wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2026 – 01:06 PM EDT

PDB ID	:	14CM / pdb_000014cm
Title	:	Structure of liver pyruvate kinase in complex with allosteric site fragment S3
Authors	:	Lulla, A.; Rodriguez Rivero, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2026-04-28
Resolution	:	1.99 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:

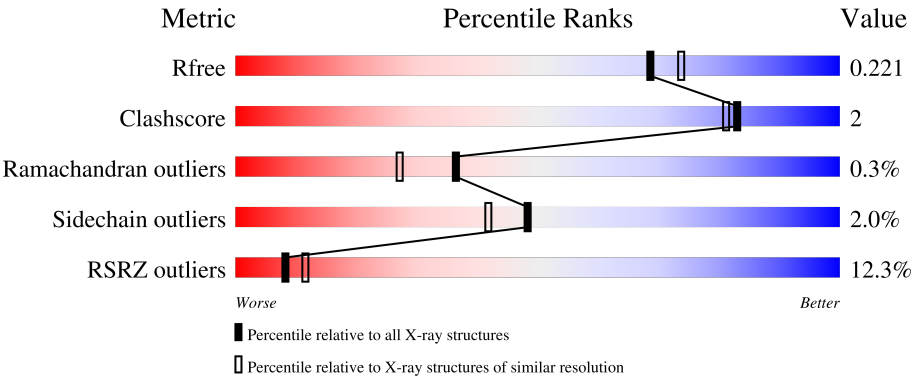
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.99 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.



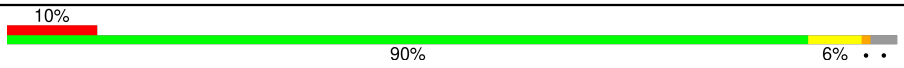
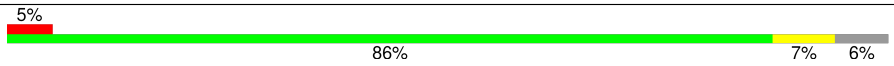
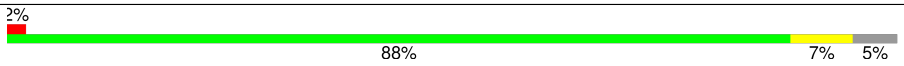
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	15% 85% 8% 6%
1	B	447	36% 89% 7%
1	C	447	6% 89% 5% 5%
1	D	447	2% 88% 6% 5%
1	E	447	17% 86% 6% 6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	602	-	X	-	-
3	OXL	B	602	-	X	-	-
3	OXL	C	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 28463 atoms, of which 120 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	11	0
			3238	2033	583	602	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	6	0
			3257	2049	584	605	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	11	0
			3253	2046	585	603	19			
1	F	432	Total	C	N	O	S	0	8	0
			3327	2094	597	616	20			
1	G	421	Total	C	N	O	S	0	5	0
			3225	2027	581	598	19			
1	H	425	Total	C	N	O	S	0	9	0
			3277	2057	597	604	19			

There are 48 discrepancies between the modelled and reference sequences:

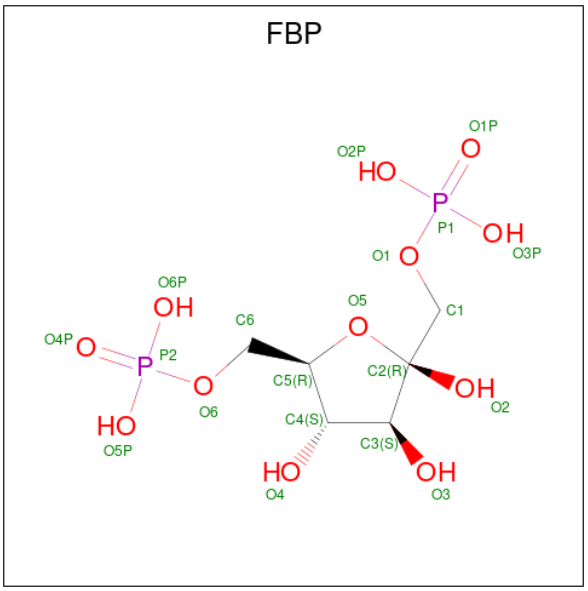
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30613
A	0	SER	-	expression tag	UNP P30613
A	12	ASP	SER	conflict	UNP P30613
A	130	GLY	-	linker	UNP P30613
A	131	SER	-	linker	UNP P30613
A	132	GLY	-	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
B	0	SER	-	expression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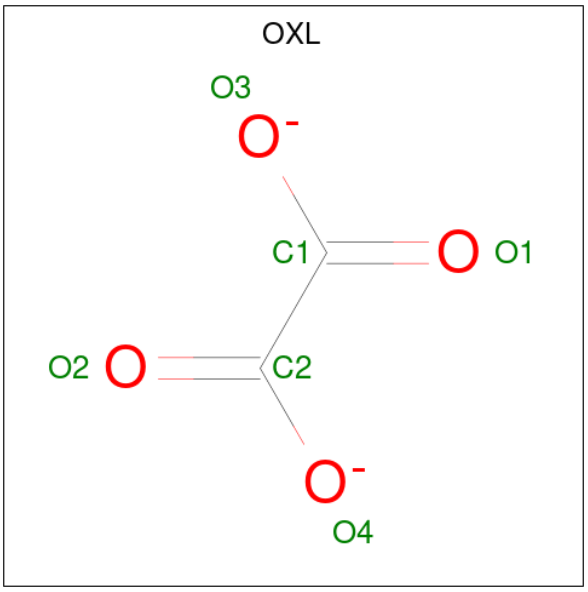
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	130	GLY	-	linker	UNP P30613
C	131	SER	-	linker	UNP P30613
C	132	GLY	-	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	12	ASP	SER	conflict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



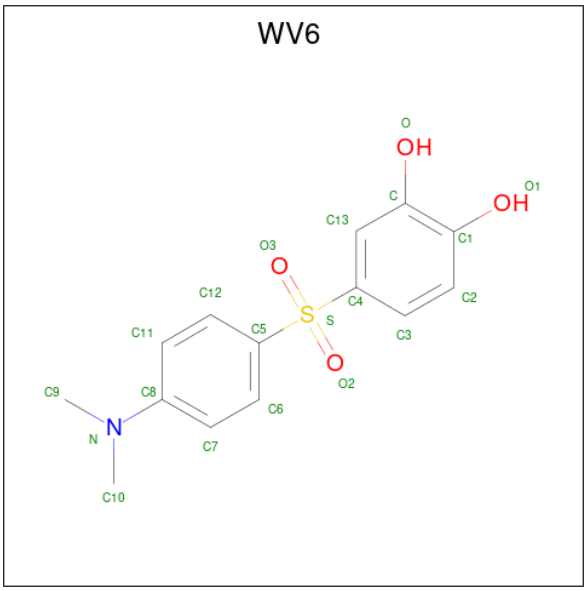
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
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 4-[4-(dimethylamino)benzene-1-sulfonyl]benzene-1,2-diol (CCD ID: WV6) (formula: $C_{14}H_{15}NO_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	30	1
			70	28	30	2	8	2		
4	B	1	Total	C	H	N	O	S	30	1
			70	28	30	2	8	2		
4	E	1	Total	C	H	N	O	S	30	1
			70	28	30	2	8	2		
4	F	1	Total	C	H	N	O	S	30	1
			70	28	30	2	8	2		

- 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	151	Total O 151 151	0	0
7	B	122	Total O 122 122	0	0
7	C	262	Total O 262 262	0	0
7	D	294	Total O 294 294	0	0
7	E	137	Total O 137 137	0	0
7	F	204	Total O 204 204	0	0
7	G	261	Total O 261 261	0	0
7	H	340	Total O 340 340	0	0

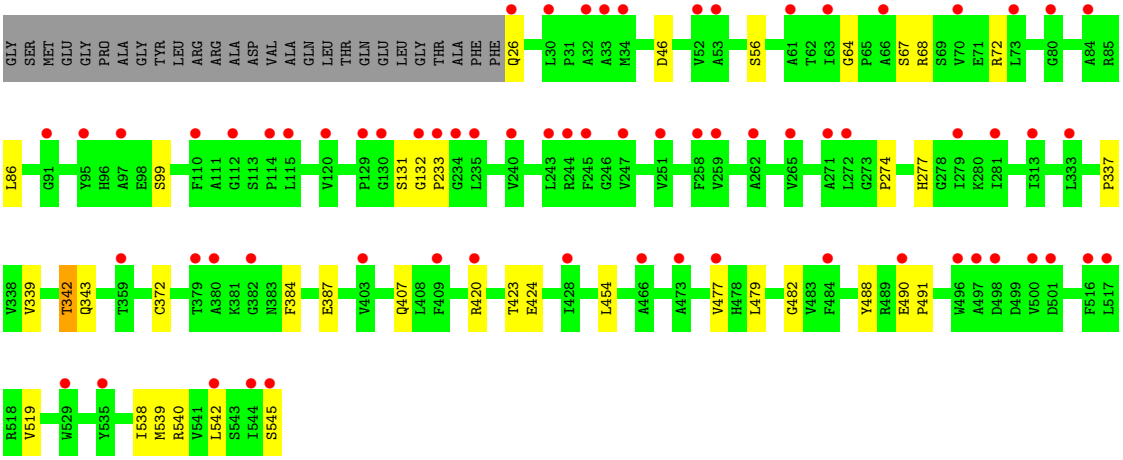
3 Residue-property plots (i)

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

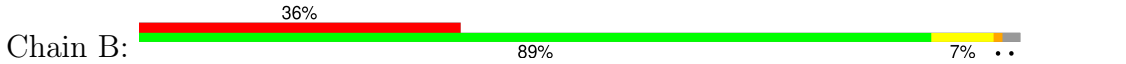
Chain A:

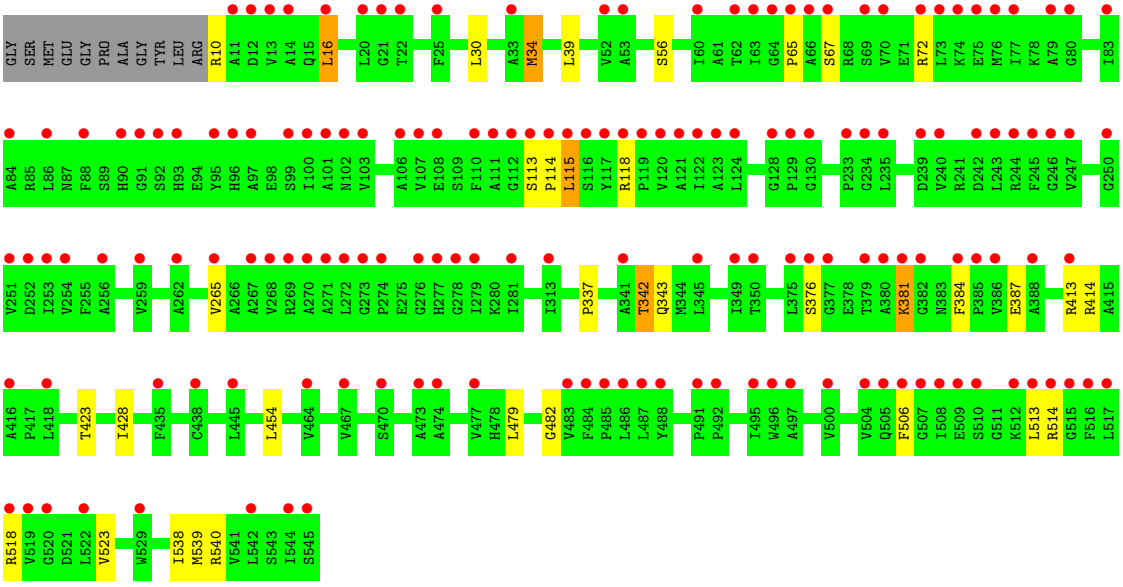




• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

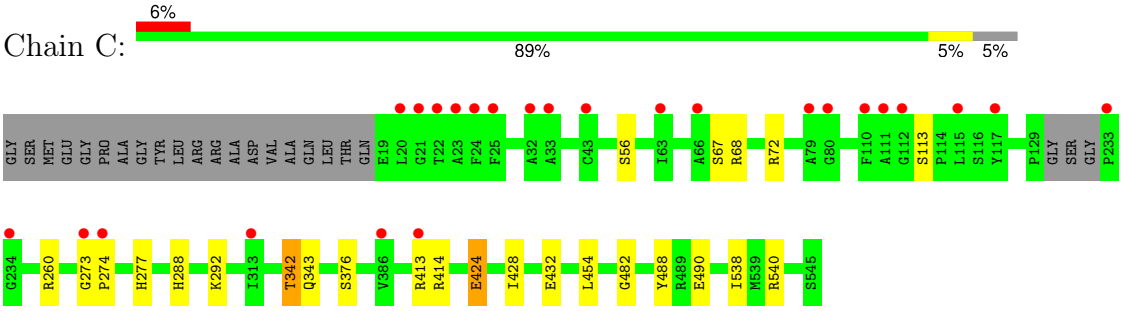
Chain B:





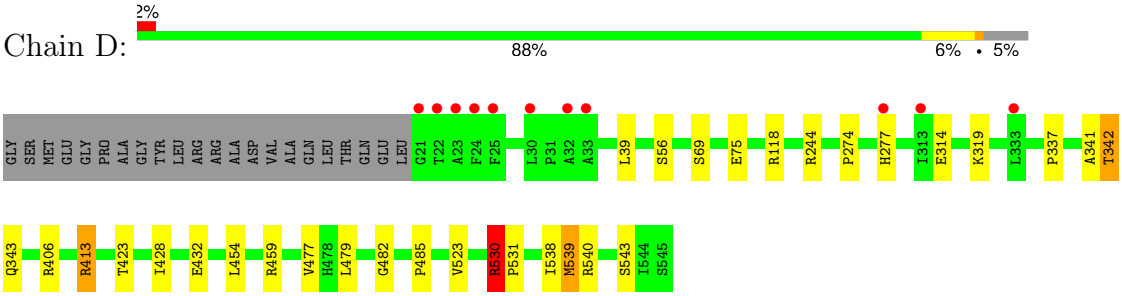
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain C:



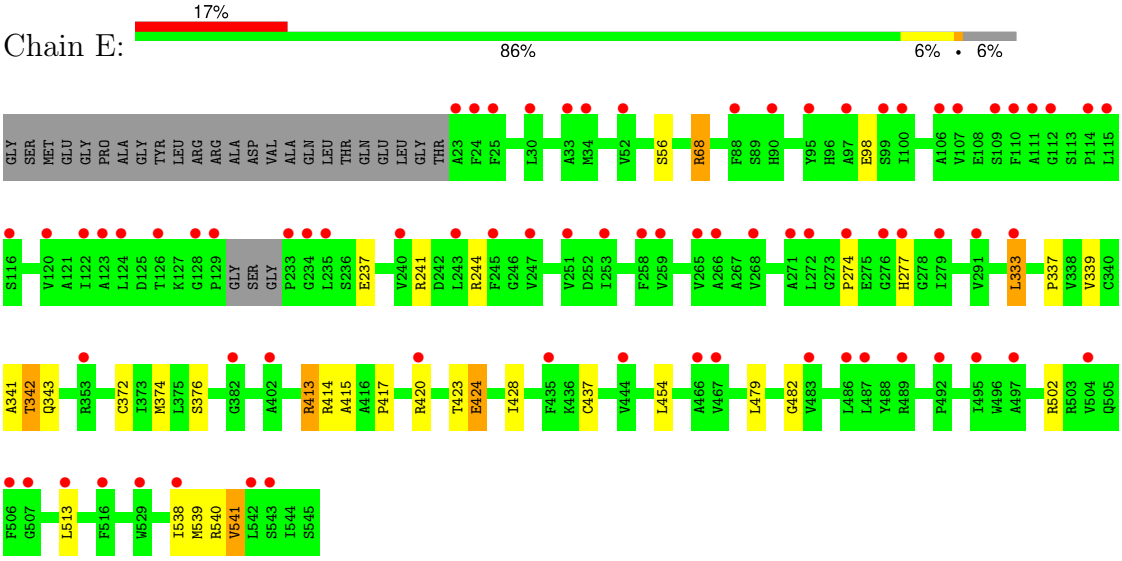
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain D:



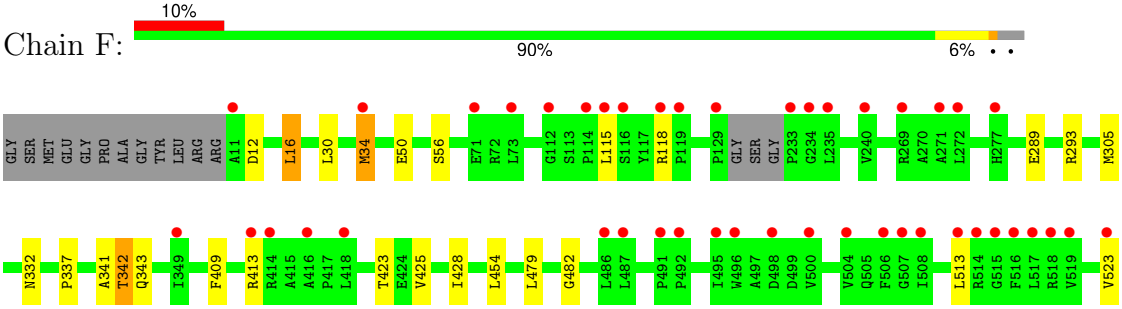
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

