wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2026 – 12:20 PM EDT

PDB ID	:	14CK / pdb_000014ck
Title	:	Structure of liver pyruvate kinase in complex with mitapivat
Authors	:	Lulla, A.; Rodriguez Rivero, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2026-04-28
Resolution	:	1.95 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:

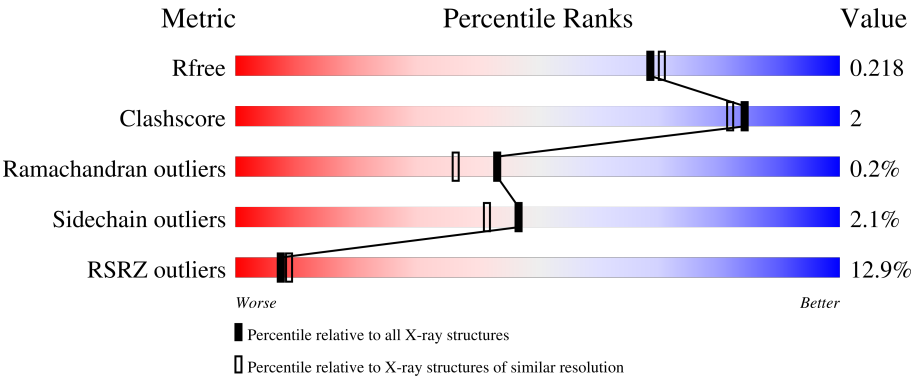
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	22% 86% 7% • 6%
1	B	447	39% 91% 6% •
1	C	447	5% 89% 6% 5%
1	D	447	3% 89% 6% 5%
1	E	447	14% 88% 6% 6%

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Mol	Chain	Length	Quality of chain
1	F	447	9% 89% 7%
1	G	447	4% 88% 6% 6%
1	H	447	3% 88% 7% 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	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 29183 atoms, of which 104 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	418	Total	C	N	O	S	0	13	0
			3238	2033	581	604	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
			3258	2048	584	607	19			
1	D	425	Total	C	N	O	S	0	8	0
			3261	2048	590	604	19			
1	E	420	Total	C	N	O	S	0	13	0
			3264	2054	585	605	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	8	0
			3246	2042	582	603	19			
1	H	425	Total	C	N	O	S	0	8	0
			3271	2053	597	602	19			

There are 48 discrepancies between the modelled and reference sequences:

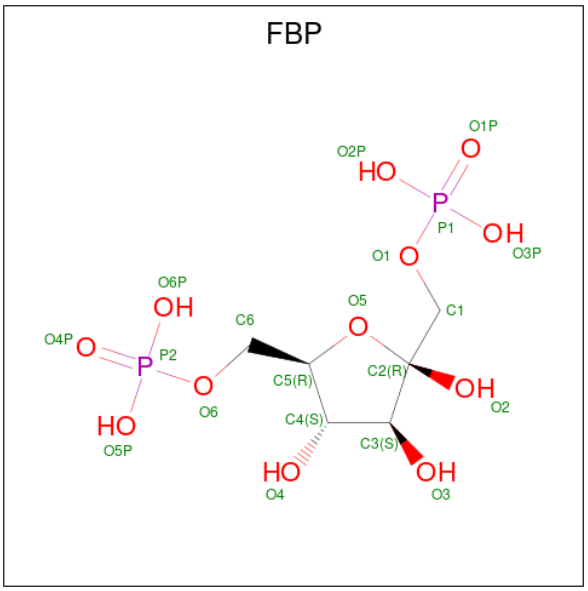
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30613
A	0	SER	-	expression tag	UNP P30613
A	12	ASP	SER	conflict	UNP P30613
A	130	GLY	-	linker	UNP P30613
A	131	SER	-	linker	UNP P30613
A	132	GLY	-	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
B	0	SER	-	expression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

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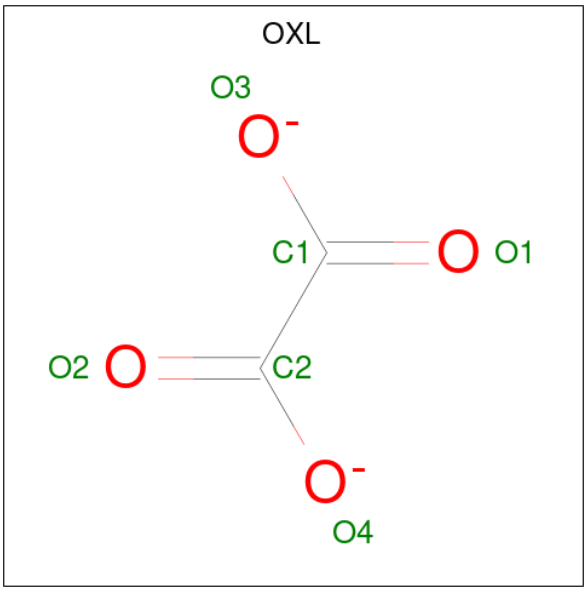
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	130	GLY	-	linker	UNP P30613
C	131	SER	-	linker	UNP P30613
C	132	GLY	-	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	12	ASP	SER	conflict	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: $C_6H_{14}O_{12}P_2$).



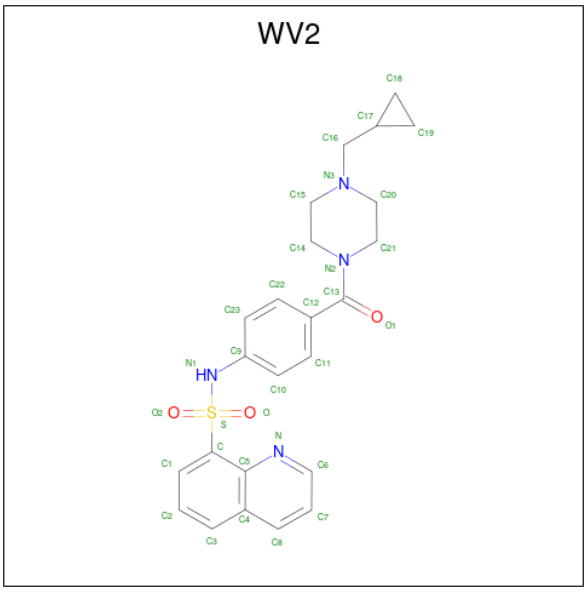
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
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 mitapivat (CCD ID: WV2) (formula: $C_{24}H_{26}N_4O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	26	0
			58	24	26	4	3	1		
4	D	1	Total	C	H	N	O	S	26	0
			58	24	26	4	3	1		
4	E	1	Total	C	H	N	O	S	26	0
			58	24	26	4	3	1		
4	H	1	Total	C	H	N	O	S	26	0
			58	24	26	4	3	1		

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

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

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

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

- Molecule 7 is water.

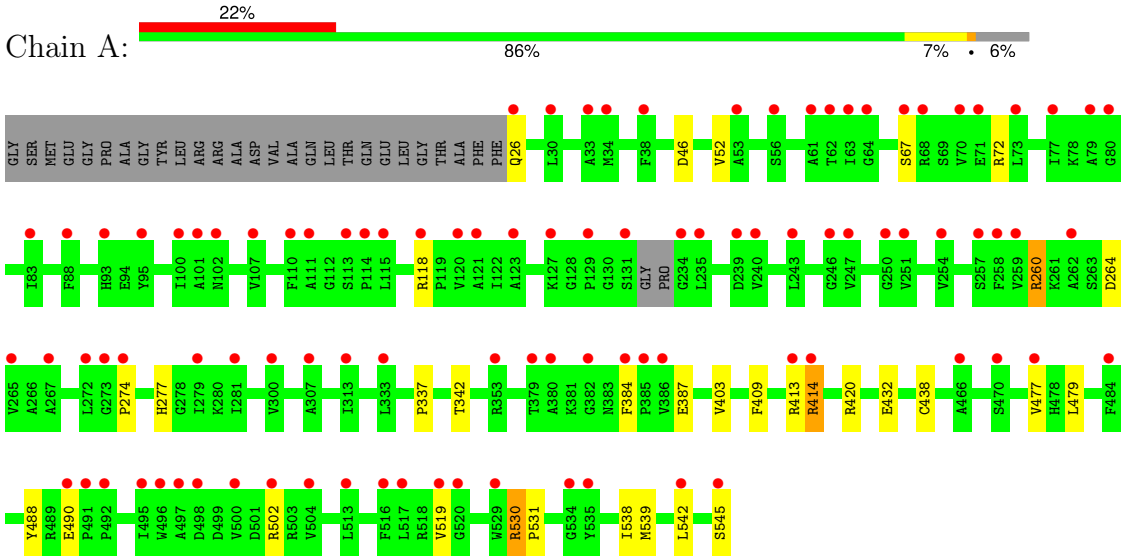
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	183	Total O 183 183	0	0
7	B	161	Total O 161 161	0	0
7	C	358	Total O 358 358	0	0
7	D	403	Total O 403 403	0	0
7	E	226	Total O 226 226	0	0
7	F	336	Total O 336 336	0	0
7	G	394	Total O 394 394	0	0
7	H	451	Total O 451 451	0	0

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.

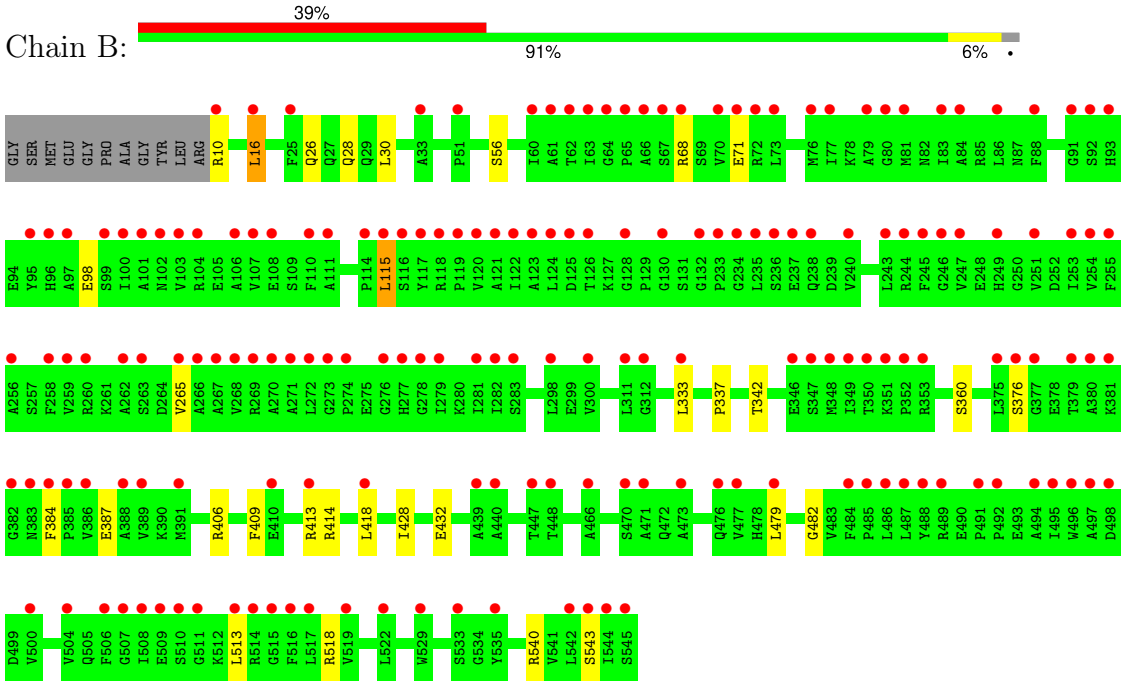
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain A:



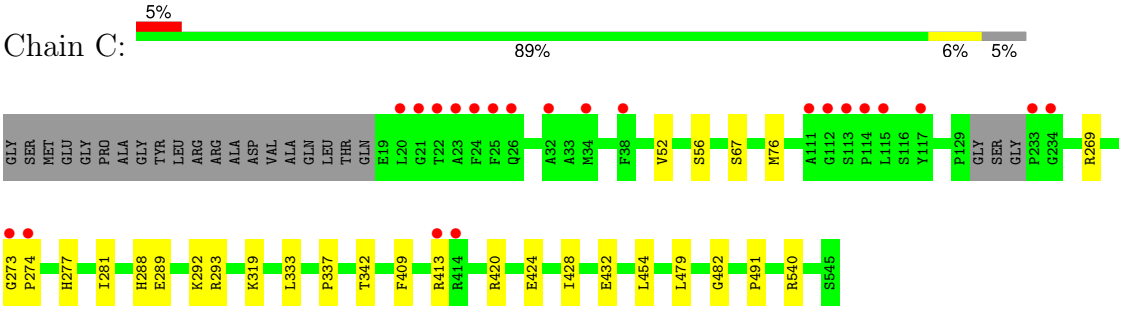
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain B:



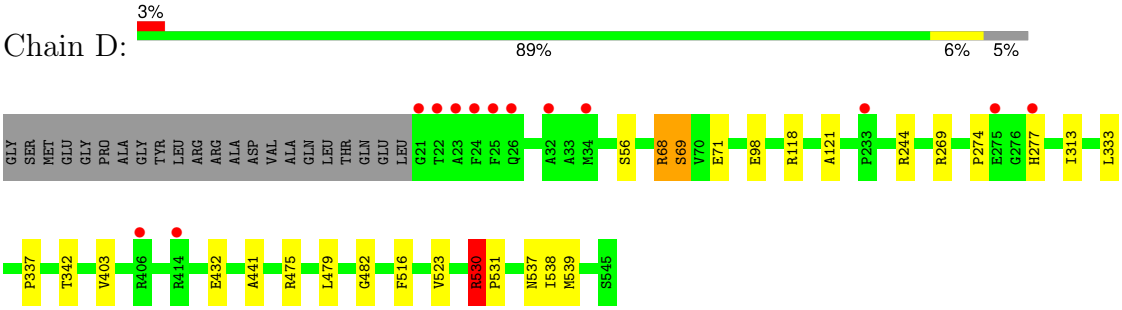
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain C:



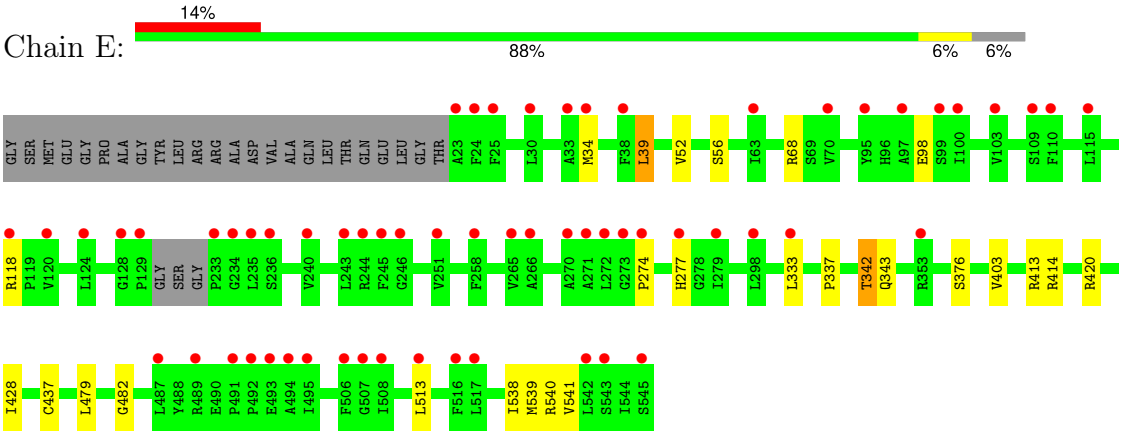
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain D:



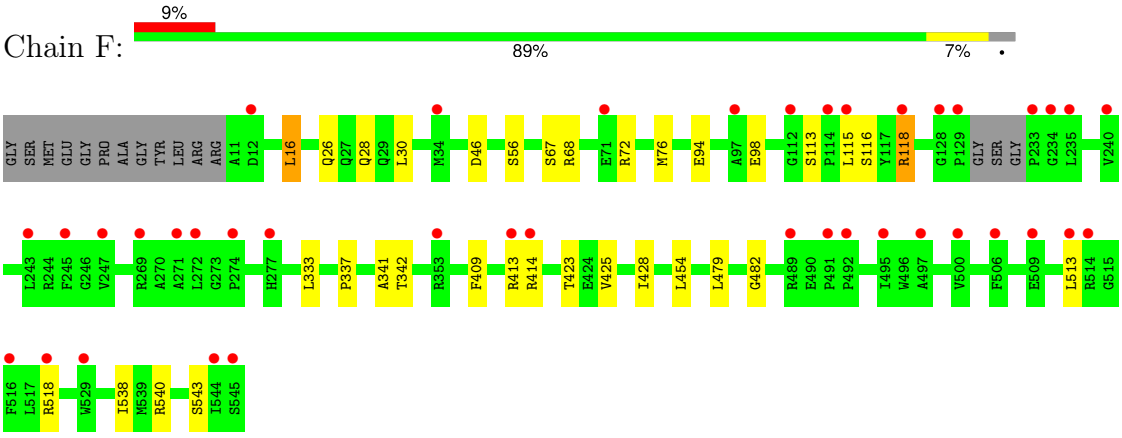
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain E:



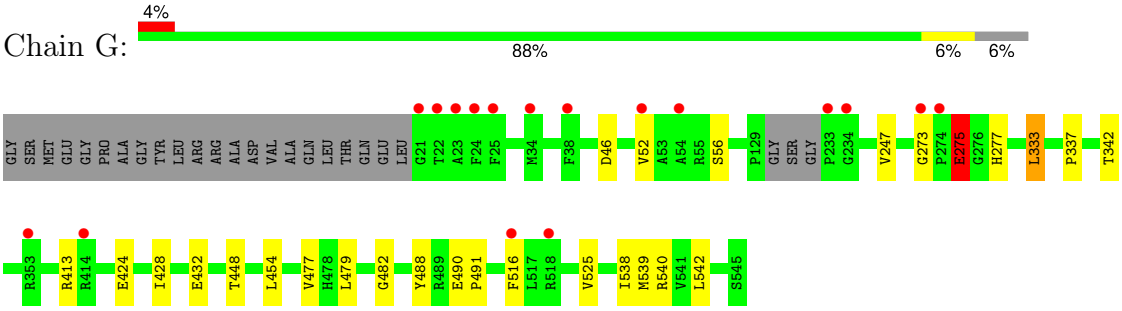
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain F:



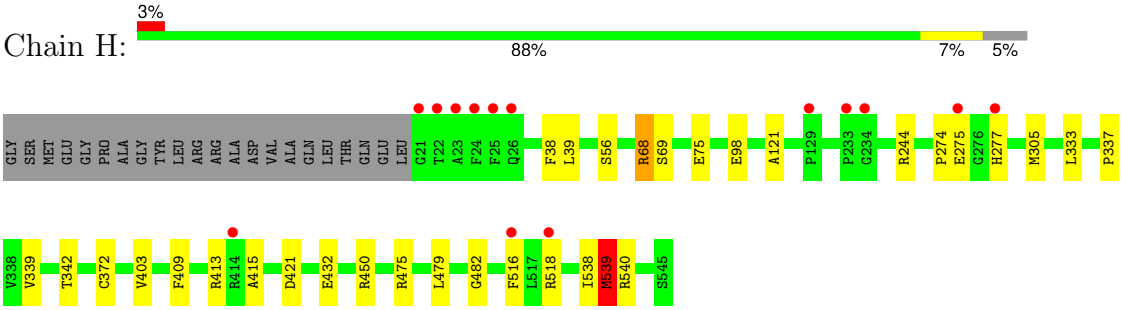
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

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	208.88Å 112.88Å 188.70Å 90.00° 91.28° 90.00°	Depositor
Resolution (Å)	188.66 – 1.95 188.66 – 1.95	Depositor EDS
% Data completeness (in resolution range)	85.9 (188.66-1.95) 85.9 (188.66-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.198 , 0.225 0.191 , 0.218	Depositor DCC
R_{free} test set	13526 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29183	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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 38.66 % 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 3.5669e-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, MG, OXL, WV2, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.67	0/3328	0.96	1/4497 (0.0%)
1	B	0.71	2/3429 (0.1%)	0.99	0/4636
1	C	0.77	0/3333	0.97	1/4505 (0.0%)
1	D	0.81	0/3341	0.99	3/4517 (0.1%)
1	E	0.66	1/3358 (0.0%)	0.96	0/4538
1	F	0.73	0/3405	0.99	4/4603 (0.1%)
1	G	0.81	1/3324 (0.0%)	1.00	3/4493 (0.1%)
1	H	0.86	2/3348 (0.1%)	0.98	1/4525 (0.0%)
All	All	0.75	6/26866 (0.0%)	0.98	13/36314 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376[A]	SER	CA-C	6.38	1.55	1.52
1	B	376[B]	SER	CA-C	6.38	1.55	1.52
1	G	491	PRO	CA-C	5.69	1.55	1.52
1	H	305	MET	SD-CE	-5.37	1.66	1.79
1	H	539	MET	SD-CE	-5.19	1.66	1.79

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	275	GLU	CB-CG-CD	6.82	124.19	112.60
1	H	516	PHE	CA-CB-CG	6.40	120.20	113.80
1	F	113	SER	N-CA-C	5.84	113.48	108.22
1	F	46	ASP	CA-CB-CG	5.80	118.41	112.60
1	G	516	PHE	CA-CB-CG	5.65	119.45	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	3238	0	3312	16	0
1	B	3350	0	3417	18	0
1	C	3258	0	3314	17	0
1	D	3261	0	3321	16	0
1	E	3264	0	3331	13	0
1	F	3327	0	3399	17	0
1	G	3246	0	3308	16	0
1	H	3271	0	3335	25	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	32	26	0	1	0
4	D	32	26	0	1	0
4	E	32	26	0	1	0
4	H	32	26	0	7	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

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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	183	0	0	0	0
7	B	161	0	0	0	0
7	C	358	0	0	2	1
7	D	403	0	0	1	1
7	E	226	0	0	0	0
7	F	336	0	0	0	0
7	G	394	0	0	0	0
7	H	451	0	0	2	0
All	All	29079	104	26817	120	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 120 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:540:ARG:HG2	1:H:538:ILE:HG12	1.65	0.77
1:H:409:PHE:O	1:H:413:ARG:HG2	1.84	0.77
1:E:420[B]:ARG:HG3	1:F:16:LEU:HD11	1.67	0.76
1:A:538:ILE:HG12	1:B:540:ARG:HG2	1.69	0.74
1:B:115:LEU:HG	1:B:513:LEU:HB3	1.71	0.72

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:C:1000:HOH:O	7:D:781:HOH:O[4_545]	2.00	0.20

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/447 (96%)	423 (99%)	3 (1%)	1 (0%)	43	36
1	B	442/447 (99%)	437 (99%)	4 (1%)	1 (0%)	43	36
1	C	427/447 (96%)	422 (99%)	4 (1%)	1 (0%)	43	36
1	D	431/447 (96%)	428 (99%)	2 (0%)	1 (0%)	43	36
1	E	429/447 (96%)	425 (99%)	3 (1%)	1 (0%)	43	36
1	F	436/447 (98%)	432 (99%)	3 (1%)	1 (0%)	43	36
1	G	426/447 (95%)	420 (99%)	5 (1%)	1 (0%)	43	36
1	H	431/447 (96%)	427 (99%)	3 (1%)	1 (0%)	43	36
All	All	3449/3576 (96%)	3414 (99%)	27 (1%)	8 (0%)	43	36

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	THR
1	F	342	THR
1	H	342	THR
1	A	342	THR
1	C	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	345/352 (98%)	334 (97%)	11 (3%)	34	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	353/352 (100%)	342 (97%)	11 (3%)	35	26
1	C	344/352 (98%)	341 (99%)	3 (1%)	70	70
1	D	344/352 (98%)	338 (98%)	6 (2%)	53	49
1	E	347/352 (99%)	337 (97%)	10 (3%)	37	29
1	F	351/352 (100%)	343 (98%)	8 (2%)	44	38
1	G	343/352 (97%)	339 (99%)	4 (1%)	63	61
1	H	344/352 (98%)	339 (98%)	5 (2%)	57	54
All	All	2771/2816 (98%)	2713 (98%)	58 (2%)	47	41

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

Mol	Chain	Res	Type
1	D	333	LEU
1	H	69	SER
1	E	333	LEU
1	H	68	ARG
1	G	52	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	405	HIS
1	H	28	GLN
1	F	27	GLN
1	H	407	GLN
1	G	277	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OXL	G	602	5	5,5,5	2.80	3 (60%)	6,6,6	1.71	2 (33%)
2	FBP	C	601	-	18,20,20	0.70	0	21,32,32	0.57	0
2	FBP	H	601	-	18,20,20	0.65	0	21,32,32	0.64	0
4	WV2	H	603	-	36,36,36	0.49	0	52,52,52	0.86	2 (3%)
2	FBP	A	601	-	18,20,20	0.42	0	21,32,32	0.58	0
3	OXL	D	602	5	5,5,5	2.60	3 (60%)	6,6,6	1.73	2 (33%)
2	FBP	F	601	-	18,20,20	0.55	0	21,32,32	0.54	0
2	FBP	G	601	-	18,20,20	0.57	0	21,32,32	0.60	0
4	WV2	D	603	-	36,36,36	0.39	0	52,52,52	0.50	0
3	OXL	B	602	5	5,5,5	2.47	3 (60%)	6,6,6	1.96	2 (33%)
3	OXL	E	602	5	5,5,5	2.25	3 (60%)	6,6,6	1.66	1 (16%)
3	OXL	H	602	5	5,5,5	2.77	3 (60%)	6,6,6	2.03	2 (33%)
2	FBP	D	601	-	18,20,20	0.56	0	21,32,32	1.05	1 (4%)
3	OXL	A	602	5	5,5,5	2.25	3 (60%)	6,6,6	2.08	2 (33%)
3	OXL	F	602	5	5,5,5	2.89	3 (60%)	6,6,6	2.21	2 (33%)
3	OXL	C	602	5	5,5,5	2.56	3 (60%)	6,6,6	2.07	2 (33%)
2	FBP	E	601	-	18,20,20	0.64	0	21,32,32	0.60	0
4	WV2	E	603	-	36,36,36	0.33	0	52,52,52	0.54	0
2	FBP	B	601	-	18,20,20	0.36	0	21,32,32	0.79	1 (4%)
4	WV2	A	603	-	36,36,36	0.38	0	52,52,52	0.57	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
3	OXL	G	602	5	-	4/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
4	WV2	H	603	-	-	1/23/35/35	1/5/5/5
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	5	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
4	WV2	D	603	-	-	0/23/35/35	0/5/5/5
3	OXL	B	602	5	-	4/4/4/4	-
3	OXL	E	602	5	-	4/4/4/4	-
3	OXL	H	602	5	-	4/4/4/4	-
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	5	-	4/4/4/4	-
3	OXL	F	602	5	-	0/4/4/4	-
3	OXL	C	602	5	-	4/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
4	WV2	E	603	-	-	0/23/35/35	0/5/5/5
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
4	WV2	A	603	-	-	3/23/35/35	1/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	OXL	O2-C2	4.64	1.34	1.22
3	F	602	OXL	C2-C1	4.40	1.62	1.54
3	F	602	OXL	O2-C2	4.26	1.33	1.22
3	C	602	OXL	O2-C2	4.13	1.32	1.22
3	H	602	OXL	C2-C1	4.05	1.61	1.54

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	602	OXL	O4-C2-C1	3.90	120.40	112.83
3	A	602	OXL	O4-C2-C1	3.85	120.30	112.83
3	C	602	OXL	O4-C2-C1	3.84	120.27	112.83
2	D	601	FBP	O6-P2-O4P	3.56	116.07	106.44
3	F	602	OXL	O4-C2-C1	3.55	119.71	112.83

There are no chirality outliers.

