Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2026 – 12:38 PM EDT

PDB ID	:	14CO / pdb_000014co
Title	:	Structure of liver pyruvate kinase in complex with allosteric activator 8a
Authors	:	Lulla, A.; Rodriguez Rivero, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2026-04-28
Resolution	:	1.89 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:

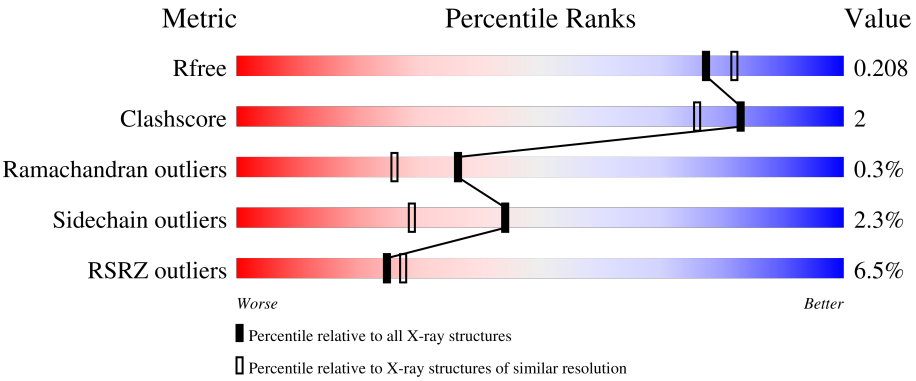
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.89 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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

Mol	Chain	Length	Quality of chain
1	A	447	10% 87% 7% • 6%
1	B	447	13% 91% 6% ••
1	C	447	4% 90% 5% 5%
1	D	447	3% 89% 6% • 5%
1	E	447	6% 88% 5% 6%

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Mol	Chain	Length	Quality of chain
1	F	447	6% 90% 6%
1	G	447	4% 89% 7%
1	H	447	3% 88% 7% 5%

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

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

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 29210 atoms, of which 106 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	421	Total	C	N	O	S	0	13	0
			3267	2055	587	605	20			
1	B	436	Total	C	N	O	S	3	8	0
			3350	2104	604	622	20			
1	C	425	Total	C	N	O	S	0	10	0
			3284	2068	588	609	19			
1	D	425	Total	C	N	O	S	0	8	0
			3261	2048	590	604	19			
1	E	419	Total	C	N	O	S	0	14	0
			3265	2054	587	604	20			
1	F	433	Total	C	N	O	S	0	8	0
			3338	2100	601	617	20			
1	G	430	Total	C	N	O	S	0	10	0
			3311	2082	593	617	19			
1	H	425	Total	C	N	O	S	0	9	0
			3269	2053	593	604	19			

There are 48 discrepancies between the modelled and reference sequences:

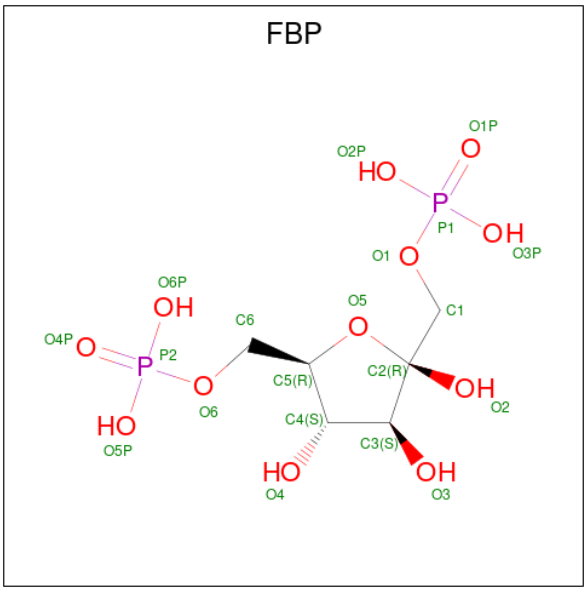
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30613
A	0	SER	-	expression tag	UNP P30613
A	12	ASP	SER	conflict	UNP P30613
A	130	GLY	-	linker	UNP P30613
A	131	SER	-	linker	UNP P30613
A	132	GLY	-	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
B	0	SER	-	expression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

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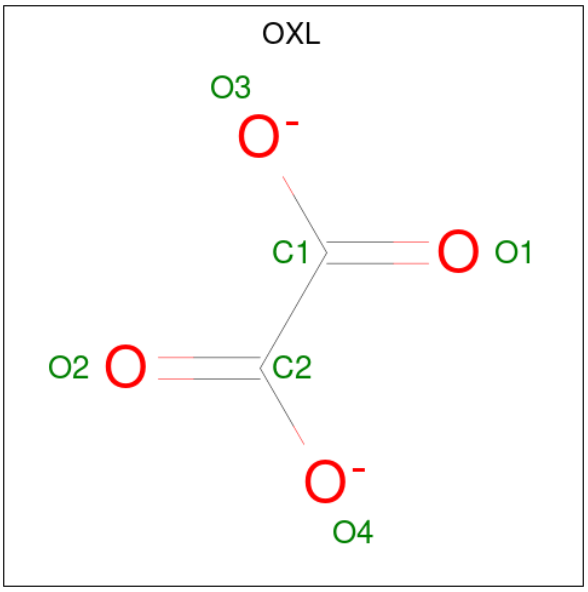
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	130	GLY	-	linker	UNP P30613
C	131	SER	-	linker	UNP P30613
C	132	GLY	-	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	12	ASP	SER	conflict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



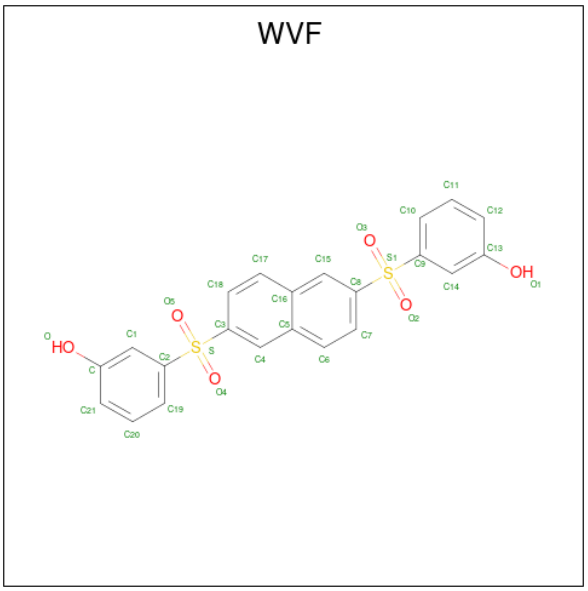
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
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	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is 3,3'-(naphthalene-2,6-diyldisulfonyl)diphenol (CCD ID: WVF) (formula: $C_{22}H_{16}O_6S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O S 46 22 16 6 2	16	0
4	B	1	Total C H O S 46 22 16 6 2	16	0
4	E	1	Total C H O S 46 22 16 6 2	16	0
4	F	1	Total C H O S 46 22 16 6 2	16	0

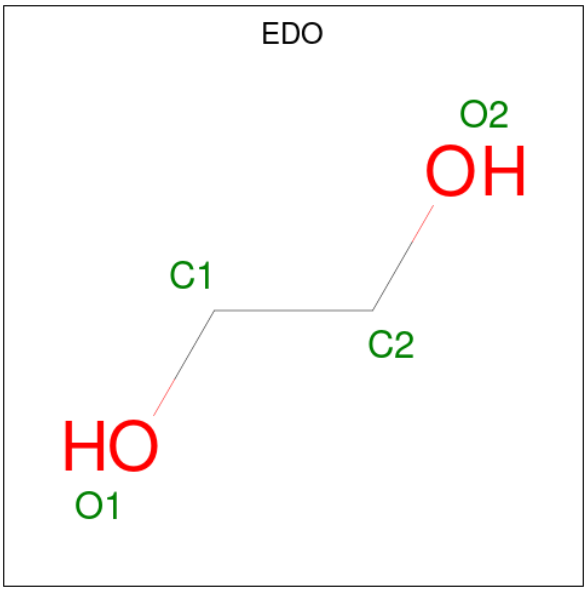
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C H O 10 2 6 2	6	0
7	C	1	Total C H O 10 2 6 2	6	0
7	D	1	Total C H O 10 2 6 2	6	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	H	O	6	0
			10	2	6	2		
7	F	1	Total	C	H	O	6	0
			10	2	6	2		
7	G	1	Total	C	H	O	6	0
			10	2	6	2		
7	H	1	Total	C	H	O	6	0
			10	2	6	2		

- Molecule 8 is water.