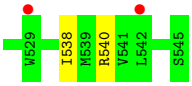
Chain E:



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

Chain F:

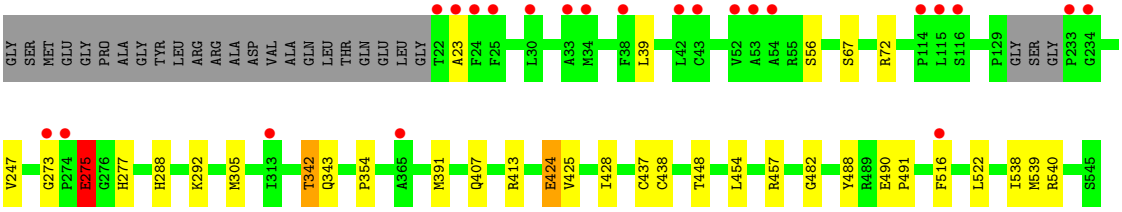




• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain G:

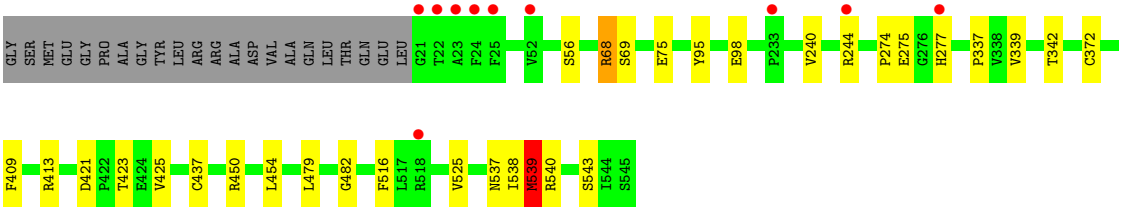




• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

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	208.50Å 113.30Å 188.78Å 90.00° 91.56° 90.00°	Depositor
Resolution (Å)	188.71 – 1.99 188.71 – 1.99	Depositor EDS
% Data completeness (in resolution range)	66.7 (188.71-1.99) 66.7 (188.71-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.204 , 0.232 0.193 , 0.221	Depositor DCC
R_{free} test set	9908 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28463	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 49.00 % 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 7.9363e-05. 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: MG, FBP, WV6, OXL, 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	0.68	0/3324	1.01	1/4494 (0.0%)
1	B	0.71	2/3429 (0.1%)	1.01	0/4636
1	C	0.79	1/3329 (0.0%)	1.02	0/4500
1	D	0.81	2/3341 (0.1%)	1.04	3/4517 (0.1%)
1	E	0.67	1/3341 (0.0%)	1.00	1/4516 (0.0%)
1	F	0.74	1/3405 (0.0%)	1.03	4/4603 (0.1%)
1	G	0.84	3/3294 (0.1%)	1.04	2/4452 (0.0%)
1	H	0.83	1/3357 (0.0%)	1.04	1/4537 (0.0%)
All	All	0.76	11/26820 (0.0%)	1.02	12/36255 (0.0%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	539	MET	SD-CE	-7.50	1.60	1.79
1	G	23	ALA	CA-C	6.96	1.62	1.52
1	C	376	SER	CA-C	6.79	1.55	1.52
1	G	491	PRO	CA-C	6.68	1.55	1.51
1	D	459	ARG	CA-CB	5.75	1.56	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	541	VAL	N-CA-CB	5.95	118.17	111.21
1	G	275	GLU	CB-CG-CD	5.62	122.16	112.60
1	G	516	PHE	CA-CB-CG	5.60	119.40	113.80
1	F	341	ALA	CA-C-N	5.60	132.23	121.54
1	F	341	ALA	C-N-CA	5.60	132.23	121.54

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	3313	19	0
1	B	3350	0	3417	17	0
1	C	3257	0	3316	16	0
1	D	3261	0	3321	17	0
1	E	3253	0	3317	20	0
1	F	3327	0	3399	15	0
1	G	3225	0	3278	22	0
1	H	3277	0	3342	20	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	40	30	0	1	0
4	B	40	30	0	2	0
4	E	40	30	0	2	0
4	F	40	30	0	1	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	151	0	0	1	0
7	B	122	0	0	0	0
7	C	262	0	0	1	0
7	D	294	0	0	3	0
7	E	137	0	0	0	0
7	F	204	0	0	1	0
7	G	261	0	0	0	0
7	H	340	0	0	1	0
All	All	28343	120	26783	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 128 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ILE:HG12	1:B:540:ARG:HG2	1.73	0.71
1:A:420[B]:ARG:HG3	1:B:16:LEU:HD11	1.72	0.70
1:E:420[B]:ARG:HG3	1:F:16:LEU:HD11	1.73	0.70
1:G:540:ARG:HG2	1:H:538:ILE:HG12	1.72	0.69
4:F:603[A]:WV6:O2	7:F:701:HOH:O	2.10	0.69

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/447 (96%)	424 (99%)	3 (1%)	2 (0%)	24	14
1	B	442/447 (99%)	436 (99%)	5 (1%)	1 (0%)	43	35
1	C	426/447 (95%)	421 (99%)	4 (1%)	1 (0%)	43	35
1	D	431/447 (96%)	427 (99%)	3 (1%)	1 (0%)	43	35
1	E	427/447 (96%)	422 (99%)	4 (1%)	1 (0%)	43	35
1	F	436/447 (98%)	431 (99%)	4 (1%)	1 (0%)	43	35
1	G	422/447 (94%)	416 (99%)	5 (1%)	1 (0%)	43	35
1	H	432/447 (97%)	428 (99%)	3 (1%)	1 (0%)	43	35
All	All	3445/3576 (96%)	3405 (99%)	31 (1%)	9 (0%)	36	27

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	SER
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	344/352 (98%)	337 (98%)	7 (2%)	48	42
1	B	353/352 (100%)	339 (96%)	14 (4%)	28	17
1	C	343/352 (97%)	338 (98%)	5 (2%)	57	52
1	D	344/352 (98%)	335 (97%)	9 (3%)	40	32
1	E	345/352 (98%)	335 (97%)	10 (3%)	37	28
1	F	351/352 (100%)	347 (99%)	4 (1%)	65	61
1	G	339/352 (96%)	335 (99%)	4 (1%)	63	58
1	H	345/352 (98%)	340 (99%)	5 (1%)	59	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2764/2816 (98%)	2706 (98%)	58 (2%)	48 40

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

Mol	Chain	Res	Type
1	D	244[A]	ARG
1	H	275	GLU
1	E	68	ARG
1	H	69	SER
1	G	275	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	27	GLN
1	H	90	HIS
1	D	27	GLN
1	E	27	GLN
1	F	27	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	$\#\|Z\| > 2$
3	OXL	A	602	5	5,5,5	1.98	2 (40%)	6,6,6	2.03	3 (50%)
3	OXL	B	602	5	5,5,5	2.54	2 (40%)	6,6,6	1.45	1 (16%)
4	WV6	B	603[B]	-	21,21,21	0.59	1 (4%)	30,31,31	0.45	0
2	FBP	F	601	-	18,20,20	0.50	0	21,32,32	0.64	0
4	WV6	B	603[A]	-	21,21,21	0.51	0	30,31,31	0.41	0
2	FBP	E	601	-	18,20,20	0.40	0	21,32,32	0.59	0
2	FBP	G	601	-	18,20,20	0.45	0	21,32,32	0.62	0
2	FBP	D	601	-	18,20,20	0.53	0	21,32,32	0.99	1 (4%)
3	OXL	C	602	5	5,5,5	1.88	2 (40%)	6,6,6	2.35	3 (50%)
4	WV6	A	603[A]	-	21,21,21	0.50	0	30,31,31	0.48	0
4	WV6	A	603[B]	-	21,21,21	0.51	0	30,31,31	0.48	0
2	FBP	C	601	-	18,20,20	0.59	0	21,32,32	0.50	0
3	OXL	D	602	5	5,5,5	2.11	2 (40%)	6,6,6	2.74	4 (66%)
3	OXL	F	602	5	5,5,5	1.93	2 (40%)	6,6,6	2.40	3 (50%)
3	OXL	G	602	5	5,5,5	2.42	3 (60%)	6,6,6	1.10	1 (16%)
3	OXL	E	602	5	5,5,5	2.08	2 (40%)	6,6,6	2.06	2 (33%)
4	WV6	E	603[B]	-	21,21,21	0.46	0	30,31,31	0.41	0
4	WV6	E	603[A]	-	21,21,21	0.53	0	30,31,31	0.42	0
4	WV6	F	603[B]	-	21,21,21	0.57	0	30,31,31	0.47	0
4	WV6	F	603[A]	-	21,21,21	0.54	0	30,31,31	0.42	0
2	FBP	H	601	-	18,20,20	0.92	2 (11%)	21,32,32	0.81	1 (4%)
2	FBP	A	601	-	18,20,20	0.51	0	21,32,32	0.58	0
2	FBP	B	601	-	18,20,20	0.45	0	21,32,32	0.68	0
3	OXL	H	602	5	5,5,5	1.93	2 (40%)	6,6,6	1.32	1 (16%)

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	A	602	5	-	4/4/4/4	-
3	OXL	B	602	5	-	4/4/4/4	-
4	WV6	B	603[B]	-	-	0/16/16/16	0/2/2/2
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	WV6	B	603[A]	-	-	2/16/16/16	0/2/2/2
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	C	602	5	-	4/4/4/4	-
4	WV6	A	603[A]	-	-	1/16/16/16	0/2/2/2
4	WV6	A	603[B]	-	-	1/16/16/16	0/2/2/2
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	5	-	4/4/4/4	-
3	OXL	F	602	5	-	0/4/4/4	-
3	OXL	G	602	5	-	4/4/4/4	-
3	OXL	E	602	5	-	4/4/4/4	-
4	WV6	E	603[B]	-	-	2/16/16/16	0/2/2/2
4	WV6	E	603[A]	-	-	2/16/16/16	0/2/2/2
4	WV6	F	603[B]	-	-	0/16/16/16	0/2/2/2
4	WV6	F	603[A]	-	-	0/16/16/16	0/2/2/2
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	5	-	4/4/4/4	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXL	O2-C2	4.67	1.34	1.22
3	G	602	OXL	O2-C2	4.22	1.33	1.22
3	A	602	OXL	O2-C2	3.76	1.31	1.22
3	C	602	OXL	O2-C2	3.41	1.31	1.22
3	E	602	OXL	O2-C2	3.32	1.30	1.22

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	602	OXL	O4-C2-C1	4.45	121.47	112.83
3	F	602	OXL	O4-C2-C1	4.34	121.25	112.83
3	D	602	OXL	O3-C1-C2	4.18	120.94	112.83
3	D	602	OXL	O4-C2-C1	4.02	120.62	112.83
3	A	602	OXL	O4-C2-C1	3.83	120.26	112.83

There are no chirality outliers.

5 of 52 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

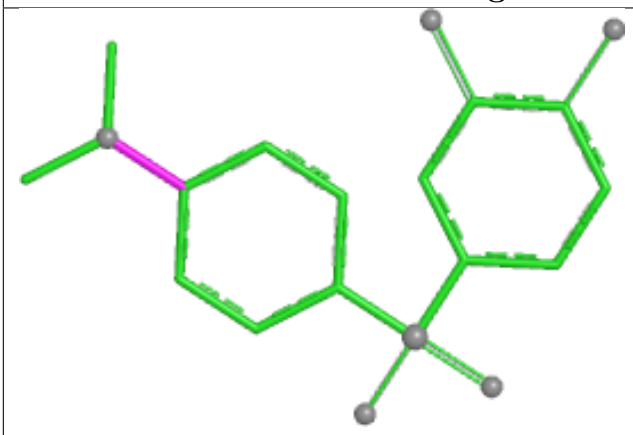
There are no ring outliers.

6 monomers are involved in 6 short contacts:

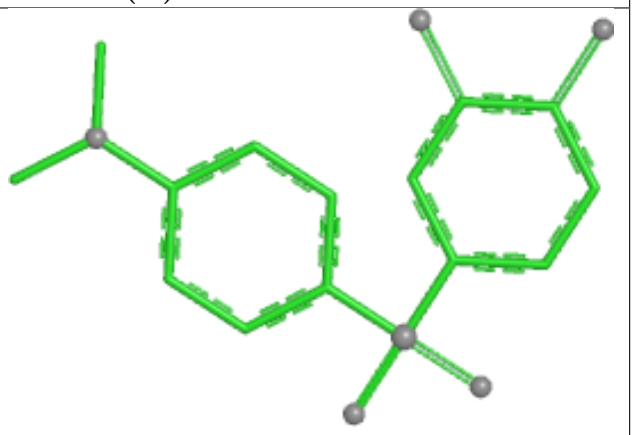
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603[B]	WV6	1	0
4	B	603[A]	WV6	1	0
4	A	603[A]	WV6	1	0
4	E	603[B]	WV6	1	0
4	E	603[A]	WV6	1	0
4	F	603[A]	WV6	1	0

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.

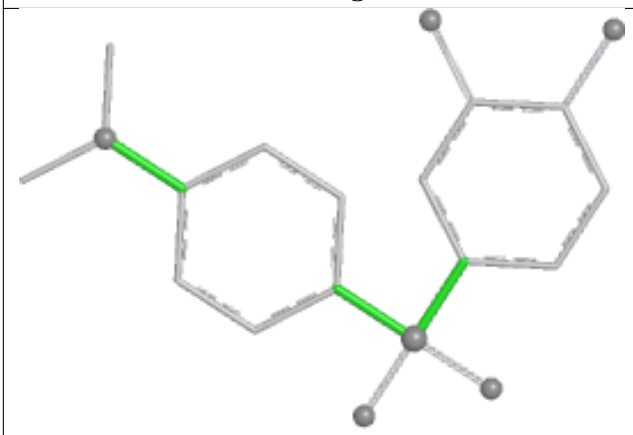
Ligand WV6 B 603 (B)