5 of 48 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	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6

All (2) ring outliers are listed below:

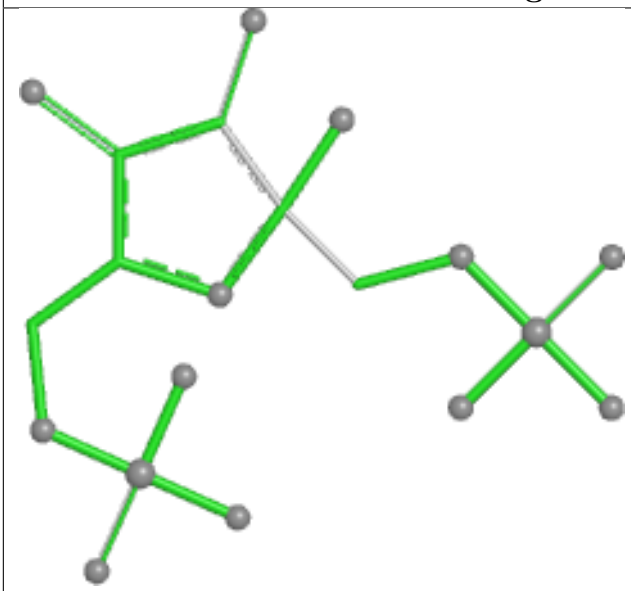
Mol	Chain	Res	Type	Atoms
4	H	603	WV2	C14-C15-C20-C21-N2-N3
4	A	603	WV2	C14-C15-C20-C21-N2-N3

4 monomers are involved in 10 short contacts:

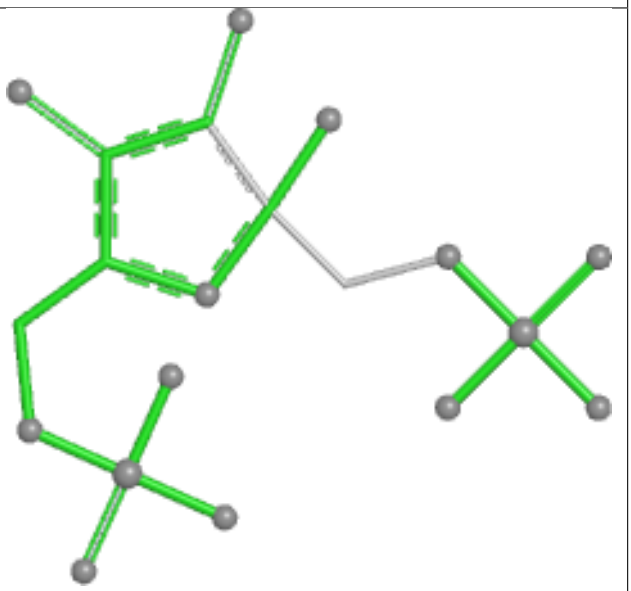
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	603	WV2	7	0
4	D	603	WV2	1	0
4	E	603	WV2	1	0
4	A	603	WV2	1	0

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.

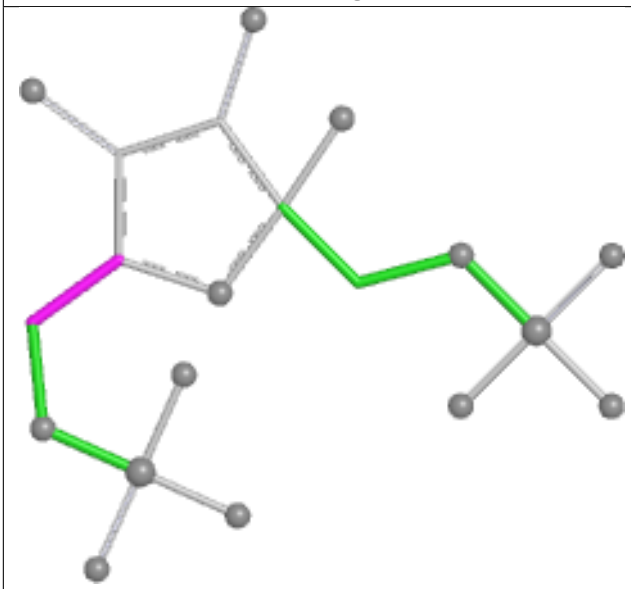
Ligand FBP C 601



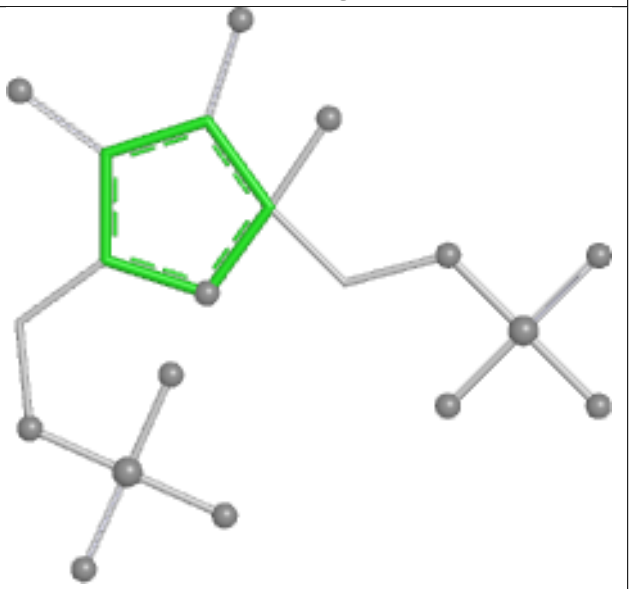
Bond lengths



Bond angles

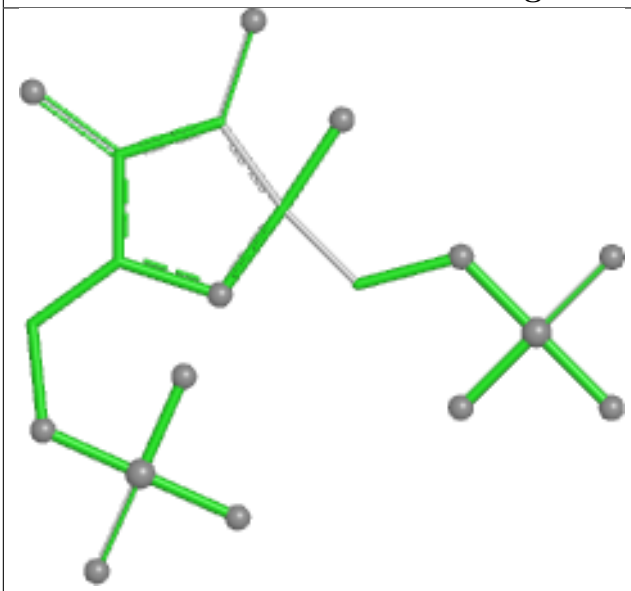


Torsions

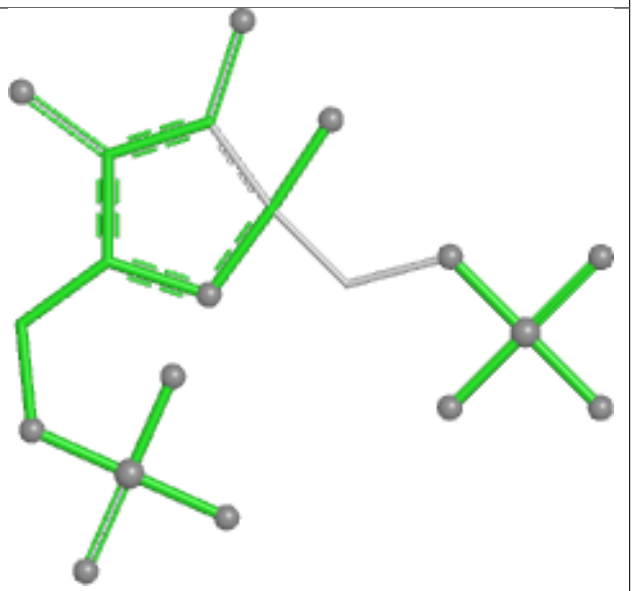


Rings

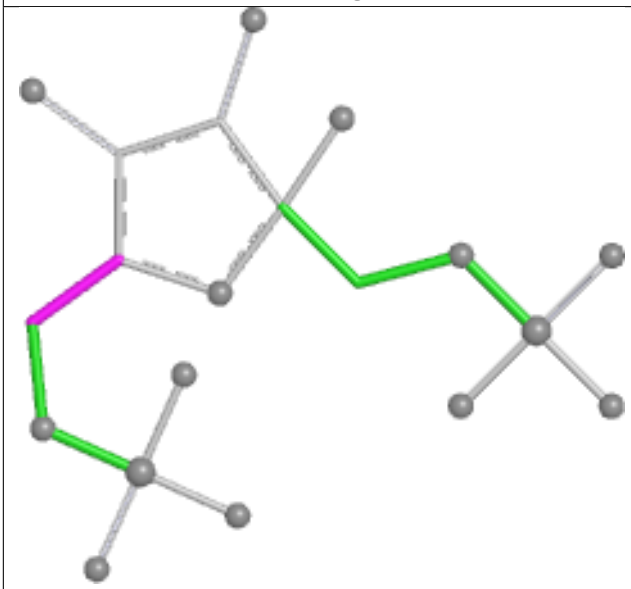
Ligand FBP H 601



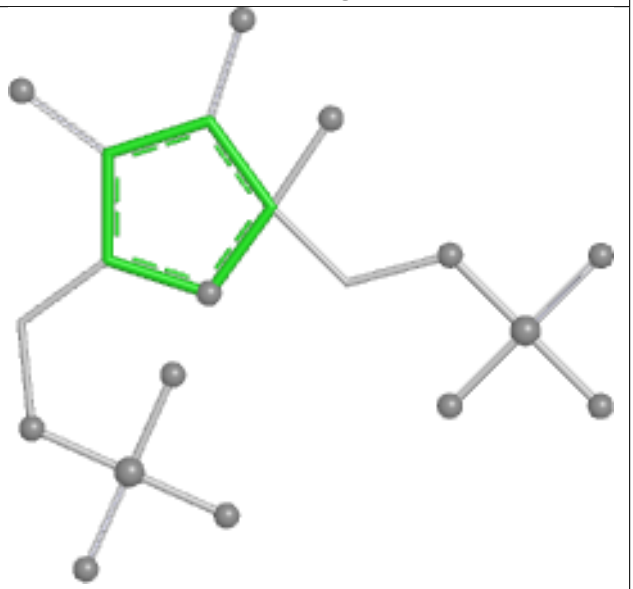
Bond lengths



Bond angles

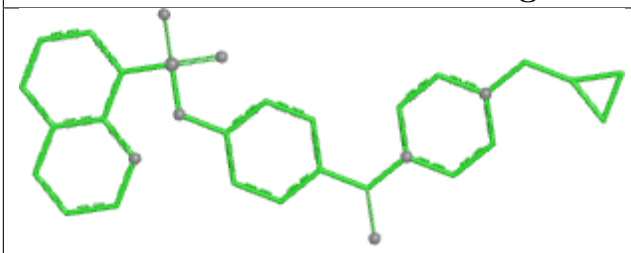


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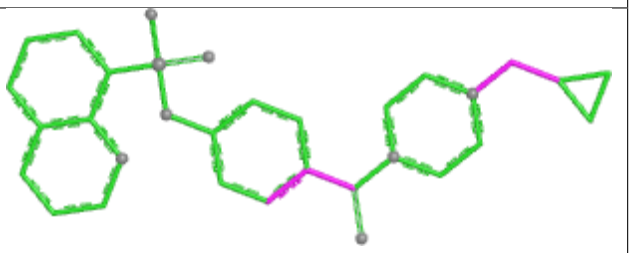


Rings

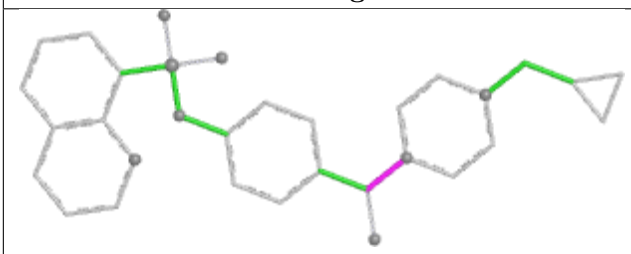
Ligand WV2 H 603



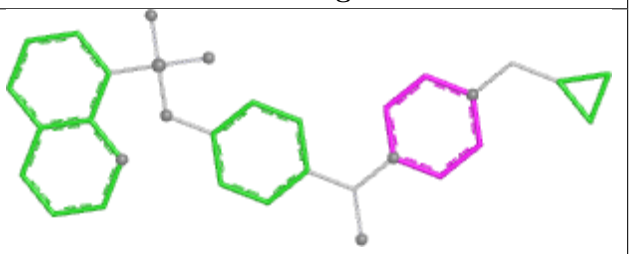
Bond lengths



Bond angles

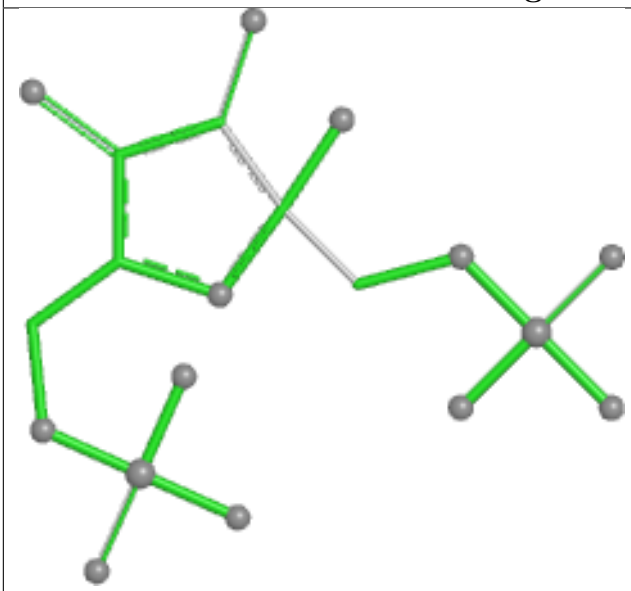


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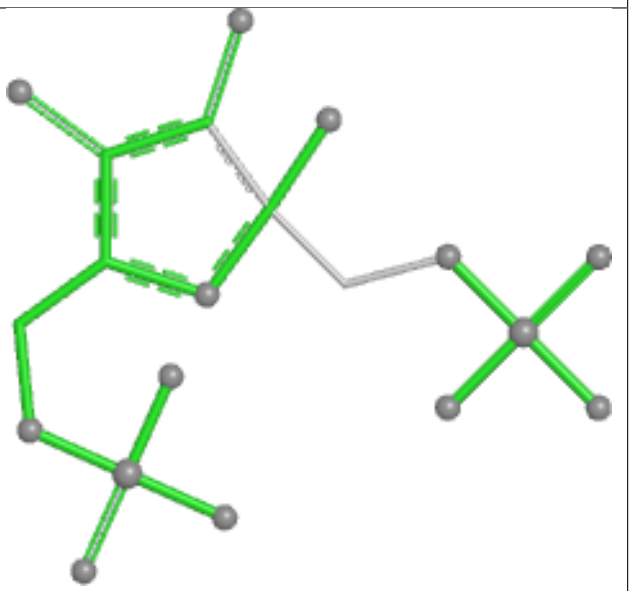


