Full wwPDB X-ray Structure Validation Report (i)

Apr 3, 2023 – 03:50 PM EDT

PDB ID	:	7FS5
Title	:	Structure of liver pyruvate kinase in complex with allosteric modulator 17
Authors	:	Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2022-12-18
Resolution	:	2.18 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

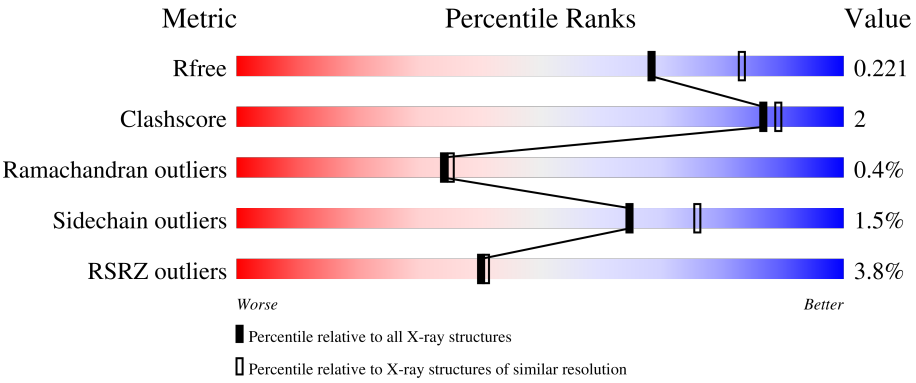
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.18 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	5% 87% 7% 6%
1	B	447	6% 91% 7%
1	C	447	2% 89% 6% 5%
1	D	447	% 88% 6% 5%
1	E	447	8% 87% 6% 6%

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Mol	Chain	Length	Quality of chain
1	F	447	4% 91% 5%
1	G	447	% 88% 6% 6%
1	H	447	2% 91% 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	F	602	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 28228 atoms, of which 76 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	6	0
			3236	2034	585	597	20			
1	B	436	Total	C	N	O	S	0	4	0
			3329	2090	604	615	20			
1	C	425	Total	C	N	O	S	0	4	0
			3247	2040	585	603	19			
1	D	425	Total	C	N	O	S	0	6	0
			3252	2042	590	601	19			
1	E	418	Total	C	N	O	S	0	5	0
			3201	2013	578	590	20			
1	F	432	Total	C	N	O	S	0	7	0
			3321	2090	597	614	20			
1	G	421	Total	C	N	O	S	0	6	0
			3231	2031	581	600	19			
1	H	425	Total	C	N	O	S	0	4	0
			3251	2040	594	598	19			

There are 64 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	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	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	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	12	ASP	SER	conflict	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	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	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	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	1	MET	-	expression tag	UNP P30613
E	2	GLU	-	expression tag	UNP P30613
E	12	ASP	SER	conflict	UNP P30613
E	228	GLY	-	linker	UNP P30613
E	229	SER	-	linker	UNP P30613
E	230	GLY	-	linker	UNP P30613
F	-1	GLY	-	expression tag	UNP P30613
F	0	SER	-	expression tag	UNP P30613
F	1	MET	-	expression tag	UNP P30613
F	2	GLU	-	expression tag	UNP P30613
F	12	ASP	SER	conflict	UNP P30613
F	228	GLY	-	linker	UNP P30613
F	229	SER	-	linker	UNP P30613
F	230	GLY	-	linker	UNP P30613
G	-1	GLY	-	expression tag	UNP P30613
G	0	SER	-	expression tag	UNP P30613
G	1	MET	-	expression tag	UNP P30613
G	2	GLU	-	expression tag	UNP P30613
G	12	ASP	SER	conflict	UNP P30613
G	130	GLY	-	linker	UNP P30613
G	131	SER	-	linker	UNP P30613

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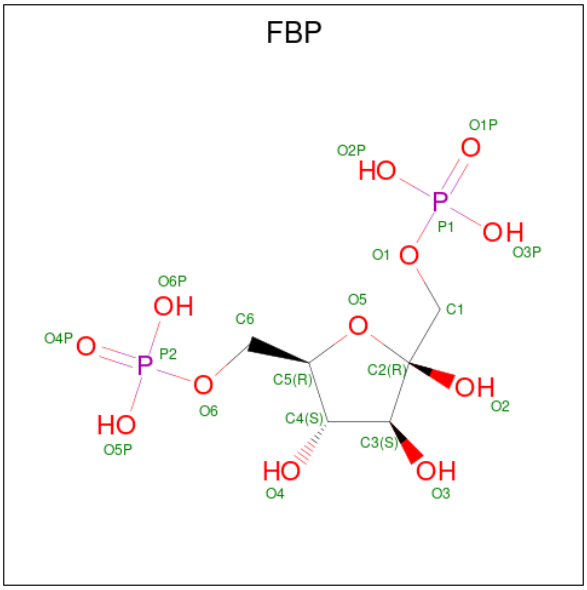
Chain	Residue	Modelled	Actual	Comment	Reference
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	130	GLY	-	linker	UNP P30613
H	131	SER	-	linker	UNP P30613
H	132	GLY	-	linker	UNP P30613

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



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

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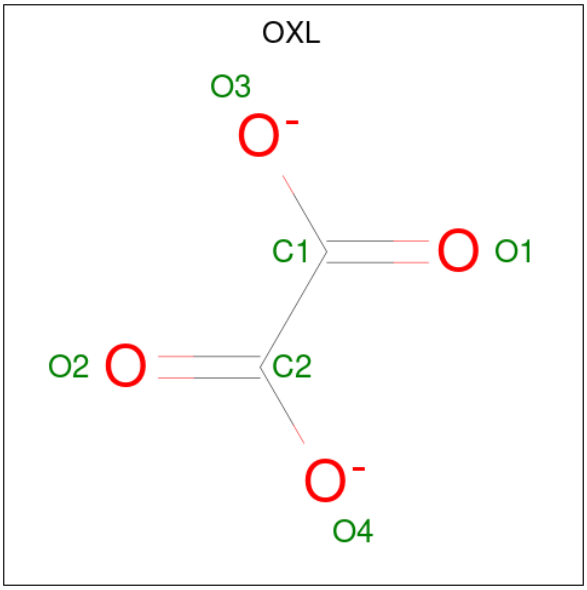
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O P 20 6 12 2	0	0
2	H	1	Total C O P 20 6 12 2	0	0

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0
3	E	1	Total C O 6 2 4	0	0
3	F	1	Total C O 6 2 4	0	0
3	G	1	Total C O 6 2 4	0	0
3	H	1	Total C O 6 2 4	0	0

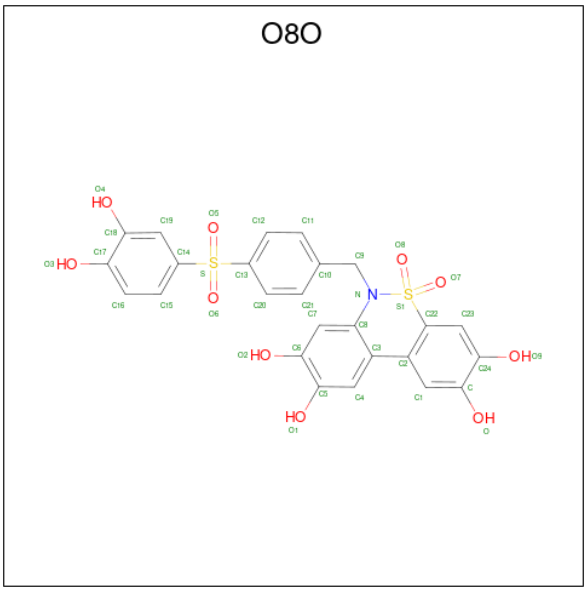
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 6 is (10aP)-6-{[4-(3,4-dihydroxybenzene-1-sulfonyl)phenyl]methyl}-2,3,8,9-tetrahydroxy-5lambda 6 -dibenzo[c,e][1,2]thiazine-5,5(6H)-dione (three-letter code: O8O) (formula: $C_{25}H_{19}NO_{10}S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	19	0
			57	25	19	1	10	2		
6	D	1	Total	C	H	N	O	S	19	0
			57	25	19	1	10	2		
6	E	1	Total	C	H	N	O	S	19	0
			57	25	19	1	10	2		
6	H	1	Total	C	H	N	O	S	19	0
			57	25	19	1	10	2		

- Molecule 7 is water.

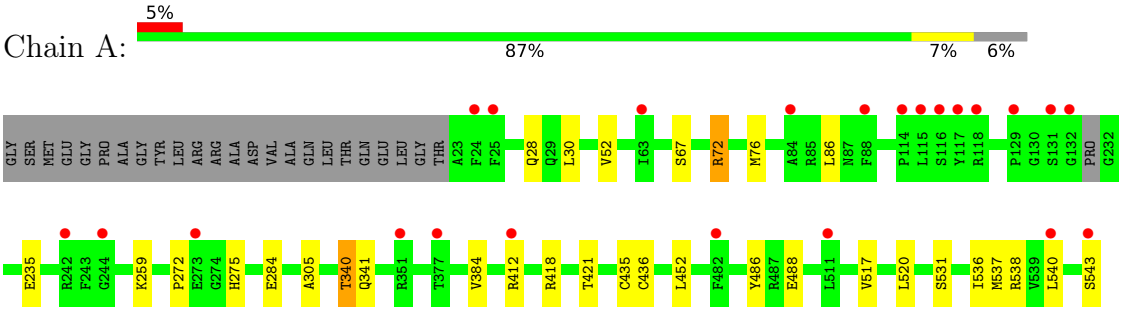
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	169	Total	O	0	0
			169	169		
7	B	153	Total	O	0	0
			153	153		
7	C	230	Total	O	0	0
			230	230		
7	D	283	Total	O	0	0
			283	283		
7	E	152	Total	O	0	0
			152	152		
7	F	173	Total	O	0	0
			173	173		
7	G	236	Total	O	0	0
			236	236		
7	H	312	Total	O	0	0
			312	312		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

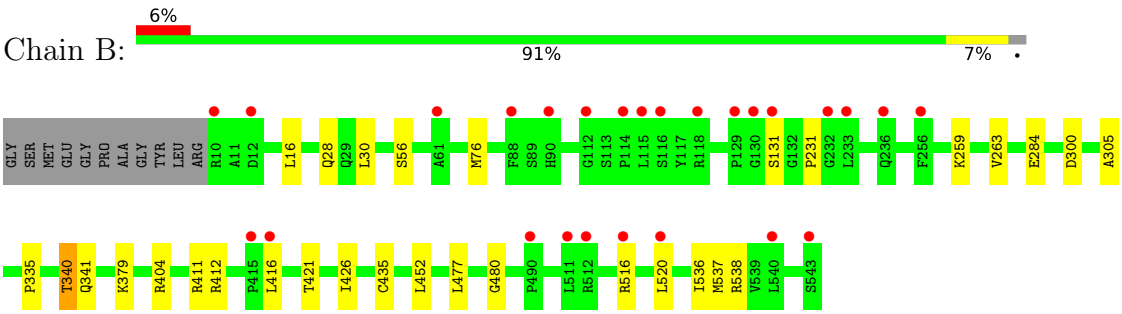
• Molecule 1: Pyruvate kinase PKLR

Chain A:



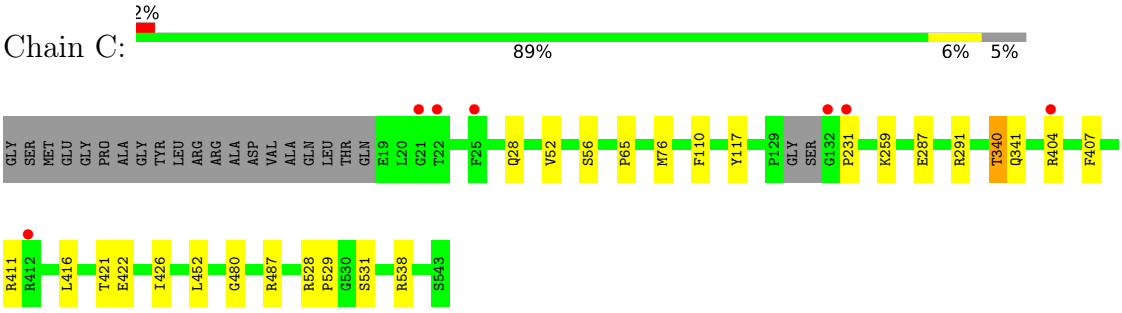
• Molecule 1: Pyruvate kinase PKLR

Chain B:



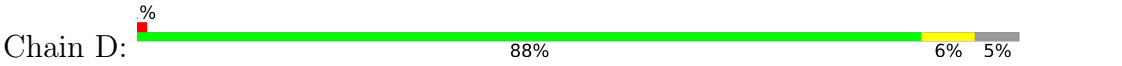
• Molecule 1: Pyruvate kinase PKLR

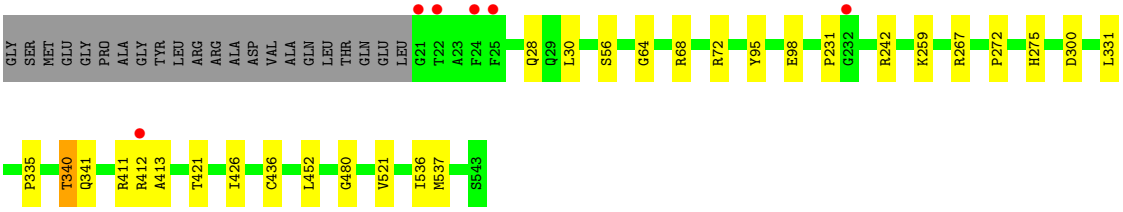
Chain C:



• Molecule 1: Pyruvate kinase PKLR

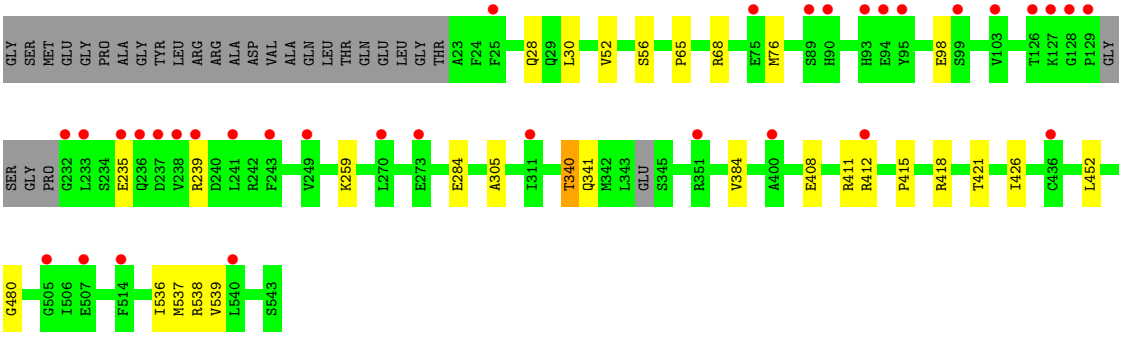
Chain D:





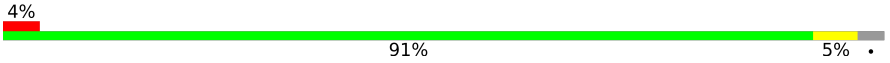
• Molecule 1: Pyruvate kinase PKLR

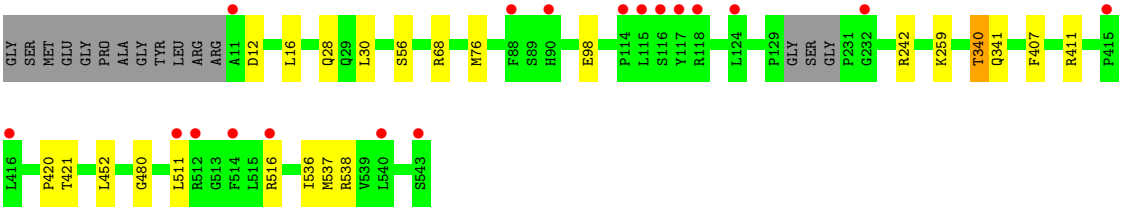
Chain E:



• Molecule 1: Pyruvate kinase PKLR

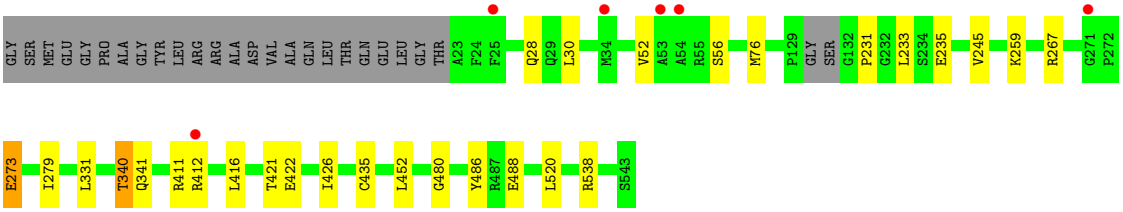
Chain F:





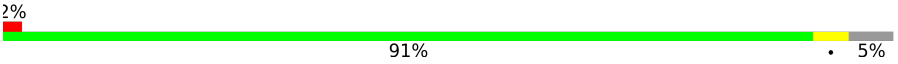
• Molecule 1: Pyruvate kinase PKLR

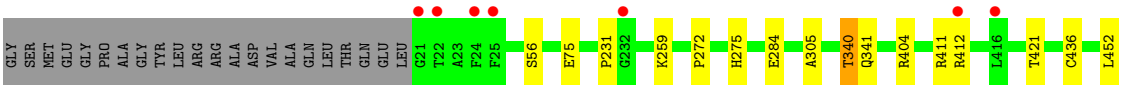
Chain G:

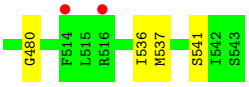


• Molecule 1: Pyruvate kinase PKLR

Chain H:






G480
F514
L515
R516
I536
M537
S541
I542
S543

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.75Å 113.24Å 189.40Å 90.00° 90.62° 90.00°	Depositor
Resolution (Å)	189.39 – 2.18 189.39 – 2.18	Depositor EDS
% Data completeness (in resolution range)	89.2 (189.39-2.18) 89.2 (189.39-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.209 , 0.234 0.199 , 0.221	Depositor DCC
R_{free} test set	10163 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.6	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	0.95	EDS
Total number of atoms	28228	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 40.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6688e-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: K, MG, OXL, O8O, FBP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/3307	0.55	0/4469
1	B	0.38	0/3396	0.53	0/4592
1	C	0.43	0/3313	0.56	0/4479
1	D	0.45	0/3326	0.56	0/4497
1	E	0.36	0/3268	0.53	0/4415
1	F	0.38	0/3396	0.53	0/4591
1	G	0.42	0/3303	0.56	0/4465
1	H	0.43	0/3316	0.55	0/4483
All	All	0.40	0/26625	0.55	0/35991

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3236	0	3300	17	0
1	B	3329	0	3394	15	0
1	C	3247	0	3299	17	0
1	D	3252	0	3311	18	0
1	E	3201	0	3264	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3321	0	3394	12	0
1	G	3231	0	3285	20	0
1	H	3251	0	3307	12	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	38	19	0	0	0
6	D	38	19	0	1	0
6	E	38	19	0	0	0
6	H	38	19	0	0	0
7	A	169	0	0	0	0
7	B	153	0	0	0	0
7	C	230	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	283	0	0	2	0
7	E	152	0	0	0	0
7	F	173	0	0	0	0
7	G	236	0	0	0	0
7	H	312	0	0	2	0
All	All	28152	76	26634	109	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.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.67	0.77
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.67	0.77
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.71	0.71
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.05	0.71
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.73	0.68
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.76	0.68
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.76	0.68
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.76	0.67
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.75	0.67
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.77	0.67
1:D:411:ARG:HG3	1:D:426:ILE:HD11	1.78	0.66
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.30	0.65
1:D:68:ARG:NH2	1:D:95:TYR:O	2.30	0.65
1:A:517:VAL:HG22	1:A:543:SER:HB3	1.79	0.64
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.79	0.64
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.79	0.63
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.80	0.63
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.70	0.59
1:A:538:ARG:HG2	1:B:536:ILE:HG12	1.83	0.59
1:E:235:GLU:O	1:E:239:ARG:HD3	2.02	0.59
1:C:538:ARG:HD3	7:C:785:HOH:O	2.03	0.58
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.66	0.58
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.85	0.58
1:C:529:PRO:HG2	1:G:235:GLU:HG2	1.85	0.58
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.87	0.57
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.87	0.57
1:D:64:GLY:O	1:D:68:ARG:HG3	2.05	0.56
1:H:541:SER:HB2	7:H:951:HOH:O	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.89	0.55
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.89	0.55
6:D:605:O8O:O6	7:D:1901:HOH:O	2.17	0.53
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.90	0.53
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.90	0.53
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.39	0.52
1:G:411:ARG:HH21	1:H:411:ARG:NH2	2.08	0.52
1:A:412:ARG:NH1	1:B:404:ARG:HH11	2.07	0.52
1:C:287:GLU:HG2	1:C:291:ARG:HD2	1.93	0.51
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.93	0.51
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.47	0.50
1:E:408:GLU:O	1:E:412:ARG:HB2	2.12	0.50
1:C:340:THR:HG22	1:C:341:GLN:HG3	1.94	0.50
1:G:28:GLN:HB3	1:G:52:VAL:HG22	1.94	0.50
1:A:28:GLN:HB3	1:A:52:VAL:HG22	1.93	0.49
1:G:267:ARG:HG2	1:G:279:ILE:CD1	2.43	0.49
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.47	0.49
1:C:416:LEU:HD13	1:D:436:CYS:SG	2.53	0.49
1:H:56:SER:HB2	1:H:480:GLY:CA	2.43	0.49
1:E:415:PRO:HB3	1:F:12:ASP:HA	1.95	0.48
1:E:418:ARG:HD3	1:F:16:LEU:HD11	1.95	0.48
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.96	0.48
1:G:56:SER:HB2	1:G:480:GLY:CA	2.43	0.47
1:E:28:GLN:HB3	1:E:52:VAL:HG22	1.96	0.47
1:C:28:GLN:HB3	1:C:52:VAL:HG22	1.96	0.47
1:C:528:ARG:HH22	1:G:233:LEU:HB3	1.79	0.47
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.49	0.47
1:H:421:THR:HG22	1:H:452:LEU:HD12	1.97	0.47
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.97	0.47
1:D:267:ARG:HD2	7:D:2155:HOH:O	2.15	0.46
1:A:436:CYS:SG	1:B:416:LEU:HD13	2.55	0.46
1:G:267:ARG:HG2	1:G:279:ILE:HD12	1.96	0.46
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.97	0.46
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.97	0.46
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.52	0.45
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.97	0.45
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.47	0.45
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.99	0.45
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.99	0.45
1:C:110:PHE:O	1:C:117:TYR:HB2	2.17	0.45
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:SER:HA	1:A:72:ARG:HG2	1.99	0.44
1:F:56:SER:HB2	1:F:480:GLY:CA	2.48	0.44
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.99	0.44
1:C:404:ARG:HD3	1:D:412:ARG:NH2	2.33	0.44
1:C:421:THR:HG22	1:C:452:LEU:HD12	2.00	0.44
1:D:331:LEU:CD1	1:D:413:ALA:HB1	2.47	0.44
1:D:411:ARG:CG	1:D:426:ILE:HD11	2.48	0.43
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.99	0.43
1:B:56:SER:HB2	1:B:480:GLY:CA	2.48	0.43
1:F:28:GLN:HG3	1:F:30:LEU:HG	2.01	0.43
1:A:28:GLN:HG3	1:A:30:LEU:HG	2.01	0.43
1:F:340:THR:HG22	1:F:341:GLN:HG3	2.01	0.43
1:C:407:PHE:O	1:C:411:ARG:HB2	2.18	0.42
1:H:284:GLU:HG2	1:H:305:ALA:HB3	2.01	0.42
1:E:76[B]:MET:HG2	1:E:384:VAL:HG22	2.02	0.42
1:D:56:SER:HB2	1:D:480:GLY:CA	2.49	0.42
1:B:300:ASP:O	1:B:335:PRO:HD2	2.20	0.42
1:G:411:ARG:HG3	1:G:426:ILE:HD11	2.02	0.42
1:E:56:SER:HB2	1:E:480:GLY:CA	2.49	0.42
1:G:435:CYS:HB2	1:G:520:LEU:HD12	2.02	0.42
1:B:28:GLN:HG3	1:B:30:LEU:HG	2.01	0.41
1:B:435:CYS:HB2	1:B:520:LEU:HD12	2.02	0.41
1:E:68:ARG:NH2	1:E:98:GLU:HB3	2.35	0.41
1:A:435:CYS:HB2	1:A:520:LEU:HD12	2.01	0.41
1:G:416:LEU:HD13	1:H:436:CYS:SG	2.60	0.41
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.34	0.41
1:D:28:GLN:HG3	1:D:30:LEU:HG	2.03	0.41
1:E:284:GLU:HG2	1:E:305:ALA:HB3	2.01	0.41
1:B:284:GLU:HG2	1:B:305:ALA:HB3	2.02	0.41
1:E:28:GLN:HG3	1:E:30:LEU:HG	2.02	0.41
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.36	0.41
1:H:340:THR:HG22	1:H:341:GLN:HG3	2.02	0.41
1:C:56:SER:HB2	1:C:480:GLY:CA	2.50	0.40
1:G:28:GLN:HG3	1:G:30:LEU:HG	2.03	0.40
1:A:284:GLU:HG2	1:A:305:ALA:HB3	2.03	0.40
1:B:335:PRO:HB3	1:B:477:LEU:O	2.22	0.40
1:C:529:PRO:CG	1:G:235:GLU:HG2	2.50	0.40
1:D:300:ASP:O	1:D:335:PRO:HD2	2.21	0.40
1:A:76[B]:MET:HG2	1:A:384:VAL:HG22	2.04	0.40
1:H:75:GLU:HG3	7:H:997:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/447 (95%)	419 (99%)	4 (1%)	1 (0%)	47	52
1	B	438/447 (98%)	434 (99%)	2 (0%)	2 (0%)	29	28
1	C	425/447 (95%)	419 (99%)	4 (1%)	2 (0%)	29	28
1	D	429/447 (96%)	425 (99%)	2 (0%)	2 (0%)	29	28
1	E	417/447 (93%)	413 (99%)	3 (1%)	1 (0%)	47	52
1	F	435/447 (97%)	431 (99%)	3 (1%)	1 (0%)	47	52
1	G	423/447 (95%)	415 (98%)	6 (1%)	2 (0%)	29	28
1	H	427/447 (96%)	422 (99%)	3 (1%)	2 (0%)	29	28
All	All	3418/3576 (96%)	3378 (99%)	27 (1%)	13 (0%)	34	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	231	PRO
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR
1	H	231	PRO
1	D	231	PRO
1	B	231	PRO
1	G	231	PRO

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	340/352 (97%)	332 (98%)	8 (2%)	49	59
1	B	349/352 (99%)	339 (97%)	10 (3%)	42	51
1	C	341/352 (97%)	335 (98%)	6 (2%)	59	70
1	D	342/352 (97%)	336 (98%)	6 (2%)	59	70
1	E	337/352 (96%)	333 (99%)	4 (1%)	71	81
1	F	350/352 (99%)	342 (98%)	8 (2%)	50	60
1	G	340/352 (97%)	335 (98%)	5 (2%)	65	76
1	H	340/352 (97%)	337 (99%)	3 (1%)	78	87
All	All	2739/2816 (97%)	2689 (98%)	50 (2%)	65	70

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	86	LEU
1	A	235	GLU
1	A	259	LYS
1	A	531	SER
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	76[A]	MET
1	B	76[B]	MET
1	B	131	SER
1	B	259	LYS
1	B	263	VAL
1	B	379	LYS
1	B	412	ARG
1	B	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	65	PRO

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Mol	Chain	Res	Type
1	C	76[A]	MET
1	C	76[B]	MET
1	C	259	LYS
1	C	487	ARG
1	C	531	SER
1	D	72	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	259	LYS
1	D	521	VAL
1	D	537	MET
1	E	65	PRO
1	E	259	LYS
1	E	537[A]	MET
1	E	537[B]	MET
1	F	76[A]	MET
1	F	76[B]	MET
1	F	242	ARG
1	F	259	LYS
1	F	511	LEU
1	F	516	ARG
1	F	537[A]	MET
1	F	537[B]	MET
1	G	76[A]	MET
1	G	76[B]	MET
1	G	259	LYS
1	G	273	GLU
1	G	331	LEU
1	H	259	LYS
1	H	412	ARG
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	FBP	H	602	-	18,20,20	0.81	0	23,32,32	0.66	0
3	OXL	H	603	4	5,5,5	1.75	2 (40%)	6,6,6	0.94	0
2	FBP	C	601	-	18,20,20	0.62	0	23,32,32	0.94	1 (4%)
6	O8O	E	605	-	42,42,42	2.12	13 (30%)	61,66,66	2.38	19 (31%)
6	O8O	D	605	-	42,42,42	2.24	11 (26%)	61,66,66	2.28	15 (24%)
3	OXL	C	602	4	5,5,5	1.91	2 (40%)	6,6,6	0.72	0
6	O8O	A	605	-	42,42,42	2.23	10 (23%)	61,66,66	2.30	18 (29%)
2	FBP	E	601	-	18,20,20	0.39	0	23,32,32	0.76	1 (4%)
3	OXL	A	602	4	5,5,5	1.96	2 (40%)	6,6,6	1.05	1 (16%)
3	OXL	G	602	4	5,5,5	1.97	2 (40%)	6,6,6	1.58	2 (33%)
2	FBP	A	601	-	18,20,20	0.61	0	23,32,32	0.74	1 (4%)
3	OXL	B	602	4	5,5,5	2.13	2 (40%)	6,6,6	0.92	0
2	FBP	F	601	-	18,20,20	0.33	0	23,32,32	0.72	0
2	FBP	D	601	-	18,20,20	0.68	1 (5%)	23,32,32	0.78	1 (4%)
6	O8O	H	601	-	42,42,42	2.38	13 (30%)	61,66,66	2.63	15 (24%)
2	FBP	G	601	-	18,20,20	0.44	0	23,32,32	0.76	1 (4%)
3	OXL	D	602	4	5,5,5	2.06	2 (40%)	6,6,6	1.60	2 (33%)
3	OXL	F	602	4	5,5,5	2.64	4 (80%)	6,6,6	1.56	2 (33%)
3	OXL	E	602	4	5,5,5	2.03	2 (40%)	6,6,6	0.79	0
2	FBP	B	601	-	18,20,20	0.68	0	23,32,32	0.73	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
2	FBP	H	602	-	-	2/13/32/32	0/1/1/1
3	OXL	H	603	4	-	0/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
6	O8O	E	605	-	-	0/16/36/36	0/4/5/5
6	O8O	D	605	-	-	0/16/36/36	0/4/5/5
3	OXL	C	602	4	-	0/4/4/4	-
6	O8O	A	605	-	-	0/16/36/36	0/4/5/5
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	4	-	1/4/4/4	-
3	OXL	G	602	4	-	0/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	1/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
6	O8O	H	601	-	-	0/16/36/36	0/4/5/5
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	4	-	0/4/4/4	-
3	OXL	F	602	4	-	0/4/4/4	-
3	OXL	E	602	4	-	0/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	605	O8O	C22-S1	-7.92	1.64	1.75
6	D	605	O8O	C22-S1	-7.81	1.64	1.75
6	A	605	O8O	C22-S1	-7.74	1.64	1.75
6	H	601	O8O	C22-S1	-7.22	1.65	1.75
6	H	601	O8O	C3-C8	6.13	1.48	1.41
6	D	605	O8O	S1-N	5.37	1.73	1.64
6	H	601	O8O	S1-N	5.31	1.73	1.64
6	H	601	O8O	C14-S	-4.73	1.69	1.77
6	A	605	O8O	C15-C14	4.72	1.46	1.38
6	A	605	O8O	S1-N	4.61	1.72	1.64
6	A	605	O8O	C14-S	-4.49	1.70	1.77
6	H	601	O8O	C9-C10	4.47	1.59	1.51
6	D	605	O8O	C3-C8	4.40	1.46	1.41
6	E	605	O8O	S1-N	4.16	1.71	1.64
6	D	605	O8O	C15-C14	3.98	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXL	O2-C2	3.92	1.33	1.22
6	A	605	O8O	C3-C8	3.84	1.45	1.41
6	D	605	O8O	C14-S	-3.66	1.71	1.77
3	E	602	OXL	O1-C1	3.63	1.32	1.22
6	A	605	O8O	C9-C10	3.63	1.58	1.51
3	C	602	OXL	O1-C1	3.60	1.32	1.22
6	E	605	O8O	C23-C22	3.53	1.44	1.39
3	A	602	OXL	O2-C2	3.51	1.32	1.22
3	D	602	OXL	O2-C2	3.46	1.31	1.22
3	F	602	OXL	O2-C2	3.34	1.31	1.22
6	D	605	O8O	C9-C10	3.28	1.57	1.51
6	E	605	O8O	C15-C14	3.26	1.44	1.38
3	G	602	OXL	O1-C1	3.19	1.31	1.22
6	E	605	O8O	C14-S	-3.15	1.72	1.77
6	H	601	O8O	C23-C22	3.14	1.44	1.39
3	F	602	OXL	O3-C1	-3.10	1.21	1.30
6	E	605	O8O	C24-C	3.06	1.45	1.40
6	E	605	O8O	C9-C10	2.96	1.56	1.51
6	A	605	O8O	C24-C	2.95	1.44	1.40
3	D	602	OXL	O4-C2	-2.94	1.22	1.30
3	G	602	OXL	O3-C1	-2.88	1.22	1.30
3	H	603	OXL	O2-C2	2.86	1.30	1.22
6	H	601	O8O	C11-C12	2.81	1.43	1.38
6	E	605	O8O	C8-N	-2.79	1.40	1.43
3	F	602	OXL	O1-C1	2.76	1.30	1.22
6	E	605	O8O	C3-C8	2.75	1.44	1.41
6	H	601	O8O	O6-S	2.69	1.49	1.44
6	D	605	O8O	C13-S	-2.68	1.72	1.77
3	E	602	OXL	O3-C1	-2.66	1.22	1.30
6	H	601	O8O	C24-C	2.64	1.44	1.40
6	A	605	O8O	C17-C18	2.62	1.44	1.40
3	B	602	OXL	O4-C2	-2.61	1.23	1.30
6	E	605	O8O	C20-C21	2.55	1.43	1.38
3	H	603	OXL	O4-C2	-2.54	1.23	1.30
3	F	602	OXL	O4-C2	-2.53	1.23	1.30
6	D	605	O8O	C20-C13	2.52	1.42	1.38
6	A	605	O8O	C23-C22	2.51	1.43	1.39
6	E	605	O8O	O5-S	2.45	1.48	1.44
3	A	602	OXL	O4-C2	-2.43	1.23	1.30
6	D	605	O8O	C1-C	2.42	1.42	1.38
3	C	602	OXL	O3-C1	-2.24	1.24	1.30
6	D	605	O8O	C5-C6	2.23	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	O8O	C8-N	-2.21	1.41	1.43
6	H	601	O8O	C2-C22	2.14	1.43	1.40
6	H	601	O8O	C15-C14	2.13	1.42	1.38
6	H	601	O8O	C12-C13	2.06	1.42	1.38
6	E	605	O8O	C19-C18	2.05	1.41	1.38
6	E	605	O8O	C2-C22	2.04	1.43	1.40
2	D	601	FBP	P2-O5P	-2.01	1.47	1.54
6	D	605	O8O	C9-N	-2.01	1.46	1.49
6	H	601	O8O	C9-N	-2.00	1.46	1.49