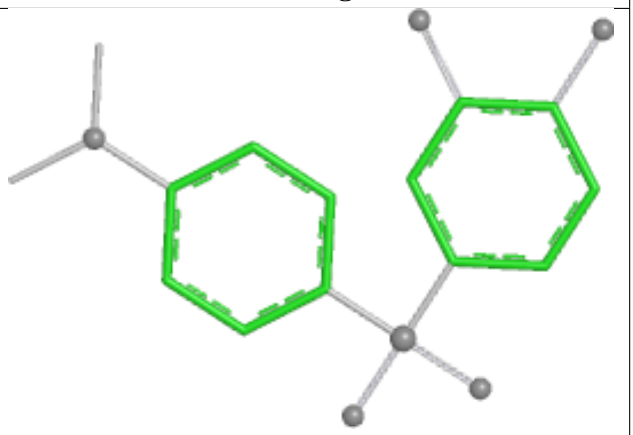
Bond lengths



Bond angles

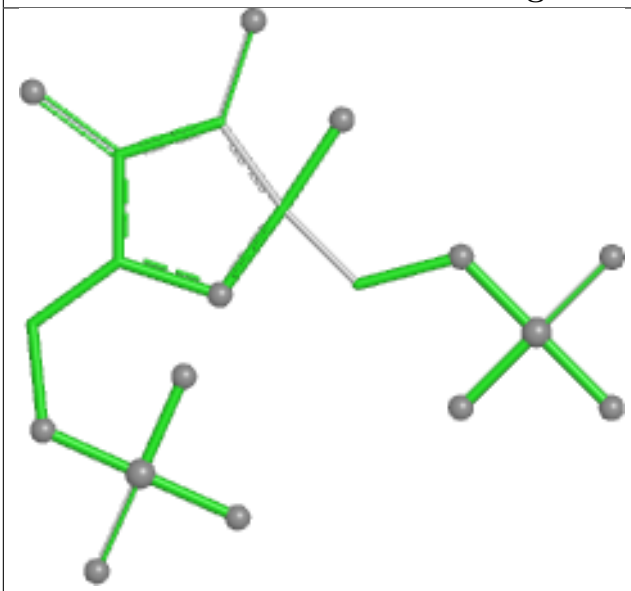


Torsions

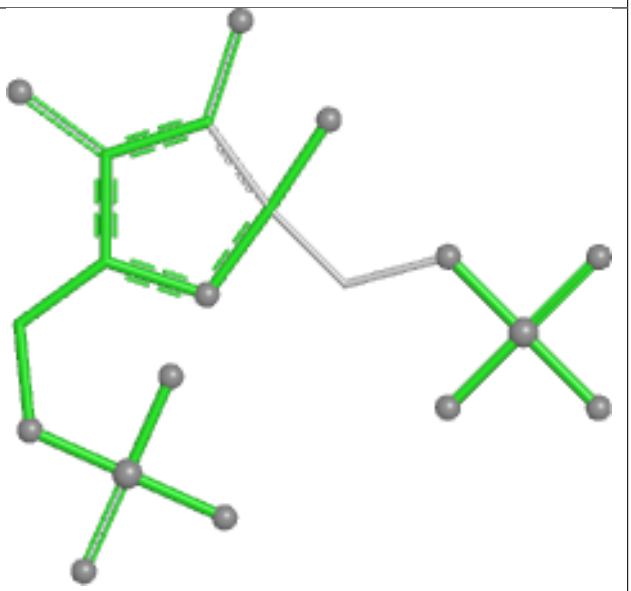


Rings

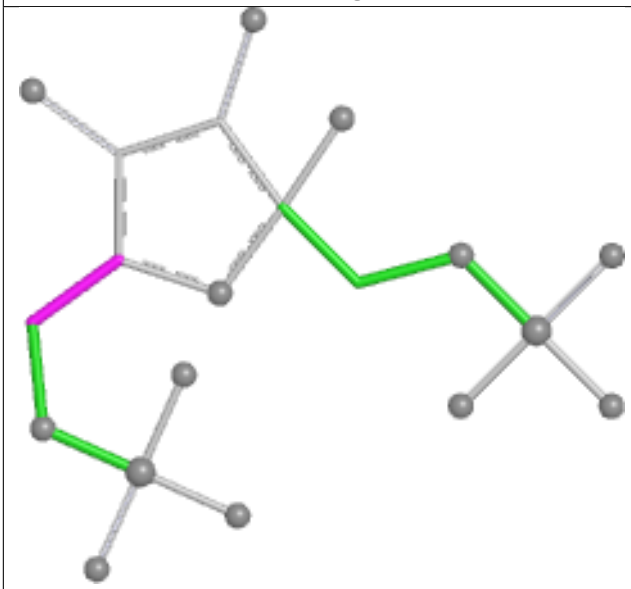
Ligand FBP F 601



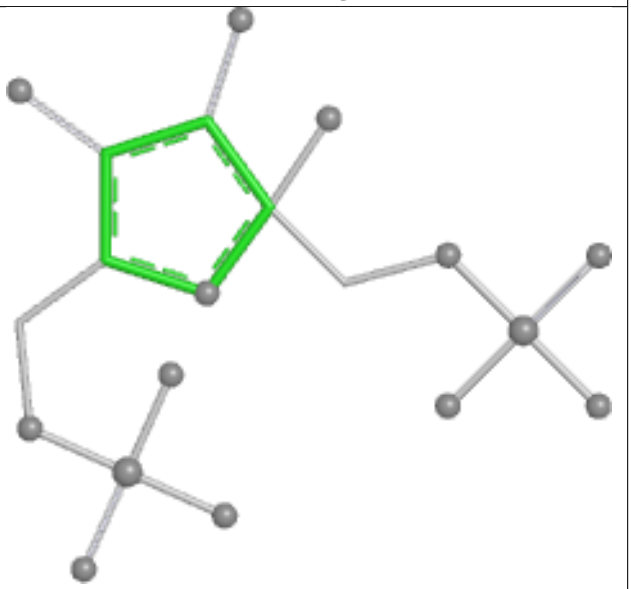
Bond lengths



Bond angles

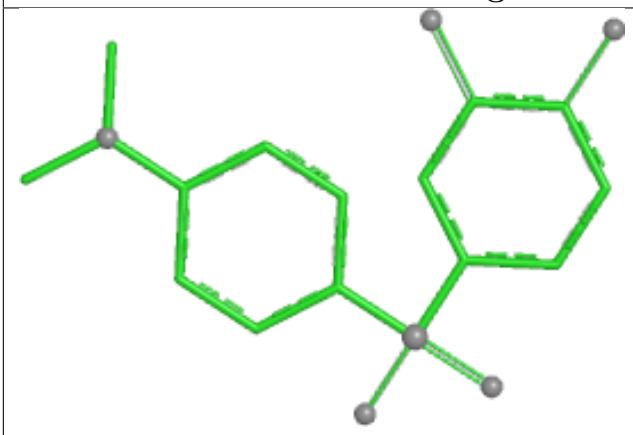


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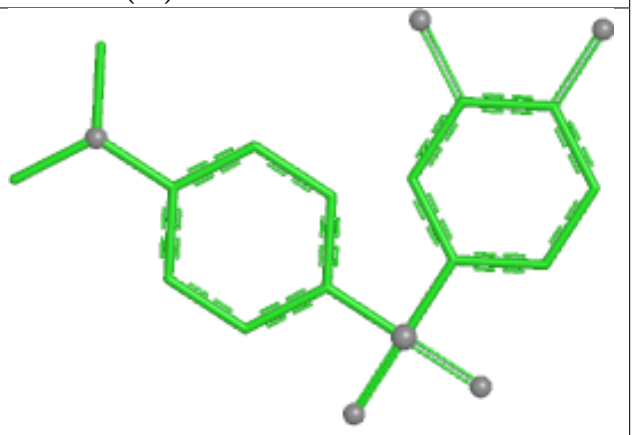


Rings

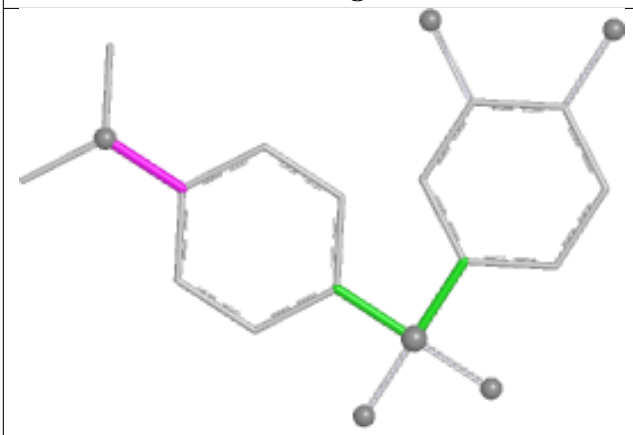
Ligand WV6 B 603 (A)



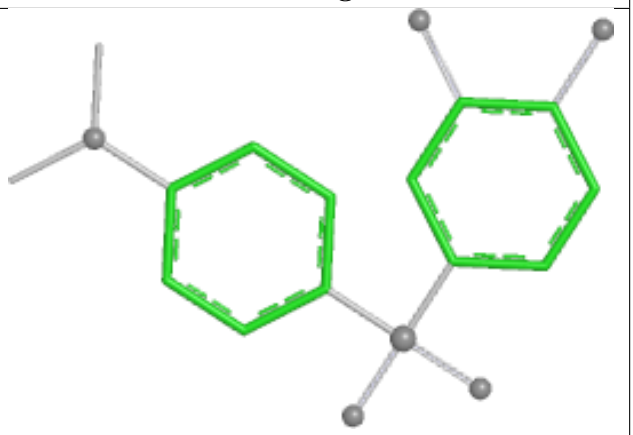
Bond lengths



Bond angles

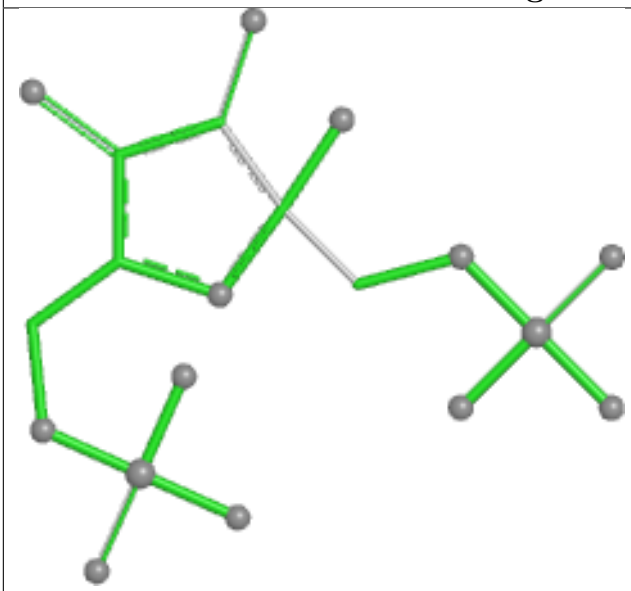


Torsions

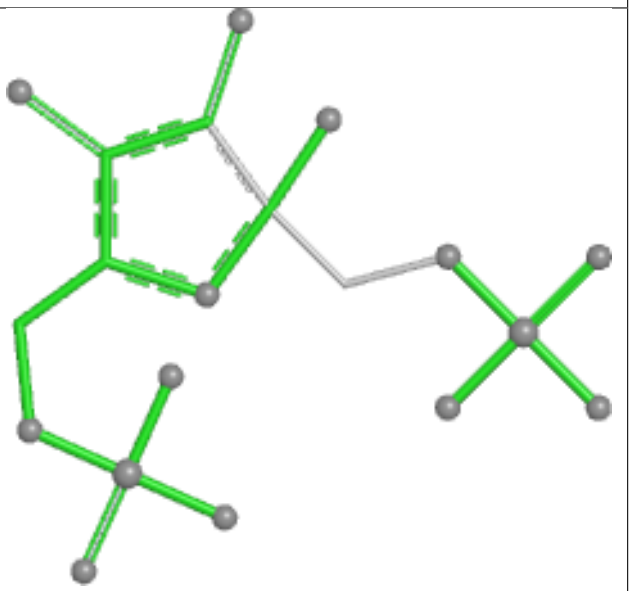


Rings

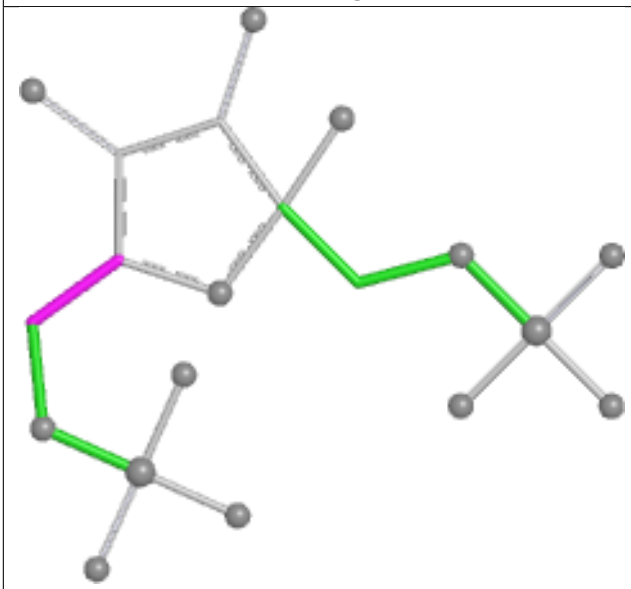
Ligand FBP E 601



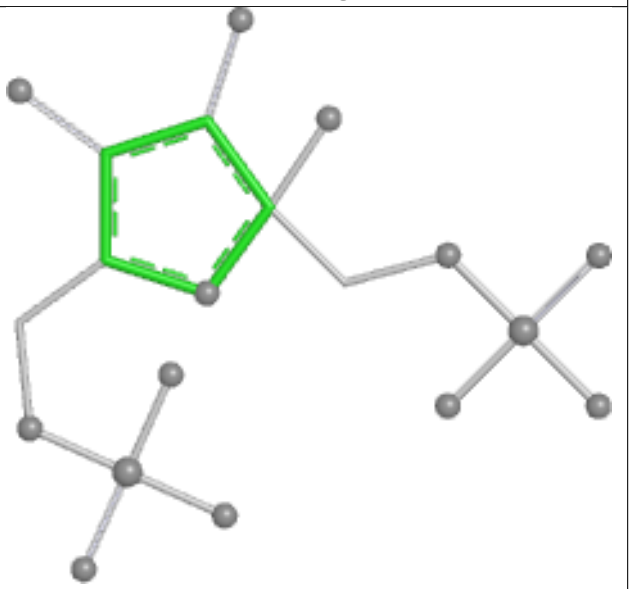
Bond lengths



Bond angles

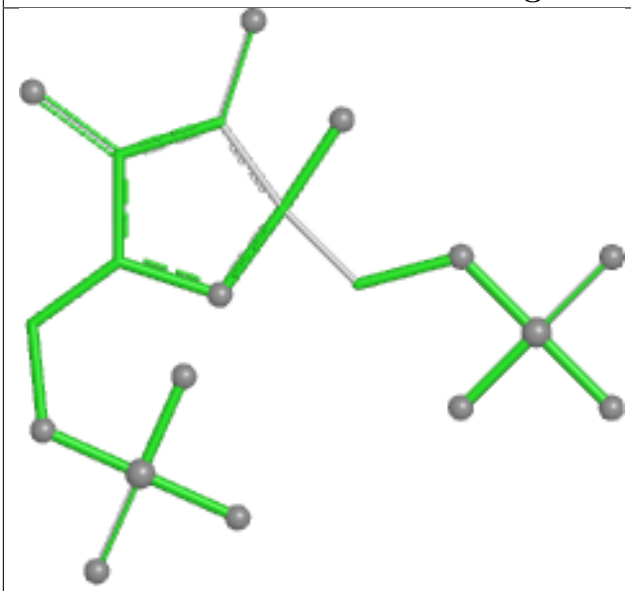


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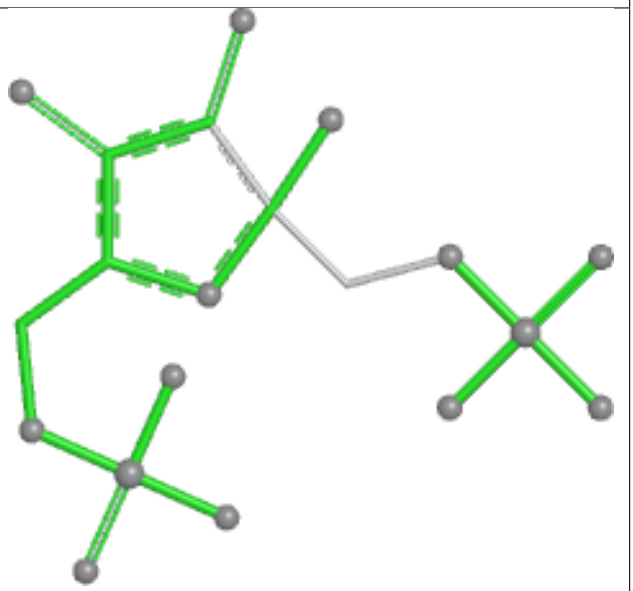