Rings

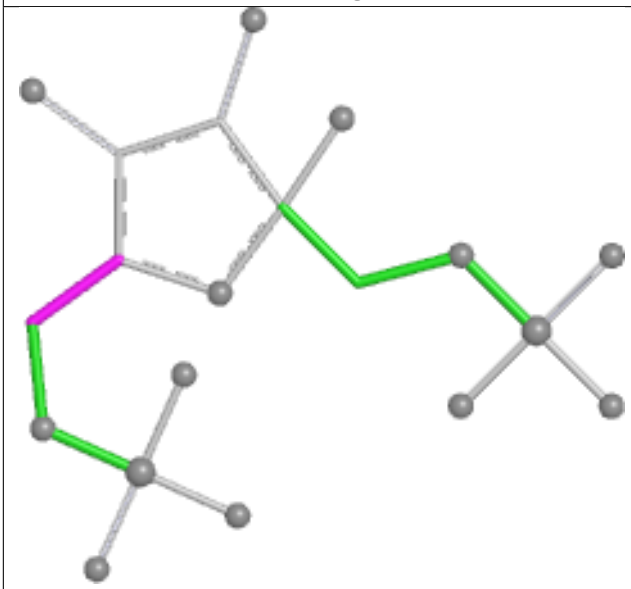
Ligand FBP A 601



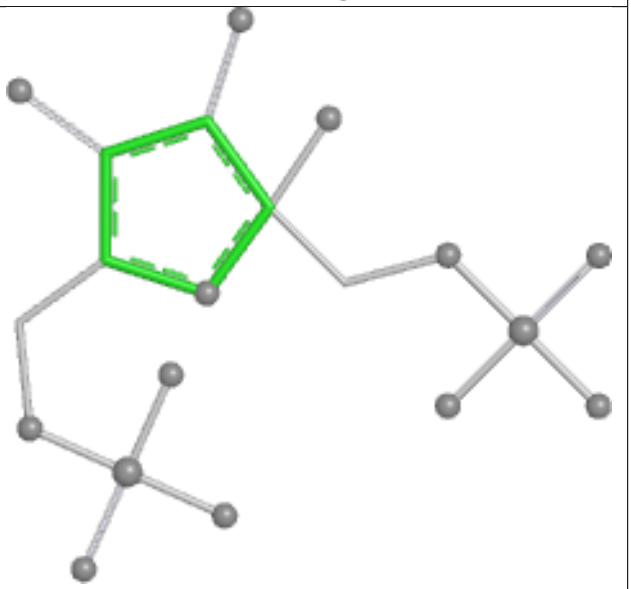
Bond lengths



Bond angles

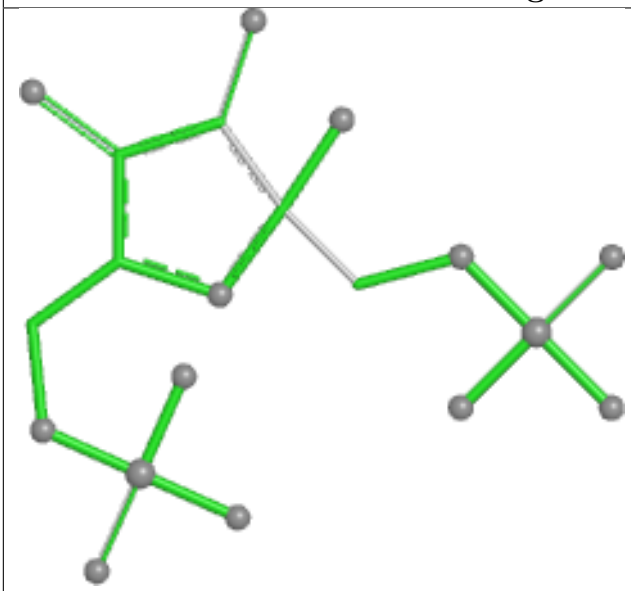


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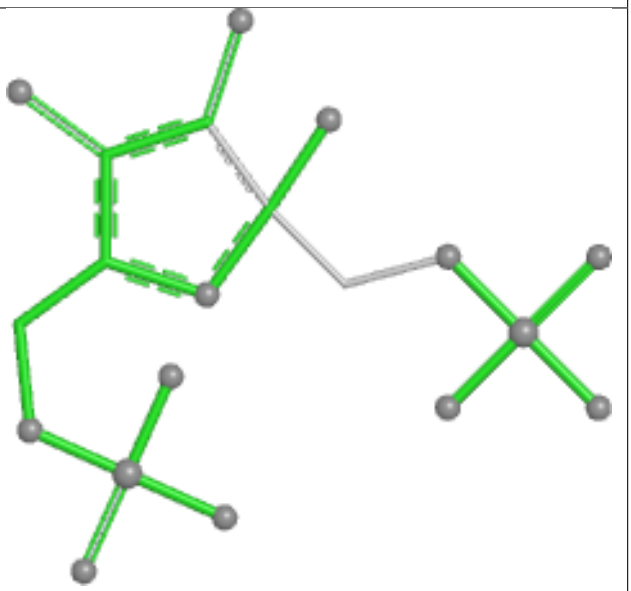


