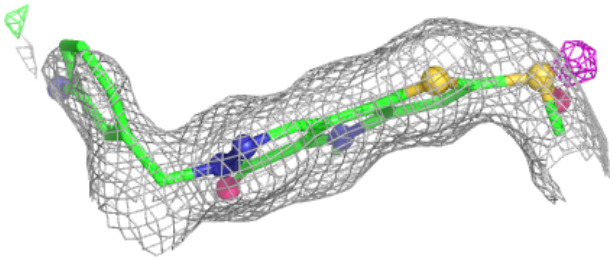


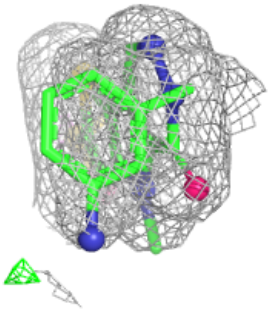


Electron density around 07T F 603 (A):

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

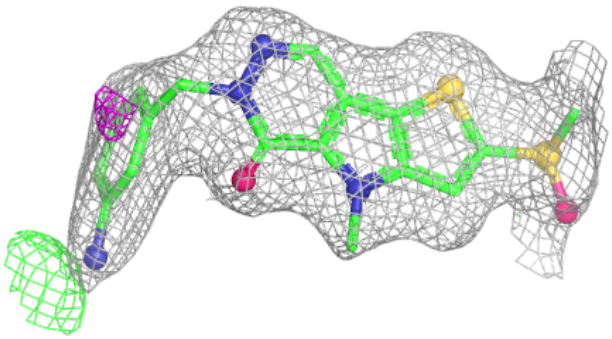


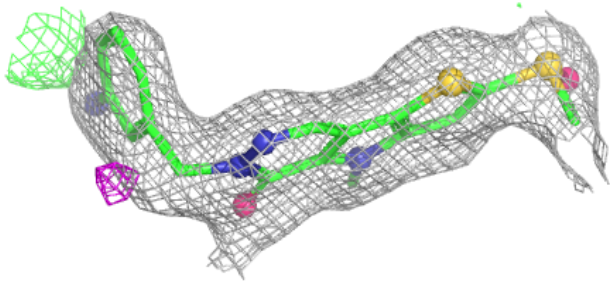


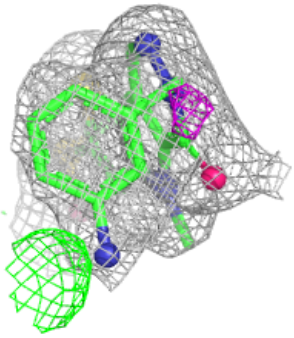


Electron density around 07T F 603 (B):

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

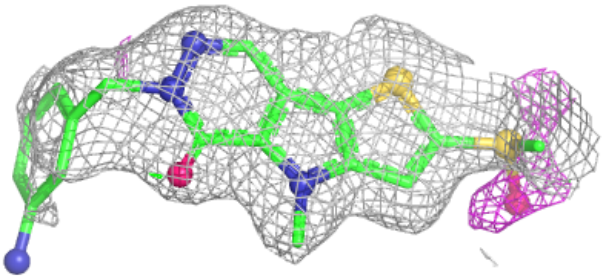


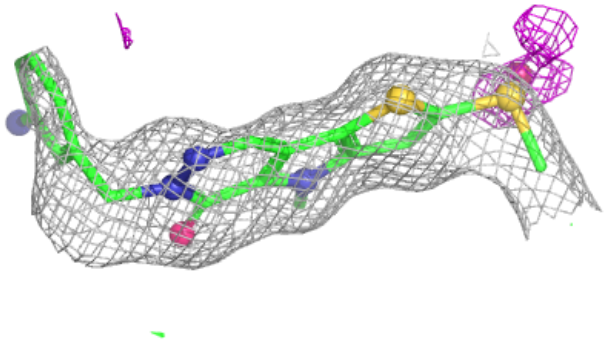


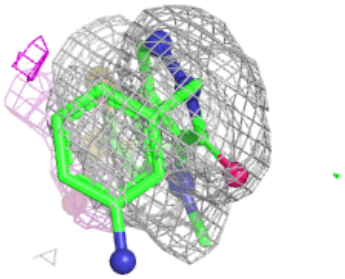


Electron density around 07T A 603 (B):