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	601	O8O	O6-S-C13	8.55	117.61	107.97
6	H	601	O8O	O8-S1-N	8.40	117.39	108.13
6	E	605	O8O	O5-S-C13	7.38	116.29	107.97
6	A	605	O8O	O8-S1-N	6.92	115.76	108.13
6	H	601	O8O	C22-S1-N	-6.75	91.49	101.82
6	D	605	O8O	O8-S1-N	6.74	115.57	108.13
6	A	605	O8O	C22-S1-N	-6.71	91.56	101.82
6	D	605	O8O	C22-S1-N	-6.51	91.86	101.82
6	A	605	O8O	O8-S1-C22	6.03	116.85	109.13
6	E	605	O8O	C22-S1-N	-5.75	93.02	101.82
6	D	605	O8O	O8-S1-C22	5.66	116.39	109.13
6	H	601	O8O	C12-C13-S	5.17	126.11	119.52
6	E	605	O8O	O8-S1-C22	4.97	115.50	109.13
6	E	605	O8O	C20-C13-S	4.91	125.78	119.52
6	H	601	O8O	O8-S1-C22	4.71	115.17	109.13
6	E	605	O8O	C12-C13-C20	-4.69	113.89	120.44
6	H	601	O8O	C12-C13-C20	-4.65	113.95	120.44
6	H	601	O8O	C21-C20-C13	4.57	124.18	119.45
6	D	605	O8O	C2-C22-S1	4.54	122.80	117.27
6	E	605	O8O	C11-C12-C13	4.50	124.11	119.45
6	A	605	O8O	O7-S1-O8	-4.50	113.07	118.59
6	E	605	O8O	C2-C22-S1	4.31	122.52	117.27
6	A	605	O8O	C12-C13-C20	-4.29	114.46	120.44
6	D	605	O8O	C12-C13-C20	-4.24	114.52	120.44
6	D	605	O8O	C20-C13-S	4.21	124.88	119.52
6	H	601	O8O	O7-S1-O8	-4.20	113.44	118.59
6	A	605	O8O	C2-C22-S1	3.96	122.09	117.27
6	H	601	O8O	C2-C22-S1	3.93	122.06	117.27
6	A	605	O8O	C20-C13-S	3.85	124.42	119.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	605	O8O	O7-S1-O8	-3.84	113.88	118.59
6	E	605	O8O	O8-S1-N	3.78	112.30	108.13
6	D	605	O8O	C16-C15-C14	3.73	123.31	119.45
6	D	605	O8O	C11-C12-C13	3.66	123.24	119.45
6	E	605	O8O	C16-C15-C14	3.59	123.16	119.45
6	A	605	O8O	C11-C12-C13	3.58	123.15	119.45
6	H	601	O8O	O5-S-C13	-3.43	104.11	107.97
6	A	605	O8O	C16-C15-C14	3.41	122.97	119.45
6	E	605	O8O	C21-C20-C13	3.36	122.92	119.45
6	E	605	O8O	O7-S1-O8	-3.35	114.47	118.59
6	D	605	O8O	O6-S-C14	-3.35	104.20	107.97
6	E	605	O8O	C15-C14-C19	-3.32	116.54	120.62
6	E	605	O8O	C19-C14-S	3.25	123.13	119.21
6	A	605	O8O	C21-C20-C13	3.15	122.71	119.45
6	D	605	O8O	C15-C14-C19	-3.12	116.79	120.62
6	E	605	O8O	O6-S-C13	-3.03	104.56	107.97
6	D	605	O8O	C21-C20-C13	2.91	122.46	119.45
6	H	601	O8O	C11-C12-C13	2.91	122.45	119.45
6	A	605	O8O	C15-C14-C19	-2.86	117.11	120.62
6	E	605	O8O	O5-S-C14	-2.82	104.80	107.97
6	H	601	O8O	C9-C10-C11	2.72	125.89	120.77
6	D	605	O8O	O1-C5-C6	2.70	125.66	118.45
6	H	601	O8O	C16-C15-C14	2.69	122.23	119.45
6	A	605	O8O	O6-S-C14	-2.62	105.02	107.97
6	A	605	O8O	O1-C5-C6	2.57	125.31	118.45
6	E	605	O8O	O3-C17-C18	2.51	125.13	118.45
2	C	601	FBP	O6-P2-O4P	2.46	113.38	106.47
3	F	602	OXL	O4-C2-C1	2.43	120.37	113.16
6	A	605	O8O	O3-C17-C18	2.41	124.88	118.45
6	E	605	O8O	O1-C5-C6	2.38	124.80	118.45
3	D	602	OXL	O4-C2-C1	2.38	120.23	113.16
2	D	601	FBP	O5P-P2-O6	2.37	113.03	106.73
6	A	605	O8O	C19-C18-C17	2.34	121.94	119.86
3	D	602	OXL	O3-C1-C2	2.33	120.08	113.16
3	G	602	OXL	O3-C1-C2	2.30	119.99	113.16
6	D	605	O8O	O3-C17-C18	2.29	124.54	118.45
2	A	601	FBP	P1-O1-C1	2.25	124.49	118.30
3	F	602	OXL	O3-C1-C2	2.24	119.81	113.16
3	G	602	OXL	O4-C2-C1	2.23	119.80	113.16
2	E	601	FBP	O3P-P1-O2P	2.23	116.16	107.64
6	E	605	O8O	O7-S1-C22	2.20	111.95	109.13
6	A	605	O8O	O6-S-C13	2.18	110.43	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	605	O8O	O-C-C24	2.16	124.22	118.45
6	A	605	O8O	C15-C16-C17	-2.14	118.30	120.50
6	D	605	O8O	O6-S-C13	2.10	110.34	107.97
6	H	601	O8O	O3-C17-C18	2.08	123.99	118.45
6	E	605	O8O	O-C-C24	2.06	123.94	118.45
3	A	602	OXL	O4-C2-C1	2.04	119.22	113.16
2	G	601	FBP	O3P-P1-O2P	2.01	115.33	107.64
6	H	601	O8O	C15-C14-C19	-2.00	118.16	120.62

There are no chirality outliers.

All (18) 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
2	F	601	FBP	C4-C5-C6-O6
2	H	602	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	G	601	FBP	O5-C5-C6-O6
2	H	602	FBP	O5-C5-C6-O6
3	A	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4

There are no ring outliers.

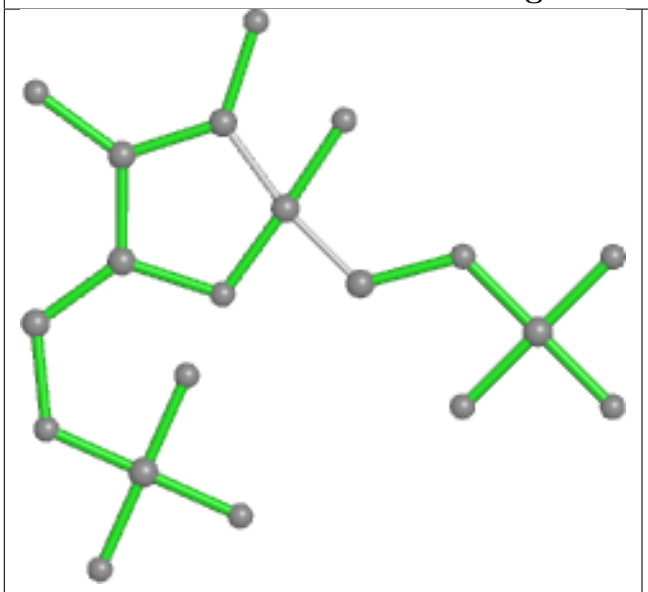
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	605	O8O	1	0

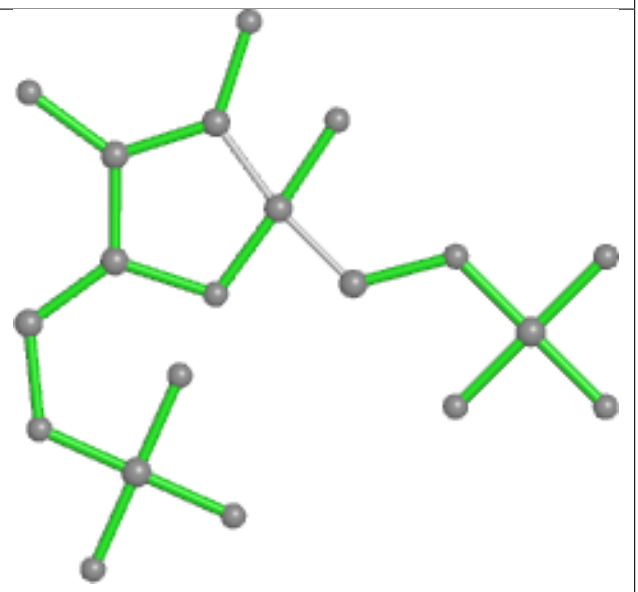
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

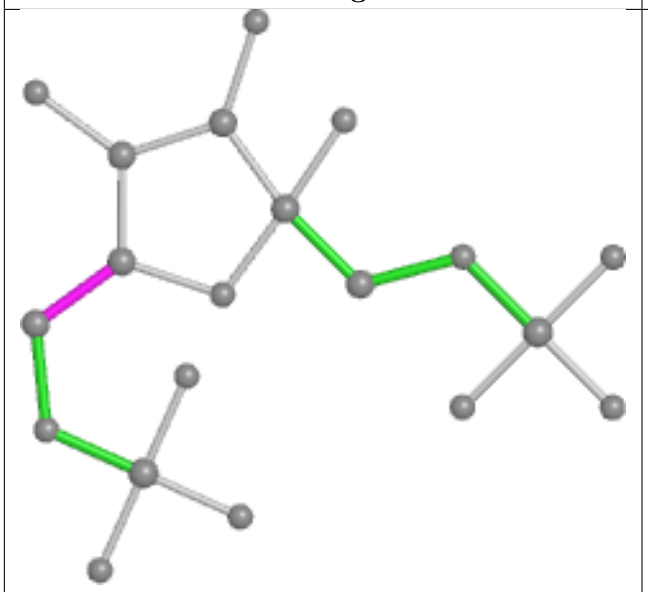
Ligand FBP H 602



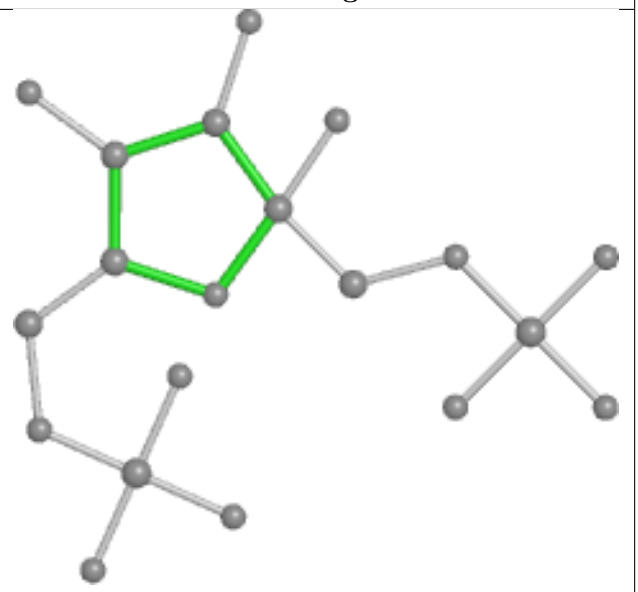
Bond lengths



Bond angles

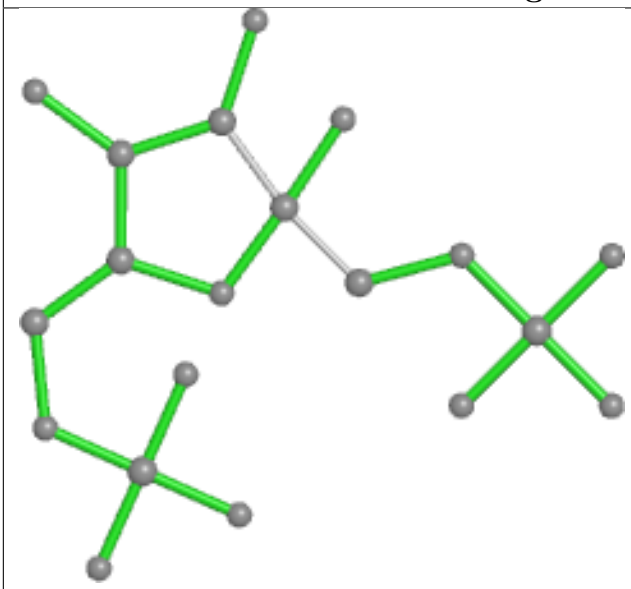


Torsions



Rings

Ligand FBP C 601



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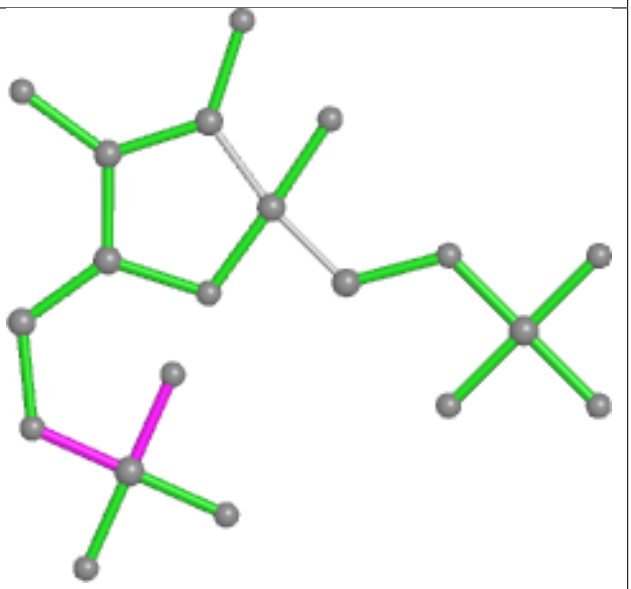