Rings

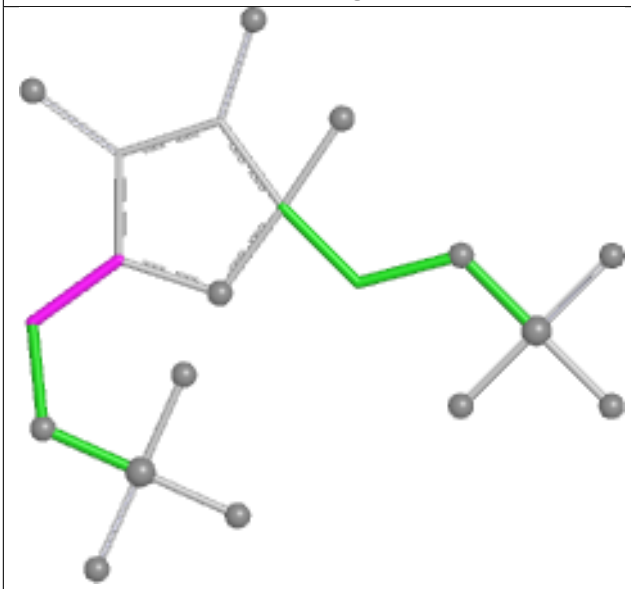
Ligand FBP F 601



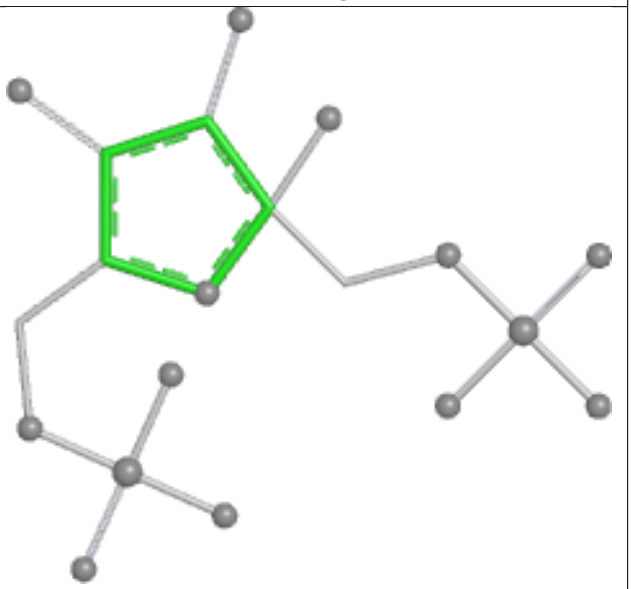
Bond lengths



Bond angles

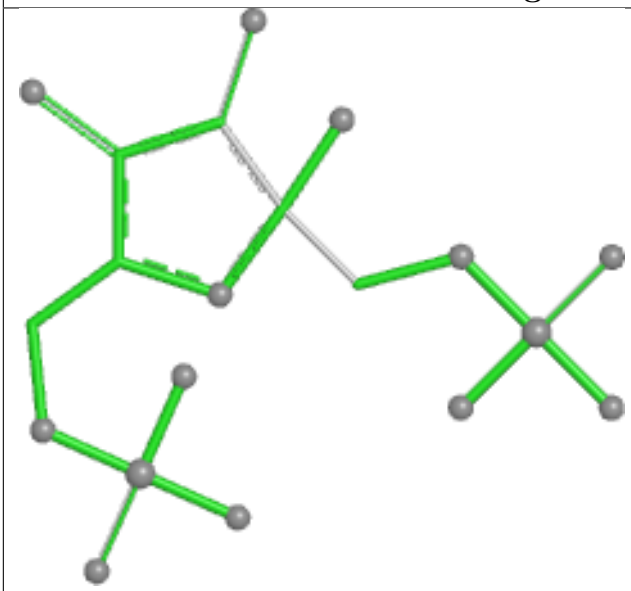


Torsions

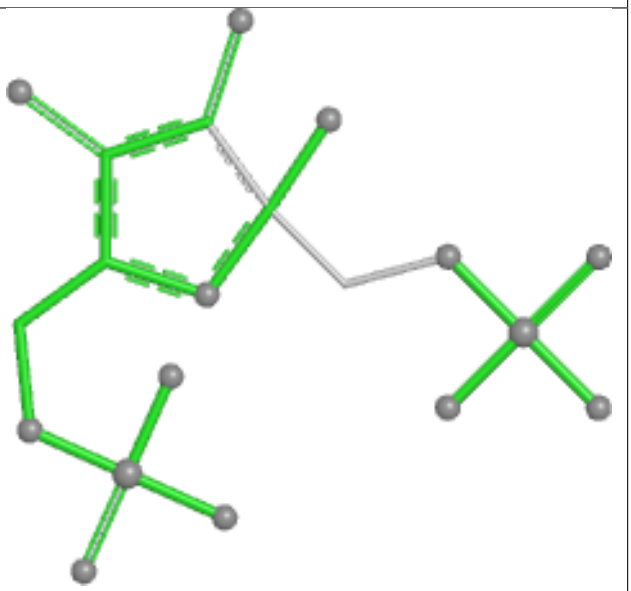


Rings

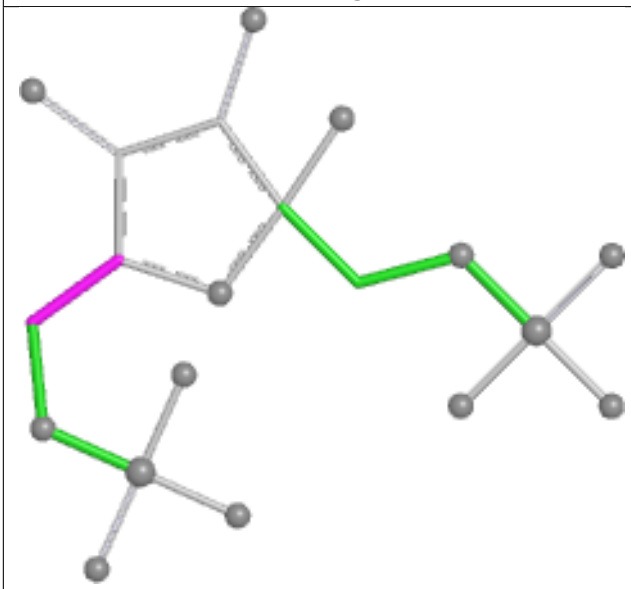
Ligand FBP G 601



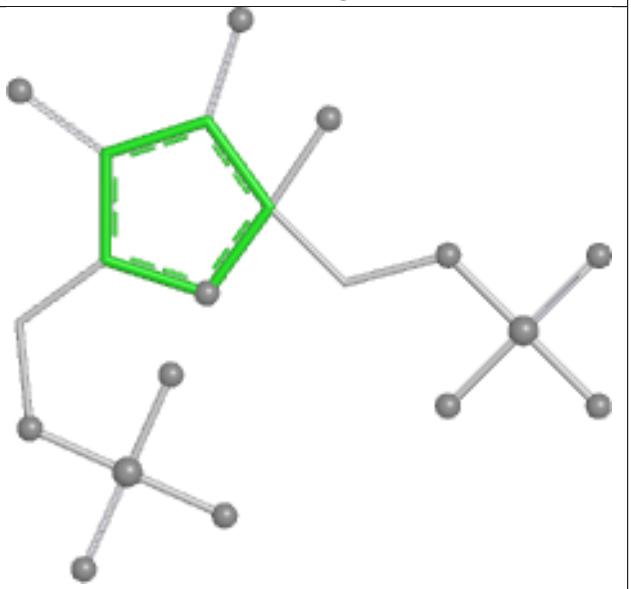
Bond lengths



Bond angles

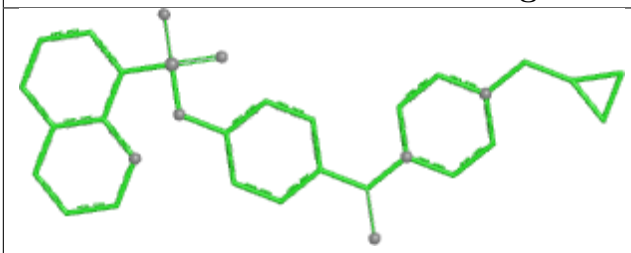


Torsions

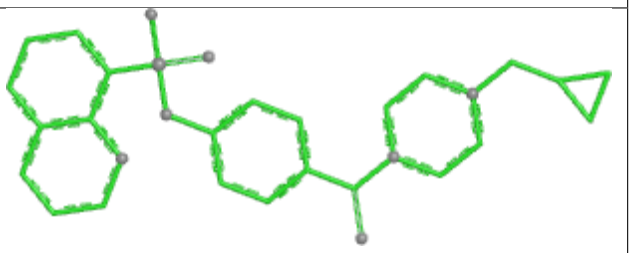


Rings

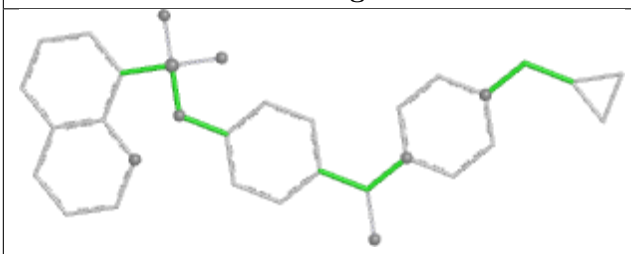
Ligand WV2 D 603



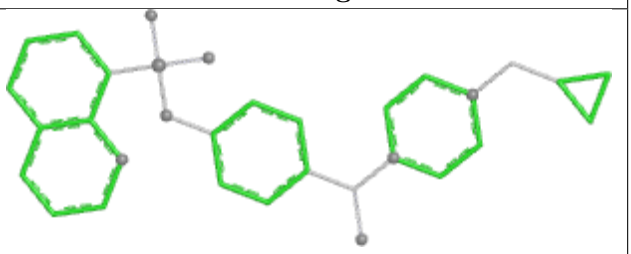
Bond lengths



Bond angles

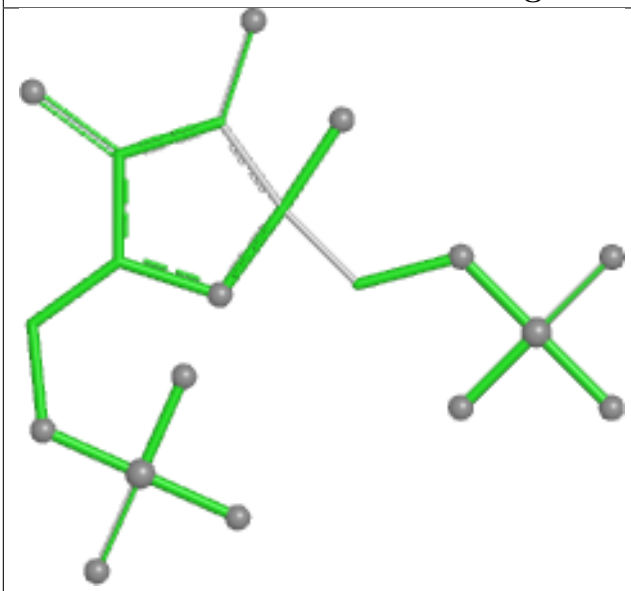


Torsions

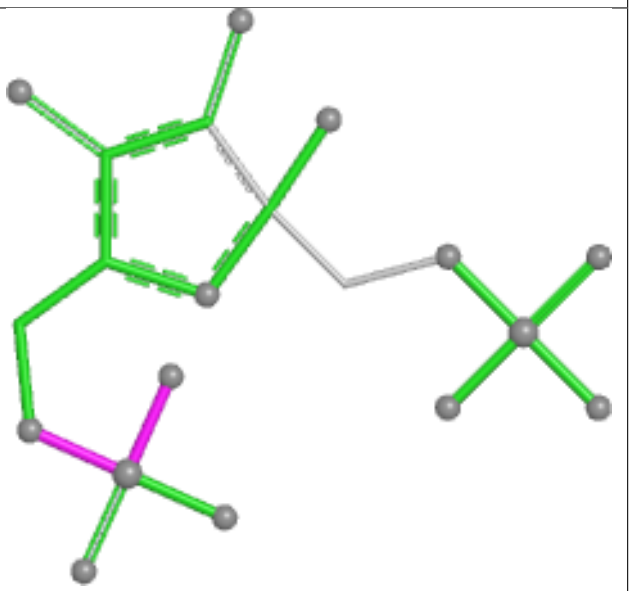


Rings

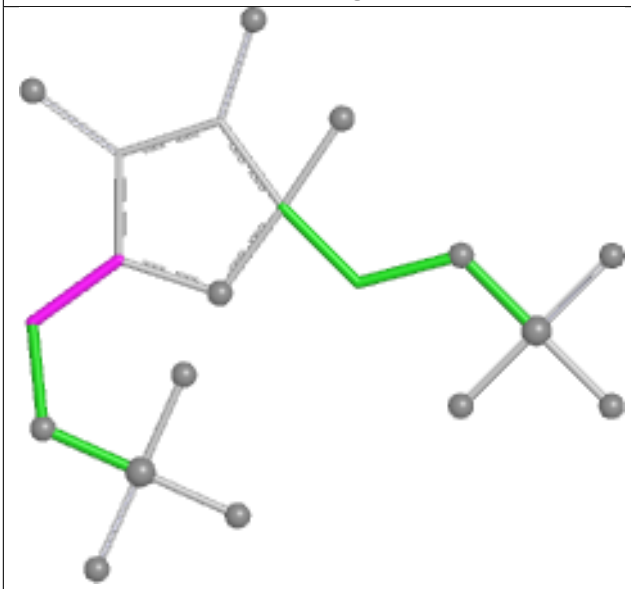
Ligand FBP D 601



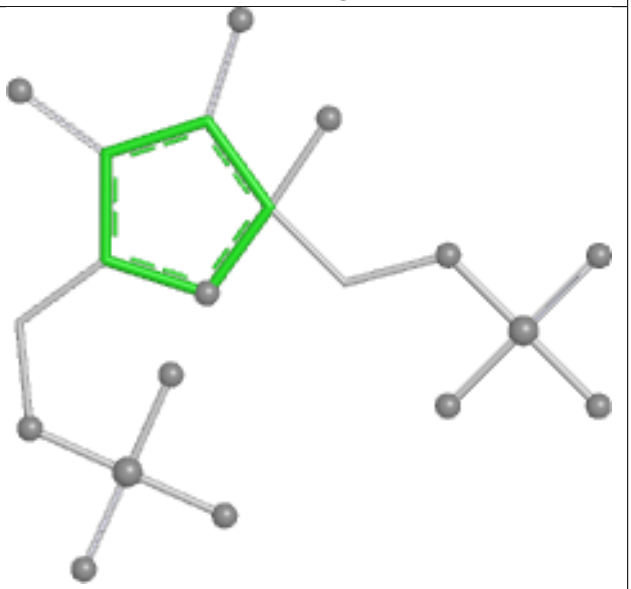
Bond lengths



Bond angles

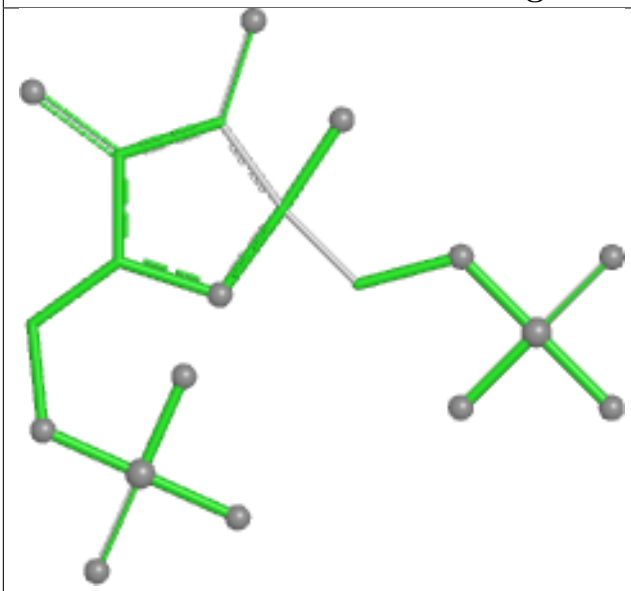


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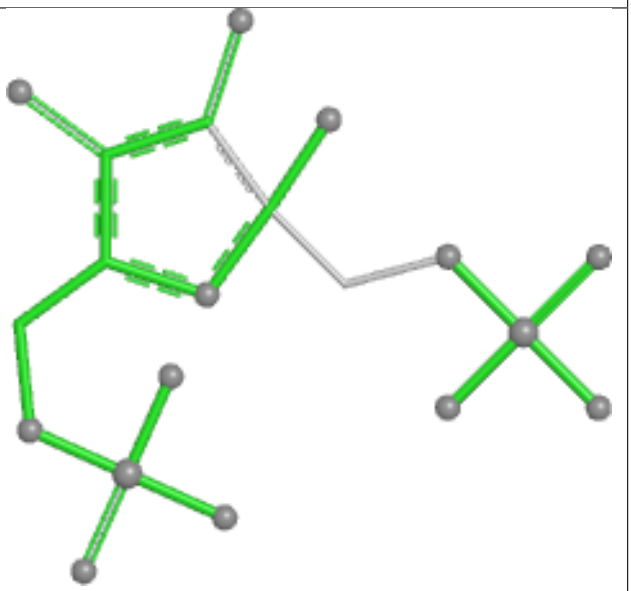


Rings

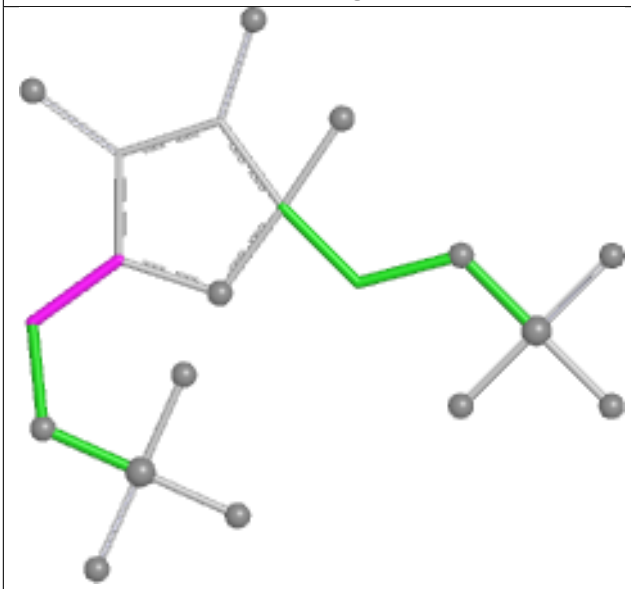
Ligand FBP E 601



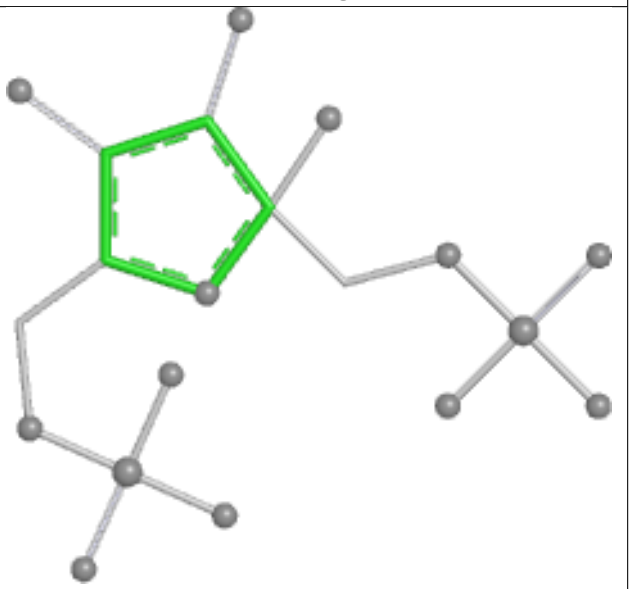
Bond lengths



Bond angles

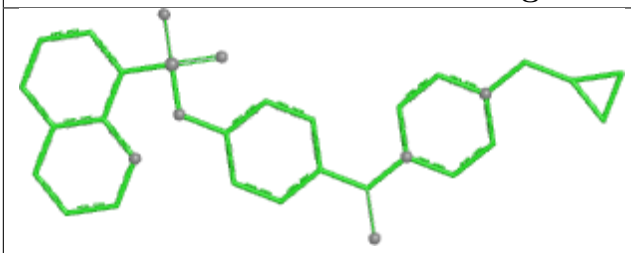


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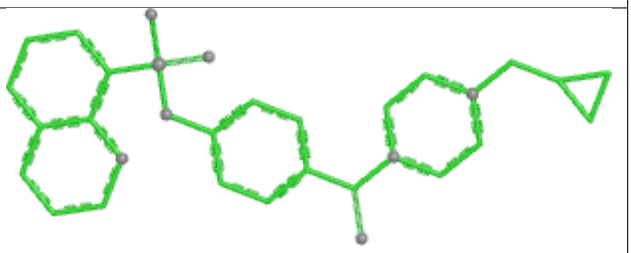