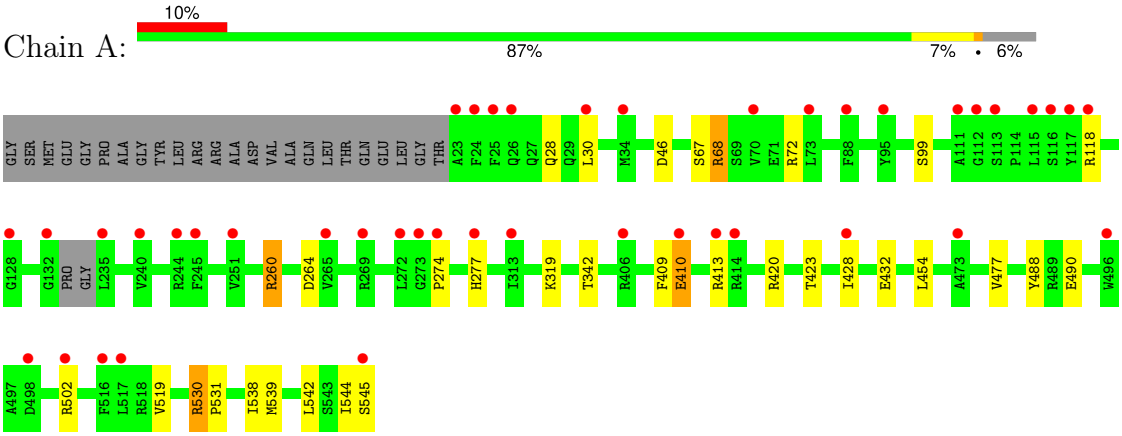
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	234	Total	O	0	0
			234	234		
8	B	224	Total	O	0	0
			224	224		
8	C	318	Total	O	0	0
			318	318		
8	D	349	Total	O	0	0
			349	349		
8	E	255	Total	O	0	0
			255	255		
8	F	297	Total	O	0	0
			297	297		
8	G	336	Total	O	0	0
			336	336		
8	H	374	Total	O	0	0
			374	374		

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.

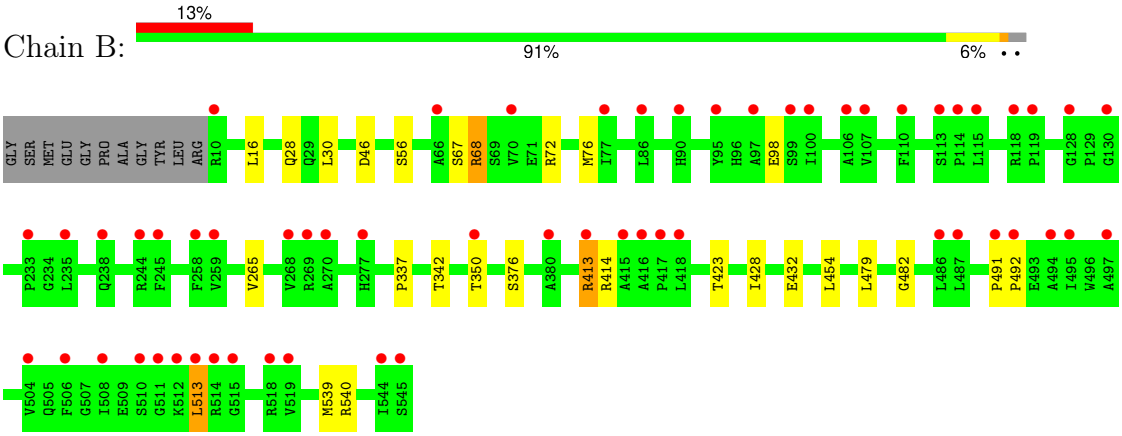
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain A:



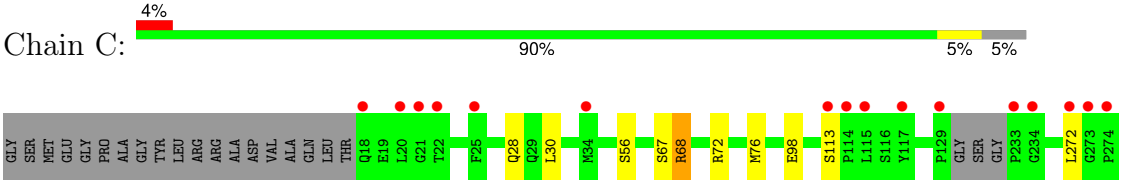
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

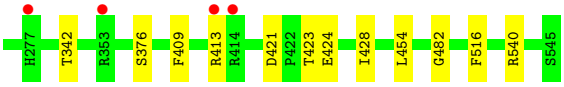
Chain B:



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

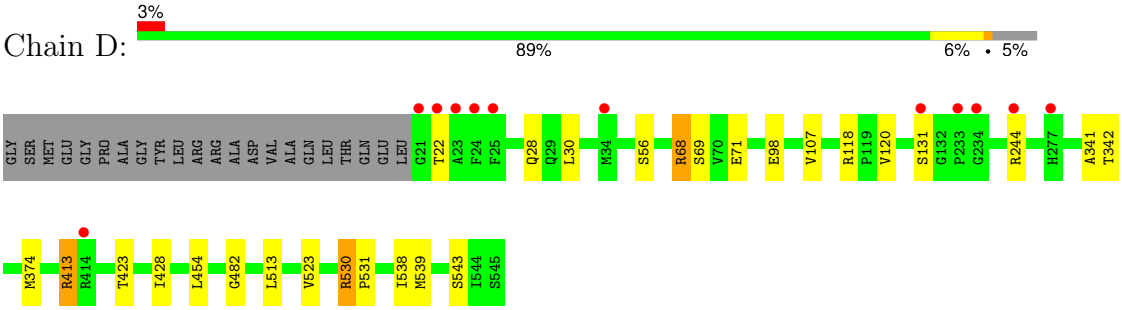
Chain C:





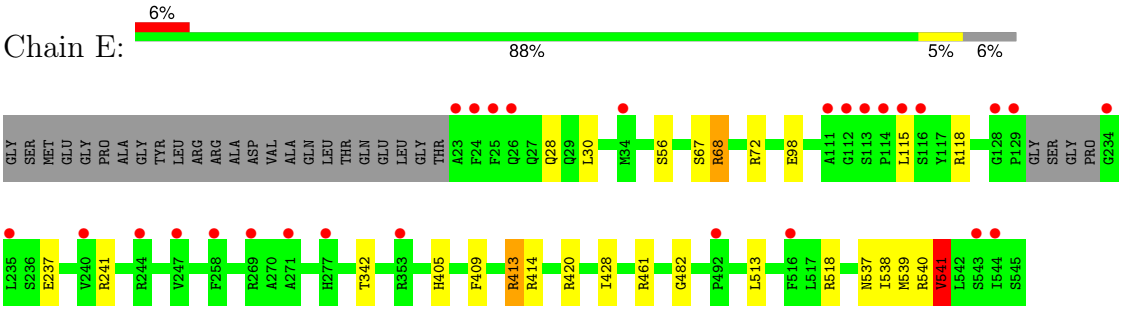
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain D:



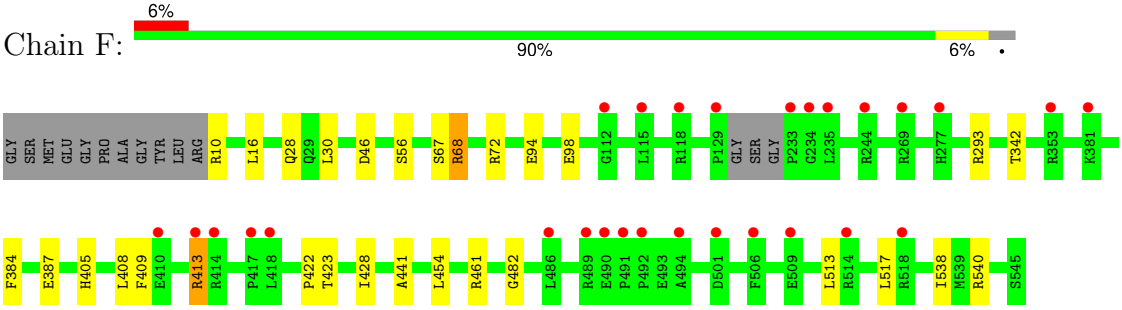
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain E:



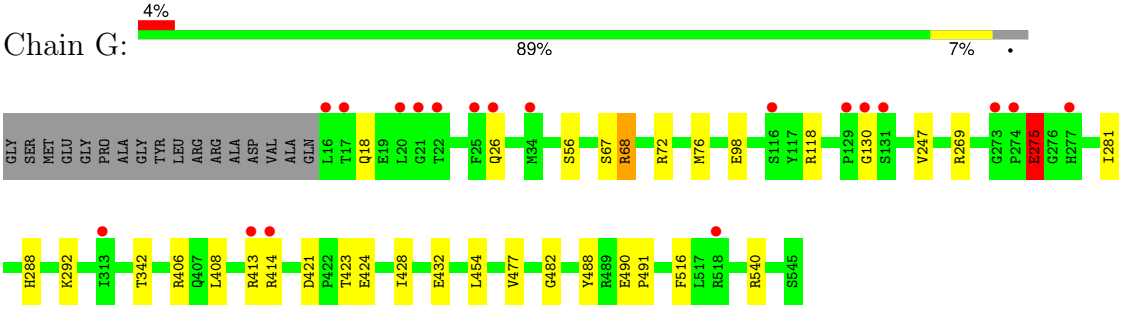
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain F:



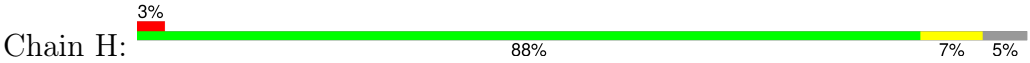
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

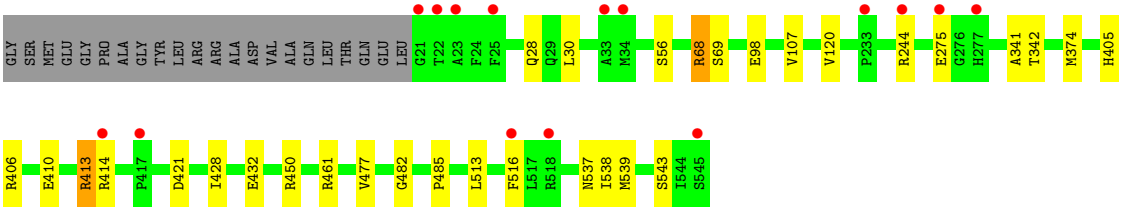
Chain G:



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

Chain H:




GLY SER MET GLU GLY PRO ALA GLY TYR LEU ARG ARG ALA ASP VAL ALA GLN LEU THR GLN GLU LEU G21 T22 A23 F24 F25 Q28 Q29 L30 A33 M34 S56 R68 S69 E98 V107 V120 P233 R244 E275 G276 H277 A341 T342 M374 H405

R406 E410 R413 R414 P417 D421 I428 E432 R450 R461 V477 G482 P485 L513 F516 L517 R518 N537 I538 M539 S543 I544 S545

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	207.43Å 112.95Å 188.28Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	188.17 – 1.89 188.17 – 1.89	Depositor EDS
% Data completeness (in resolution range)	70.6 (188.17-1.89) 70.6 (188.17-1.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.88Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.188 , 0.220 0.178 , 0.208	Depositor DCC
R_{free} test set	12149 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29210	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5297e-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: MG, OXL, EDO, K, WVF, 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	0.71	0/3359	0.97	3/4538 (0.1%)
1	B	0.75	2/3429 (0.1%)	0.98	1/4636 (0.0%)
1	C	0.80	1/3369 (0.0%)	0.97	1/4554 (0.0%)
1	D	0.81	0/3341	1.00	0/4517
1	E	0.71	0/3361	0.97	1/4541 (0.0%)
1	F	0.76	0/3416	1.00	1/4617 (0.0%)
1	G	0.81	1/3397 (0.0%)	0.98	2/4594 (0.0%)
1	H	0.84	0/3352	1.00	1/4531 (0.0%)
All	All	0.77	4/27024 (0.0%)	0.98	10/36528 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	376	SER	CA-C	8.16	1.56	1.52
1	B	376[A]	SER	CA-C	5.97	1.55	1.52
1	B	376[B]	SER	CA-C	5.97	1.55	1.52
1	G	491	PRO	CA-C	5.94	1.55	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	275	GLU	CB-CG-CD	6.26	123.25	112.60
1	E	541	VAL	N-CA-CB	6.21	118.48	111.21
1	C	516	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	46	ASP	CA-CB-CG	5.87	118.47	112.60
1	G	516	PHE	CA-CB-CG	5.85	119.65	113.80
1	B	46	ASP	CA-CB-CG	5.77	118.37	112.60
1	H	516	PHE	CA-CB-CG	5.63	119.43	113.80
1	F	46	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	544	ILE	CA-C-N	5.16	130.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	544	ILE	C-N-CA	5.16	130.98	121.70