Rings

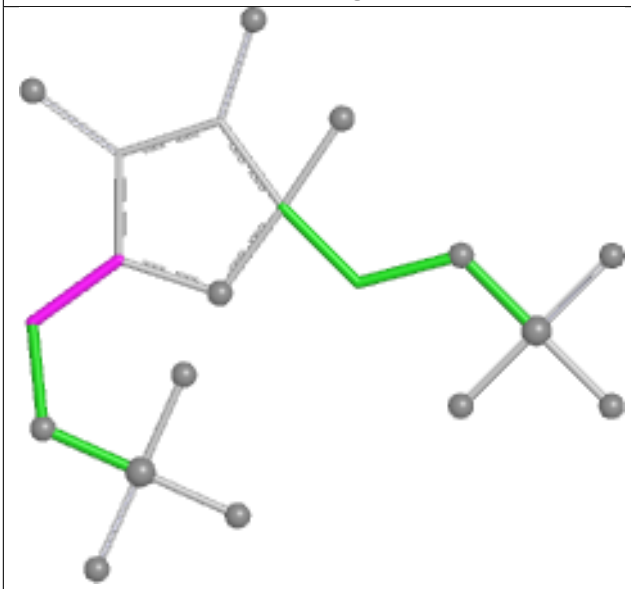
Ligand FBP G 601



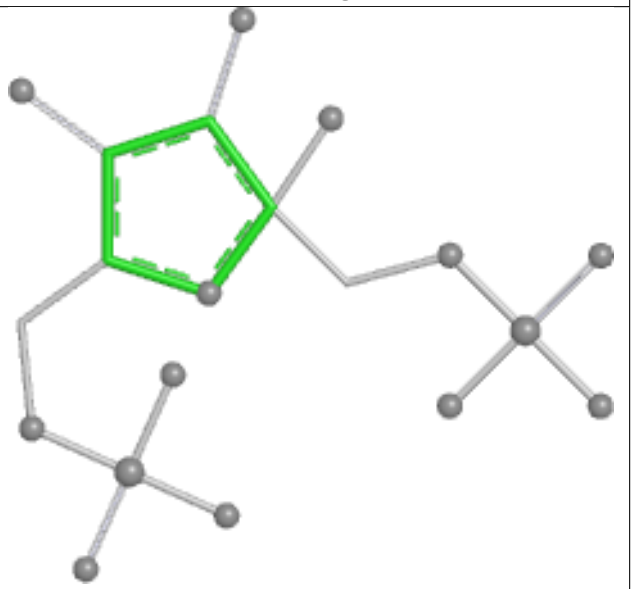
Bond lengths



Bond angles

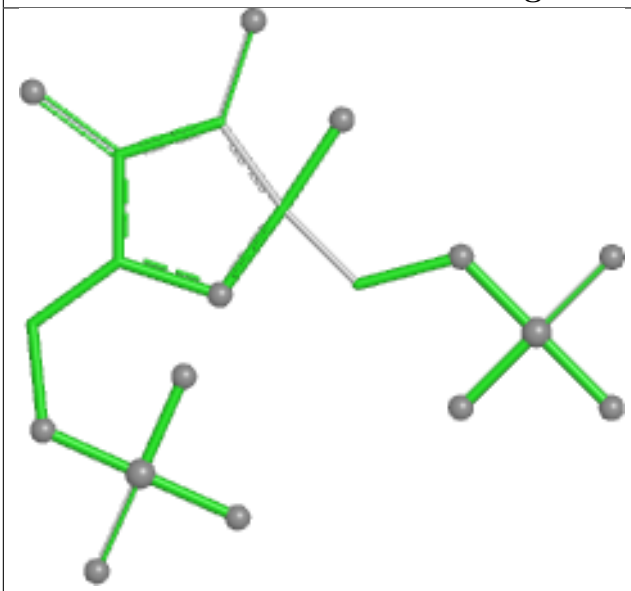


Torsions

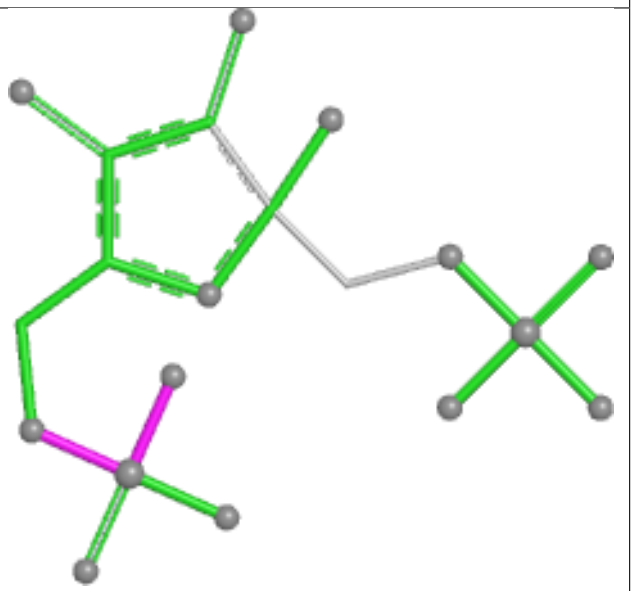


Rings

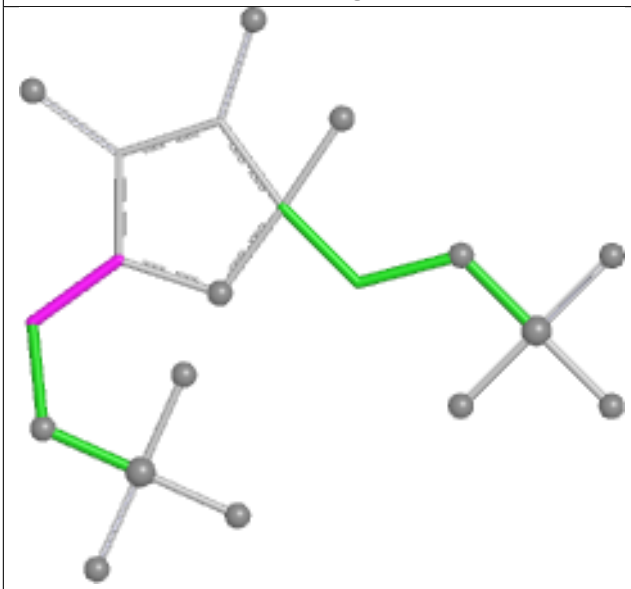
Ligand FBP D 601



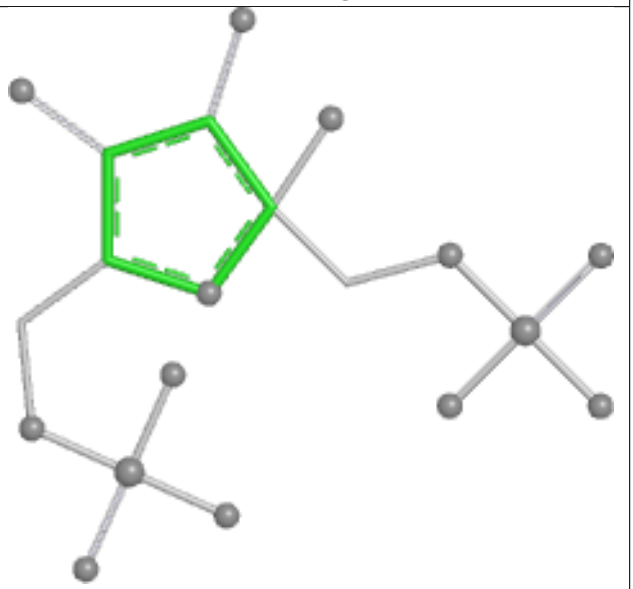
Bond lengths



Bond angles

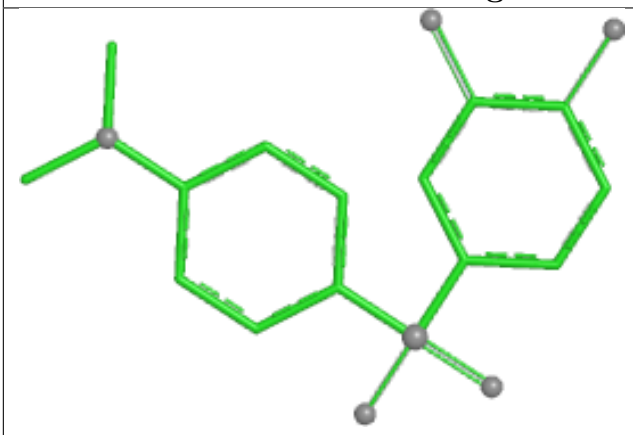


Torsions

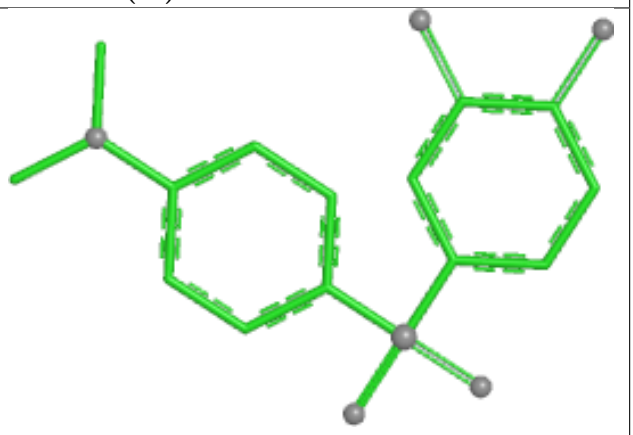


Rings

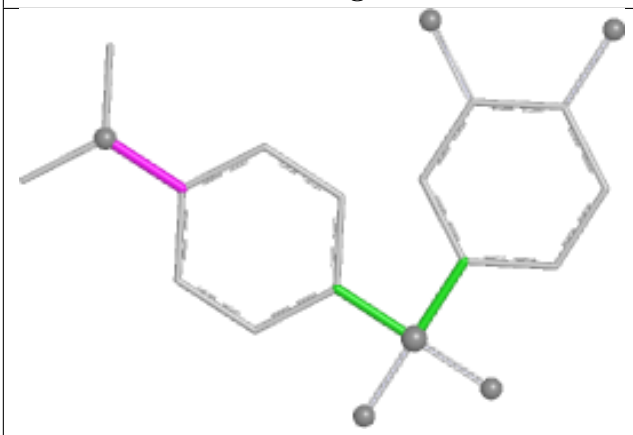
Ligand WV6 A 603 (A)



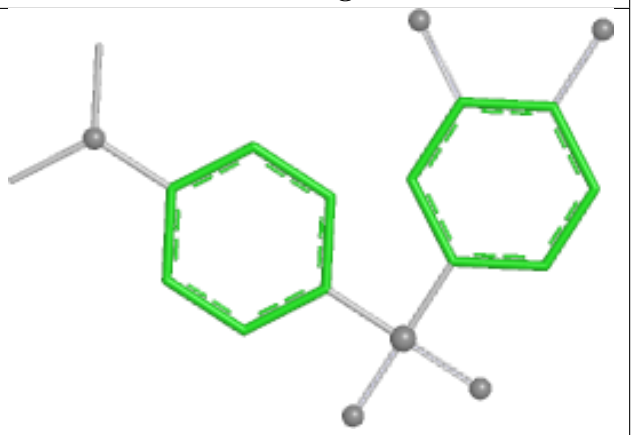
Bond lengths



Bond angles

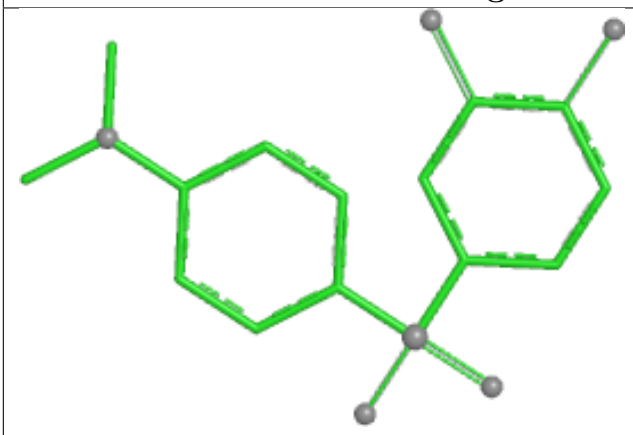


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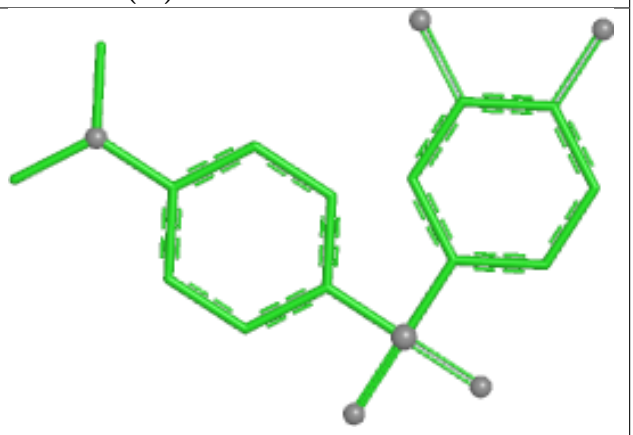


Rings

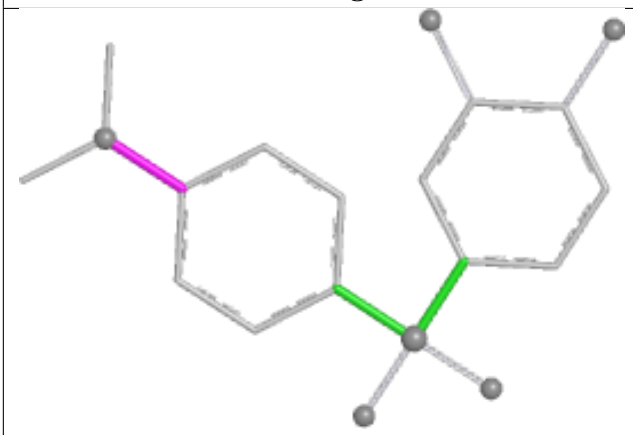
Ligand WV6 A 603 (B)



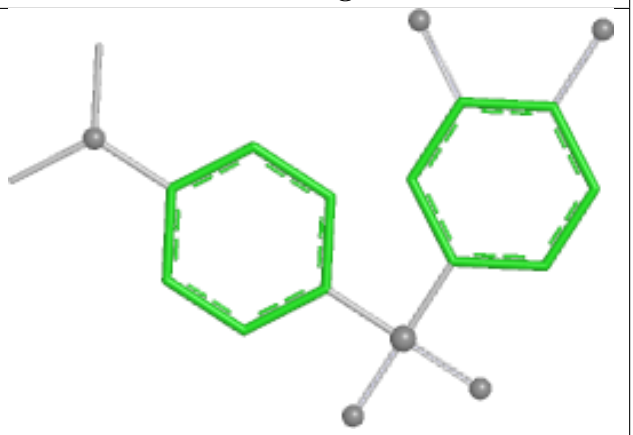
Bond lengths



Bond angles

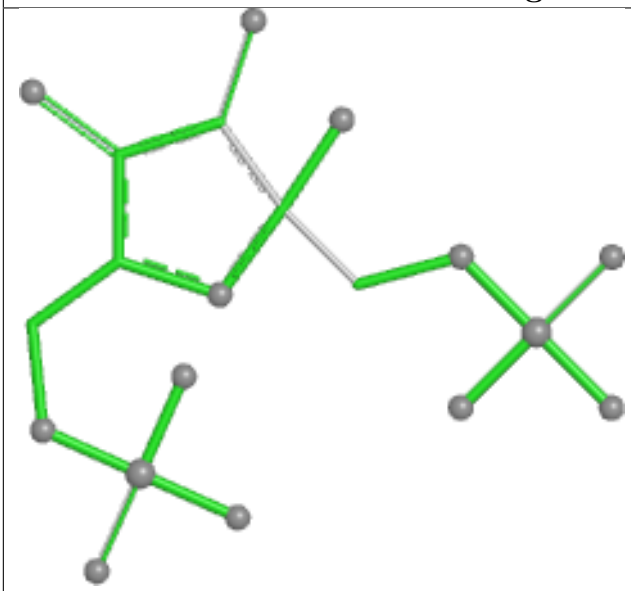


Torsions

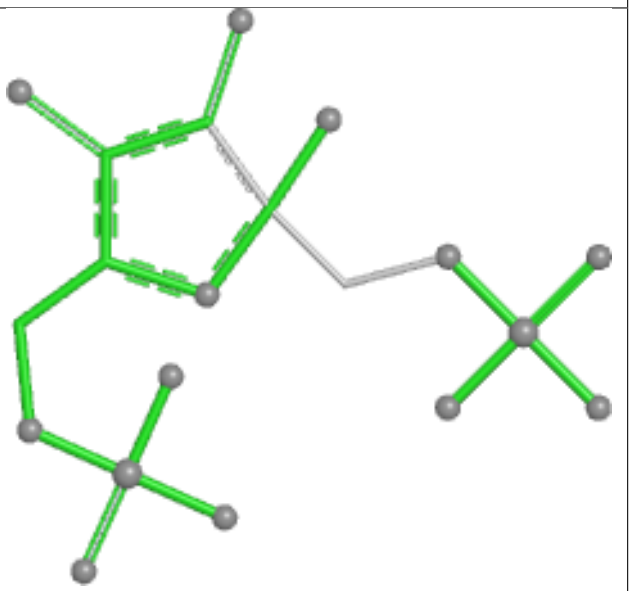


Rings

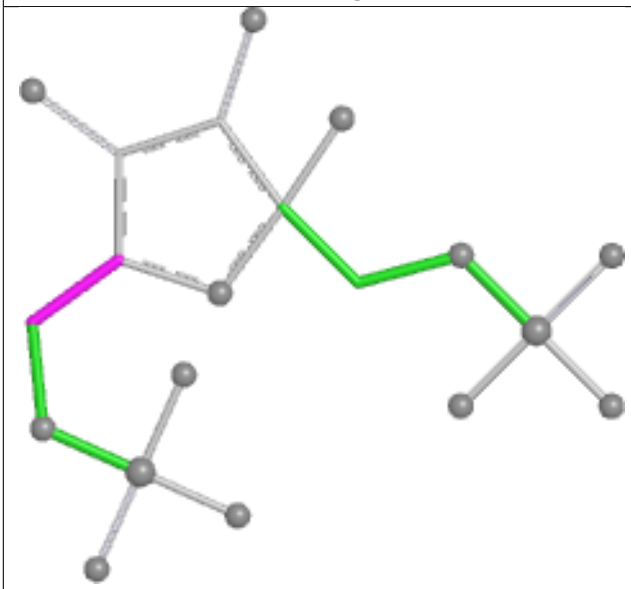
Ligand FBP C 601



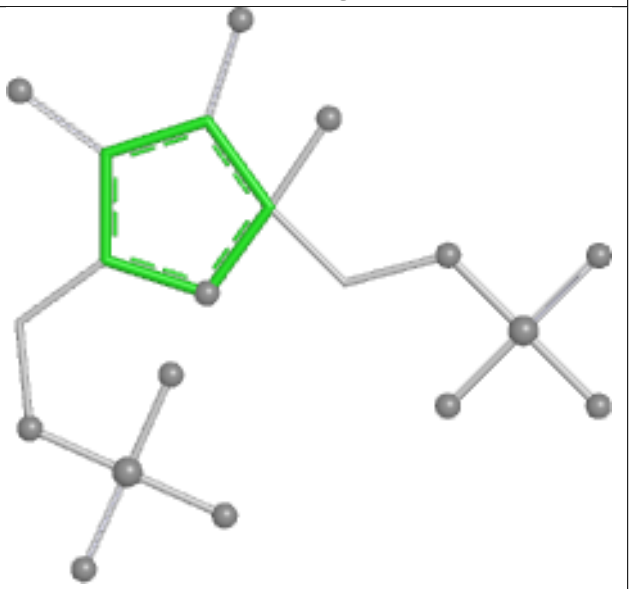
Bond lengths



Bond angles

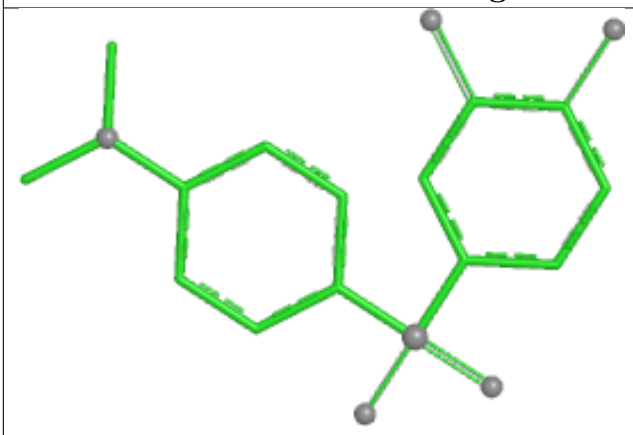


Torsions

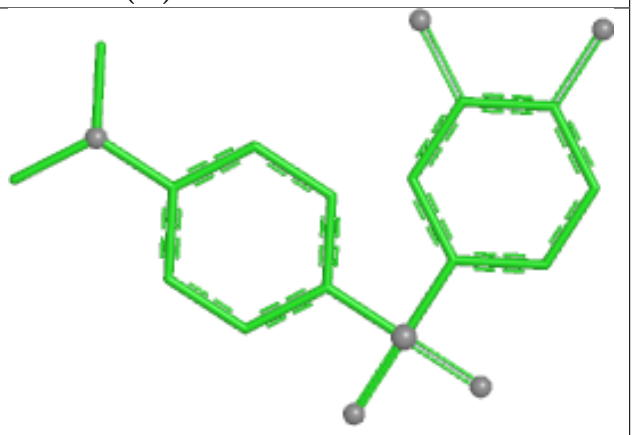


Rings

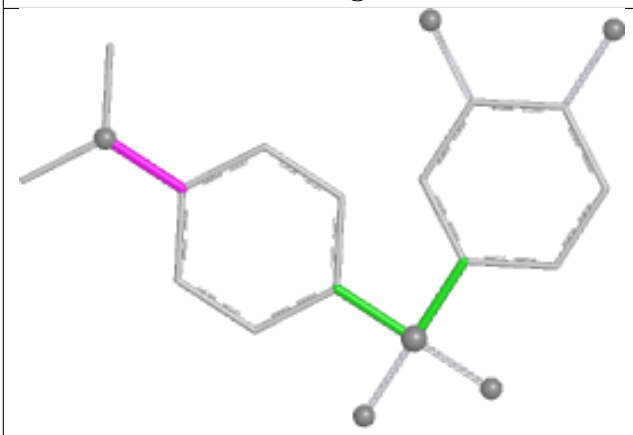
Ligand WV6 E 603 (B)