Rings

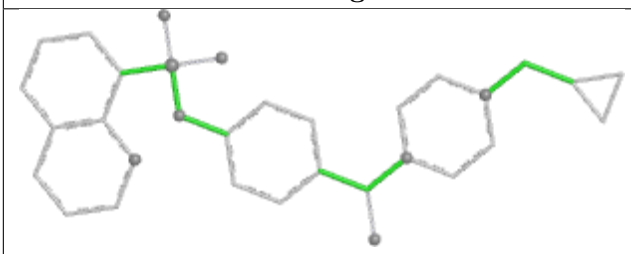
Ligand WV2 E 603



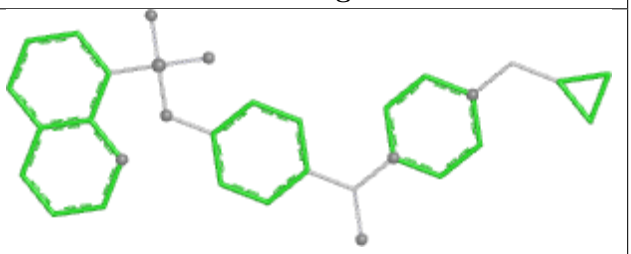
Bond lengths



Bond angles

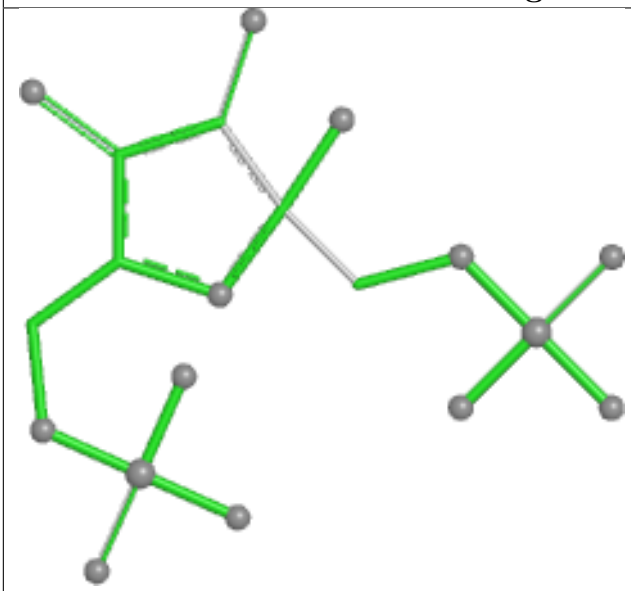


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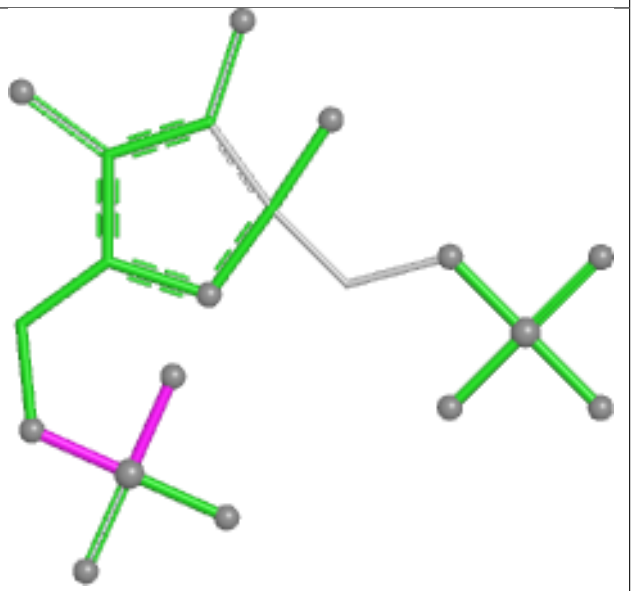


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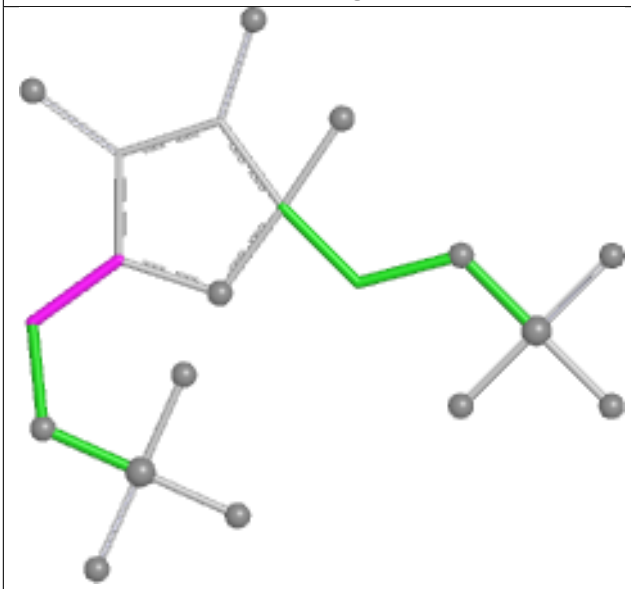
Ligand FBP B 601



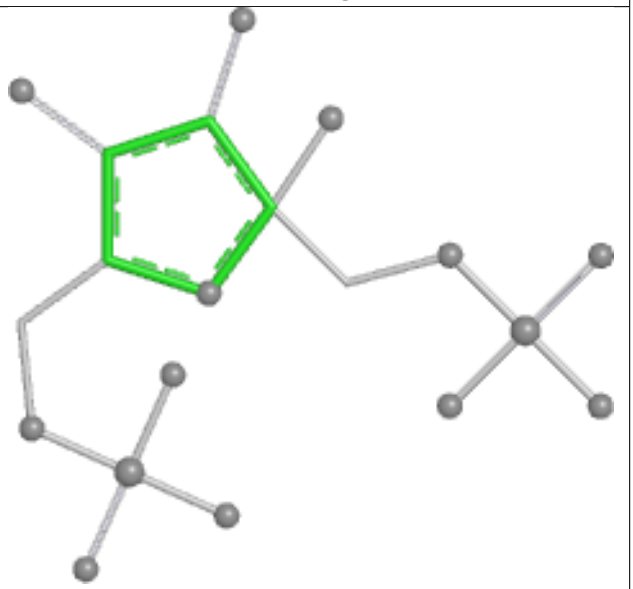
Bond lengths



Bond angles

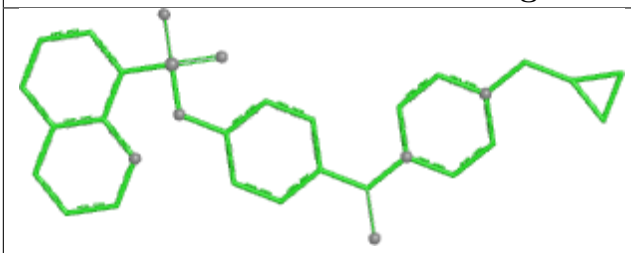


Torsions

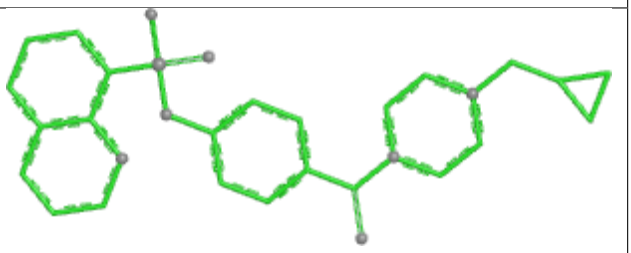


Rings

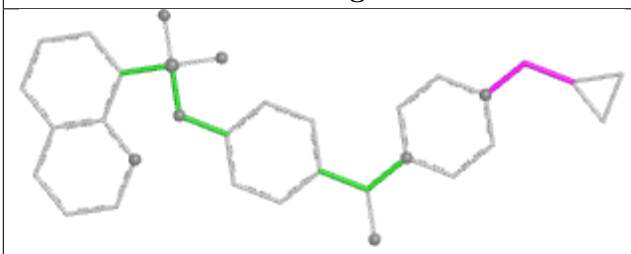
Ligand WV2 A 603



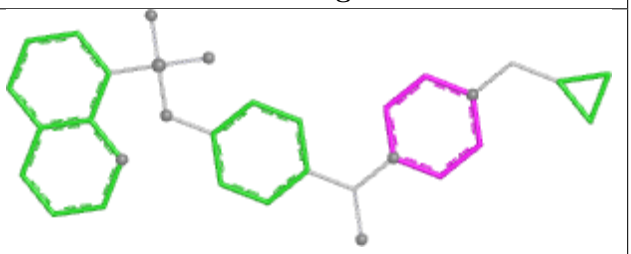
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	418/447 (93%)	1.33	97 (23%) 2 2	23, 50, 76, 92	13 (3%)
1	B	436/447 (97%)	1.84	176 (40%) 0 0	21, 52, 83, 103	8 (1%)
1	C	424/447 (94%)	0.26	22 (5%) 33 38	18, 33, 55, 93	7 (1%)
1	D	425/447 (95%)	0.08	13 (3%) 51 58	13, 29, 54, 87	8 (1%)
1	E	420/447 (93%)	0.99	61 (14%) 6 6	23, 46, 74, 85	13 (3%)
1	F	432/447 (96%)	0.56	40 (9%) 14 16	18, 37, 64, 78	8 (1%)
1	G	422/447 (94%)	0.10	17 (4%) 42 49	14, 31, 48, 73	9 (2%)
1	H	425/447 (95%)	-0.15	14 (3%) 49 55	12, 25, 47, 73	8 (1%)
All	All	3402/3576 (95%)	0.63	440 (12%) 7 9	12, 37, 71, 103	74 (2%)

The worst 5 of 440 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	273	GLY	6.9
1	B	513	LEU	6.6
1	C	273	GLY	6.4
1	B	115	LEU	5.8
1	A	234	GLY	5.8

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)

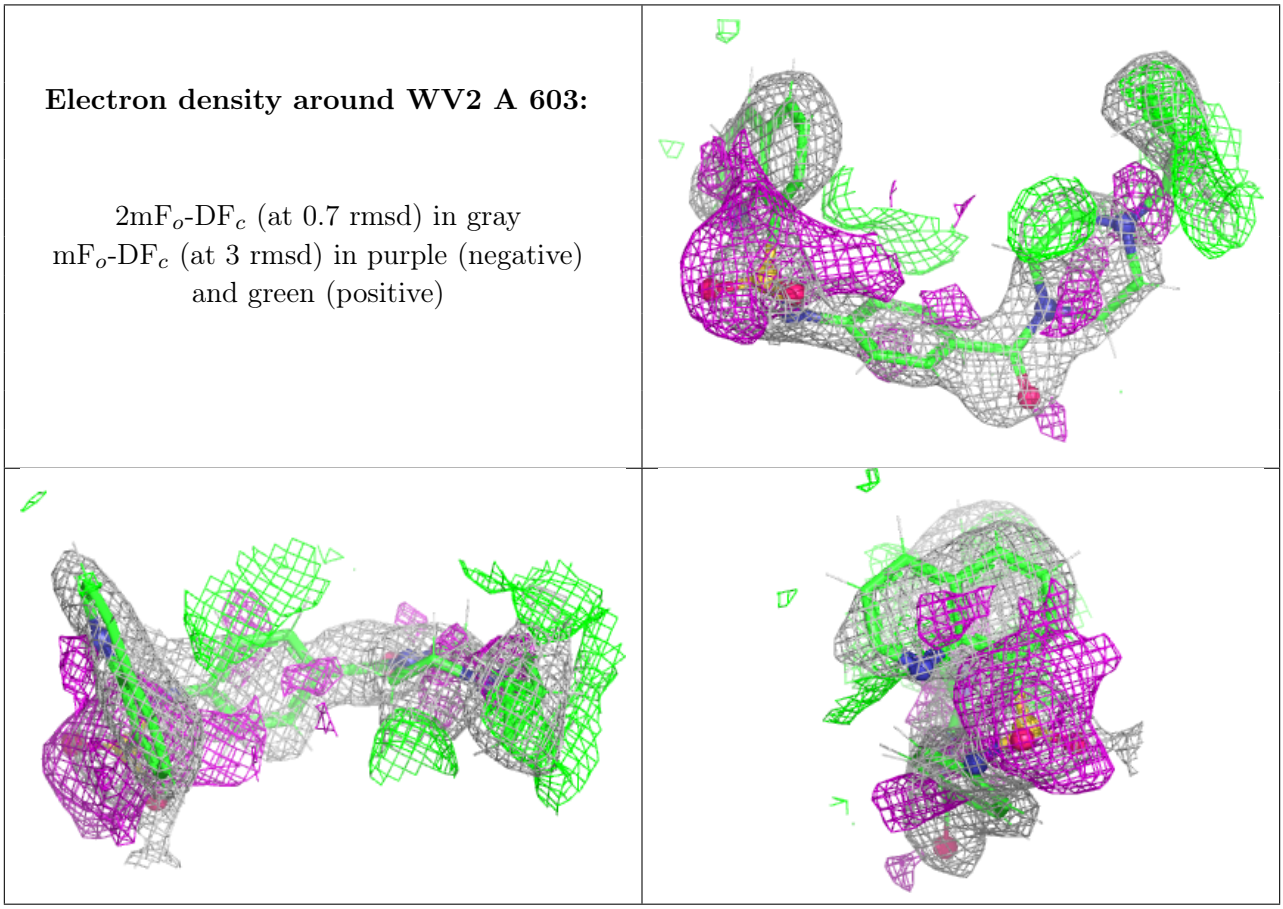
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A	602	6/6	0.75	0.21	101,102,102,102	0
3	OXL	H	602	6/6	0.75	0.17	39,40,42,43	0
4	WV2	A	603	32/32	0.75	0.23	61,62,63,63	26
4	WV2	E	603	32/32	0.79	0.20	54,55,57,57	26
5	MG	E	604	1/1	0.79	0.11	78,78,78,78	0
3	OXL	E	602	6/6	0.81	0.16	68,68,69,69	0
3	OXL	B	602	6/6	0.82	0.17	77,77,79,79	0
3	OXL	C	602	6/6	0.83	0.15	60,60,61,61	0
3	OXL	G	602	6/6	0.83	0.13	49,49,51,51	0
4	WV2	H	603	32/32	0.84	0.18	46,51,56,56	26
5	MG	A	604	1/1	0.84	0.16	102,102,102,102	0
3	OXL	F	602	6/6	0.84	0.14	54,55,56,56	0
6	K	A	605	1/1	0.87	0.26	79,79,79,79	0
6	K	E	605	1/1	0.87	0.24	75,75,75,75	0
3	OXL	D	602	6/6	0.88	0.12	53,53,54,54	0
6	K	B	604	1/1	0.91	0.15	88,88,88,88	0
2	FBP	B	601	20/20	0.91	0.11	48,49,52,52	0
4	WV2	D	603	32/32	0.92	0.12	36,39,42,42	26
2	FBP	A	601	20/20	0.92	0.09	45,46,48,49	0
6	K	F	604	1/1	0.93	0.14	69,69,69,69	0
2	FBP	E	601	20/20	0.95	0.07	41,41,43,43	0
5	MG	H	604	1/1	0.95	0.10	42,42,42,42	0
5	MG	B	603	1/1	0.95	0.07	62,62,62,62	0
6	K	C	604	1/1	0.96	0.17	49,49,49,49	0
5	MG	F	603	1/1	0.96	0.09	56,56,56,56	0
2	FBP	F	601	20/20	0.96	0.07	36,41,45,45	0
5	MG	D	604	1/1	0.98	0.07	51,51,51,51	0
5	MG	G	603	1/1	0.98	0.04	49,49,49,49	0
6	K	G	604	1/1	0.98	0.12	46,46,46,46	0
2	FBP	H	601	20/20	0.99	0.04	17,19,21,21	0
2	FBP	C	601	20/20	0.99	0.04	21,22,25,26	0
6	K	D	605	1/1	0.99	0.08	41,41,41,41	0
2	FBP	D	601	20/20	0.99	0.04	21,22,24,25	0
5	MG	C	603	1/1	0.99	0.03	56,56,56,56	0
2	FBP	G	601	20/20	0.99	0.04	21,22,23,23	0
6	K	H	605	1/1	0.99	0.08	41,41,41,41	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.