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	3267	0	3342	21	0
1	B	3350	0	3417	19	0
1	C	3284	0	3351	13	0
1	D	3261	0	3321	13	0
1	E	3265	0	3337	16	0
1	F	3338	0	3412	21	0
1	G	3311	0	3374	22	0
1	H	3269	0	3334	22	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	30	16	0	0	0
4	B	30	16	0	0	0
4	E	30	16	0	0	0
4	F	30	16	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	B	4	6	6	0	0
7	C	4	6	6	0	0
7	D	4	6	6	0	0
7	E	4	6	6	0	0
7	F	4	6	6	1	0
7	G	4	6	6	1	0
7	H	4	6	6	0	0
8	A	234	0	0	1	0
8	B	224	0	0	0	0
8	C	318	0	0	1	0
8	D	349	0	0	0	0
8	E	255	0	0	0	0
8	F	297	0	0	2	0
8	G	336	0	0	0	0
8	H	374	0	0	0	0
All	All	29104	106	27010	126	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 (126) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ARG:HG3	1:C:428:ILE:HD11	1.52	0.91
1:F:413:ARG:HG2	1:F:428:ILE:HD11	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:HG2	1:B:428:ILE:HD11	1.59	0.84
1:E:420[B]:ARG:HG3	1:F:16:LEU:HD11	1.69	0.74
1:A:538:ILE:HG12	1:B:540:ARG:HG2	1.69	0.73
1:F:409:PHE:CE2	1:F:413:ARG:NH1	2.59	0.71
1:A:409:PHE:CE2	1:A:413:ARG:NH1	2.59	0.70
1:A:413:ARG:NH2	1:B:413:ARG:NH2	2.40	0.69
1:F:413:ARG:HD2	8:F:807:HOH:O	1.90	0.69
1:A:274:PRO:HA	1:A:277:HIS:NE2	2.09	0.67
1:G:414:ARG:HH21	1:H:406:ARG:HH11	1.42	0.67
1:G:540:ARG:HG2	1:H:538:ILE:HG12	1.77	0.66
1:A:420[B]:ARG:HG3	1:B:16:LEU:HD11	1.79	0.65
1:H:413:ARG:HG2	1:H:428:ILE:HD11	1.78	0.64
1:A:420[A]:ARG:HD3	1:B:16:LEU:HD11	1.81	0.63
1:D:530:ARG:HD2	1:D:531:PRO:O	1.99	0.62
1:G:424[A]:GLU:HG2	1:G:454:LEU:HD13	1.80	0.62
1:C:540:ARG:HD3	8:C:764:HOH:O	1.99	0.61
1:C:424[A]:GLU:HG2	1:C:454:LEU:HD13	1.82	0.61
1:G:414:ARG:NH2	1:H:406:ARG:HD3	2.15	0.61
1:G:413:ARG:HG3	1:G:428:ILE:HD11	1.82	0.61
1:E:405:HIS:ND1	1:E:461:ARG:NH1	2.48	0.60
1:E:538:ILE:HG12	1:F:540:ARG:HG2	1.83	0.60
1:E:420[A]:ARG:HD3	1:F:16:LEU:HD11	1.82	0.60
1:H:68:ARG:NH2	1:H:98:GLU:HB2	2.17	0.59
1:A:530:ARG:HD2	1:A:531:PRO:O	2.02	0.59
1:F:28:GLN:O	1:F:461:ARG:NH2	2.35	0.59
1:A:67:SER:HA	1:A:72:ARG:HG2	1.84	0.59
1:C:540:ARG:HG2	1:D:538:ILE:HG12	1.83	0.59
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.18	0.58
1:H:28:GLN:O	1:H:461:ARG:NH2	2.37	0.58
1:C:413:ARG:CG	1:C:428:ILE:HD11	2.31	0.57
1:A:409:PHE:HE2	1:A:413:ARG:HH12	1.51	0.57
1:D:56:SER:HB2	1:D:482:GLY:HA2	1.87	0.57
1:E:28:GLN:O	1:E:461:ARG:NH2	2.38	0.57
1:G:56:SER:HB2	1:G:482:GLY:HA2	1.88	0.55
1:E:413:ARG:HG2	1:E:428:ILE:HD11	1.87	0.55
1:H:405:HIS:ND1	1:H:461:ARG:NH1	2.53	0.55
1:E:540:ARG:HG2	1:F:538:ILE:HG12	1.88	0.54
1:G:408:LEU:HD21	7:G:603:EDO:H11	1.88	0.54
1:D:413:ARG:HG2	1:D:428:ILE:HD11	1.90	0.54
1:E:405:HIS:CE1	1:E:461:ARG:HH11	2.25	0.54
1:A:68:ARG:HD2	1:A:99:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:SER:HB2	1:B:482:GLY:HA2	1.91	0.53
1:C:56:SER:HB2	1:C:482:GLY:HA2	1.90	0.53
1:F:56:SER:HB2	1:F:482:GLY:HA2	1.91	0.53
1:H:68:ARG:HH22	1:H:98:GLU:HB2	1.73	0.52
1:H:56:SER:HB2	1:H:482:GLY:HA2	1.93	0.51
1:A:260:ARG:HG2	1:A:264:ASP:OD2	2.11	0.51
1:F:67:SER:HA	1:F:72:ARG:HG2	1.93	0.51
1:E:237:GLU:O	1:E:241:ARG:HD3	2.12	0.49
1:A:410:GLU:HG2	1:A:413:ARG:HH21	1.77	0.49
1:F:408:LEU:HD21	7:F:604:EDO:H11	1.94	0.49
1:E:56:SER:HB2	1:E:482:GLY:HA2	1.94	0.48
1:C:421:ASP:OD2	1:C:424[A]:GLU:HG3	2.13	0.48
1:E:541:VAL:HG22	1:F:422:PRO:HB3	1.96	0.47
1:B:423:THR:HG22	1:B:454:LEU:HD12	1.97	0.47
1:G:423:THR:HG22	1:G:454:LEU:HD12	1.97	0.46
1:D:56:SER:HB2	1:D:482:GLY:CA	2.45	0.46
1:G:247:VAL:CG1	1:G:275:GLU:HG2	2.45	0.46
1:C:67:SER:HA	1:C:72:ARG:HG2	1.97	0.46
1:G:68:ARG:NH2	1:G:98[A]:GLU:HB2	2.31	0.46
1:H:537:ASN:OD1	1:H:538:ILE:HG13	2.16	0.45
1:A:319:LYS:NZ	8:A:704:HOH:O	2.49	0.45
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.81	0.45
1:G:269:ARG:HG2	1:G:281:ILE:CD1	2.47	0.45
1:A:413:ARG:NH2	1:B:413:ARG:CZ	2.80	0.45
1:G:67:SER:HA	1:G:72:ARG:HG2	1.98	0.45
1:A:488:TYR:CZ	1:A:490[B]:GLU:HB2	2.52	0.45
1:F:405:HIS:ND1	1:F:461:ARG:NH1	2.60	0.45
1:A:519:VAL:HG13	1:A:545:SER:HB3	1.97	0.45
1:D:423:THR:HG22	1:D:454:LEU:HD12	1.99	0.44
1:E:67:SER:HA	1:E:72:ARG:HG2	1.98	0.44
1:C:67:SER:HB2	1:C:76[B]:MET:SD	2.58	0.44
1:A:28:GLN:HG3	1:A:30:LEU:HG	2.00	0.44
1:C:423:THR:HG22	1:C:454:LEU:HD12	2.00	0.44
1:G:288:HIS:CE1	1:G:292:LYS:HG3	2.53	0.44
1:G:406:ARG:HD3	1:H:414:ARG:CZ	2.47	0.44
1:B:68:ARG:NH2	1:B:98:GLU:HB3	2.33	0.44
1:B:67:SER:HB2	1:B:76[B]:MET:SD	2.58	0.44
1:F:56:SER:HB2	1:F:482:GLY:CA	2.47	0.44
1:G:432[A]:GLU:OE1	1:H:432[A]:GLU:OE1	2.35	0.44
1:G:67:SER:HB2	1:G:76[B]:MET:SD	2.58	0.44
1:G:421:ASP:OD2	1:G:424[A]:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLU:CD	1:B:413:ARG:HD2	2.43	0.43
1:C:68:ARG:NH2	1:C:98[A]:GLU:HB2	2.32	0.43
1:E:409:PHE:O	1:E:413:ARG:HB2	2.17	0.43
1:G:488:TYR:CZ	1:G:490:GLU:HB2	2.54	0.43
1:B:67:SER:HA	1:B:72:ARG:HG2	1.99	0.43
1:A:432:GLU:OE2	1:B:432[A]:GLU:OE1	2.36	0.43
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.32	0.43
1:B:56:SER:HB2	1:B:482:GLY:CA	2.48	0.43
1:F:384:PHE:HB3	1:F:387:GLU:HB2	2.01	0.43
1:H:56:SER:HB2	1:H:482:GLY:CA	2.49	0.43
1:F:28:GLN:HG3	1:F:30:LEU:HG	2.01	0.43
1:H:28:GLN:HG3	1:H:30:LEU:HG	1.99	0.43
1:H:341:ALA:HB1	1:H:374:MET:HE2	2.01	0.43
1:D:28:GLN:HG3	1:D:30:LEU:HG	2.01	0.42
1:A:423:THR:HG22	1:A:454:LEU:HD12	2.02	0.42
1:G:414:ARG:HH21	1:H:406:ARG:NH1	2.13	0.42
1:F:405:HIS:CE1	1:F:461:ARG:HH11	2.36	0.42
1:F:413:ARG:CD	8:F:807:HOH:O	2.60	0.42
1:G:68:ARG:NH2	1:G:98[B]:GLU:HB3	2.35	0.42
1:D:107:VAL:HG21	1:D:120:VAL:HB	2.02	0.42
1:E:537:ASN:OD1	1:E:538:ILE:HG13	2.20	0.41
1:G:56:SER:HB2	1:G:482:GLY:CA	2.49	0.41
1:B:491:PRO:HA	1:B:492:PRO:HD3	1.97	0.41
1:H:477:VAL:CG2	1:H:485:PRO:HB3	2.50	0.41
1:D:71[B]:GLU:CD	1:D:71[B]:GLU:H	2.26	0.41
1:D:341:ALA:HB1	1:D:374:MET:HE2	2.03	0.41
1:E:68:ARG:NH2	1:E:98:GLU:HB3	2.35	0.41
1:G:414:ARG:HD2	1:H:410:GLU:OE2	2.19	0.41
1:B:28:GLN:HG3	1:B:30:LEU:HG	2.02	0.41
1:C:28:GLN:HG3	1:C:30:LEU:HG	2.02	0.41
1:C:409:PHE:O	1:C:413:ARG:HB2	2.20	0.41
1:F:423:THR:HG22	1:F:454:LEU:HD12	2.03	0.41
1:H:30:LEU:HD23	1:H:30:LEU:HA	1.98	0.41
1:H:107:VAL:HG21	1:H:120:VAL:HB	2.03	0.41
1:B:337:PRO:HB3	1:B:479:LEU:O	2.21	0.41
1:E:28:GLN:HG3	1:E:30:LEU:HG	2.03	0.41
1:A:432:GLU:OE2	1:B:432[B]:GLU:OE1	2.39	0.40
1:D:413:ARG:CG	1:D:428:ILE:HD11	2.49	0.40
1:H:405:HIS:CE1	1:H:461:ARG:HH11	2.37	0.40
1:F:441:ALA:HB3	1:F:517:LEU:HD21	2.03	0.40
1:H:421:ASP:OD2	1:H:450:ARG:NH2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:LEU:HD13	1:B:513:LEU:HA	1.97	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	430/447 (96%)	424 (99%)	5 (1%)	1 (0%)	43	34
1	B	442/447 (99%)	435 (98%)	6 (1%)	1 (0%)	43	34
1	C	431/447 (96%)	425 (99%)	5 (1%)	1 (0%)	43	34
1	D	431/447 (96%)	425 (99%)	5 (1%)	1 (0%)	43	34
1	E	429/447 (96%)	423 (99%)	5 (1%)	1 (0%)	43	34
1	F	437/447 (98%)	433 (99%)	3 (1%)	1 (0%)	43	34
1	G	438/447 (98%)	428 (98%)	8 (2%)	2 (0%)	24	13
1	H	432/447 (97%)	427 (99%)	4 (1%)	1 (0%)	43	34
All	All	3470/3576 (97%)	3420 (99%)	41 (1%)	9 (0%)	36	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	130	GLY
1	A	342	THR
1	B	342	THR
1	C	342	THR
1	D	342	THR
1	E	342	THR
1	F	342	THR
1	G	342	THR
1	H	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	347/352 (99%)	336 (97%)	11 (3%)	34	17
1	B	353/352 (100%)	345 (98%)	8 (2%)	44	29
1	C	348/352 (99%)	344 (99%)	4 (1%)	65	56
1	D	344/352 (98%)	331 (96%)	13 (4%)	29	13
1	E	347/352 (99%)	337 (97%)	10 (3%)	37	20
1	F	352/352 (100%)	346 (98%)	6 (2%)	53	40
1	G	351/352 (100%)	345 (98%)	6 (2%)	53	40
1	H	345/352 (98%)	336 (97%)	9 (3%)	40	24
All	All	2787/2816 (99%)	2720 (98%)	67 (2%)	44	27