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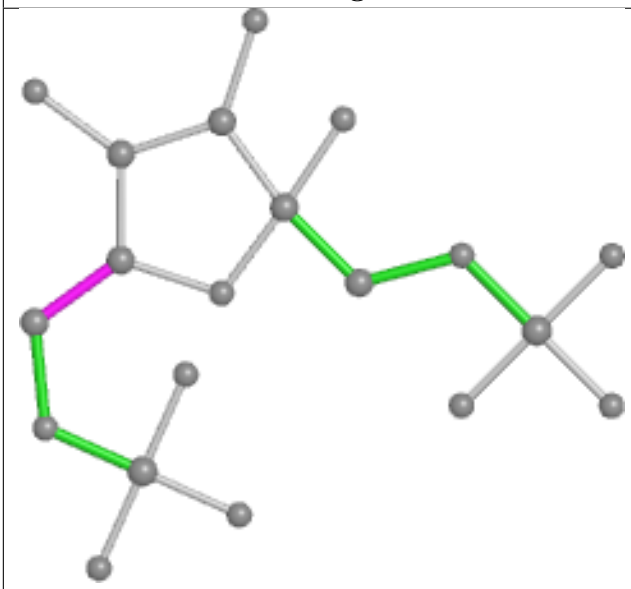

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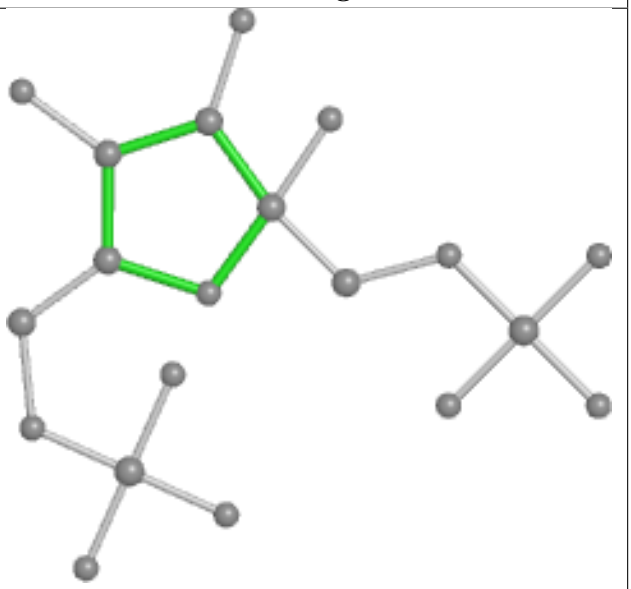
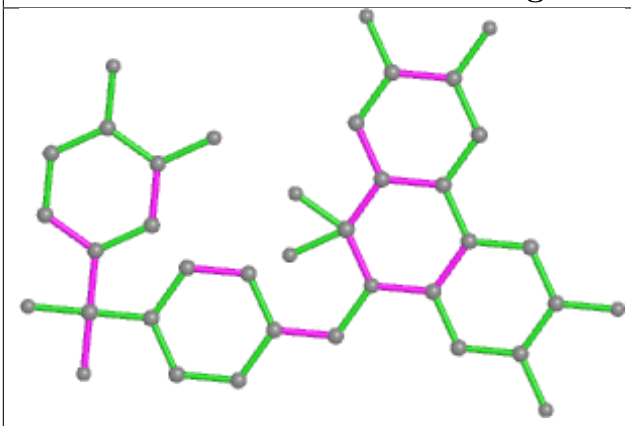


Rings

Ligand O8O E 605



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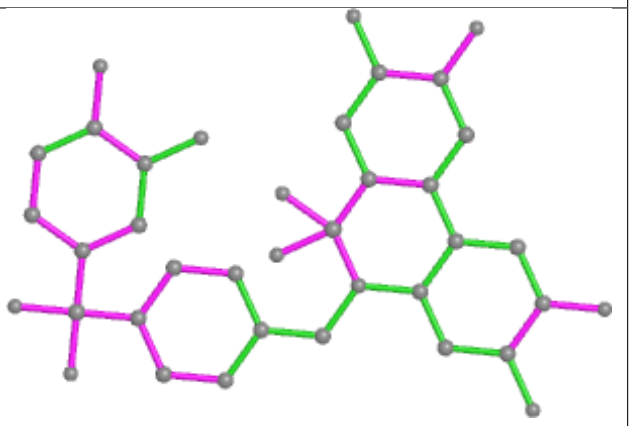

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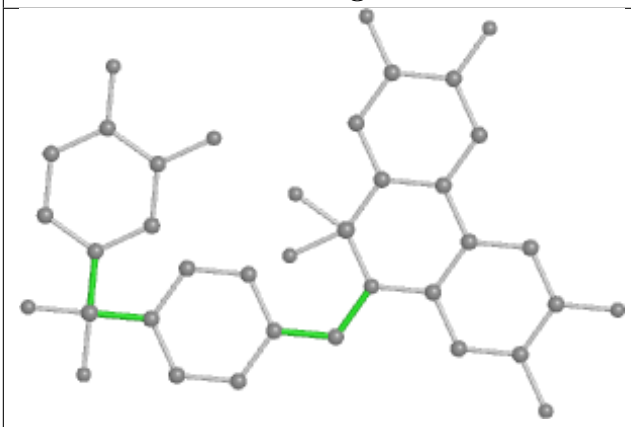

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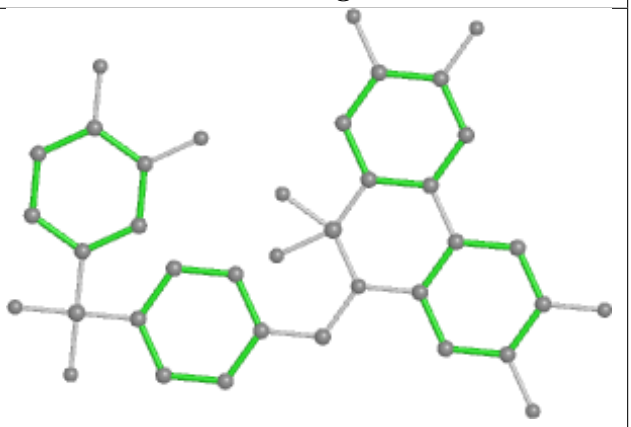
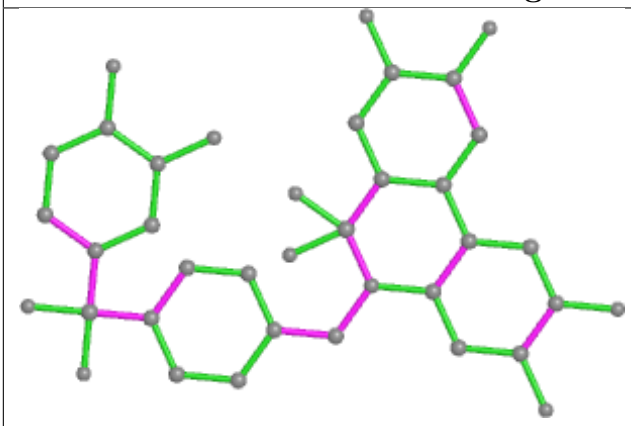


Rings

Ligand O8O D 605



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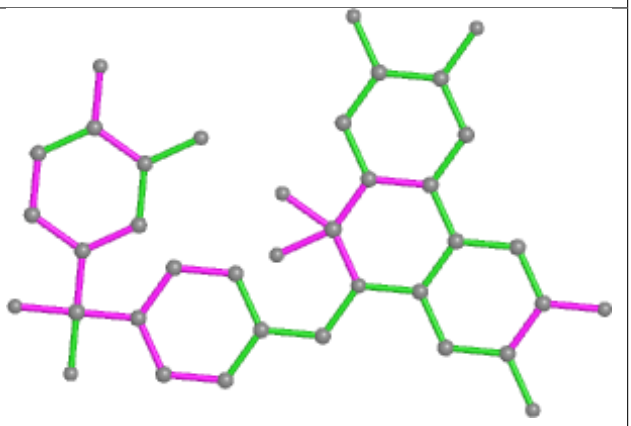

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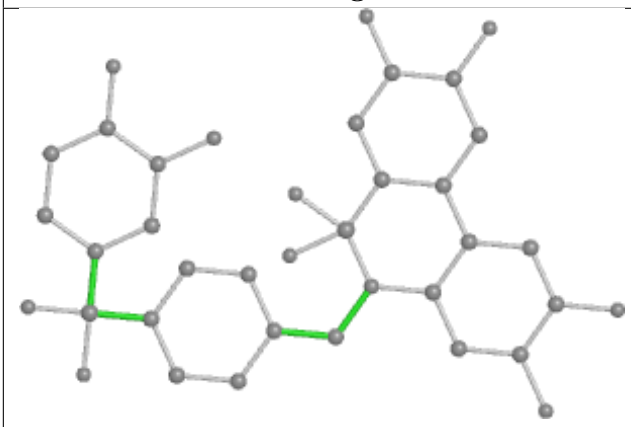

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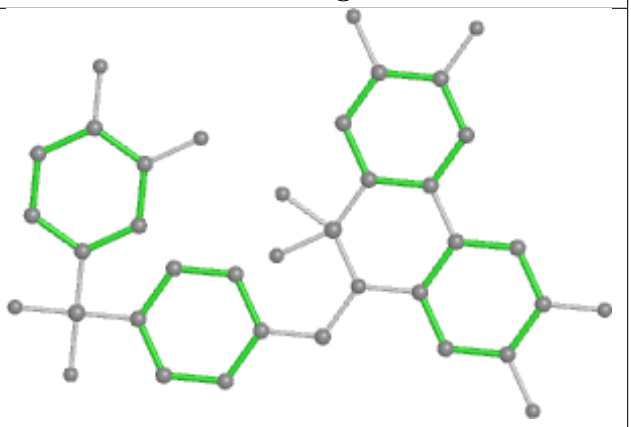
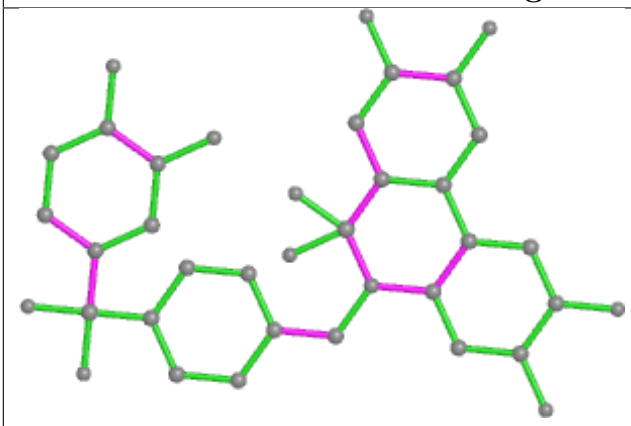


Rings

Ligand O8O A 605



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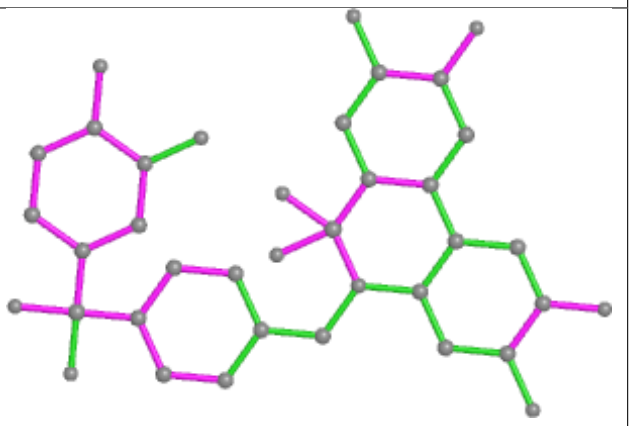

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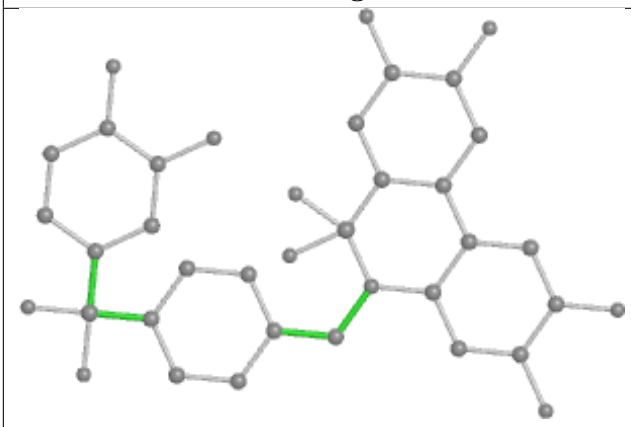

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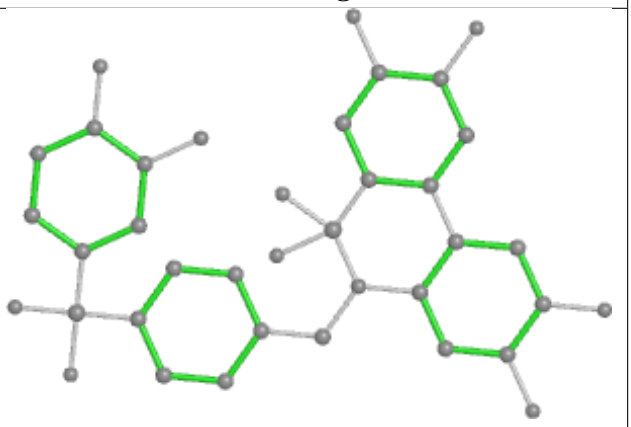
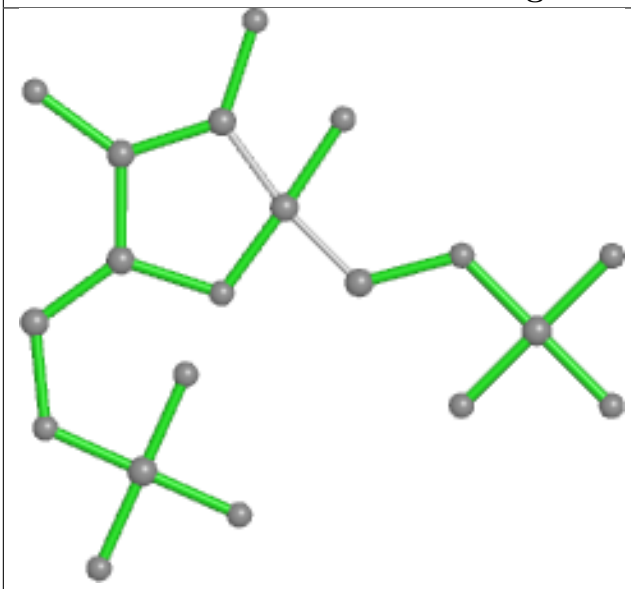