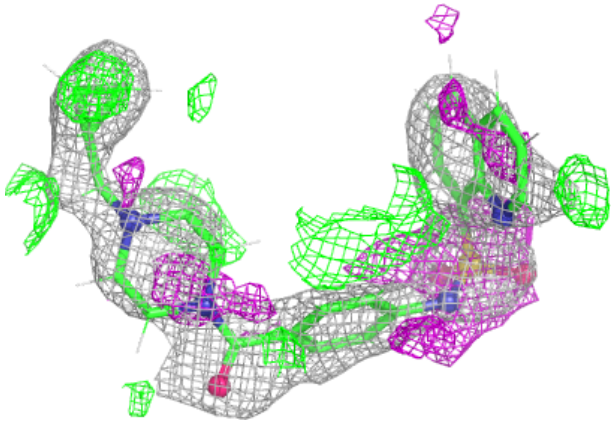
Electron density around WV2 A 603:

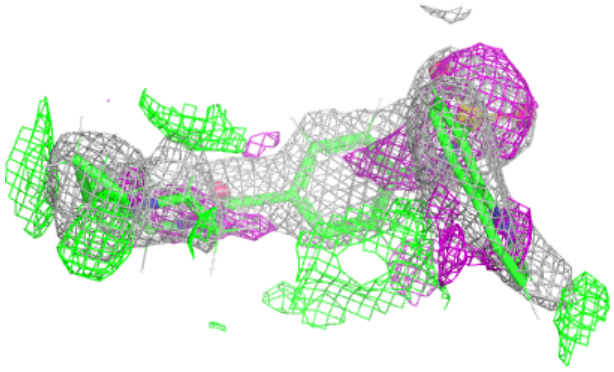
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

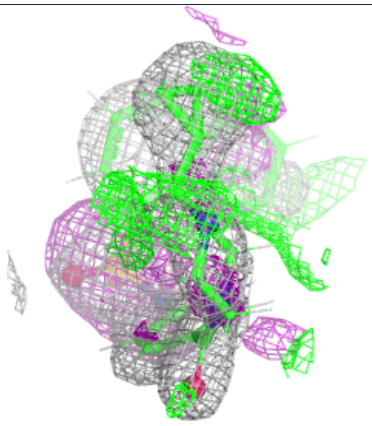


Electron density around WV2 E 603:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

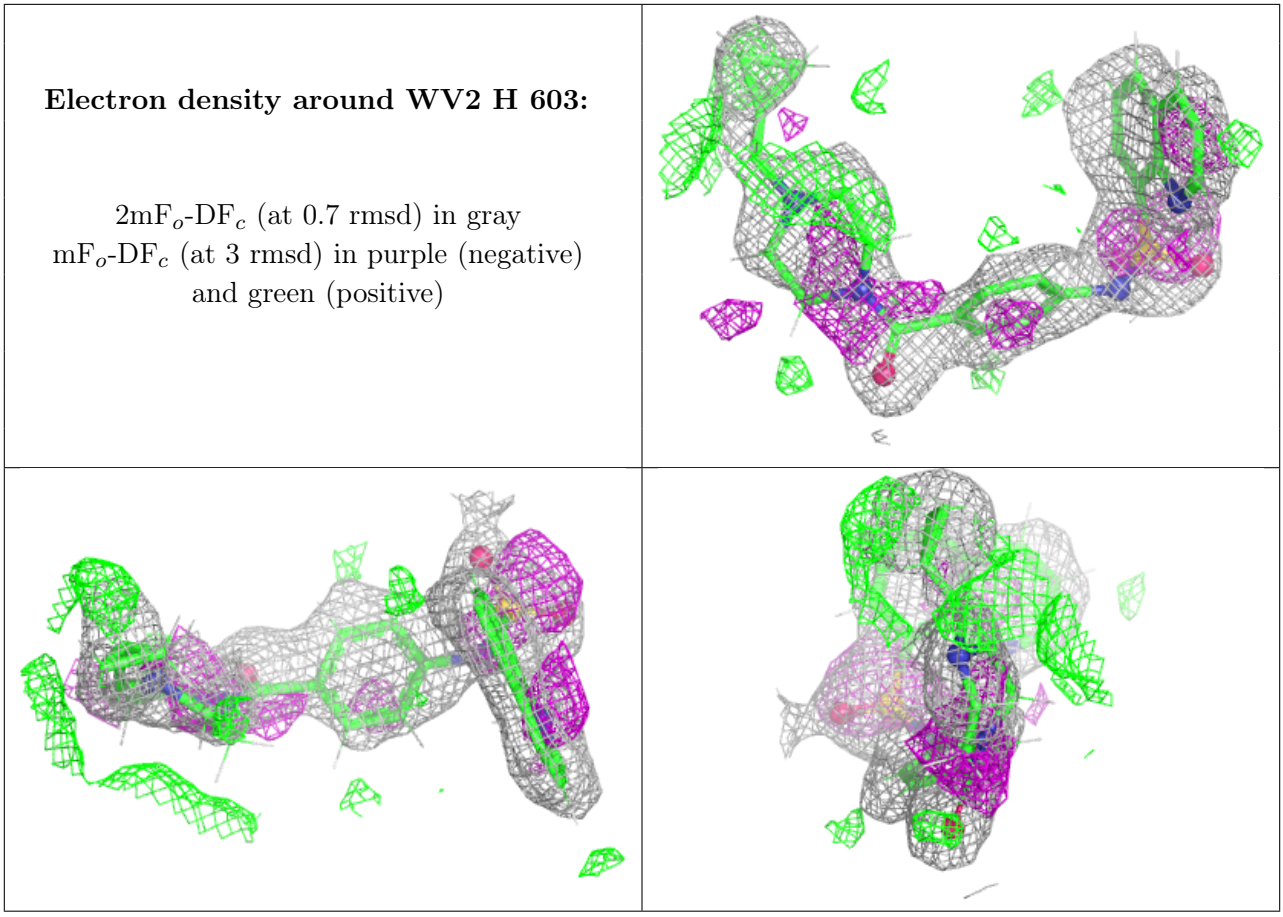






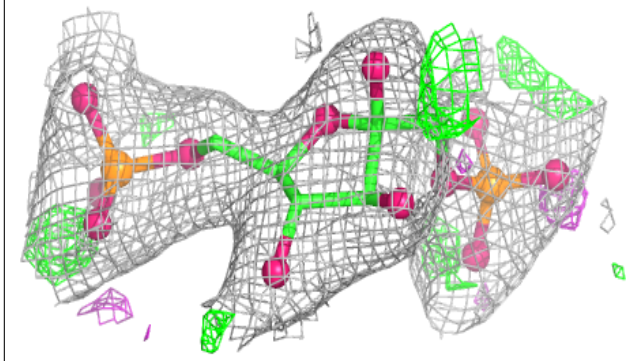
Electron density around WV2 H 603:

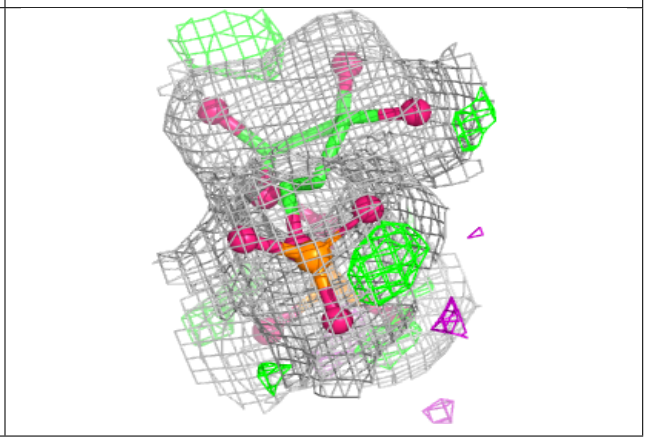
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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FBP B 601:

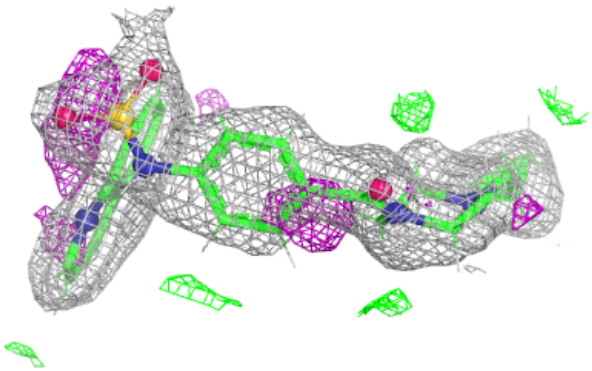
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

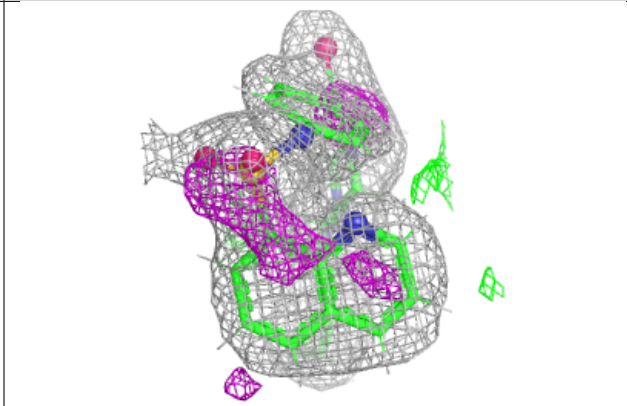




Electron density around WV2 D 603:

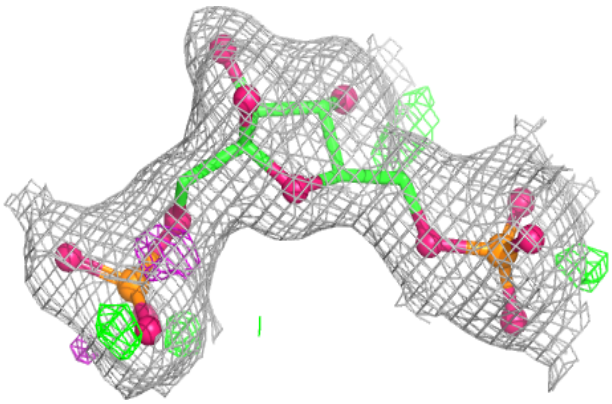
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

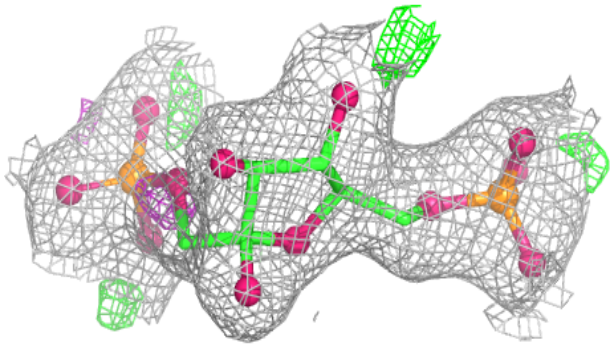


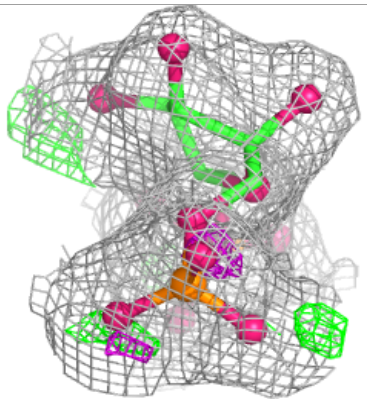


Electron density around FBP A 601:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

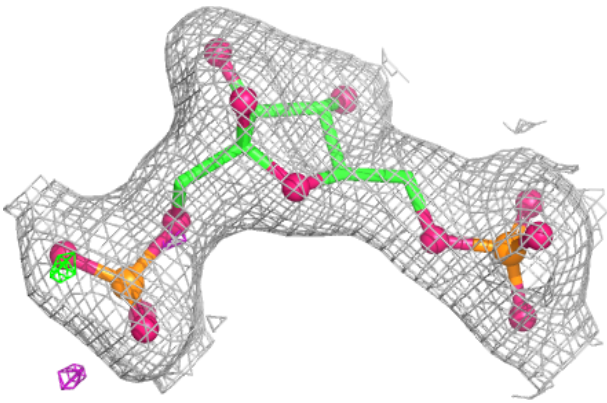


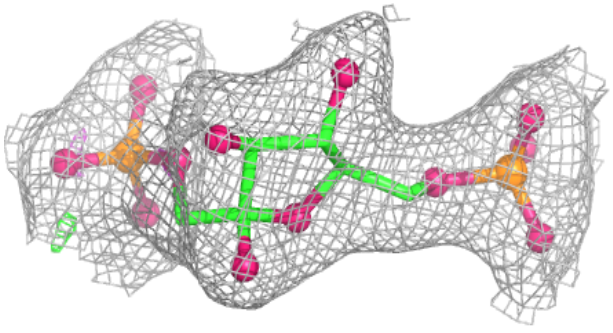


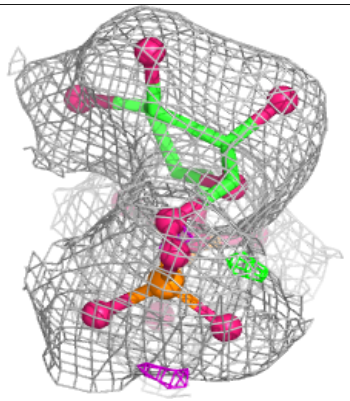


Electron density around FBP E 601:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