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	118	ARG
1	A	260	ARG
1	A	410	GLU
1	A	428	ILE
1	A	477	VAL
1	A	502	ARG
1	A	530	ARG
1	A	539[A]	MET
1	A	539[B]	MET
1	A	542	LEU
1	B	68	ARG
1	B	265	VAL
1	B	350	THR
1	B	413	ARG
1	B	414	ARG
1	B	513	LEU
1	B	539[A]	MET
1	B	539[B]	MET

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Mol	Chain	Res	Type
1	C	68	ARG
1	C	113	SER
1	C	272[A]	LEU
1	C	272[B]	LEU
1	D	22	THR
1	D	68	ARG
1	D	69	SER
1	D	118	ARG
1	D	131	SER
1	D	244[A]	ARG
1	D	244[B]	ARG
1	D	413	ARG
1	D	513	LEU
1	D	523	VAL
1	D	530	ARG
1	D	539	MET
1	D	543	SER
1	E	68	ARG
1	E	115	LEU
1	E	118	ARG
1	E	413	ARG
1	E	414	ARG
1	E	513	LEU
1	E	518	ARG
1	E	539[A]	MET
1	E	539[B]	MET
1	E	541	VAL
1	F	10	ARG
1	F	68	ARG
1	F	94	GLU
1	F	293	ARG
1	F	413	ARG
1	F	513	LEU
1	G	18	GLN
1	G	26	GLN
1	G	68	ARG
1	G	118	ARG
1	G	275	GLU
1	G	477	VAL
1	H	68	ARG
1	H	69	SER
1	H	244[A]	ARG

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Mol	Chain	Res	Type
1	H	244[B]	ARG
1	H	275	GLU
1	H	413	ARG
1	H	513	LEU
1	H	539	MET
1	H	543	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	27	GLN
1	C	90	HIS
1	C	472	GLN
1	D	27	GLN
1	D	90	HIS
1	G	18	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 43 ligands modelled in this entry, 16 are monoatomic - leaving 27 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	G	601	-	18,20,20	0.43	0	21,32,32	0.65	0
3	OXL	D	602	5	5,5,5	2.18	2 (40%)	6,6,6	2.02	2 (33%)
2	FBP	E	601	-	18,20,20	0.58	0	21,32,32	0.67	0
2	FBP	A	601	-	18,20,20	0.47	0	21,32,32	0.63	0
3	OXL	F	602	5	5,5,5	2.02	1 (20%)	6,6,6	2.44	3 (50%)
7	EDO	H	603	-	3,3,3	0.39	0	2,2,2	0.22	0
7	EDO	C	603	-	3,3,3	0.41	0	2,2,2	0.38	0
3	OXL	H	602	5	5,5,5	1.80	2 (40%)	6,6,6	1.83	2 (33%)
7	EDO	E	603	-	3,3,3	0.33	0	2,2,2	0.31	0
2	FBP	B	601	-	18,20,20	0.45	0	21,32,32	0.72	0
3	OXL	G	602	5	5,5,5	2.43	2 (40%)	6,6,6	1.67	2 (33%)
4	WVF	E	604	-	33,33,33	0.28	0	48,50,50	0.42	0
7	EDO	F	604	-	3,3,3	0.21	0	2,2,2	0.40	0
2	FBP	D	601	-	18,20,20	0.62	0	21,32,32	1.02	1 (4%)
7	EDO	B	603	-	3,3,3	0.16	0	2,2,2	0.20	0
4	WVF	B	604	-	33,33,33	0.27	0	48,50,50	0.41	0
3	OXL	C	602	5	5,5,5	1.81	1 (20%)	6,6,6	2.22	2 (33%)
7	EDO	D	603	-	3,3,3	0.30	0	2,2,2	0.25	0
3	OXL	E	602	5	5,5,5	2.21	2 (40%)	6,6,6	1.36	1 (16%)
3	OXL	A	602	5	5,5,5	1.86	2 (40%)	6,6,6	2.35	3 (50%)
4	WVF	F	603	-	33,33,33	0.33	0	48,50,50	0.41	0
2	FBP	C	601	-	18,20,20	0.67	0	21,32,32	0.63	0
2	FBP	H	601	-	18,20,20	0.68	0	21,32,32	0.75	1 (4%)
4	WVF	A	603	-	33,33,33	0.27	0	48,50,50	0.39	0
3	OXL	B	602	5	5,5,5	2.24	2 (40%)	6,6,6	1.64	2 (33%)
2	FBP	F	601	-	18,20,20	0.46	0	21,32,32	0.61	0
7	EDO	G	603	-	3,3,3	0.31	0	2,2,2	0.32	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	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	5	-	4/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXL	F	602	5	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	H	603	-	-	0/1/1/1	-
7	EDO	C	603	-	-	0/1/1/1	-
3	OXL	H	602	5	-	4/4/4/4	-
7	EDO	E	603	-	-	1/1/1/1	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	G	602	5	-	4/4/4/4	-
4	WVF	E	604	-	-	0/24/24/24	0/4/4/4
7	EDO	F	604	-	-	0/1/1/1	-
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
7	EDO	B	603	-	-	0/1/1/1	-
4	WVF	B	604	-	-	0/24/24/24	0/4/4/4
3	OXL	C	602	5	-	4/4/4/4	-
7	EDO	D	603	-	-	0/1/1/1	-
3	OXL	E	602	5	-	4/4/4/4	-
3	OXL	A	602	5	-	4/4/4/4	-
4	WVF	F	603	-	-	0/24/24/24	0/4/4/4
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
4	WVF	A	603	-	-	0/24/24/24	0/4/4/4
3	OXL	B	602	5	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
7	EDO	G	603	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	OXL	O2-C2	4.84	1.34	1.22
3	B	602	OXL	O2-C2	4.11	1.32	1.22
3	F	602	OXL	O2-C2	3.98	1.32	1.22
3	E	602	OXL	O4-C2	-3.51	1.21	1.30
3	A	602	OXL	O2-C2	3.47	1.31	1.22
3	D	602	OXL	O2-C2	3.42	1.31	1.22
3	C	602	OXL	O2-C2	3.41	1.31	1.22
3	E	602	OXL	O2-C2	3.12	1.30	1.22
3	D	602	OXL	O4-C2	-2.96	1.22	1.30
3	H	602	OXL	O4-C2	-2.93	1.22	1.30
3	B	602	OXL	O4-C2	-2.72	1.23	1.30
3	H	602	OXL	O2-C2	2.48	1.28	1.22
3	G	602	OXL	O4-C2	-2.42	1.24	1.30
3	A	602	OXL	O4-C2	-2.17	1.24	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	OXL	O4-C2-C1	4.47	121.50	112.83
3	C	602	OXL	O4-C2-C1	4.38	121.33	112.83
3	A	602	OXL	O4-C2-C1	4.34	121.24	112.83
3	H	602	OXL	O4-C2-C1	3.88	120.35	112.83
3	D	602	OXL	O4-C2-C1	3.19	119.01	112.83
2	D	601	FBP	O6-P2-O4P	2.97	114.48	106.44
3	F	602	OXL	O2-C2-C1	-2.96	114.46	120.63
3	D	602	OXL	O3-C1-C2	2.93	118.51	112.83
3	A	602	OXL	O2-C2-C1	-2.88	114.62	120.63
3	C	602	OXL	O2-C2-C1	-2.84	114.72	120.63
3	G	602	OXL	O4-C2-C1	2.71	118.09	112.83
3	B	602	OXL	O3-C1-C2	2.69	118.05	112.83
3	G	602	OXL	O3-C1-C2	2.60	117.88	112.83
3	B	602	OXL	O4-C2-C1	2.58	117.83	112.83
3	F	602	OXL	O3-C1-C2	2.53	117.74	112.83
3	E	602	OXL	O4-C2-C1	2.44	117.56	112.83
3	A	602	OXL	O3-C1-C2	2.38	117.45	112.83
2	H	601	FBP	O6-P2-O4P	2.34	112.76	106.44
3	H	602	OXL	O2-C2-C1	-2.06	116.35	120.63