Rings

Ligand FBP E 601



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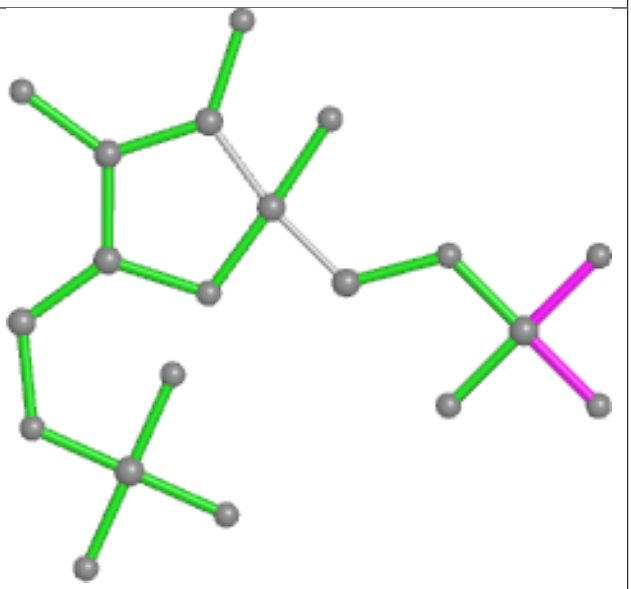

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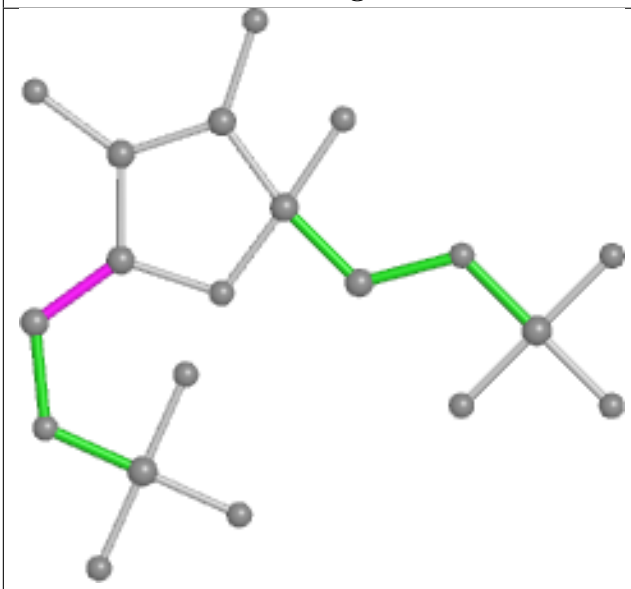

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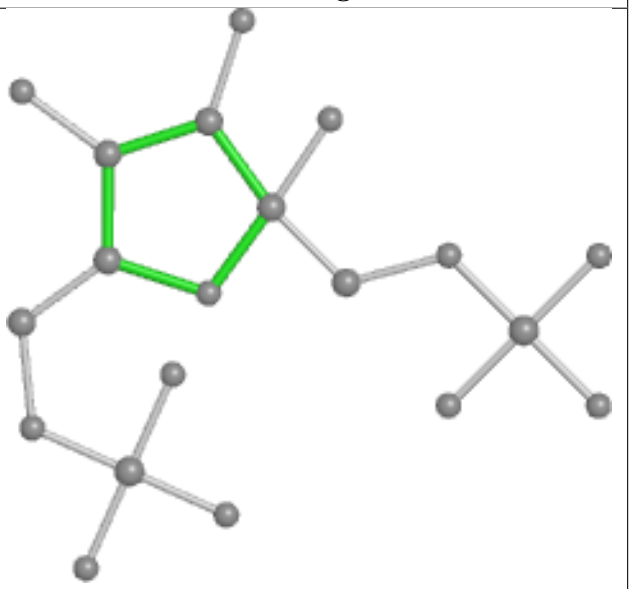
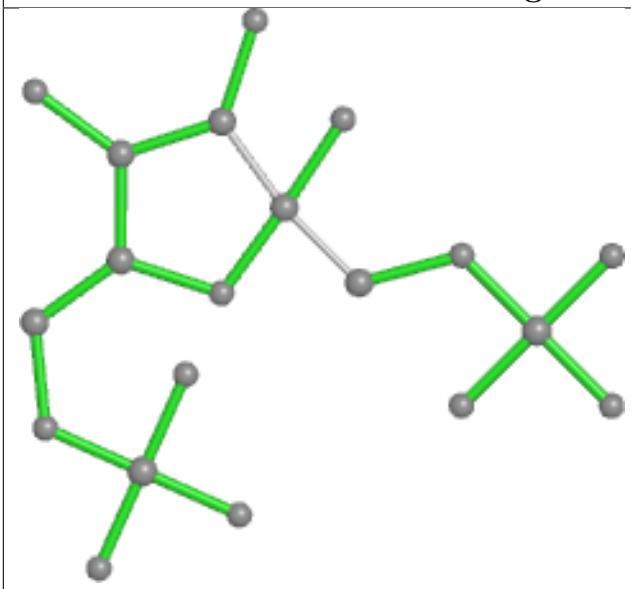
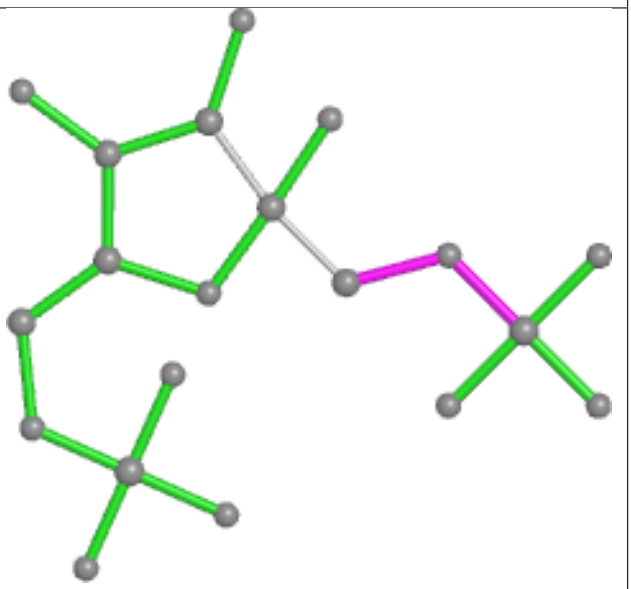