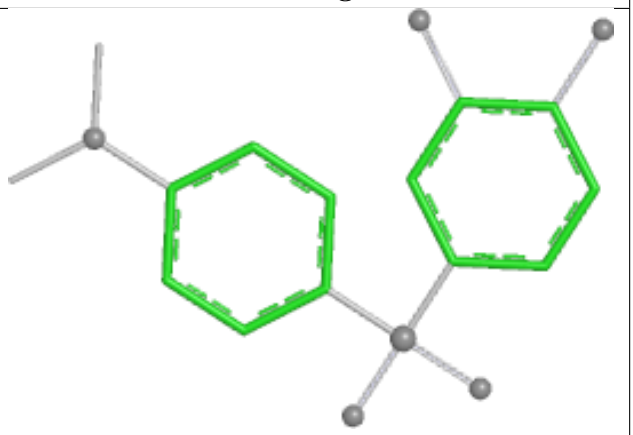
Bond lengths



Bond angles

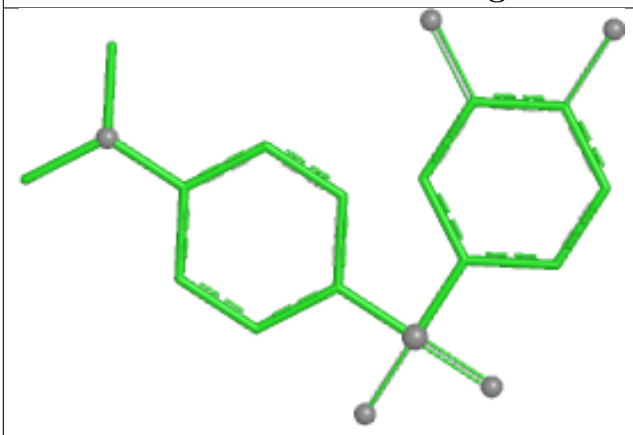


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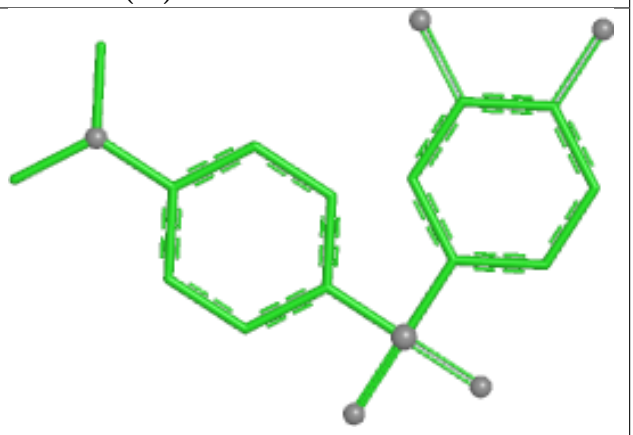


Rings

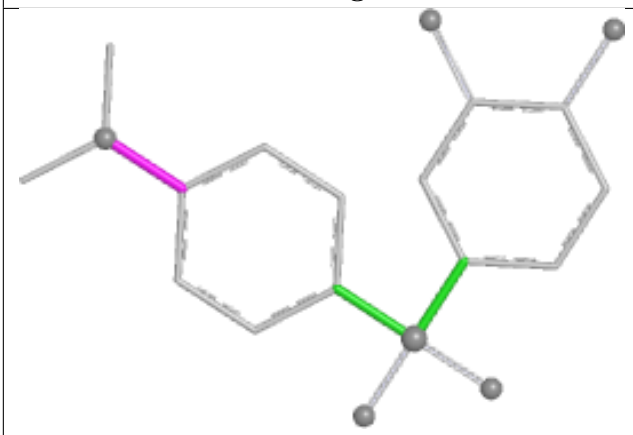
Ligand WV6 E 603 (A)



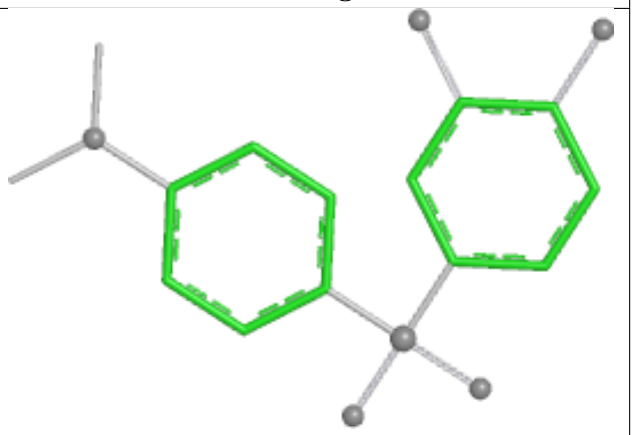
Bond lengths



Bond angles

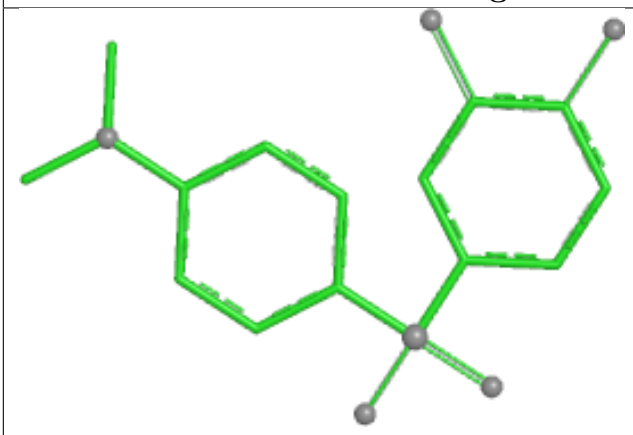


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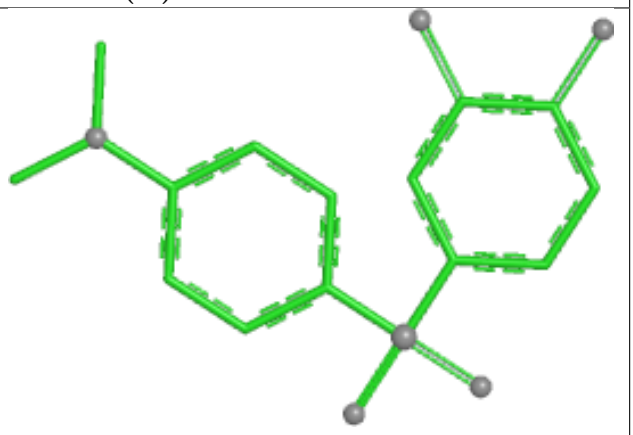


Rings

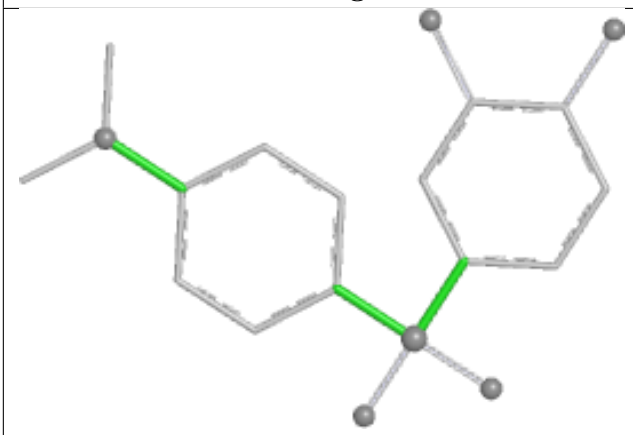
Ligand WV6 F 603 (B)



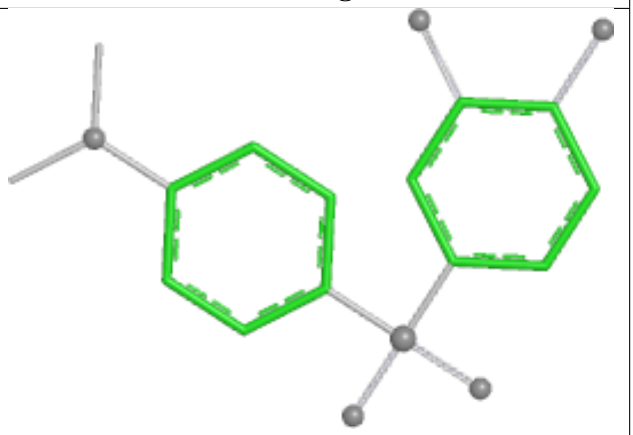
Bond lengths



Bond angles

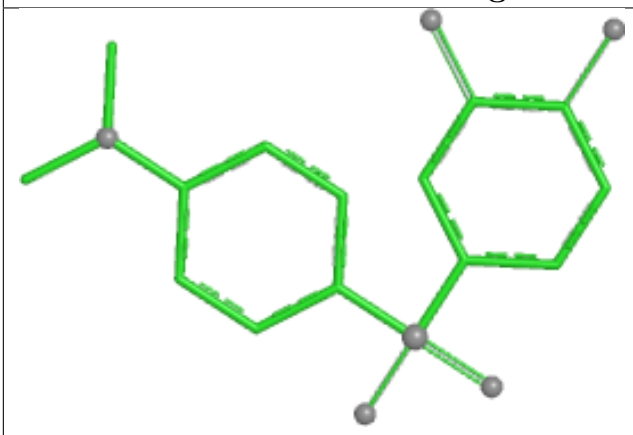


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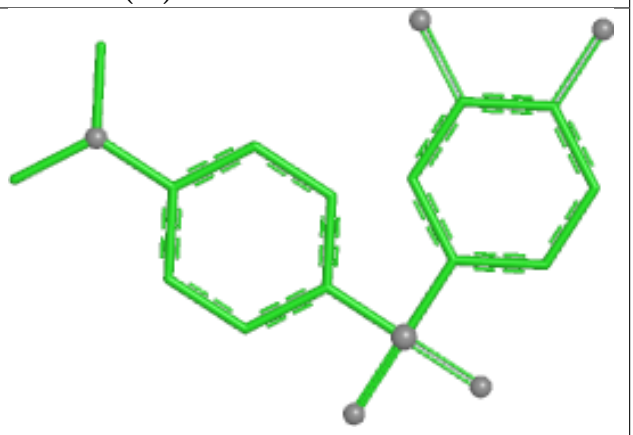


Rings

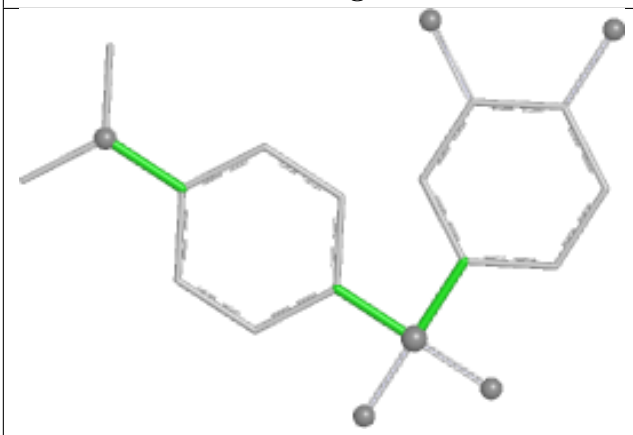
Ligand WV6 F 603 (A)



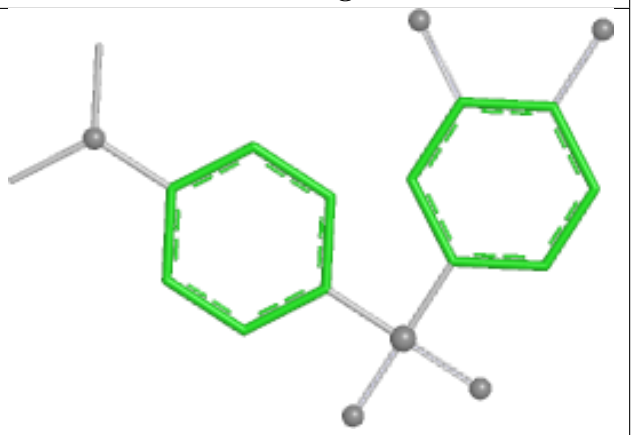
Bond lengths



Bond angles

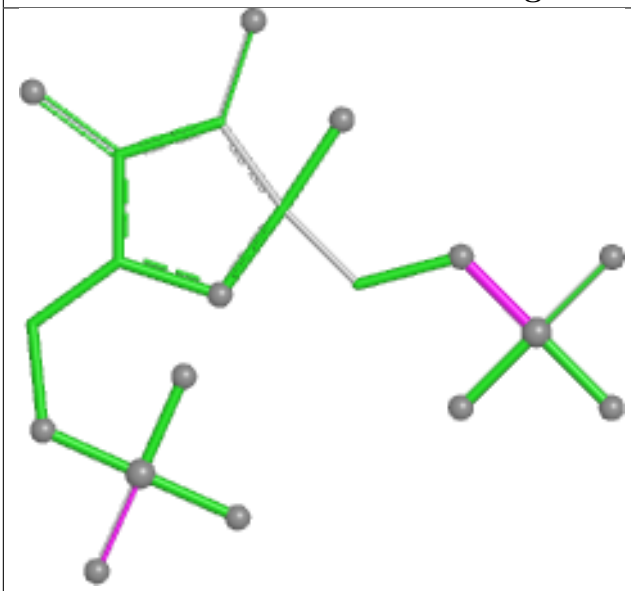


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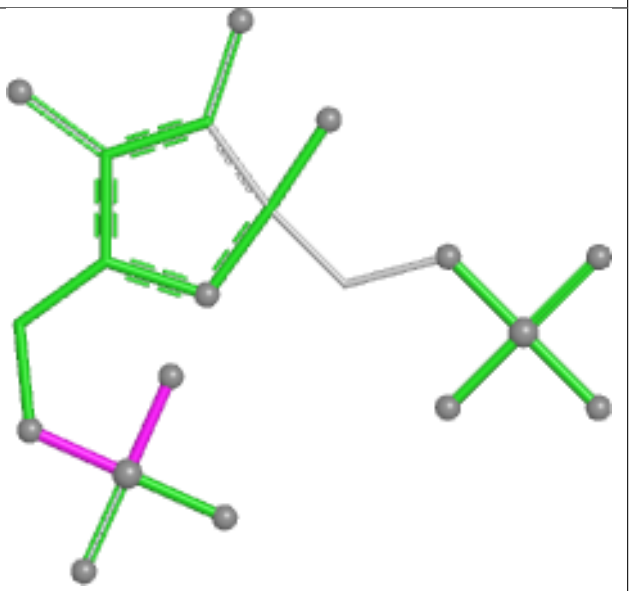