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	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	G	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
2	B	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	601	FBP	O5-C5-C6-O6
3	H	602	OXL	O3-C1-C2-O4

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Mol	Chain	Res	Type	Atoms
3	A	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
3	A	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
7	E	603	EDO	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	E	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O1-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O2

There are no ring outliers.

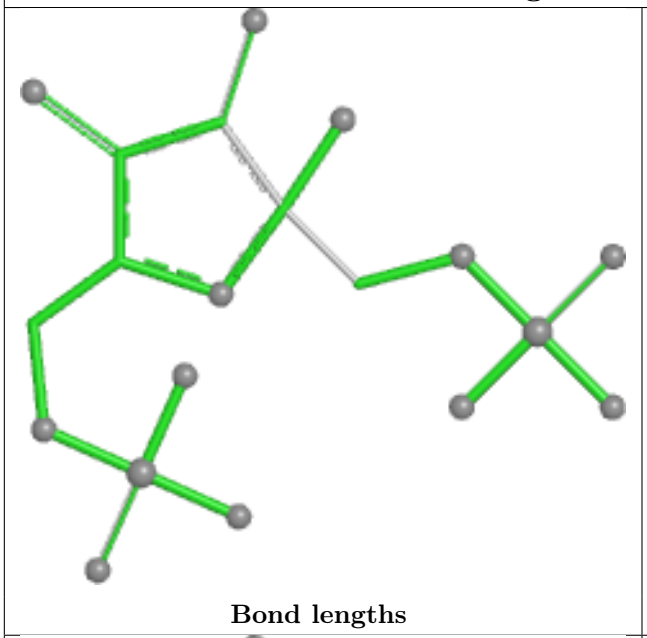
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	604	EDO	1	0
7	G	603	EDO	1	0

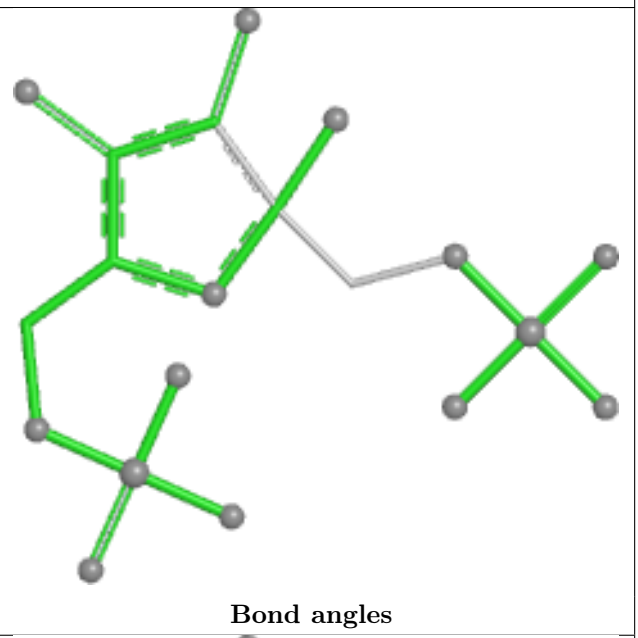
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