Rings

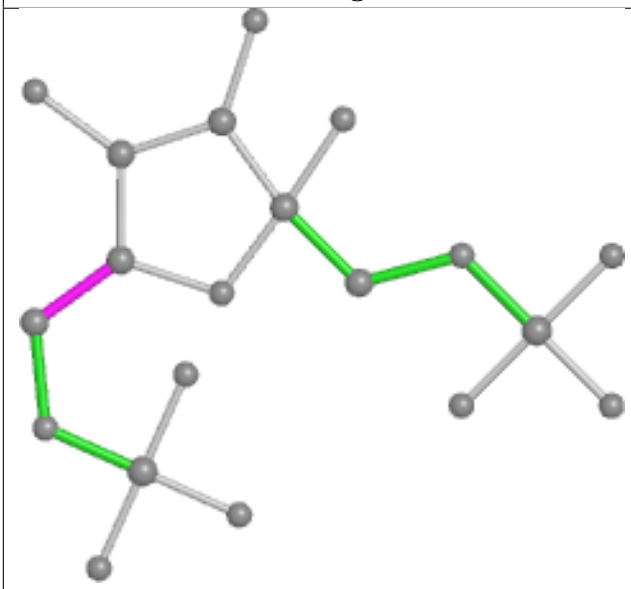
Ligand FBP A 601



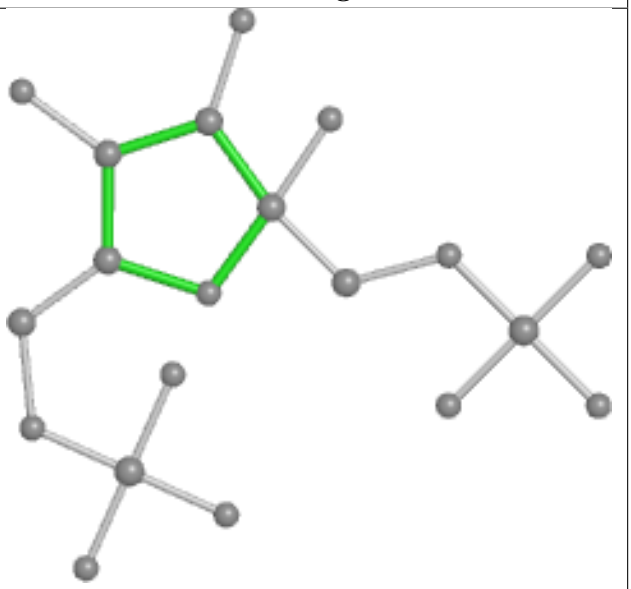
Bond lengths



Bond angles

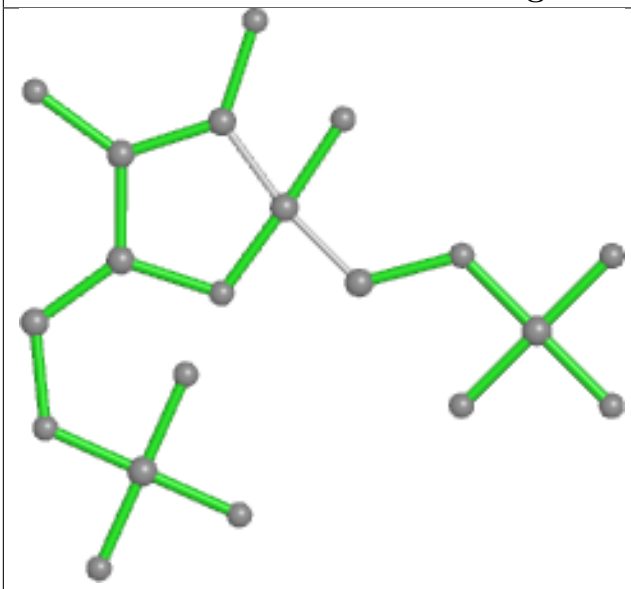


Torsions

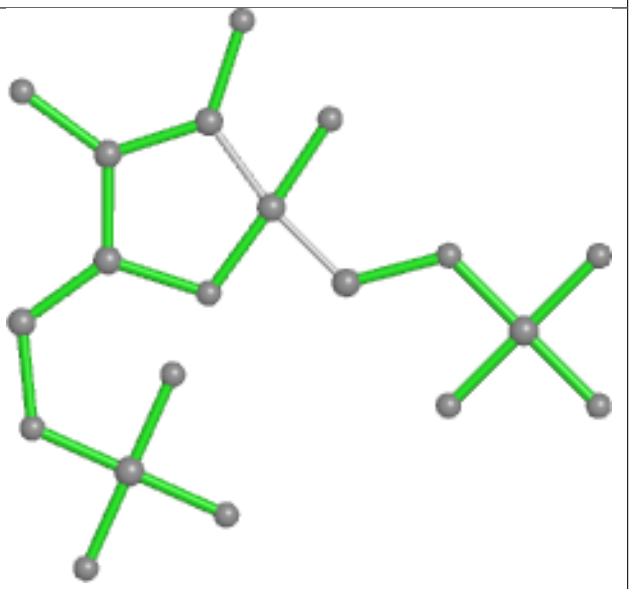


Rings

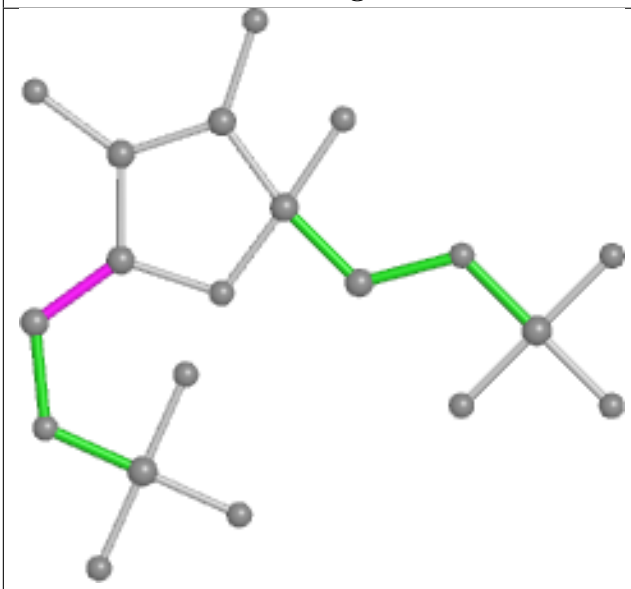
Ligand FBP F 601



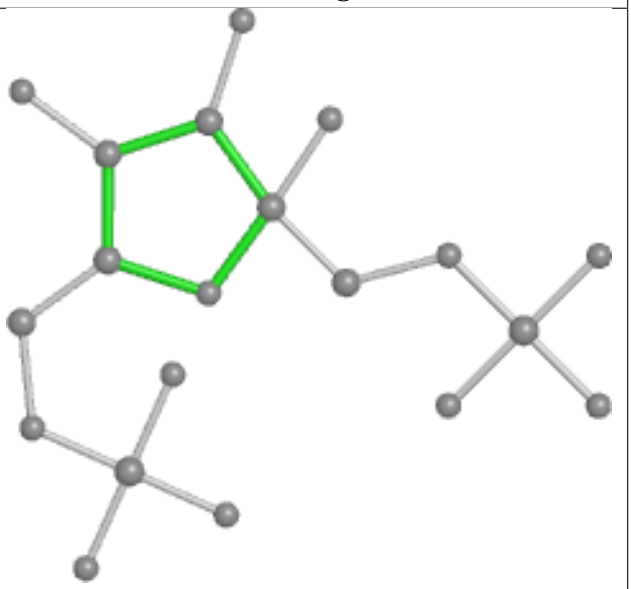
Bond lengths



Bond angles

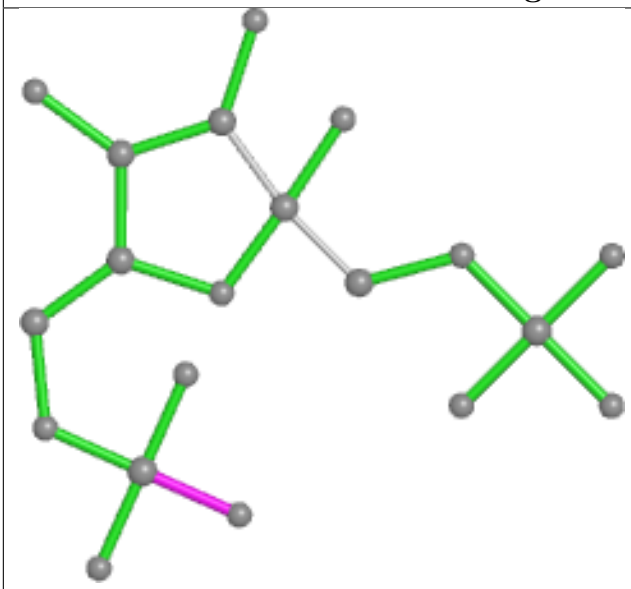


Torsions

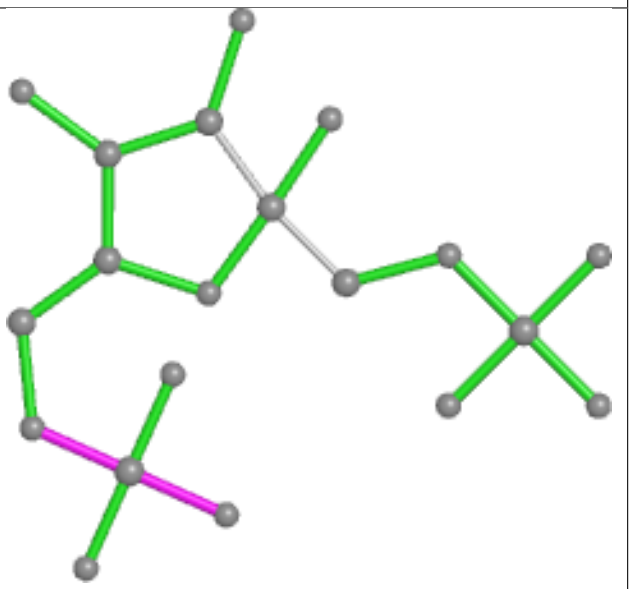


Rings

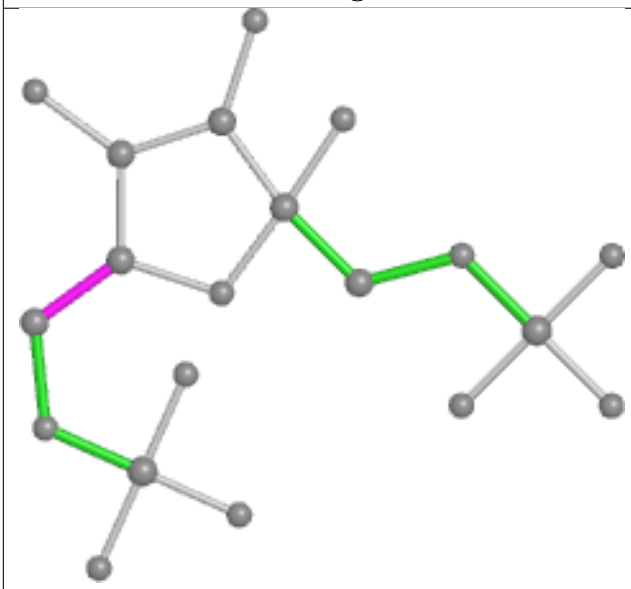
Ligand FBP D 601



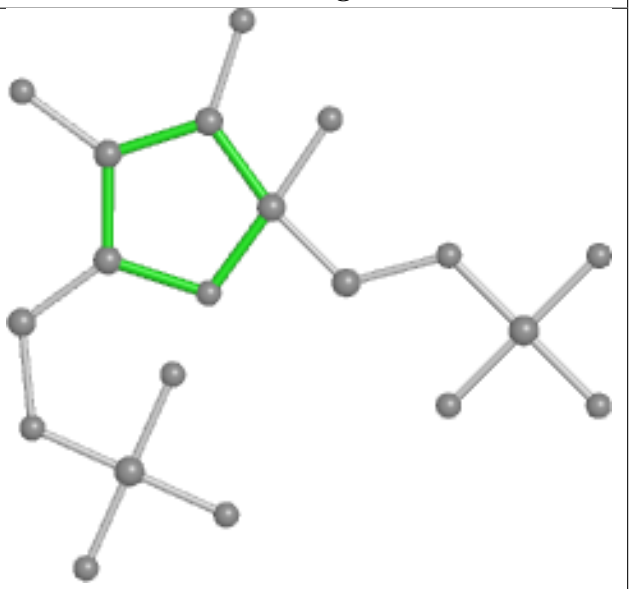
Bond lengths



Bond angles

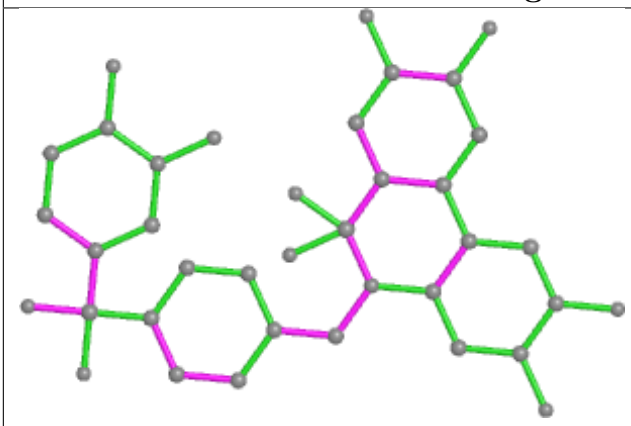


Torsions

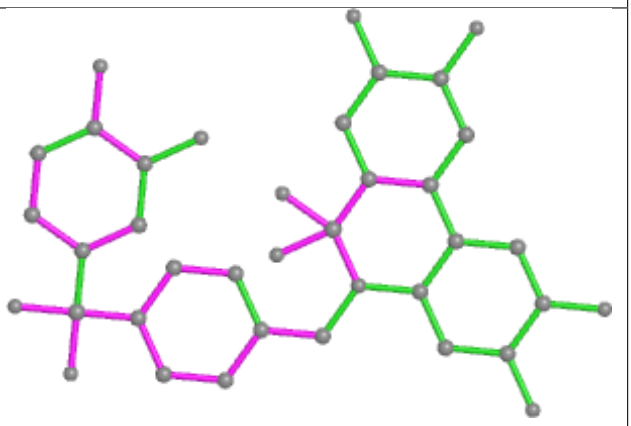


Rings

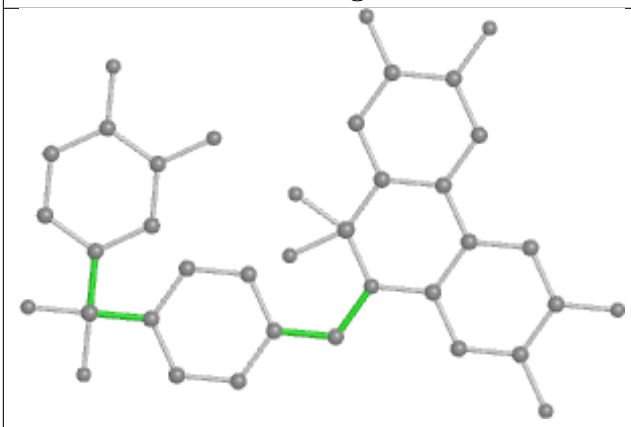
Ligand O8O H 601



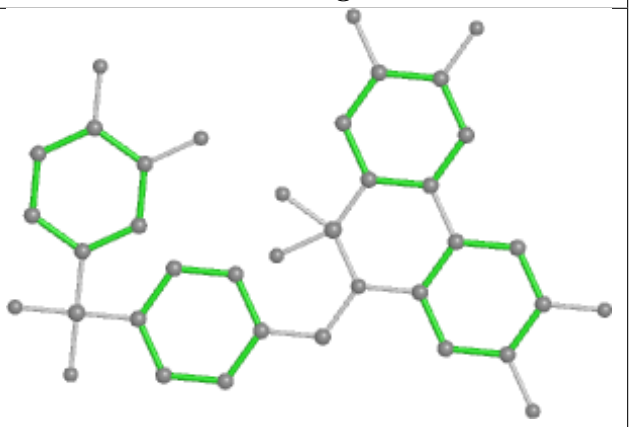
Bond lengths



Bond angles

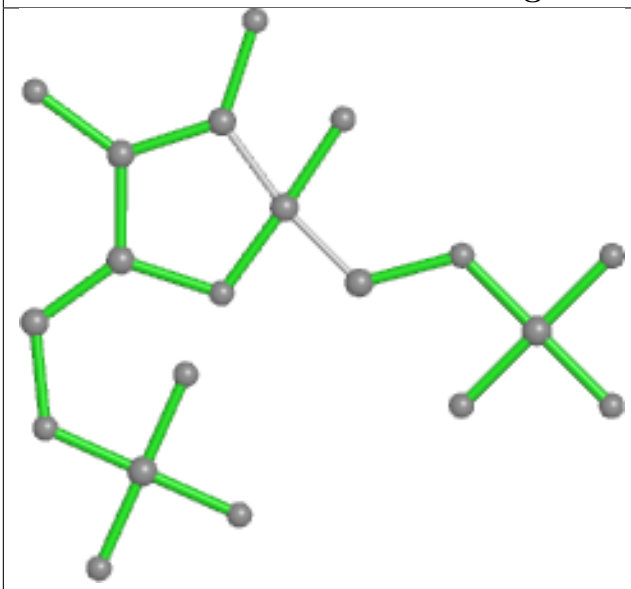


Torsions

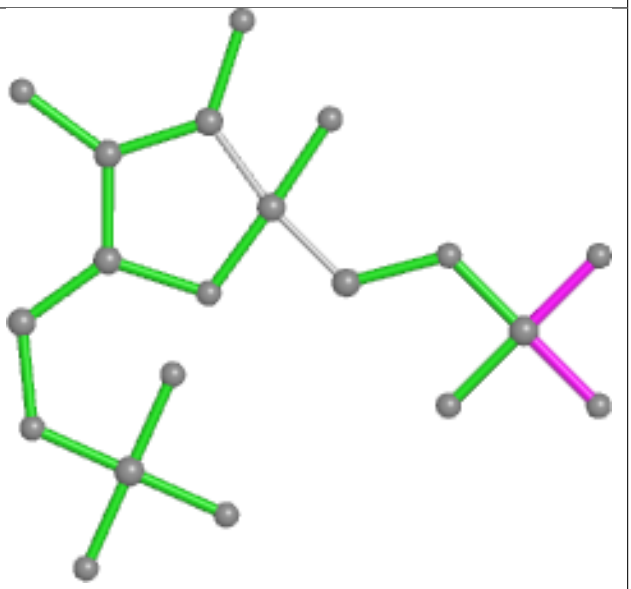


Rings

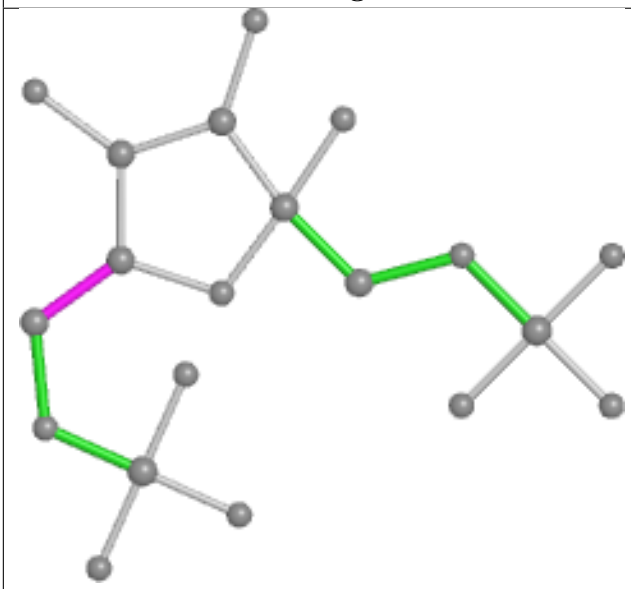
Ligand FBP G 601



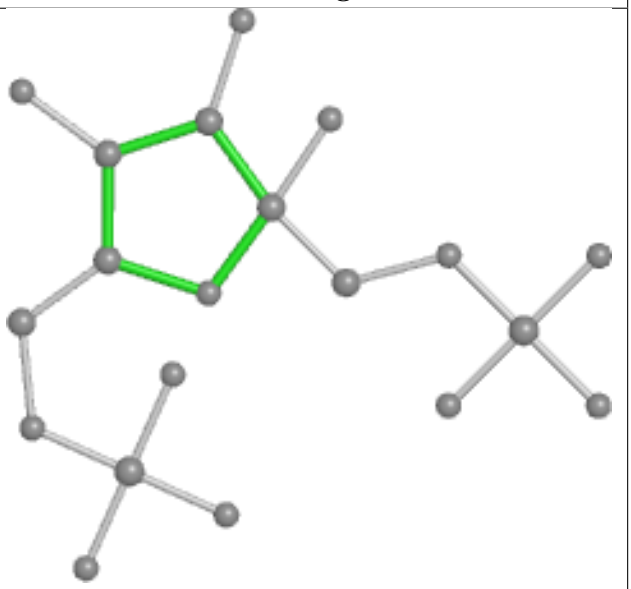
Bond lengths



Bond angles

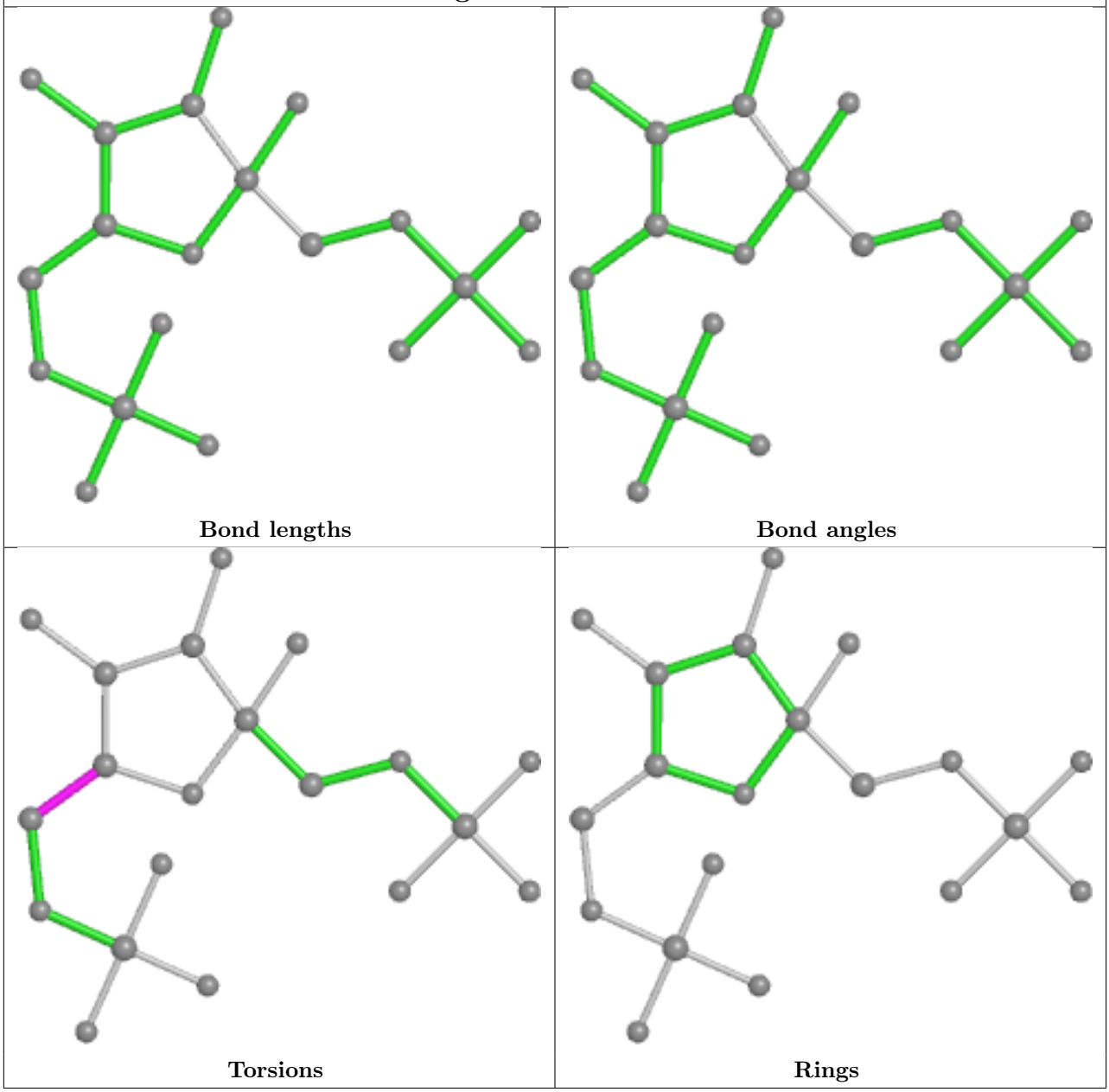


Torsions



Rings

Ligand FBP B 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	422/447 (94%)	0.38	23 (5%) 25 26	42, 56, 82, 98	0
1	B	436/447 (97%)	0.38	26 (5%) 21 23	36, 54, 86, 102	0
1	C	425/447 (95%)	0.16	7 (1%) 72 72	32, 45, 68, 112	0
1	D	425/447 (95%)	0.18	6 (1%) 75 75	31, 40, 62, 103	0
1	E	418/447 (93%)	0.47	34 (8%) 12 12	42, 58, 88, 109	0
1	F	432/447 (96%)	0.31	18 (4%) 36 37	37, 53, 82, 98	0
1	G	421/447 (94%)	0.12	6 (1%) 75 75	33, 44, 62, 82	1 (0%)
1	H	425/447 (95%)	0.15	9 (2%) 63 64	32, 41, 63, 84	0
All	All	3404/3576 (95%)	0.27	129 (3%) 40 41	31, 49, 80, 112	1 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	11.8
1	D	25	PHE	9.2
1	D	22	THR	9.1
1	A	25	PHE	8.4
1	E	25	PHE	7.4
1	B	115	LEU	7.1
1	F	511	LEU	5.9
1	H	25	PHE	5.7
1	G	25	PHE	5.6
1	F	115	LEU	5.3
1	F	116	SER	5.0
1	H	21	GLY	4.9
1	A	63	ILE	4.9
1	C	25	PHE	4.8
1	E	89	SER	4.5
1	A	114	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	270	LEU	4.4
1	B	130	GLY	4.3
1	F	11	ALA	4.2
1	B	10	ARG	4.0
1	A	273	GLU	3.8
1	E	243	PHE	3.8
1	A	540	LEU	3.7
1	E	412	ARG	3.7
1	H	516	ARG	3.6
1	D	24	PHE	3.6
1	D	21	GLY	3.5
1	F	416	LEU	3.5
1	B	232	GLY	3.4
1	A	118	ARG	3.3
1	C	22	THR	3.3
1	B	116	SER	3.3
1	B	88	PHE	3.3
1	B	236	GLN	3.3
1	F	516	ARG	3.3
1	A	482	PHE	3.2
1	E	540	LEU	3.2
1	E	129	PRO	3.2
1	H	412	ARG	3.2
1	D	232	GLY	3.1
1	E	90	HIS	3.1
1	A	24	PHE	3.1
1	A	129	PRO	3.1
1	B	416	LEU	3.1
1	A	511	LEU	3.1
1	F	514	PHE	3.0
1	B	131	SER	3.0
1	C	412	ARG	3.0
1	H	22	THR	3.0
1	F	232	GLY	3.0
1	B	233	LEU	2.9
1	H	232	GLY	2.9
1	A	88	PHE	2.9
1	B	516	ARG	2.9
1	B	12	ASP	2.9
1	D	412	ARG	2.8
1	B	540[A]	LEU	2.8
1	F	512	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	311	ILE	2.7
1	A	543	SER	2.7
1	A	412	ARG	2.7
1	F	90	HIS	2.7
1	F	117	TYR	2.7
1	E	103	VAL	2.7
1	B	543	SER	2.7
1	E	351	ARG	2.7
1	E	236	GLN	2.6
1	E	94	GLU	2.6
1	E	95	TYR	2.6
1	F	114	PRO	2.6
1	A	131	SER	2.6
1	H	514	PHE	2.6
1	B	114	PRO	2.6
1	C	132	GLY	2.6
1	B	490	PRO	2.5
1	A	84	ALA	2.5
1	A	242	ARG	2.5
1	E	75	GLU	2.5
1	A	116	SER	2.5
1	E	126	THR	2.4
1	B	415	PRO	2.4
1	E	232	GLY	2.4
1	F	543	SER	2.4
1	B	256	PHE	2.4
1	G	412	ARG	2.4