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

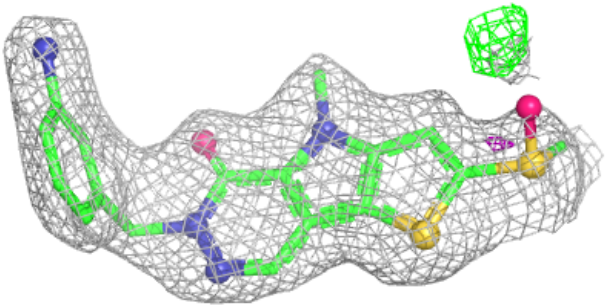


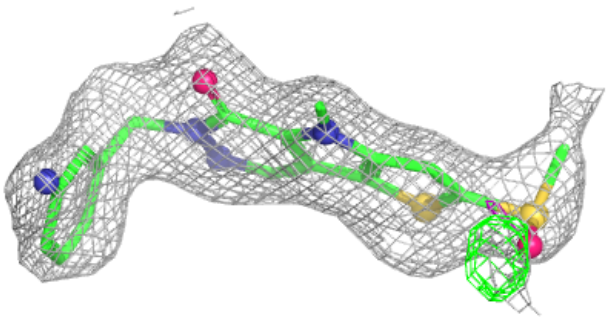


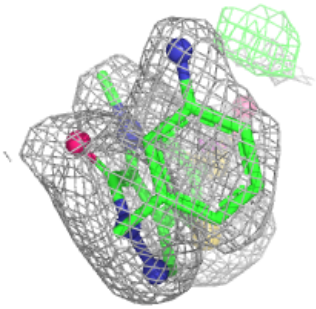


Electron density around 07T B 603 (A):

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

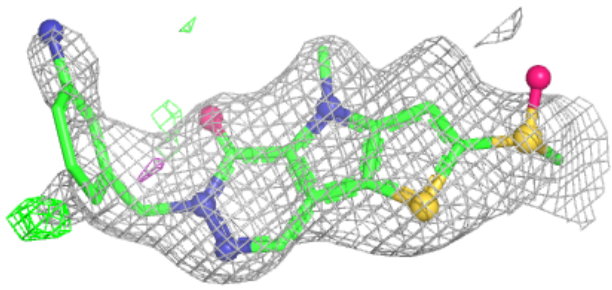


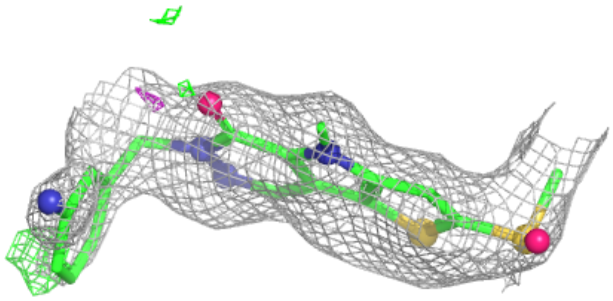


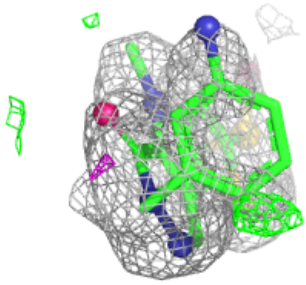


Electron density around 07T B 603 (B):