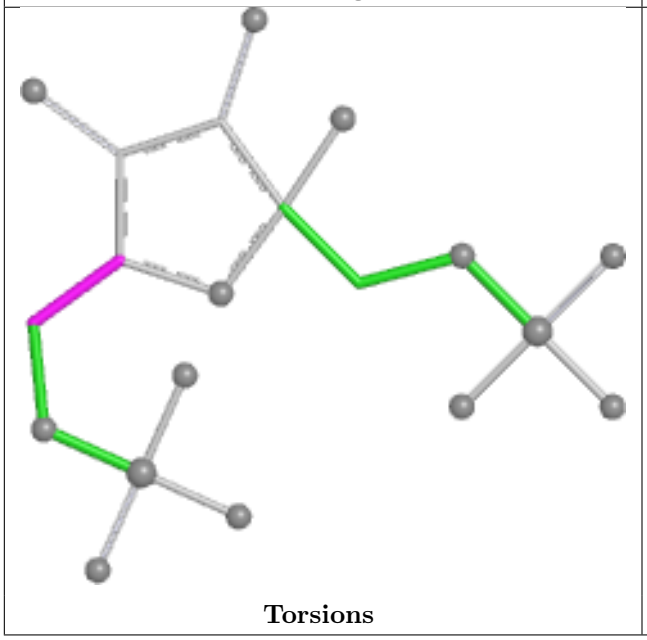
Ligand FBP G 601



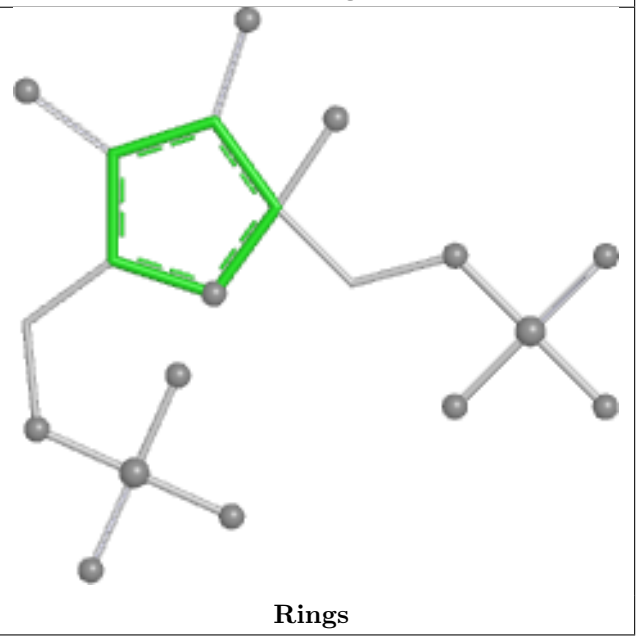
Bond lengths



Bond angles

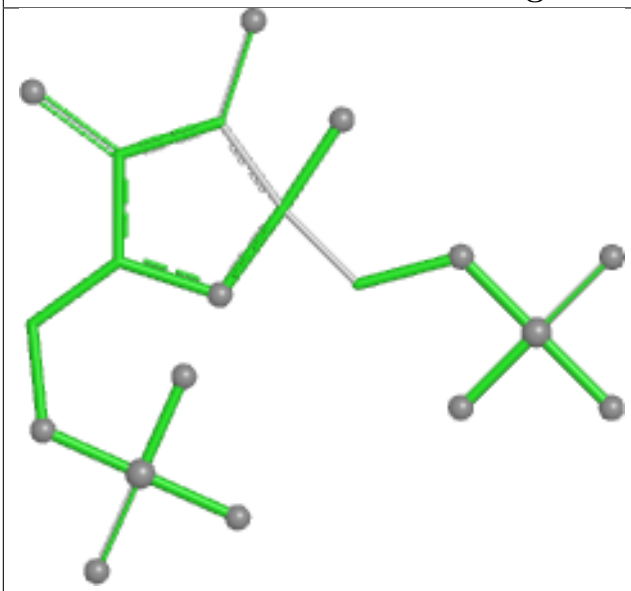


Torsions

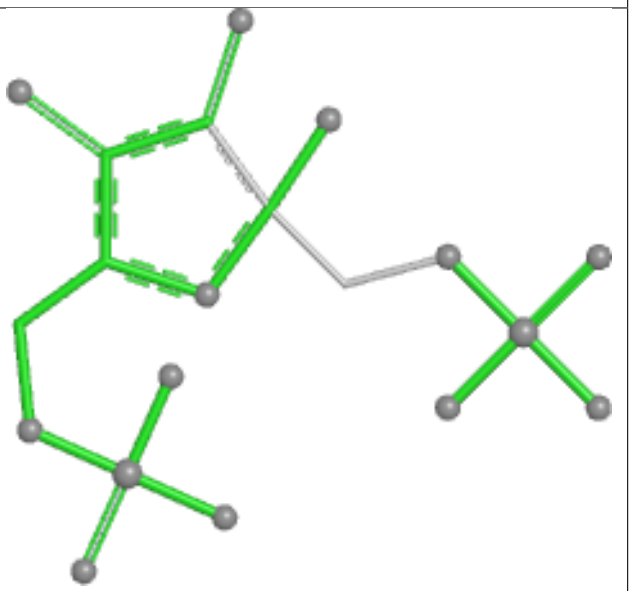


Rings

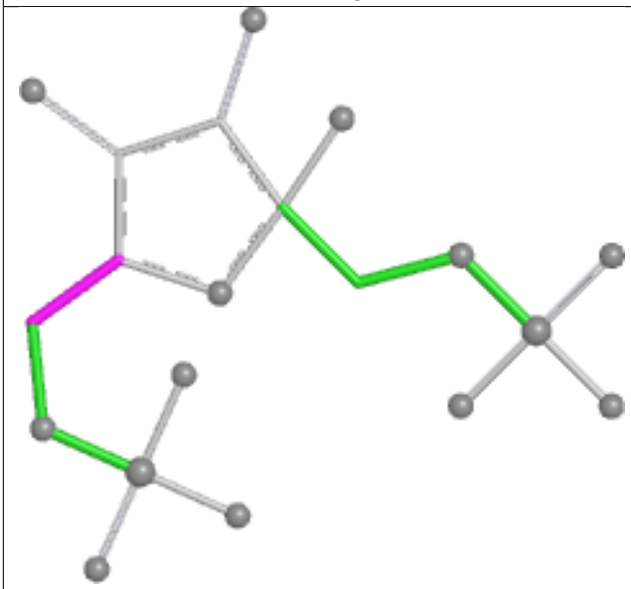
Ligand FBP E 601



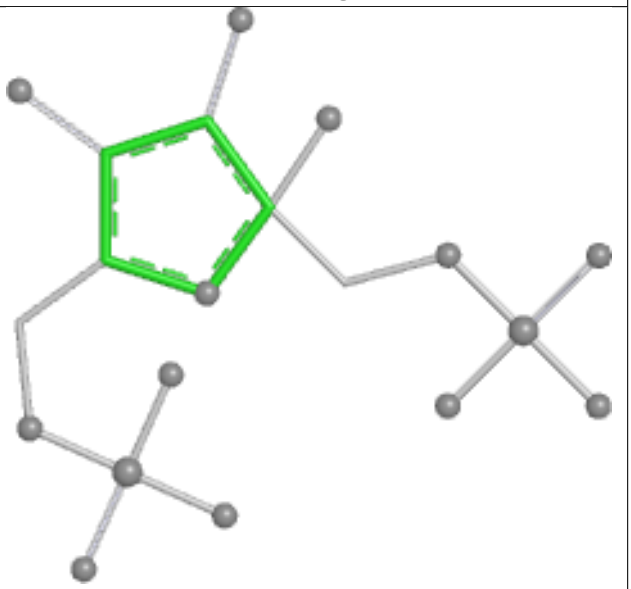
Bond lengths



Bond angles

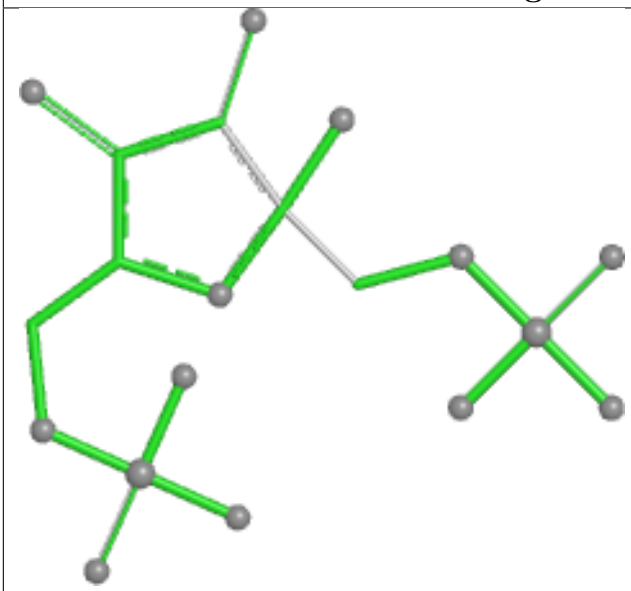


Torsions

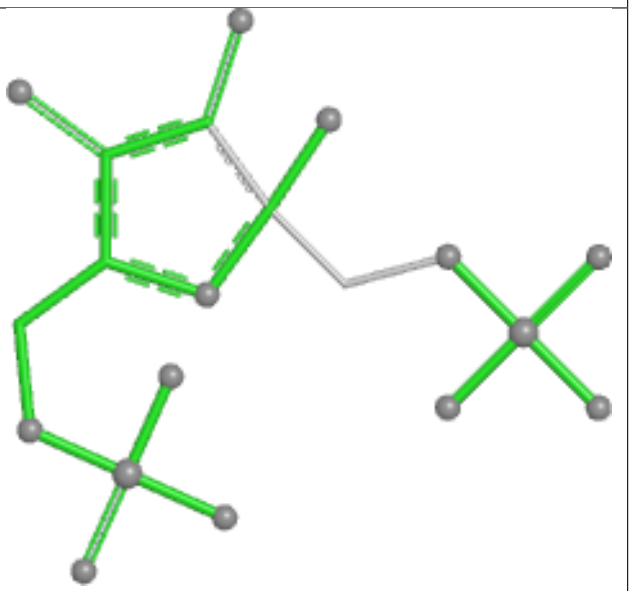


Rings

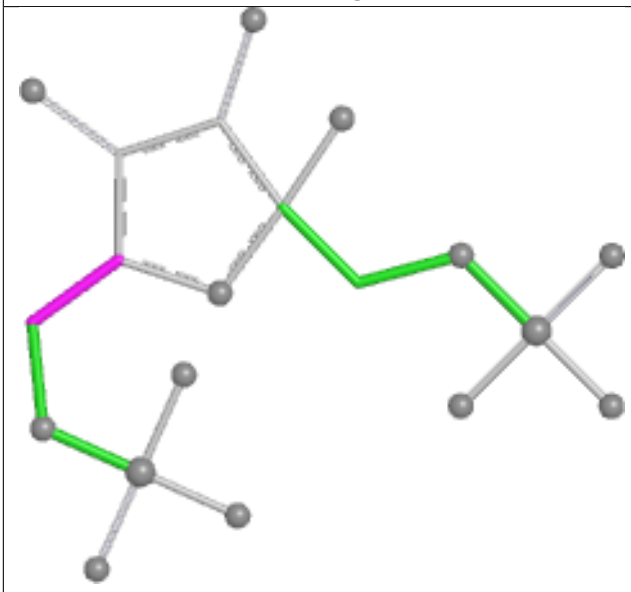
Ligand FBP A 601



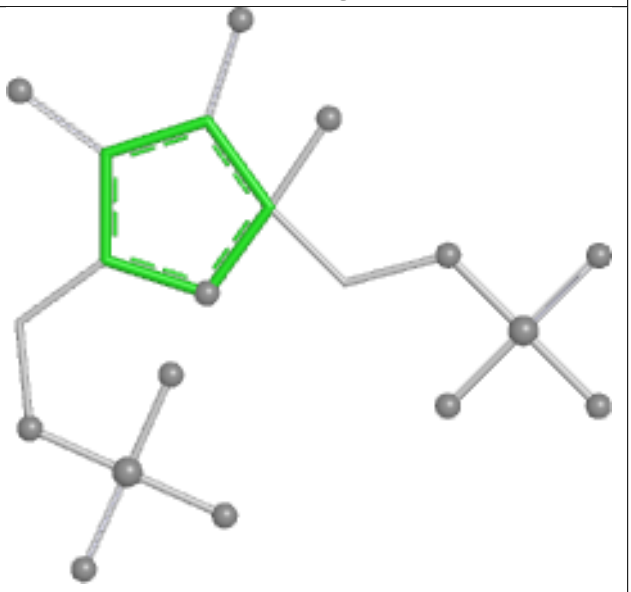