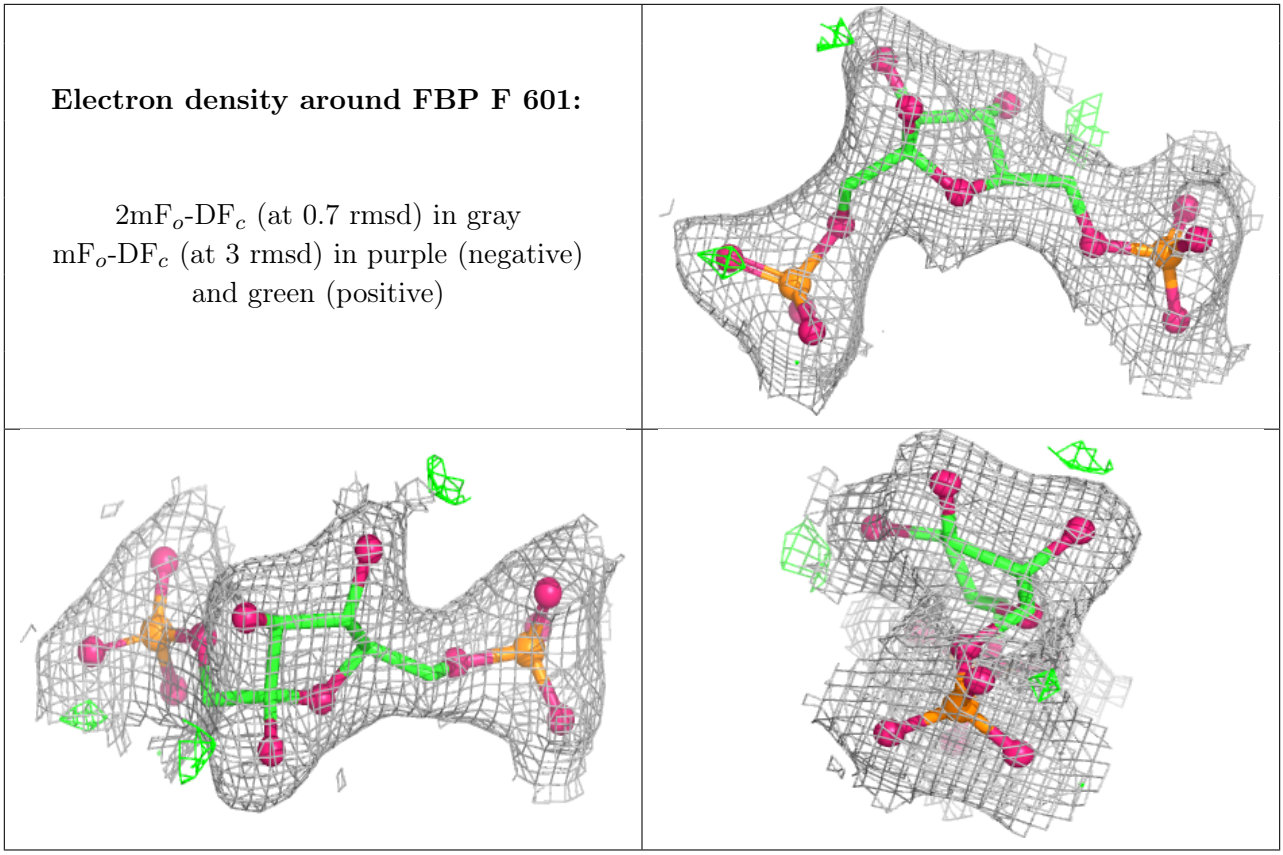






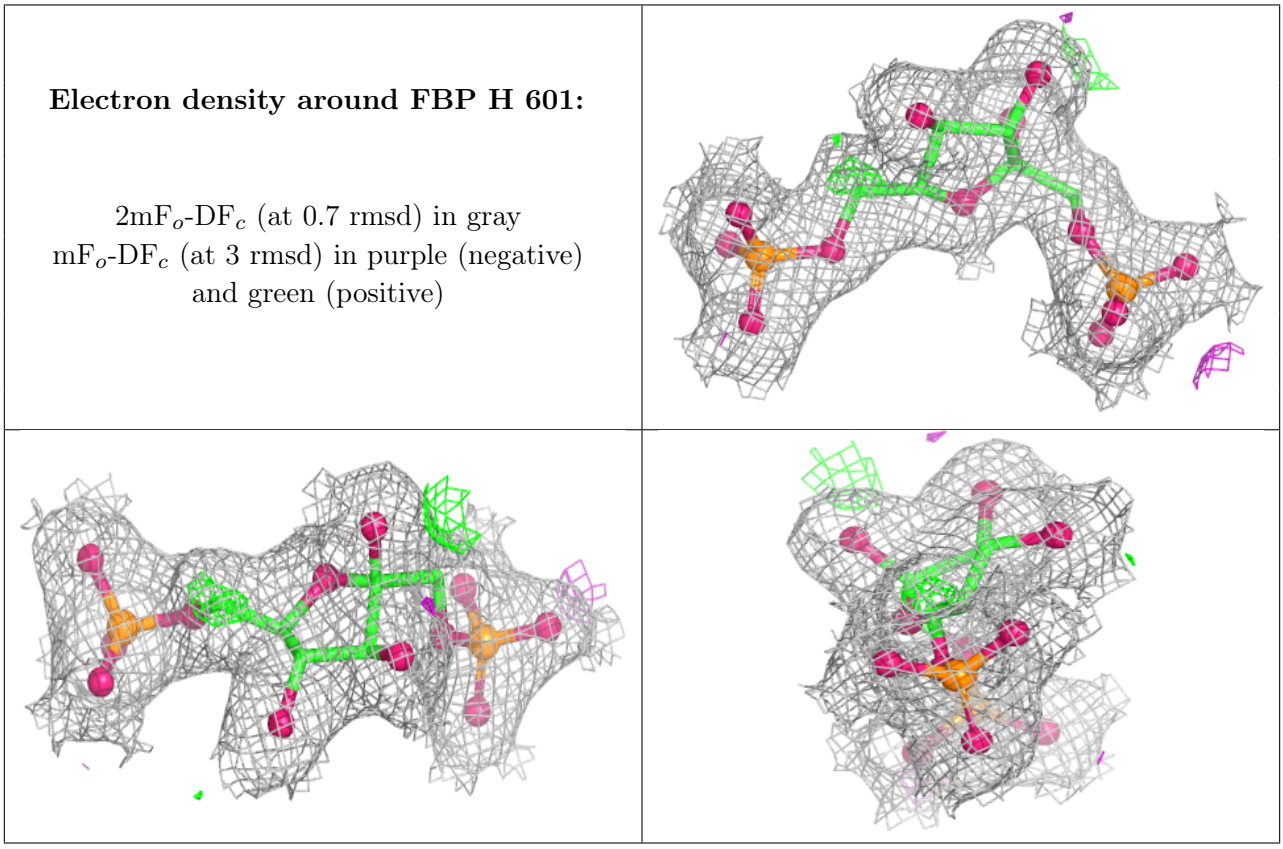
Electron density around FBP F 601:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



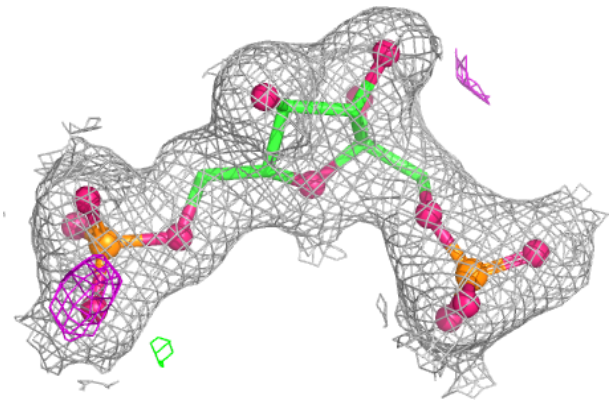
Electron density around FBP H 601:

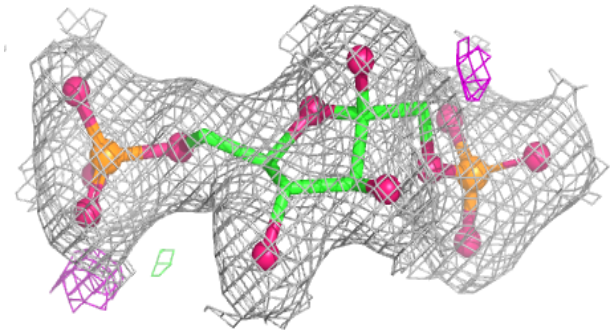
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

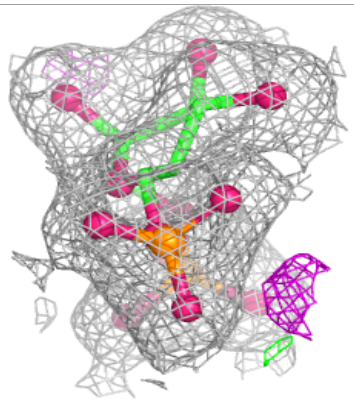


Electron density around FBP C 601:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

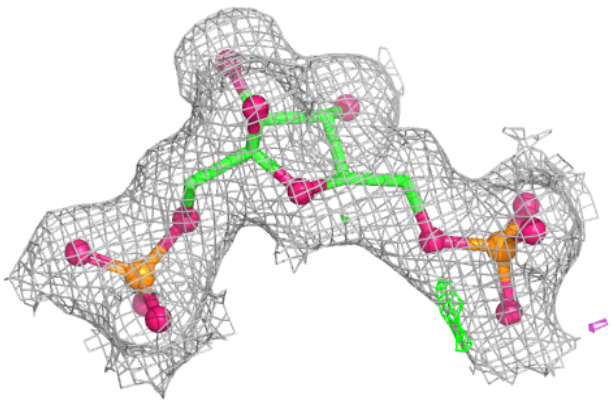


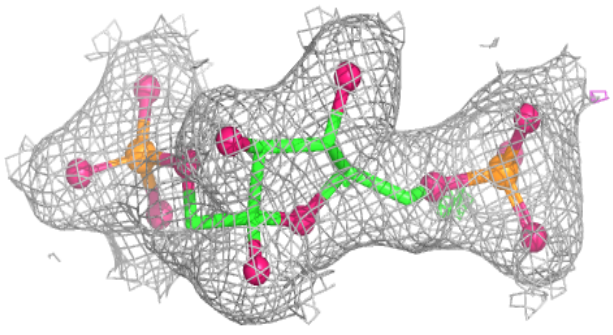


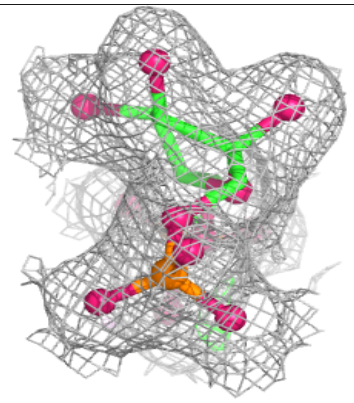


Electron density around FBP D 601:

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

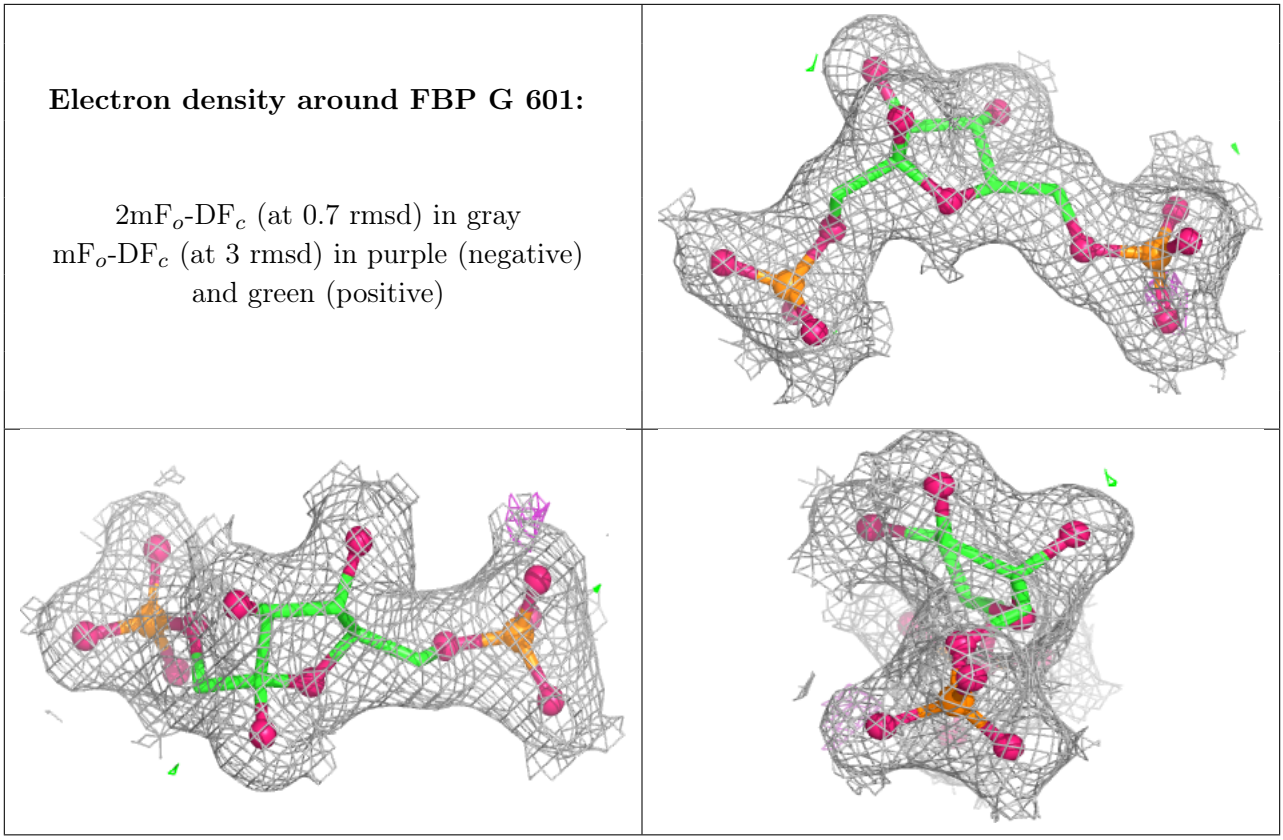






Electron density around FBP G 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.