Rings

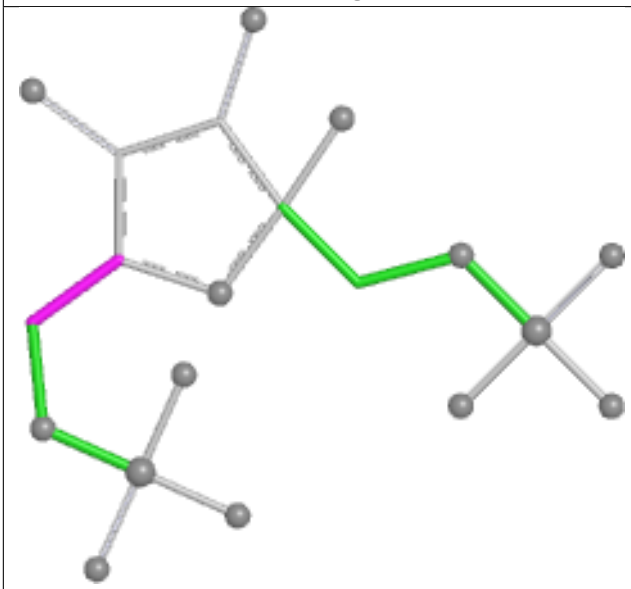
Ligand FBP H 601



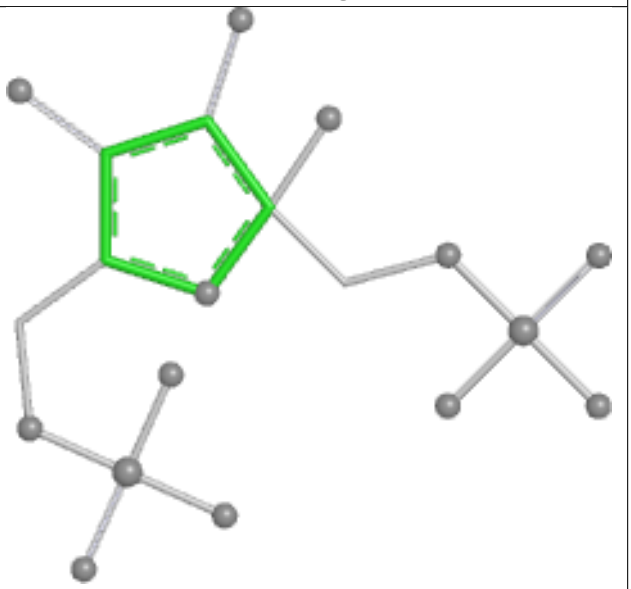
Bond lengths



Bond angles

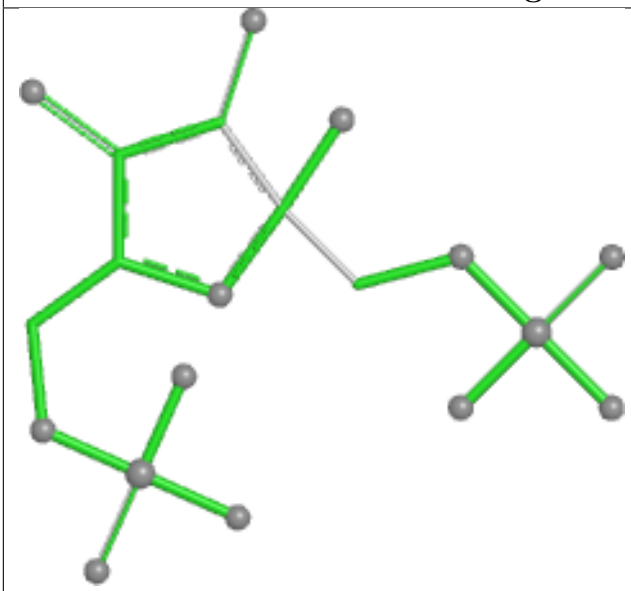


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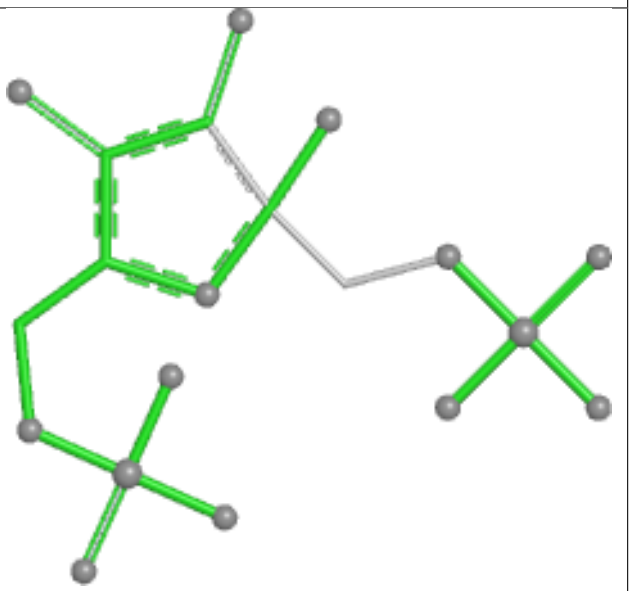


Rings

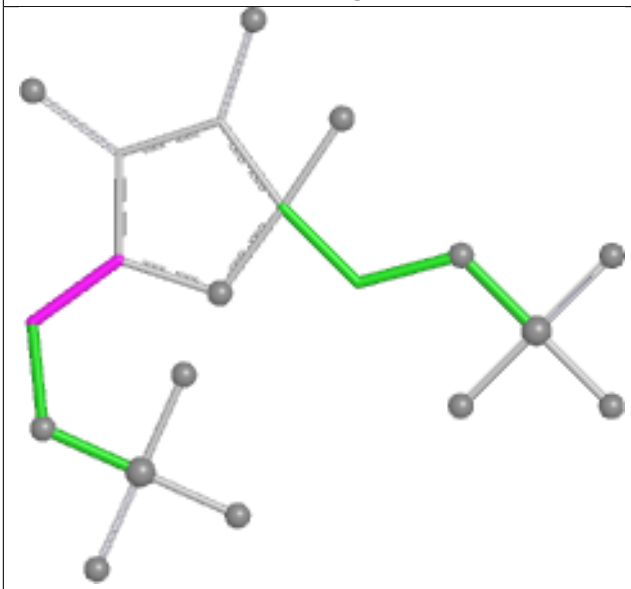
Ligand FBP A 601



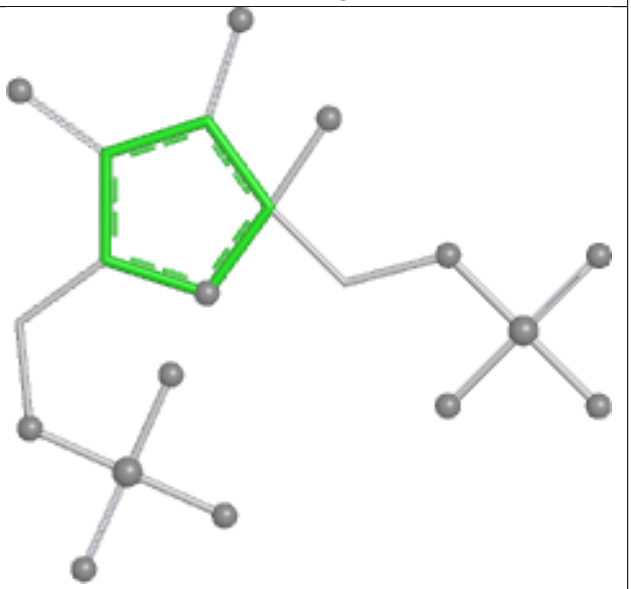
Bond lengths



Bond angles

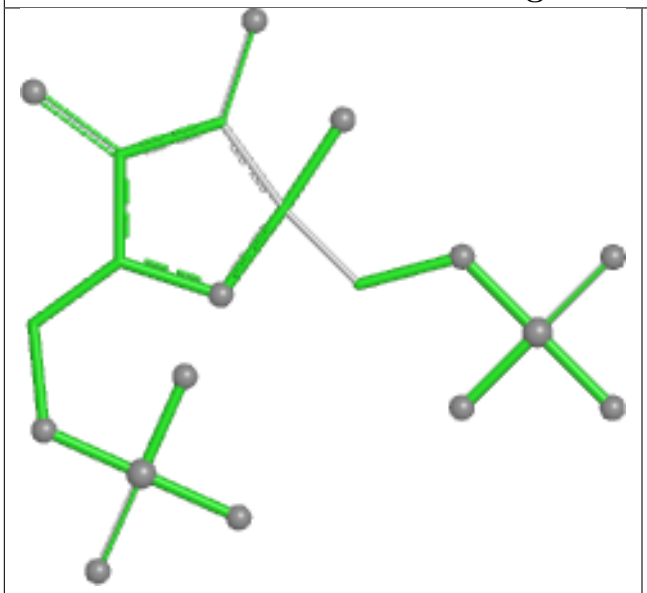


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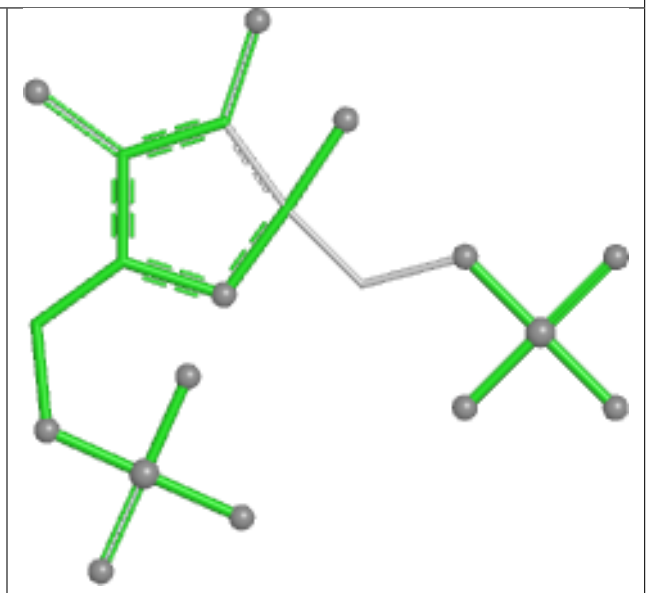


Rings

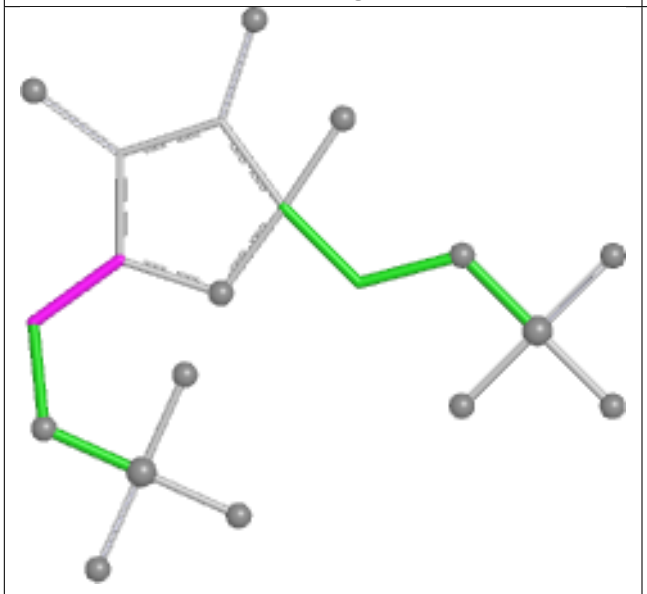
Ligand FBP B 601



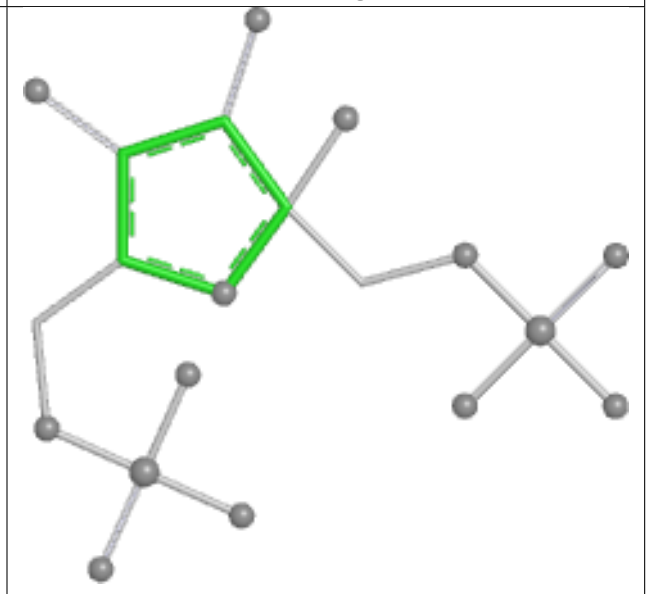
Bond lengths



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%)	1.18	69 (16%) 4 5	32, 59, 88, 109	11 (2%)
1	B	436/447 (97%)	1.73	160 (36%) 1 1	28, 61, 98, 114	8 (1%)
1	C	424/447 (94%)	0.53	25 (5%) 28 37	22, 45, 70, 122	6 (1%)
1	D	425/447 (95%)	0.17	11 (2%) 57 67	18, 38, 63, 116	8 (1%)
1	E	420/447 (93%)	1.21	75 (17%) 3 4	32, 60, 90, 104	11 (2%)
1	F	432/447 (96%)	0.77	46 (10%) 11 15	27, 49, 78, 96	8 (1%)
1	G	421/447 (94%)	0.35	23 (5%) 30 39	25, 41, 63, 96	6 (1%)
1	H	425/447 (95%)	-0.00	10 (2%) 59 69	17, 35, 59, 110	9 (2%)
All	All	3403/3576 (95%)	0.74	419 (12%) 8 11	17, 49, 86, 122	67 (1%)

The worst 5 of 419 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	513	LEU	7.7
1	E	277[A]	HIS	6.8
1	B	115	LEU	6.4
1	F	233	PRO	5.9
1	C	20	LEU	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
4	WV6	F	603[A]	20/20	0.81	0.23	44,45,47,47	35
4	WV6	F	603[B]	20/20	0.81	0.23	48,50,50,50	35
6	K	E	605	1/1	0.81	0.33	104,104,104,104	0
4	WV6	A	603[B]	20/20	0.83	0.27	49,51,52,52	35
4	WV6	A	603[A]	20/20	0.83	0.27	60,62,63,63	35
3	OXL	E	602	6/6	0.85	0.13	78,78,78,79	0
4	WV6	E	603[B]	20/20	0.86	0.24	53,56,57,57	35
4	WV6	E	603[A]	20/20	0.86	0.24	57,57,58,58	35
4	WV6	B	603[B]	20/20	0.88	0.21	49,52,53,53	35
6	K	B	605	1/1	0.88	0.13	79,79,79,79	0
4	WV6	B	603[A]	20/20	0.88	0.21	48,50,50,50	35
5	MG	E	604	1/1	0.91	0.10	65,65,65,65	0
6	K	A	605	1/1	0.91	0.17	104,104,104,104	0
3	OXL	A	602	6/6	0.91	0.10	64,64,65,66	0
5	MG	A	604	1/1	0.91	0.11	68,68,68,68	0
2	FBP	B	601	20/20	0.92	0.10	59,60,64,65	0
3	OXL	B	602	6/6	0.93	0.08	51,52,52,53	0
5	MG	B	604	1/1	0.93	0.09	73,73,73,73	0
2	FBP	E	601	20/20	0.93	0.09	57,58,59,60	0
2	FBP	F	601	20/20	0.94	0.09	49,55,60,60	0
3	OXL	G	602	6/6	0.94	0.08	45,46,47,47	0
6	K	C	604	1/1	0.95	0.18	67,67,67,67	0
3	OXL	C	602	6/6	0.95	0.07	55,56,56,57	0
6	K	F	605	1/1	0.95	0.07	92,92,92,92	0
6	K	G	604	1/1	0.95	0.21	71,71,71,71	0
3	OXL	F	602	6/6	0.96	0.06	50,51,53,53	0
3	OXL	D	602	6/6	0.96	0.06	40,42,42,43	0
3	OXL	H	602	6/6	0.96	0.07	40,40,41,41	0
2	FBP	A	601	20/20	0.96	0.07	52,54,55,55	0
5	MG	D	603	1/1	0.98	0.04	39,39,39,39	0
6	K	D	604	1/1	0.98	0.09	55,55,55,55	0
2	FBP	C	601	20/20	0.98	0.05	32,33,36,36	0
2	FBP	D	601	20/20	0.98	0.04	29,31,34,34	0
2	FBP	G	601	20/20	0.98	0.05	30,32,35,36	0
5	MG	F	604	1/1	0.99	0.02	42,42,42,42	0
5	MG	G	603	1/1	0.99	0.03	37,37,37,37	0
5	MG	H	603	1/1	0.99	0.06	40,40,40,40	0

Continued on next page...