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

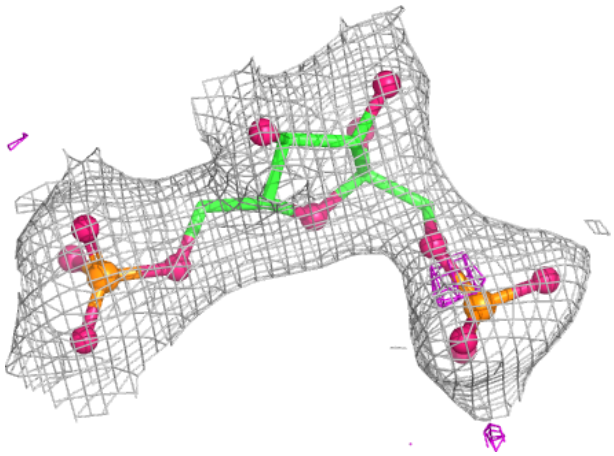


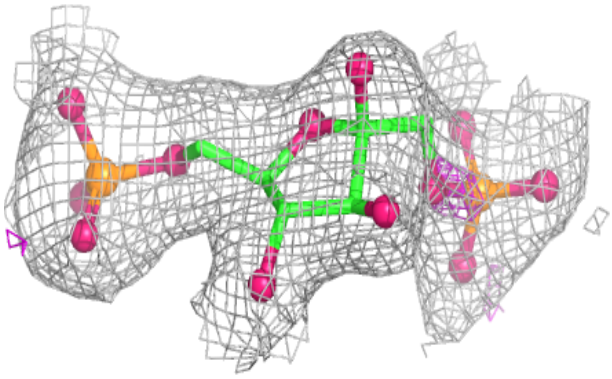


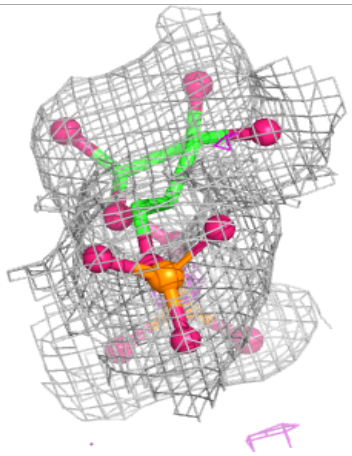


Electron density around FBP B 601:

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

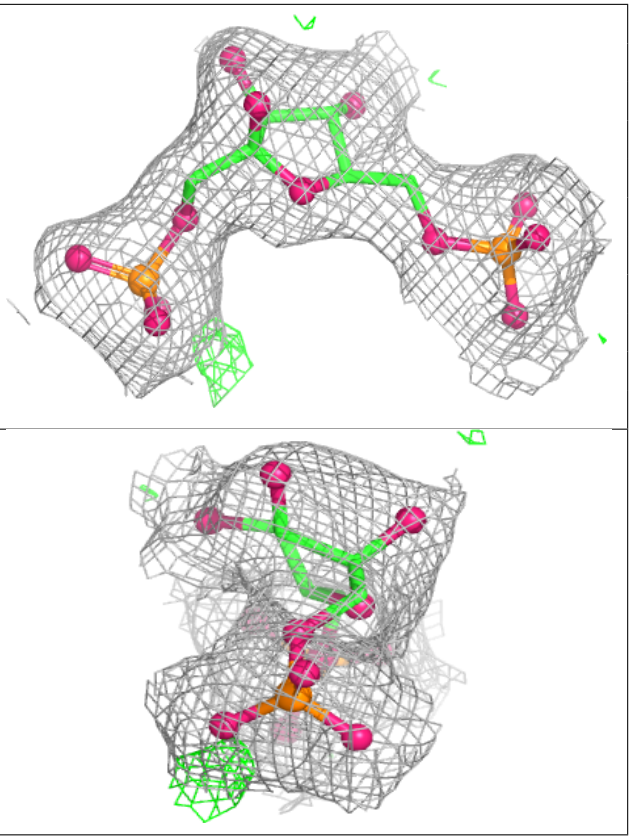






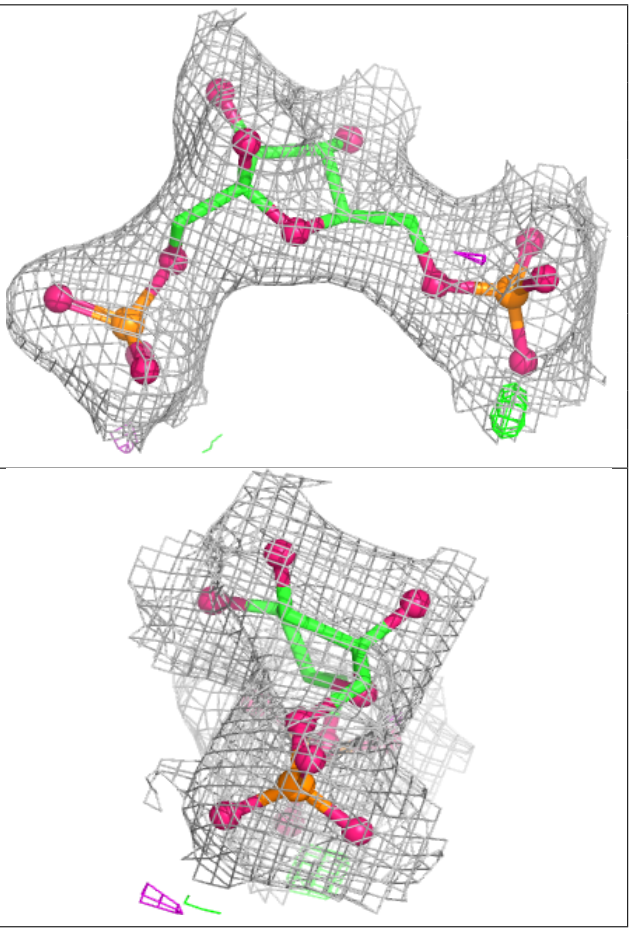
Electron density around FBP A 601:

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



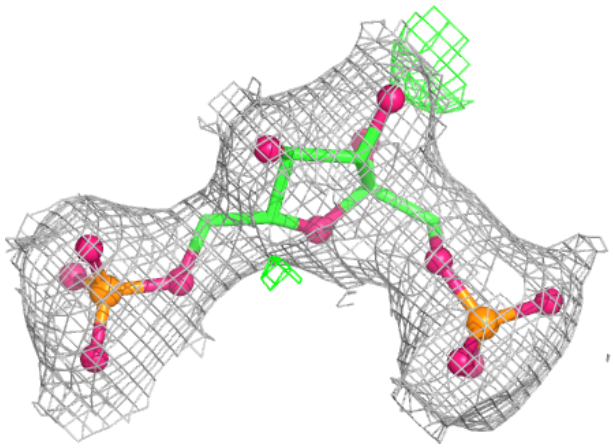
Electron density around FBP F 601:

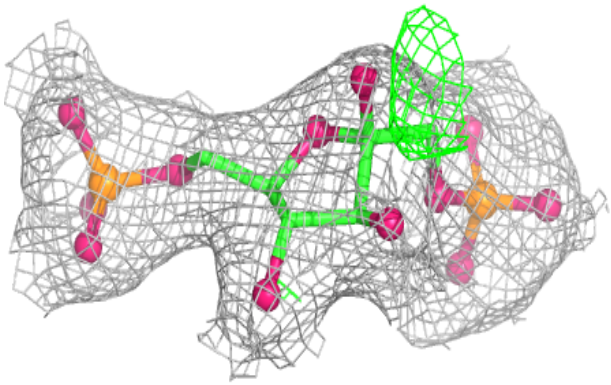
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

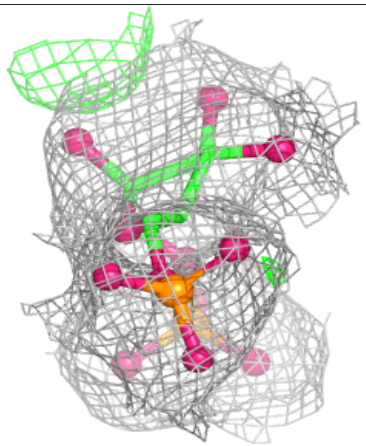


Electron density around FBP E 601:

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

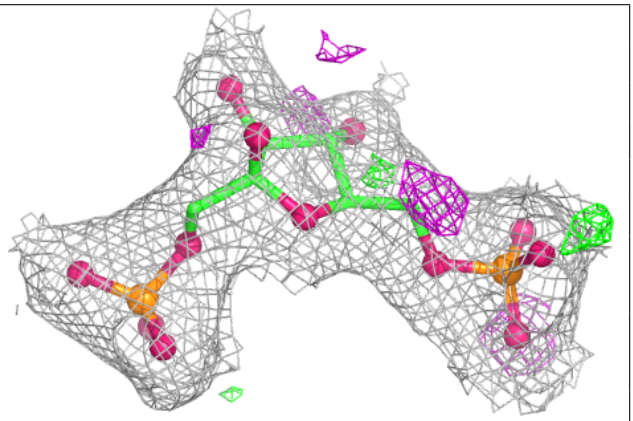


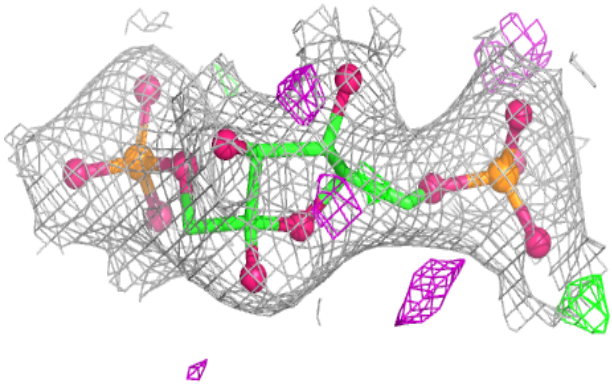


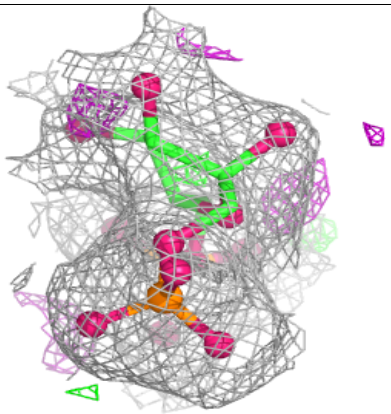


Electron density around FBP G 601:

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

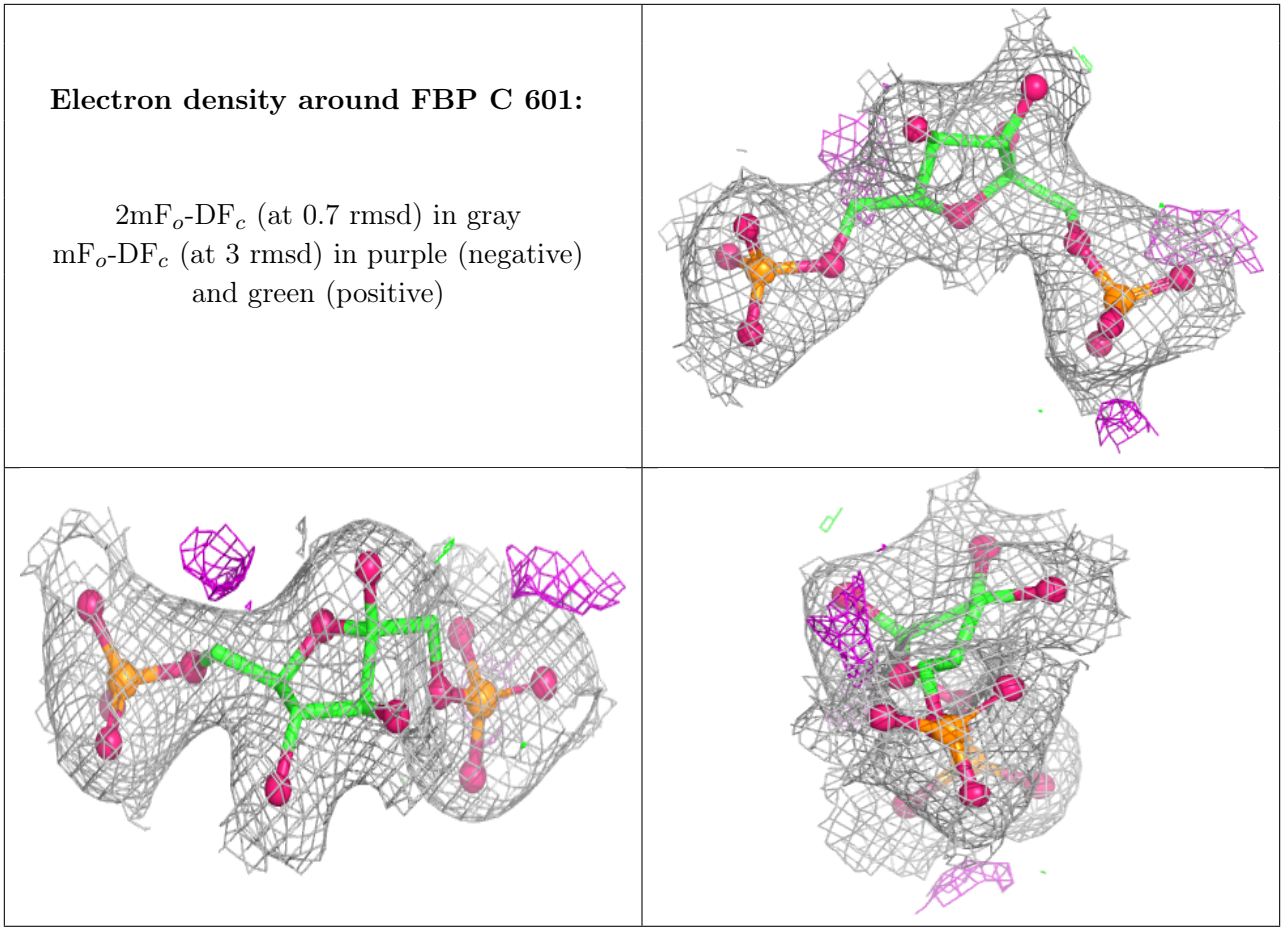






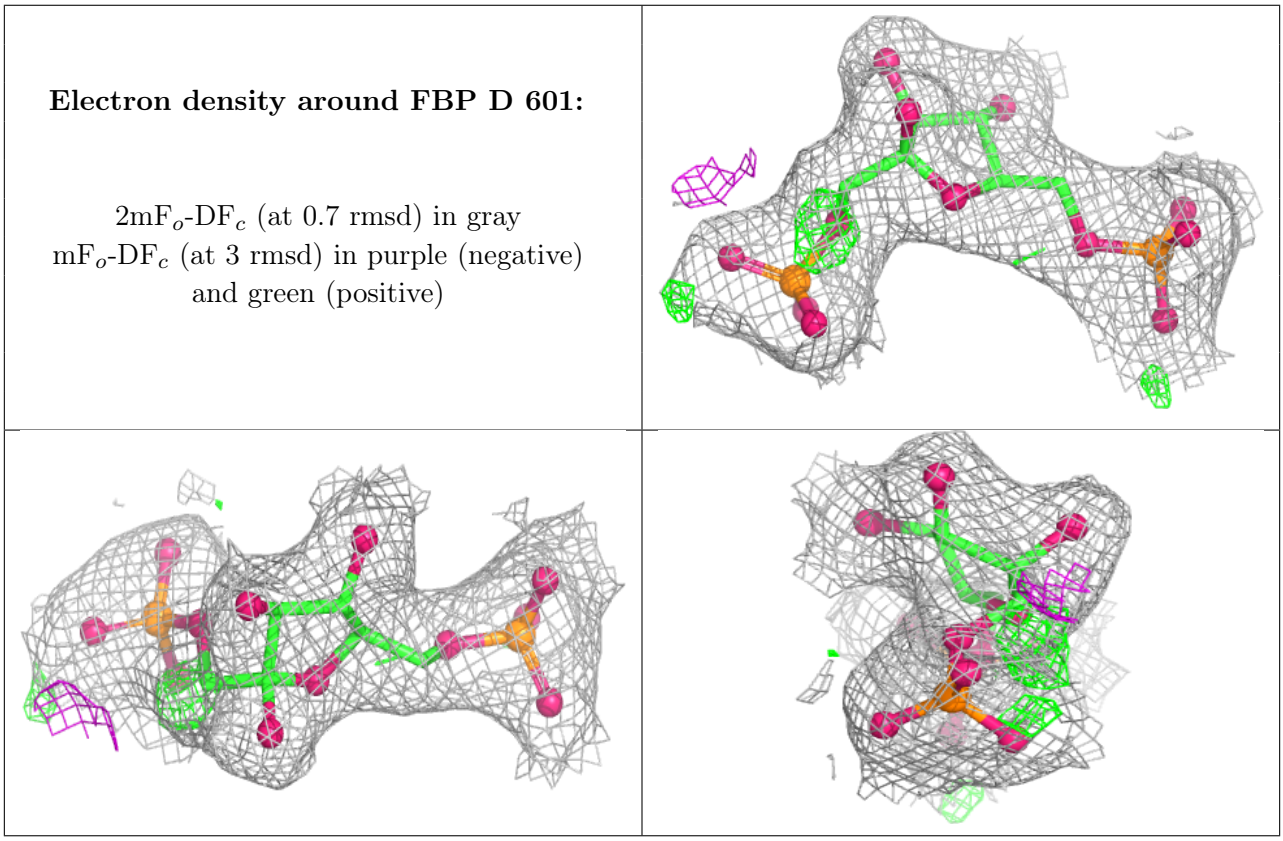
Electron density around FBP C 601:

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



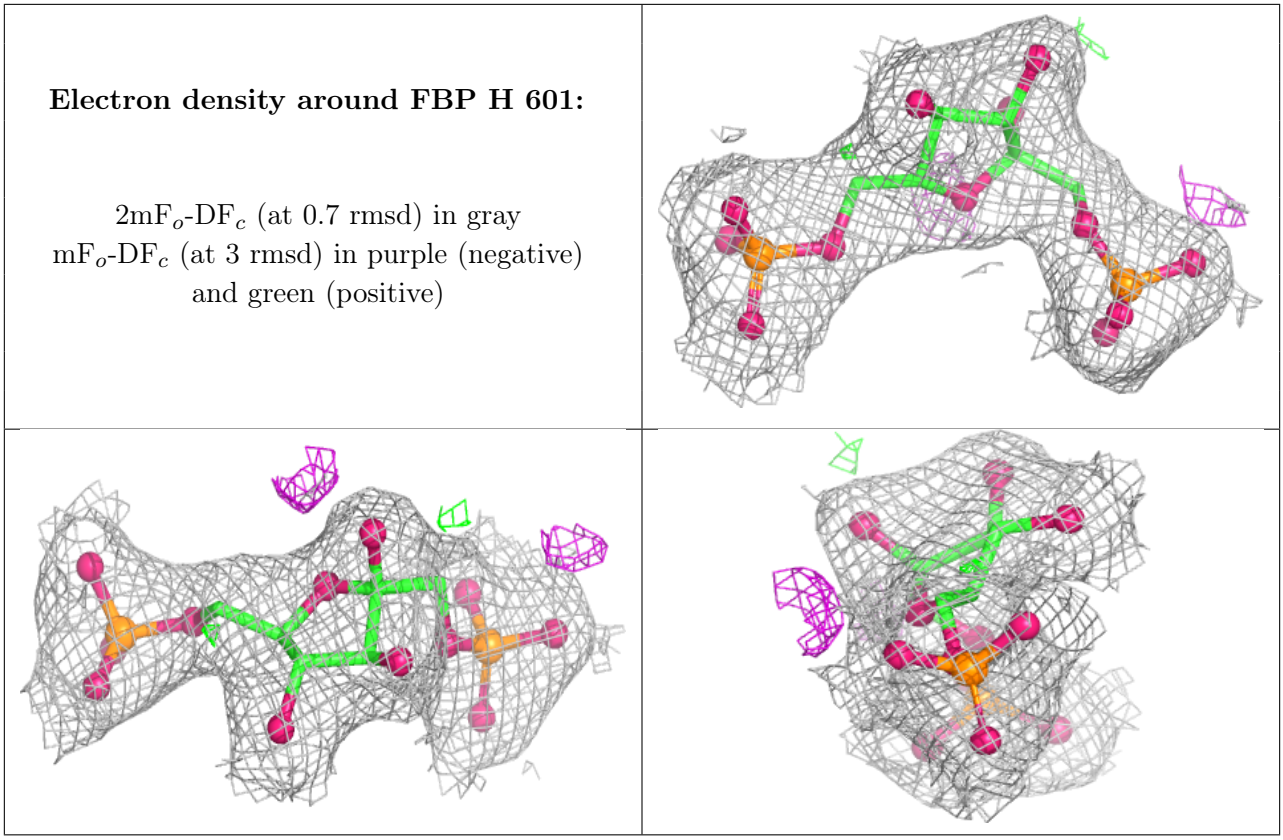
Electron density around FBP D 601:

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



Electron density around FBP 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)



6.5 Other polymers (i)

There are no such residues in this entry.