1	E	505	GLY	2.4
1	F	88	PHE	2.3
1	B	129	PRO	2.3
1	E	93	HIS	2.3
1	B	511	LEU	2.3
1	B	520	LEU	2.3
1	B	512	ARG	2.3
1	E	249	VAL	2.2
1	E	128	GLY	2.2
1	E	127	LYS	2.2
1	E	233	LEU	2.2
1	E	241	LEU	2.2
1	B	118	ARG	2.2
1	G	54	ALA	2.2
1	B	90	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	231	PRO	2.2
1	E	273	GLU	2.1
1	G	34	MET	2.1
1	A	244	GLY	2.1
1	E	235	GLU	2.1
1	C	21	GLY	2.1
1	G	53	ALA	2.1
1	B	61	ALA	2.1
1	E	400	ALA	2.1
1	E	237	ASP	2.1
1	F	118	ARG	2.1
1	E	514	PHE	2.1
1	F	540[A]	LEU	2.1
1	F	415	PRO	2.1
1	A	351	ARG	2.1
1	A	132	GLY	2.1
1	B	112	GLY	2.1
1	E	507	GLU	2.0
1	A	117	TYR	2.0
1	E	436	CYS	2.0
1	E	238	VAL	2.0
1	H	24	PHE	2.0
1	E	99	SER	2.0
1	A	377	THR	2.0
1	F	124	LEU	2.0
1	H	416	LEU	2.0
1	C	404	ARG	2.0
1	E	239	ARG	2.0
1	G	271	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

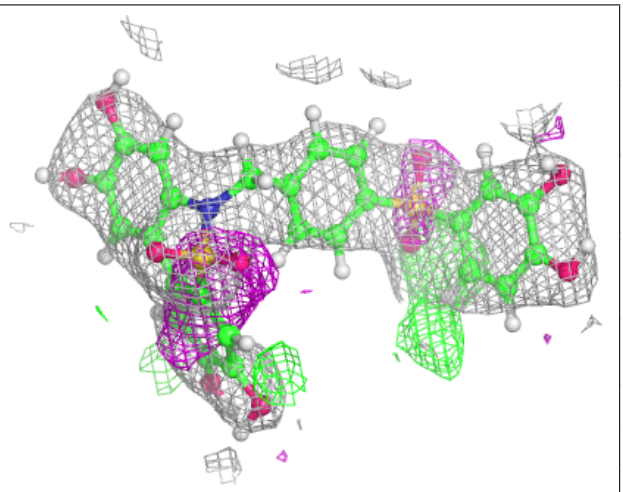
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

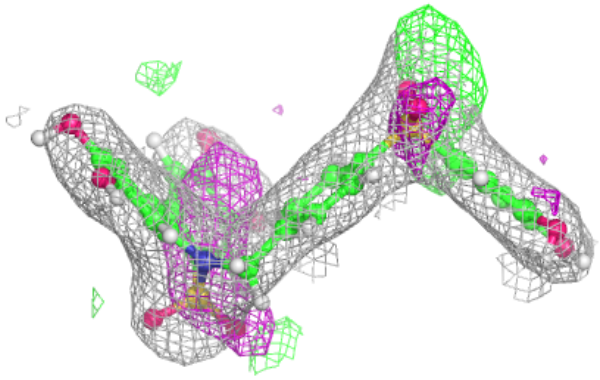
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OXL	A	602	6/6	0.86	0.31	77,77,77,77	0
6	O8O	E	605	38/38	0.86	0.20	56,63,67,69	19
5	K	E	604	1/1	0.87	0.62	105,105,105,105	0
6	O8O	H	601	38/38	0.87	0.17	47,53,56,57	19
5	K	D	604	1/1	0.88	0.07	60,60,60,60	0
6	O8O	A	605	38/38	0.90	0.15	51,57,62,62	19
5	K	F	604	1/1	0.90	0.18	91,91,91,91	0
5	K	H	605	1/1	0.90	0.06	66,66,66,66	0
4	MG	C	603	1/1	0.91	0.21	31,31,31,31	0
6	O8O	D	605	38/38	0.94	0.16	47,50,54,55	19
4	MG	H	604	1/1	0.94	0.21	30,30,30,30	0
3	OXL	G	602	6/6	0.94	0.14	50,50,51,52	0
4	MG	B	603	1/1	0.95	0.12	43,43,43,43	0
3	OXL	F	602	6/6	0.95	0.23	68,69,69,70	0
4	MG	D	603	1/1	0.95	0.25	33,33,33,33	0
3	OXL	B	602	6/6	0.95	0.14	64,65,66,66	0
3	OXL	C	602	6/6	0.96	0.15	49,50,50,50	0
5	K	G	604	1/1	0.96	0.10	69,69,69,69	0
3	OXL	H	603	6/6	0.96	0.20	54,55,55,55	0
5	K	A	604	1/1	0.96	0.25	83,83,83,83	0
5	K	B	604	1/1	0.96	0.19	90,90,90,90	0
3	OXL	D	602	6/6	0.96	0.20	54,55,55,56	0
2	FBP	F	601	20/20	0.96	0.12	52,56,61,61	0
2	FBP	A	601	20/20	0.97	0.13	47,48,51,51	0
4	MG	F	603	1/1	0.97	0.13	42,42,42,42	0
5	K	C	604	1/1	0.97	0.20	75,75,75,75	0
2	FBP	B	601	20/20	0.97	0.12	52,53,57,58	0
2	FBP	H	602	20/20	0.98	0.15	34,37,39,41	0
3	OXL	E	602	6/6	0.98	0.12	66,66,67,67	0
4	MG	E	603	1/1	0.98	0.18	34,34,34,34	0
4	MG	A	603	1/1	0.98	0.14	42,42,42,42	0
4	MG	G	603	1/1	0.98	0.18	28,28,28,28	0
2	FBP	E	601	20/20	0.98	0.12	52,54,57,57	0
2	FBP	G	601	20/20	0.99	0.14	33,35,37,37	0
2	FBP	C	601	20/20	0.99	0.14	33,34,39,41	0
2	FBP	D	601	20/20	0.99	0.15	33,36,38,39	0

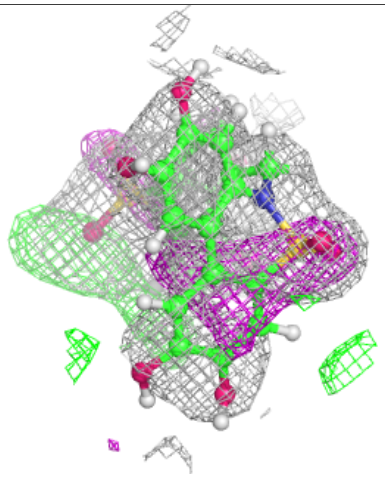
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around O8O E 605:

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

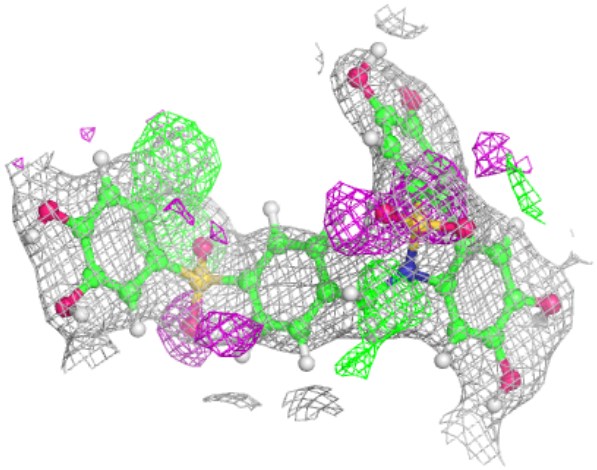


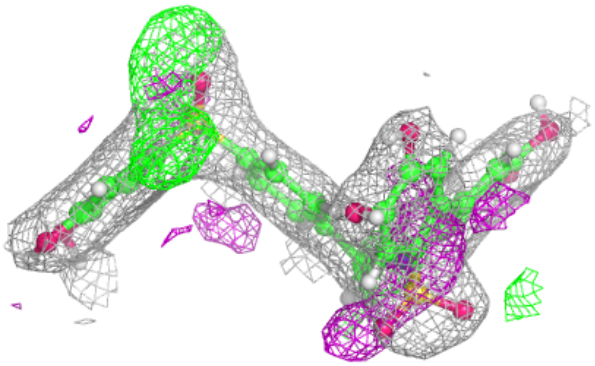


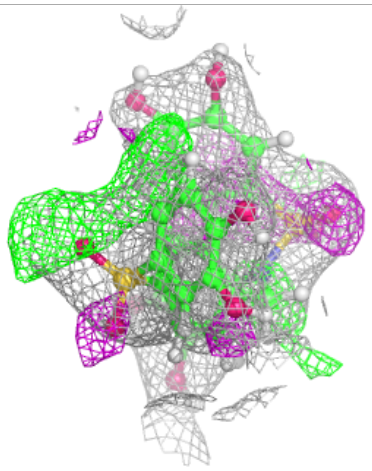


Electron density around O8O H 601:

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

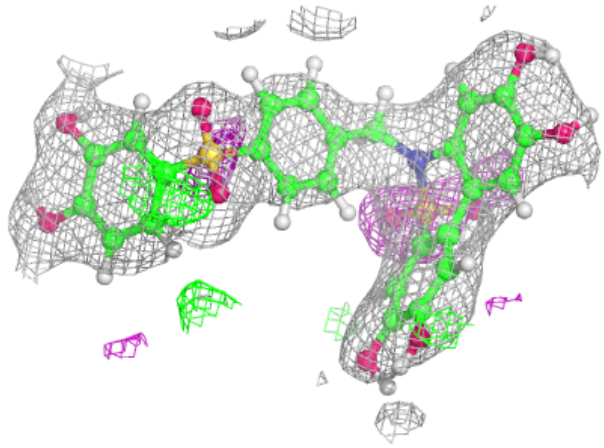


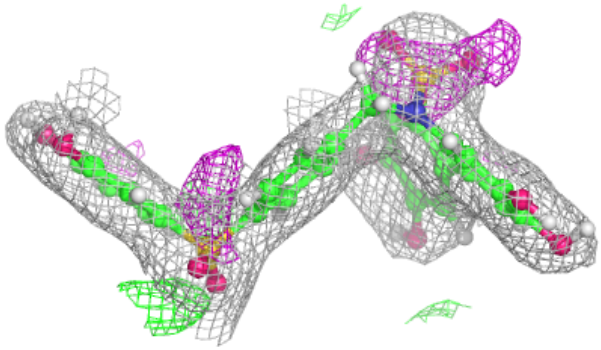


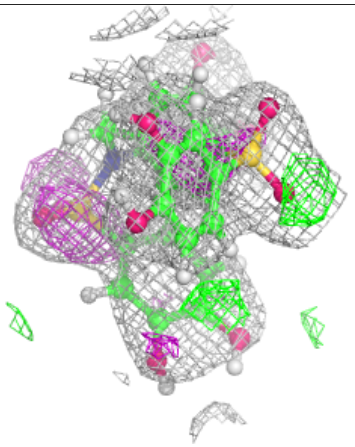


Electron density around O8O A 605:

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

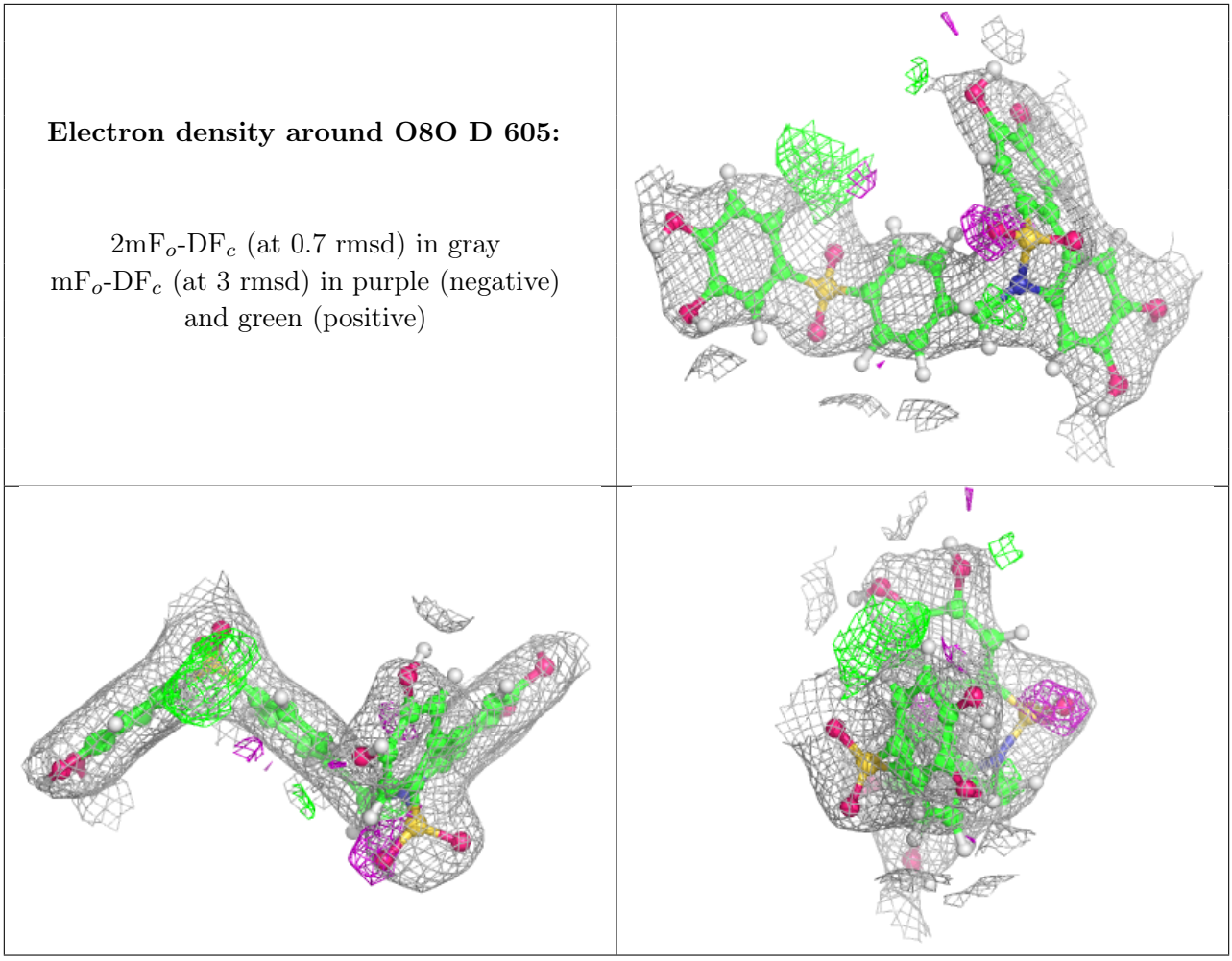






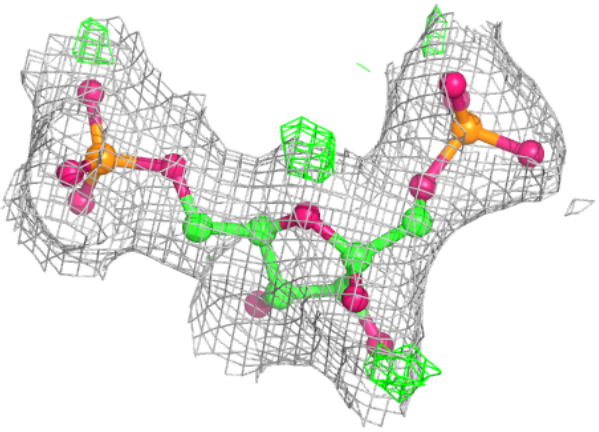
Electron density around O8O D 605:

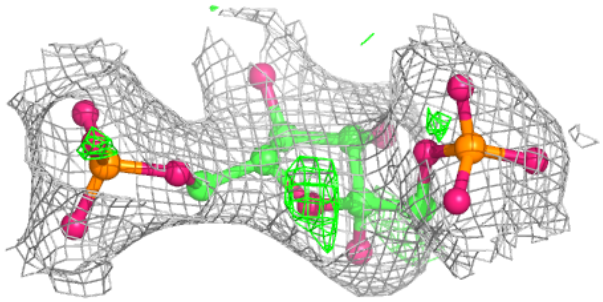
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

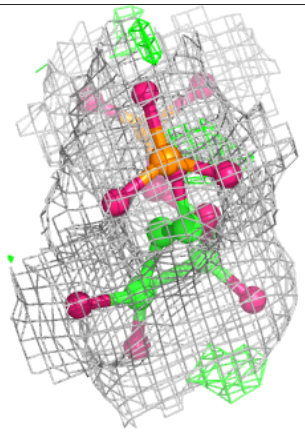


Electron density around FBP F 601:

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

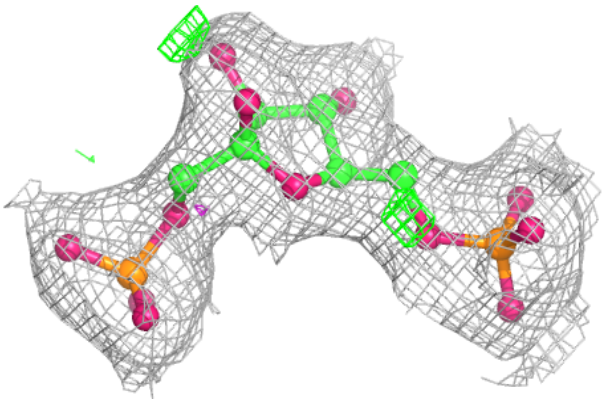


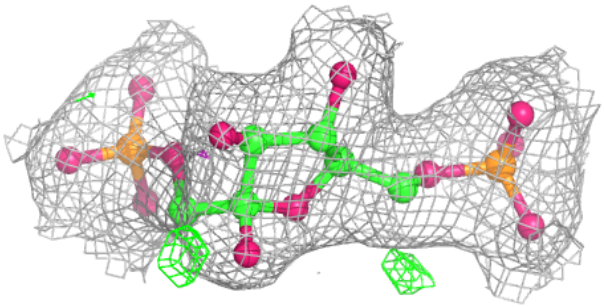


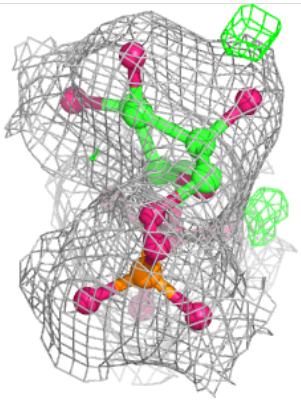


Electron density around FBP A 601:

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

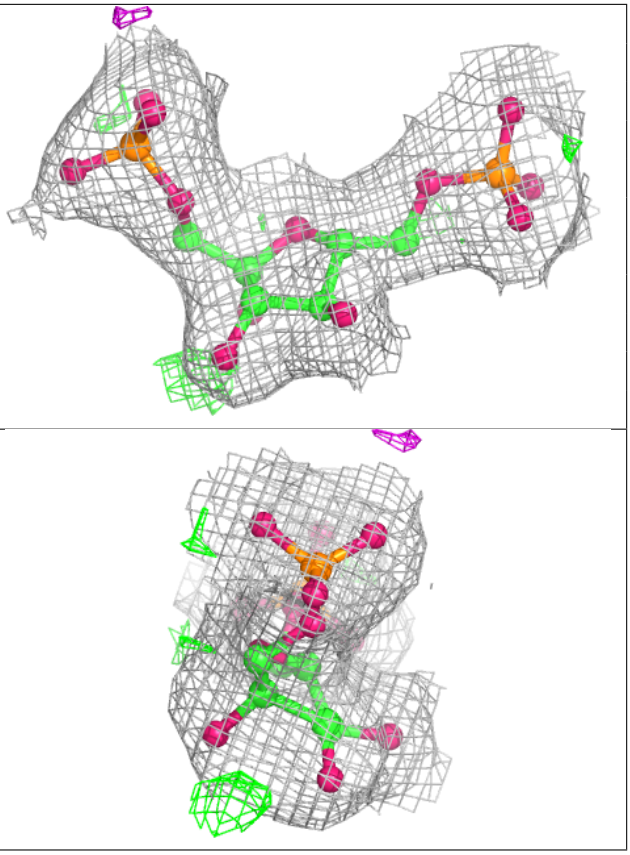






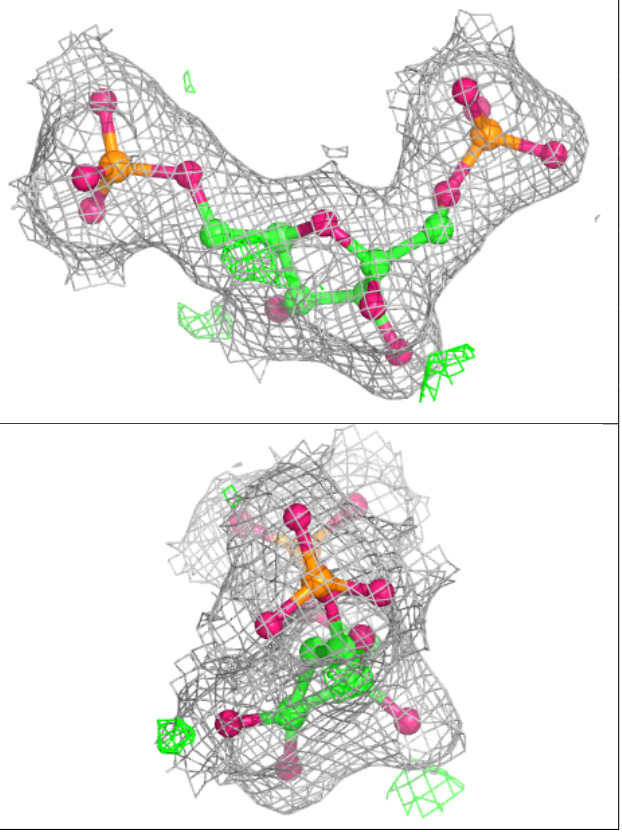
Electron density around FBP B 601:

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



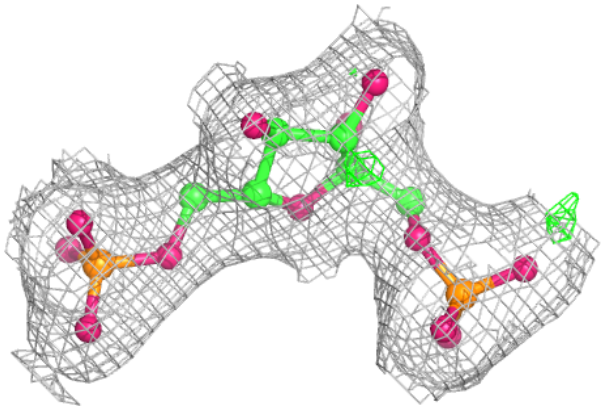
Electron density around FBP H 602:

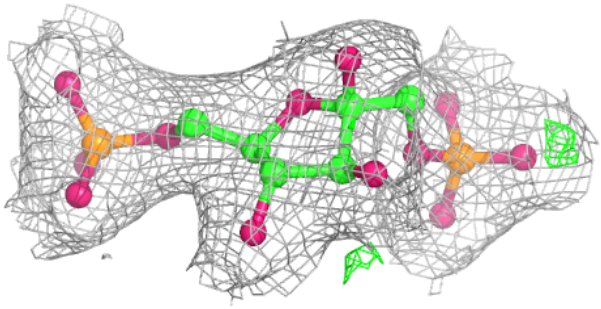
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

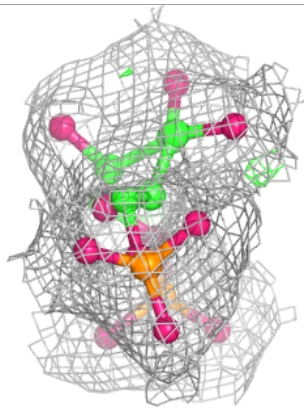


Electron density around FBP E 601:

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

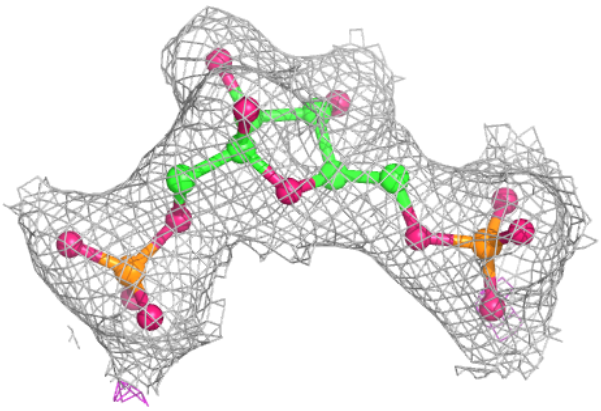


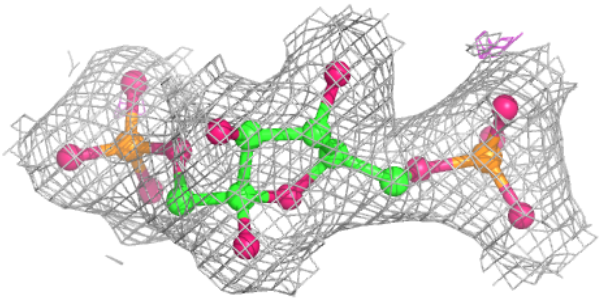


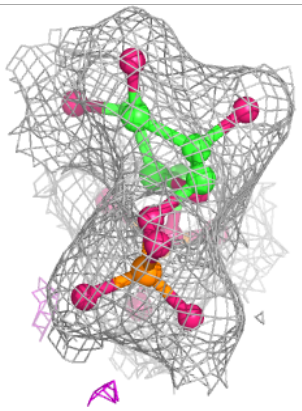


Electron density around FBP G 601:

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

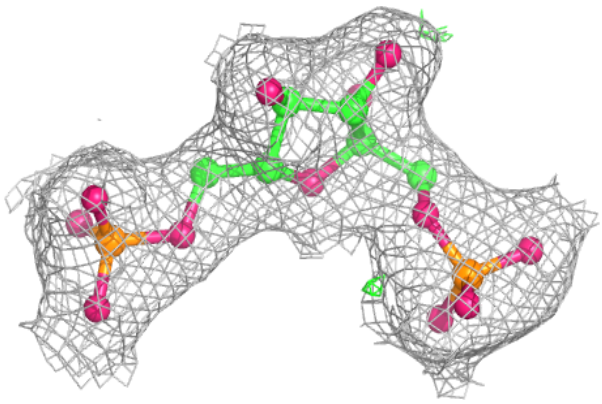


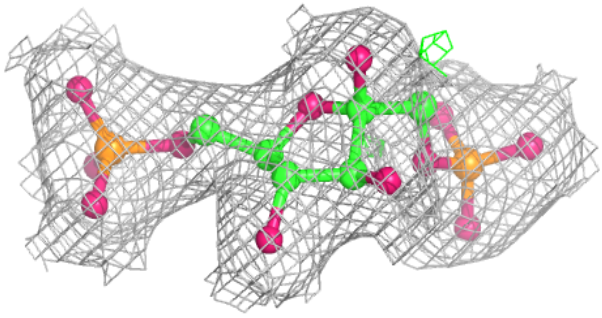


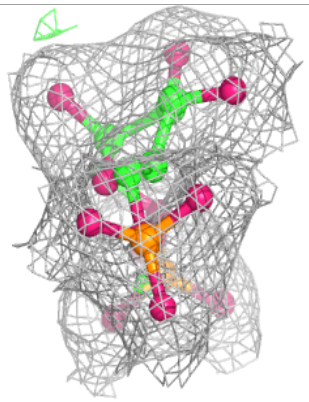


Electron density around FBP C 601:

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

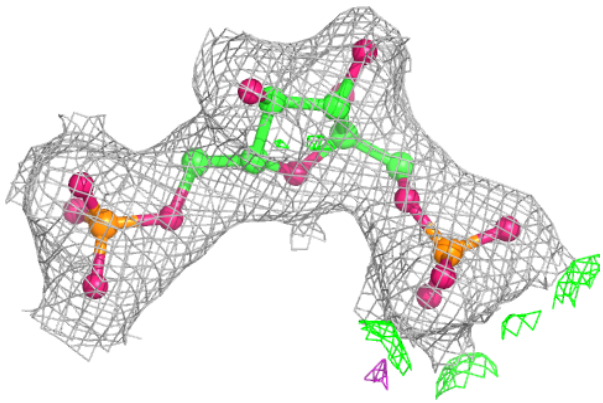


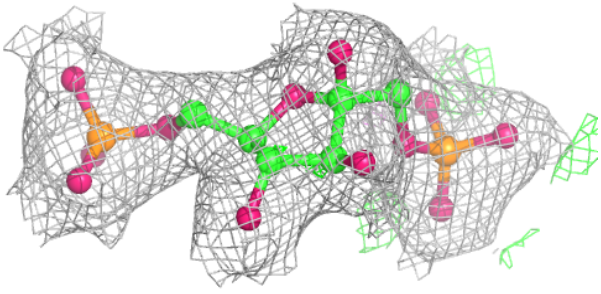


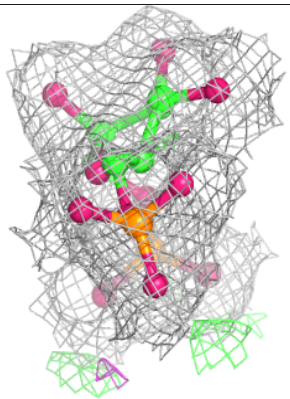


Electron density around FBP D 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.