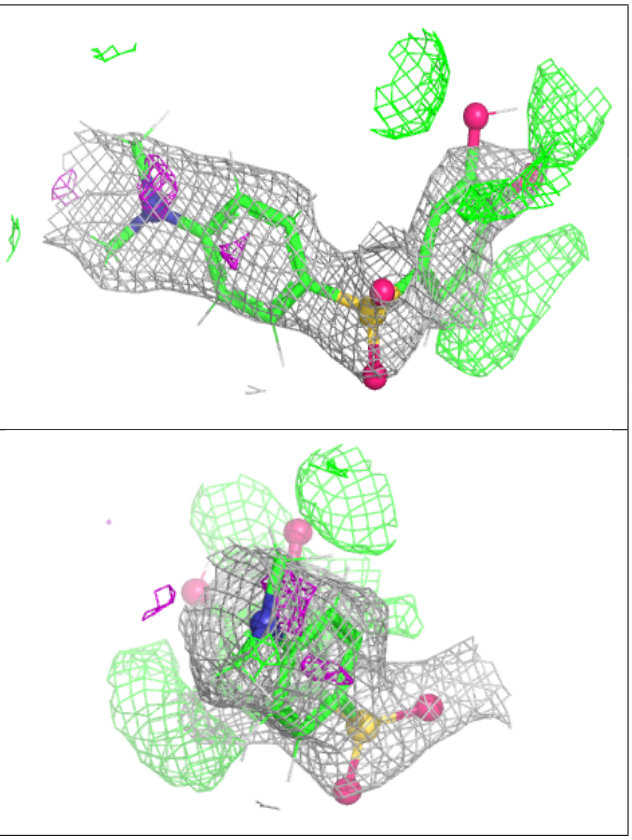
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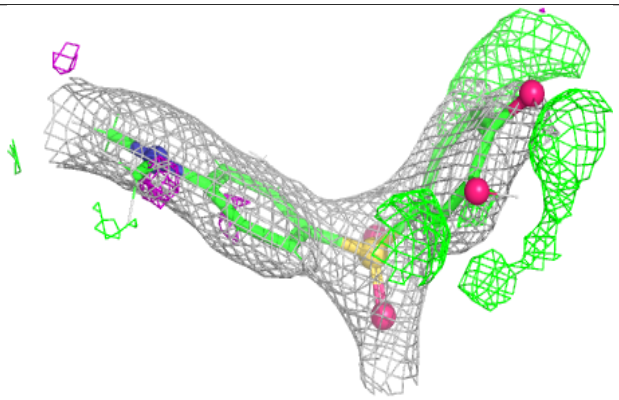
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FBP	H	601	20/20	0.99	0.04	25,27,31,31	0
5	MG	C	603	1/1	0.99	0.02	49,49,49,49	0
6	K	H	604	1/1	0.99	0.16	55,55,55,55	0

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 WV6 F 603 (A):

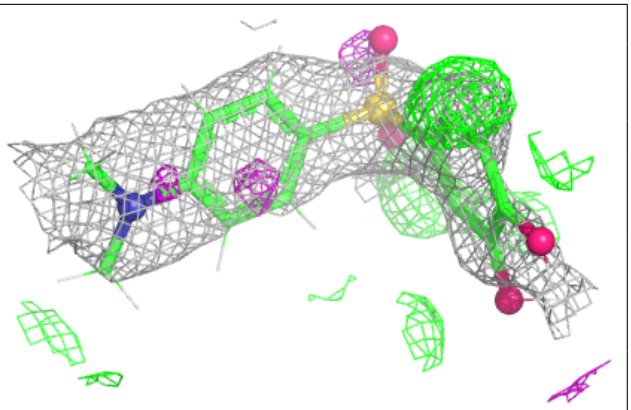
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

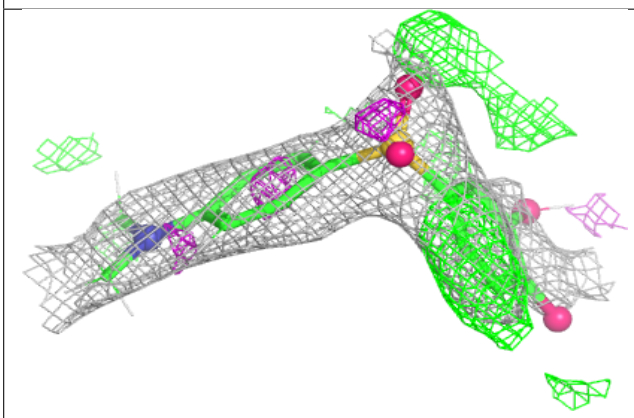


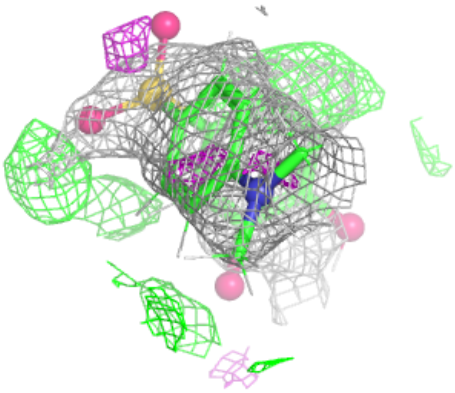


Electron density around WV6 F 603 (B):

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

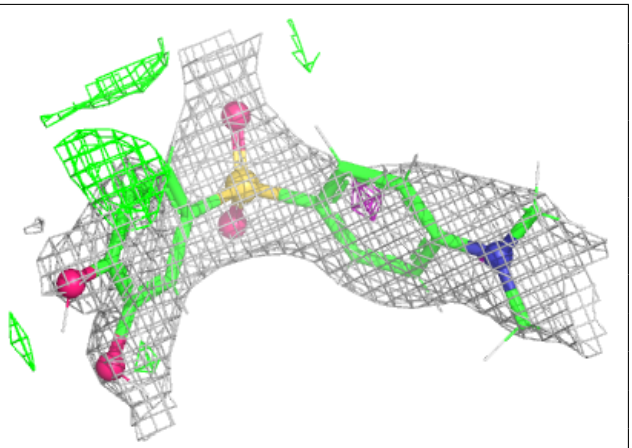


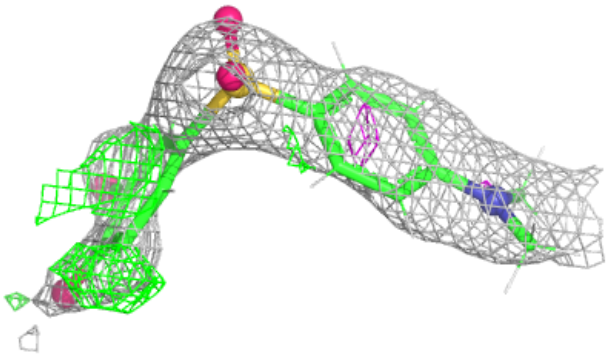


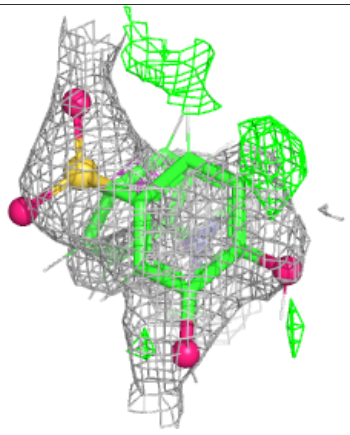


Electron density around WV6 A 603 (B):

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

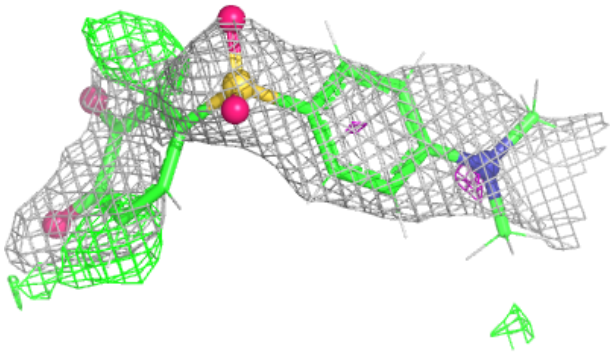


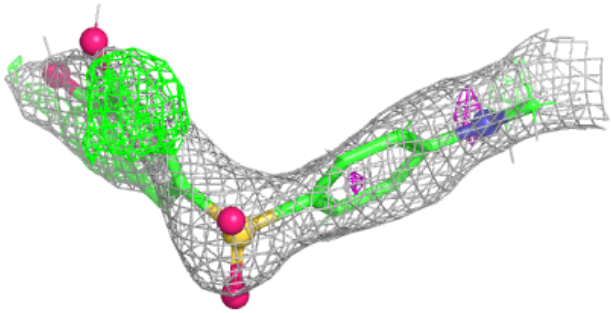


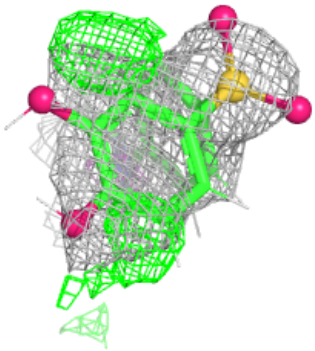


Electron density around WV6 A 603 (A):

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

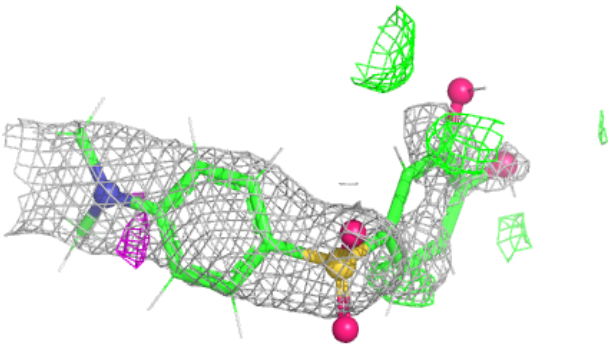


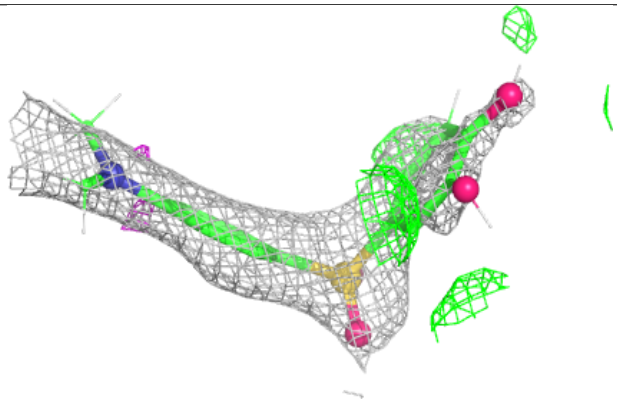


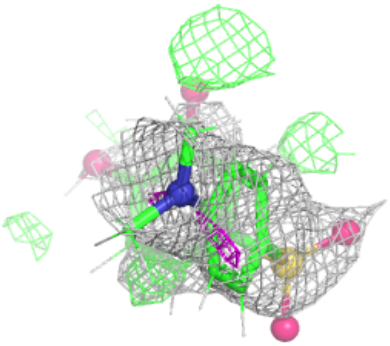


Electron density around WV6 E 603 (B):

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

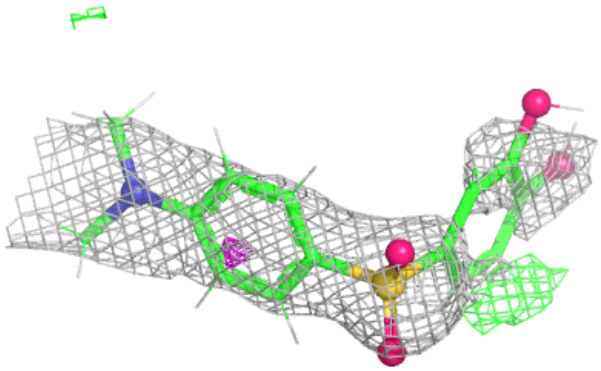


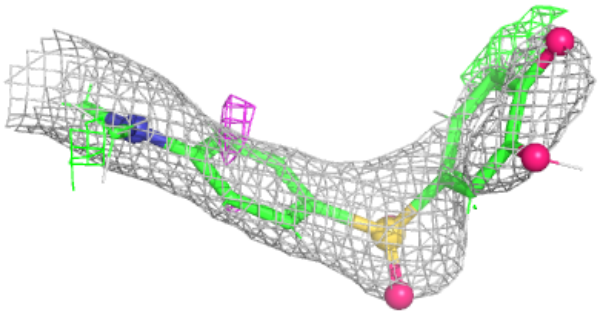


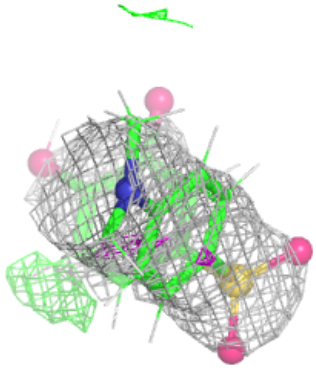


Electron density around WV6 E 603 (A):

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

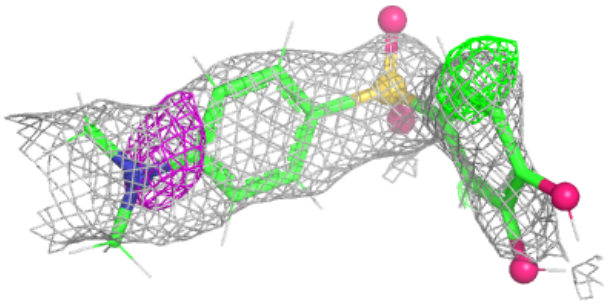


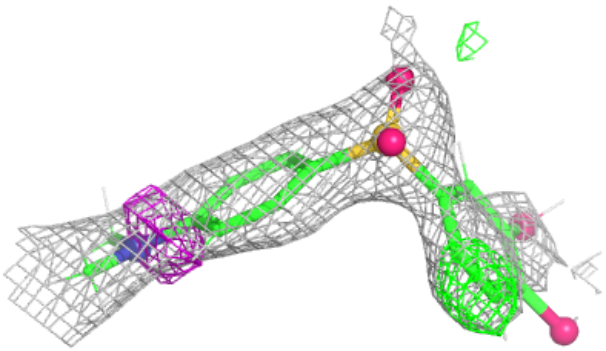


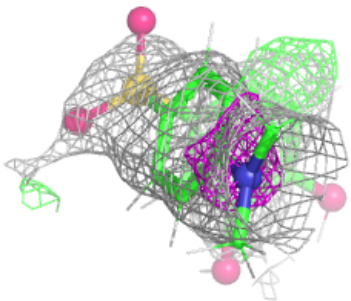


Electron density around WV6 B 603 (B):

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

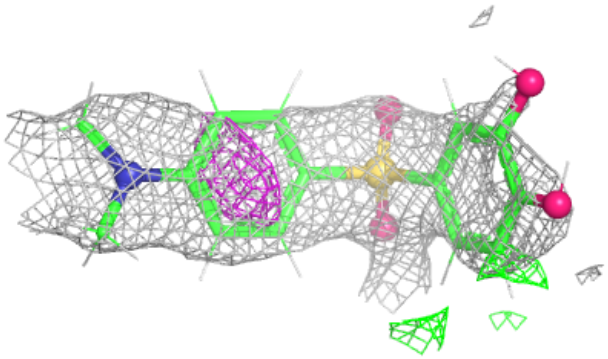


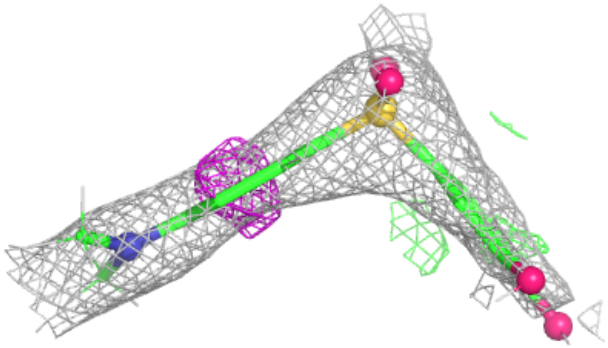


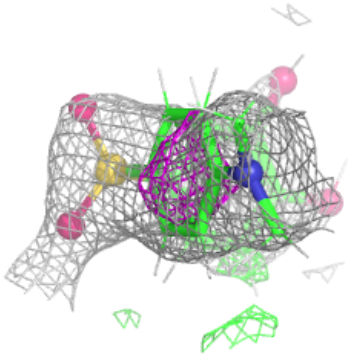


Electron density around WV6 B 603 (A):

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

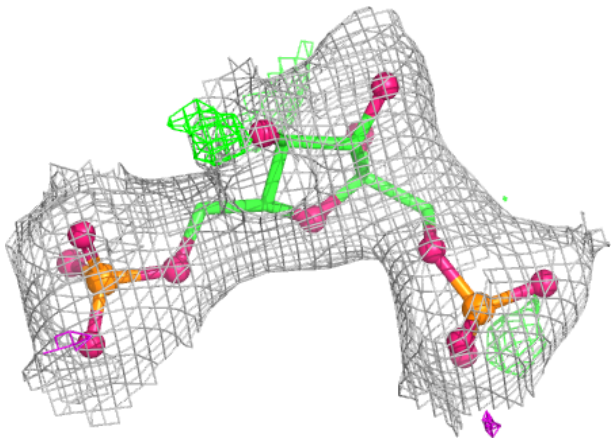


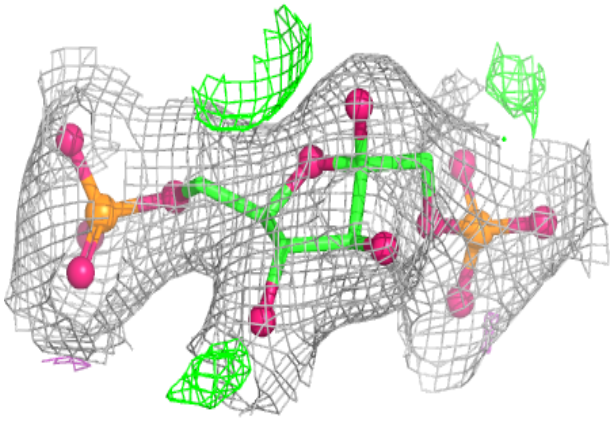


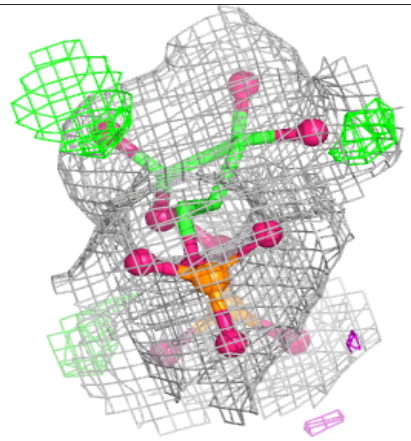


Electron density around FBP B 601:

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

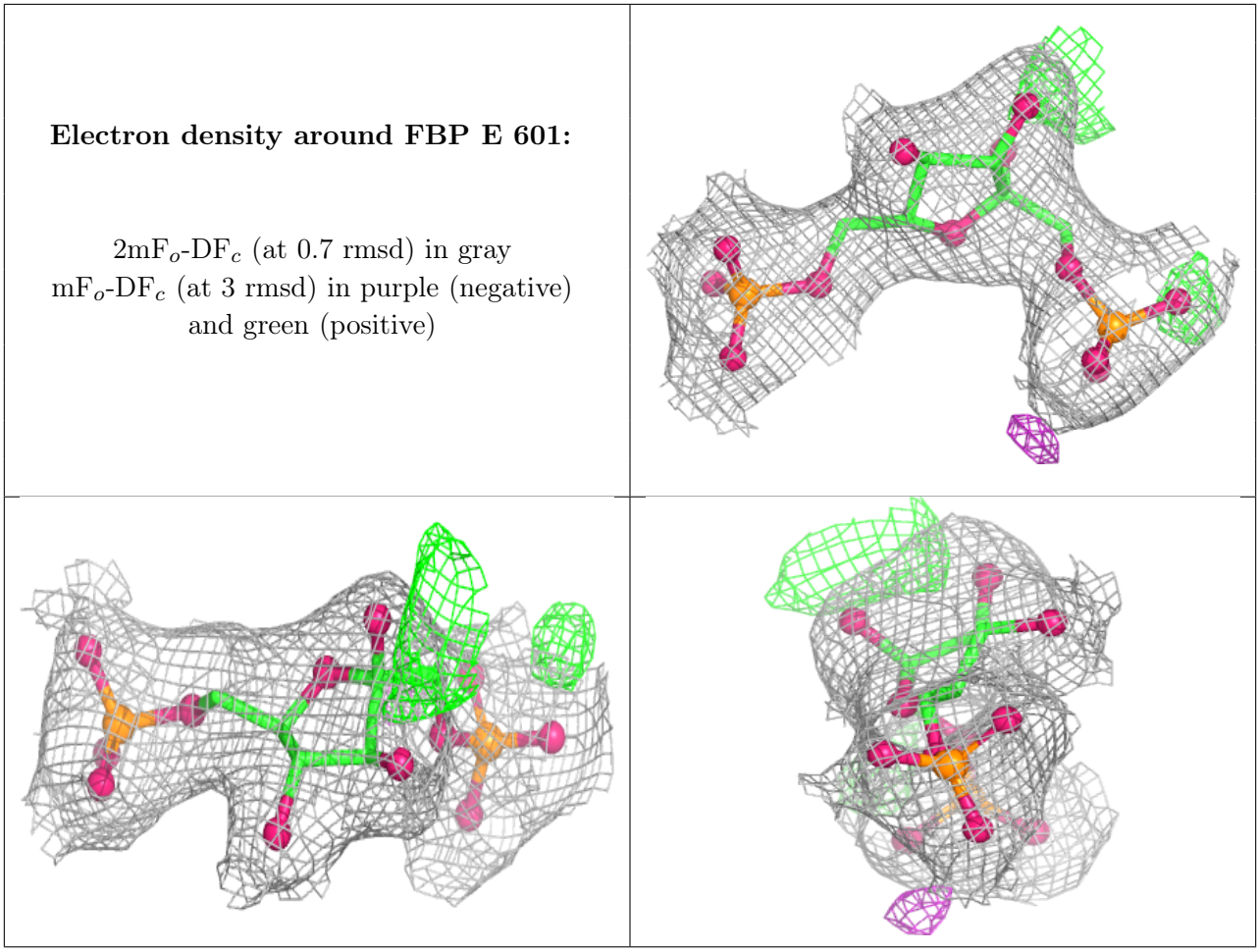






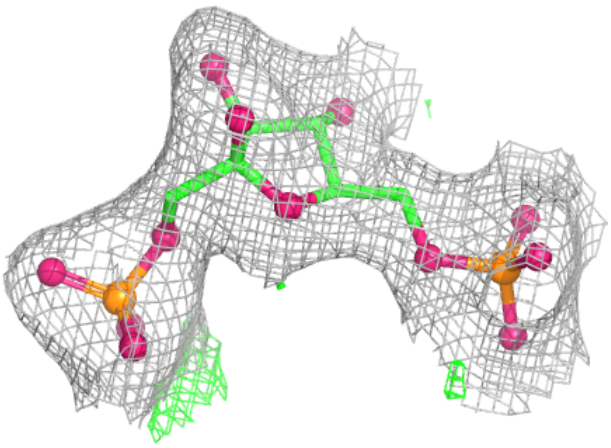
Electron density around FBP E 601:

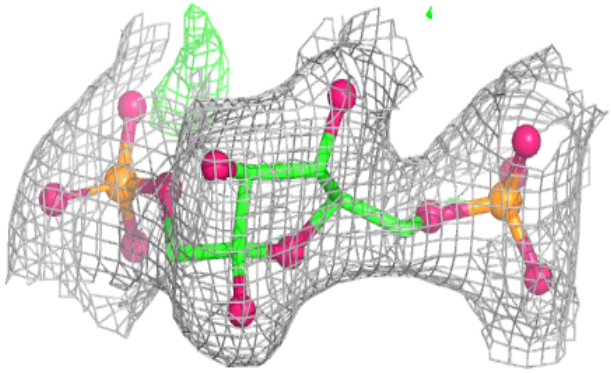
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

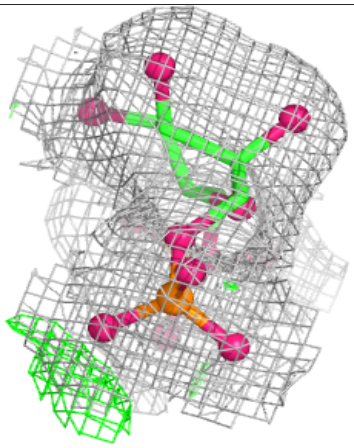


Electron density around FBP F 601:

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

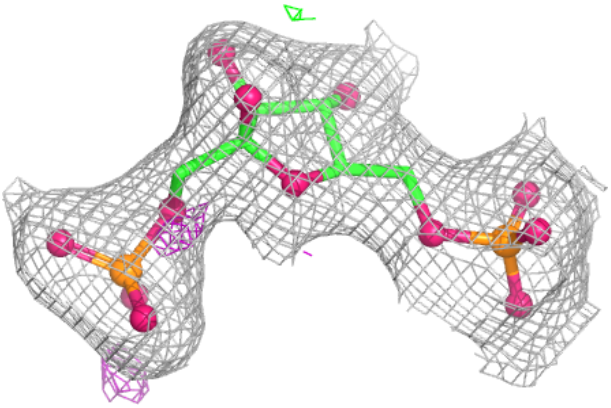


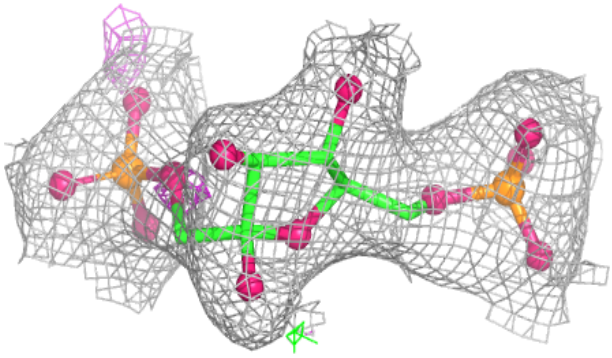


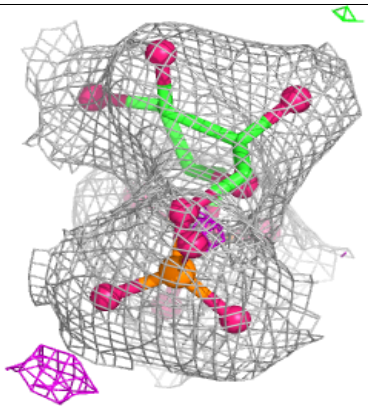


Electron density around FBP A 601:

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

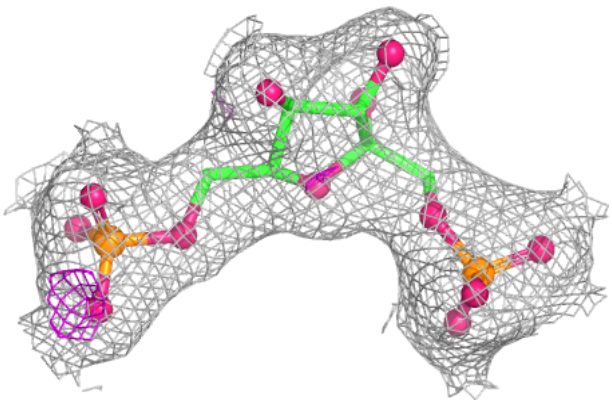


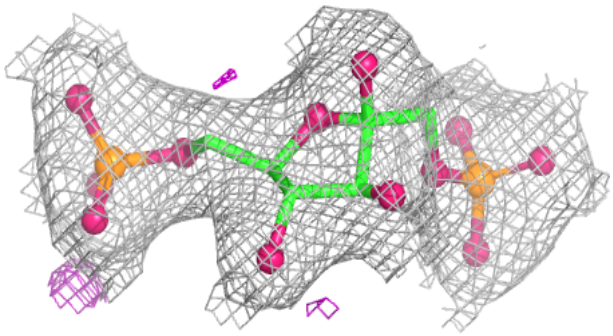


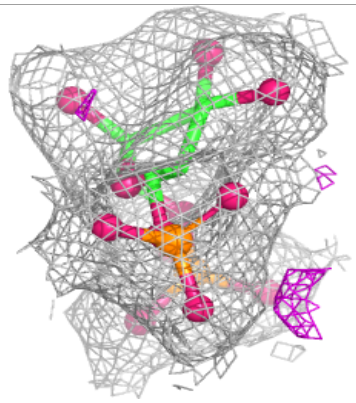


Electron density around FBP C 601:

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

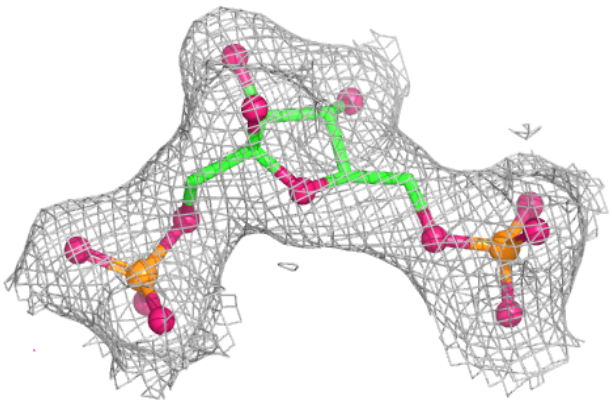


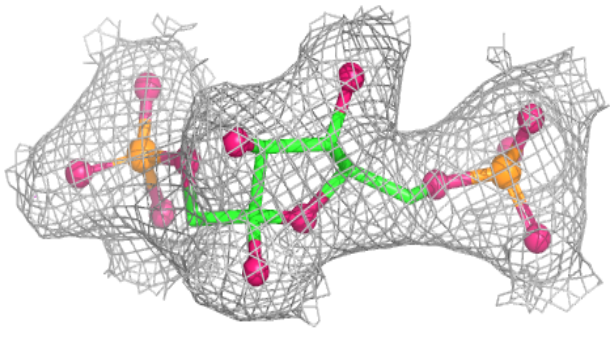


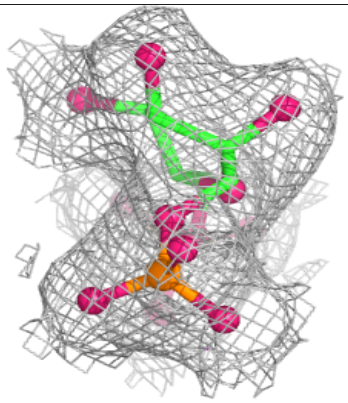


Electron density around FBP D 601:

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

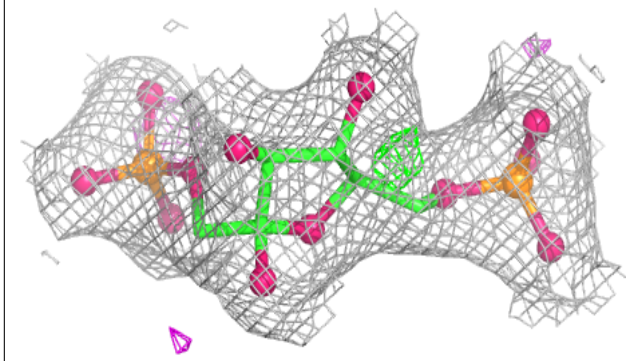


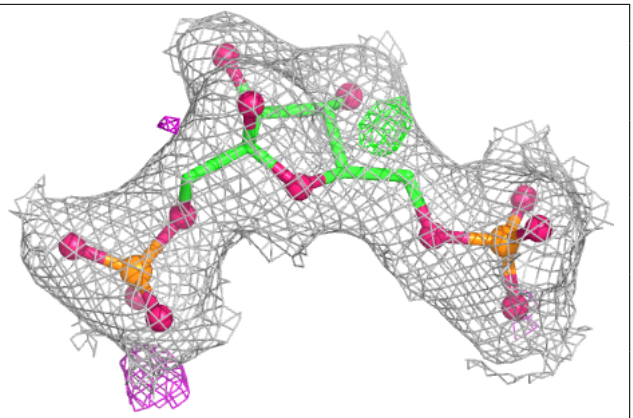


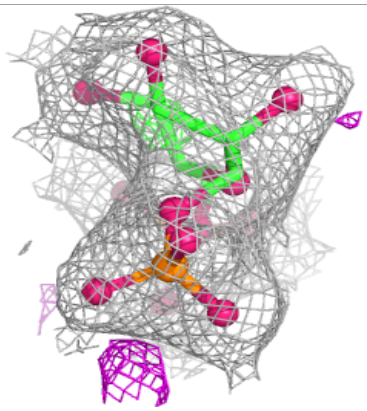


Electron density around FBP G 601:

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

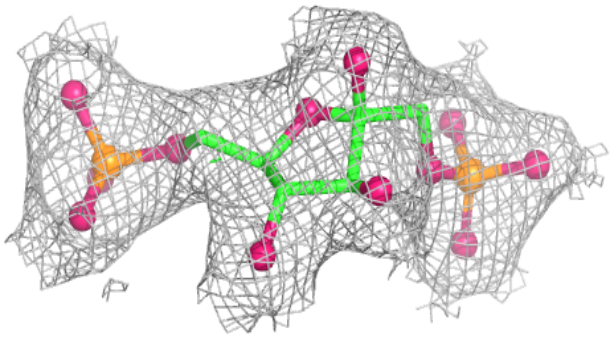


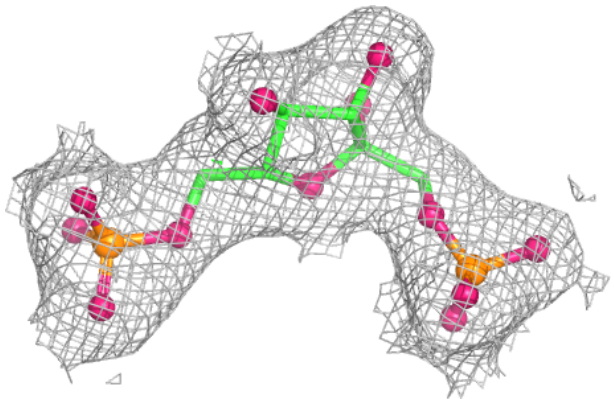


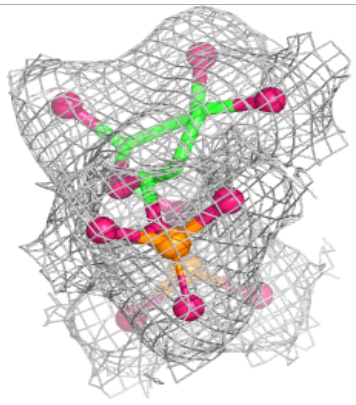


Electron density around FBP H 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.