Bond lengths



Bond angles

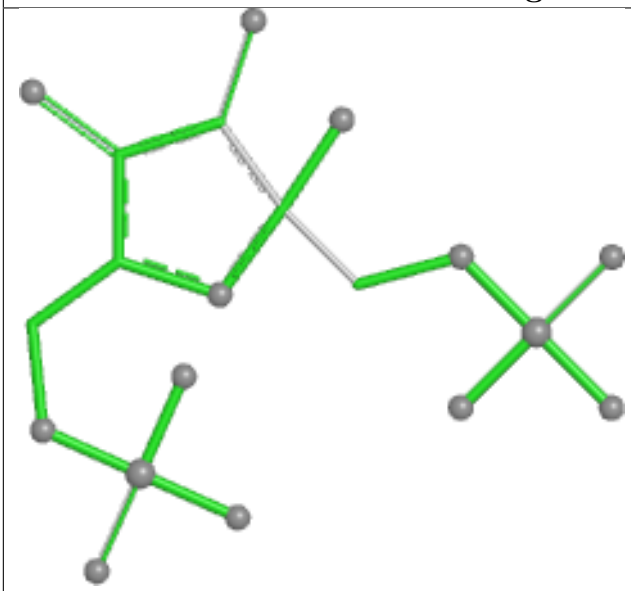


Torsions

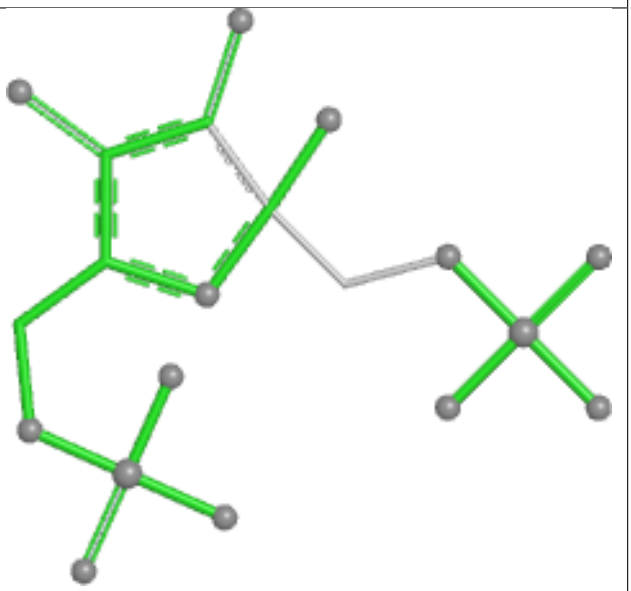


Rings

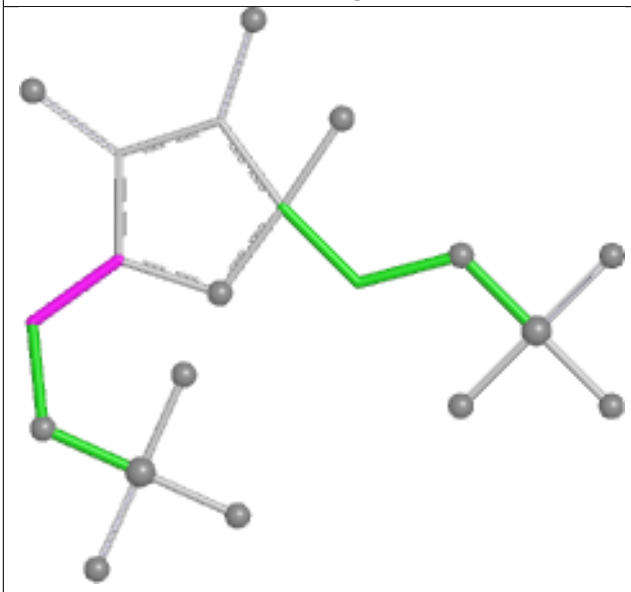
Ligand FBP B 601



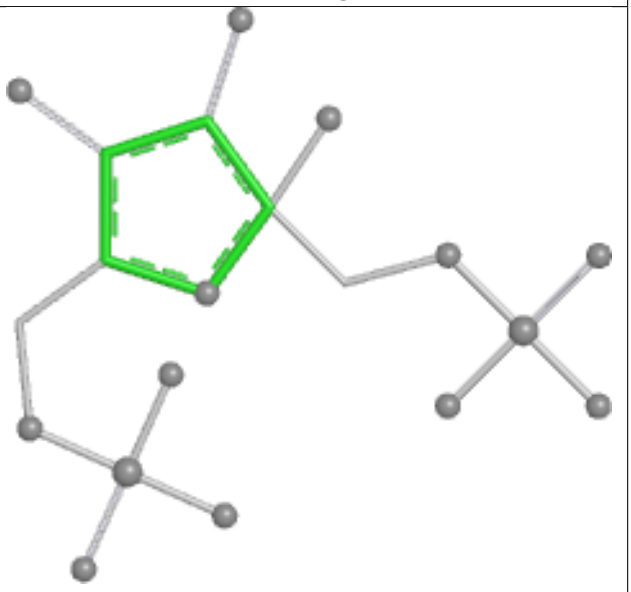
Bond lengths



Bond angles

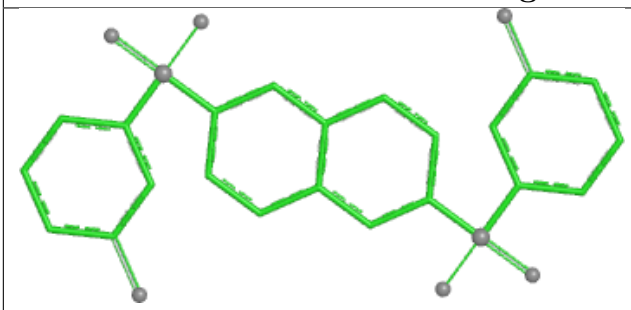


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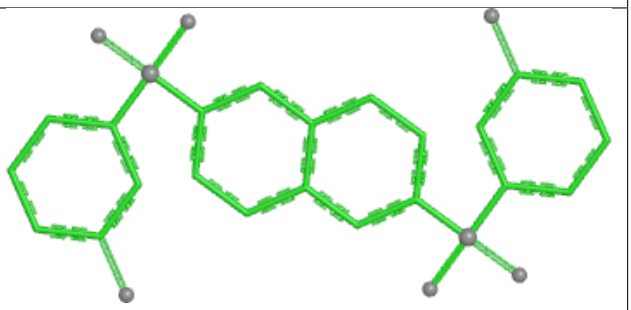


Rings

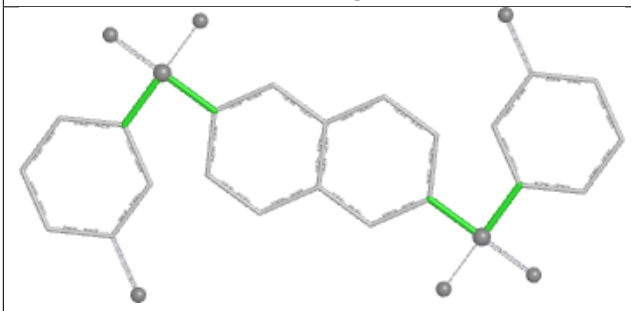
Ligand WVF E 604



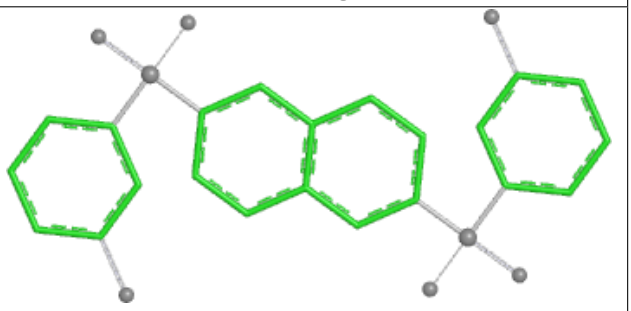
Bond lengths



Bond angles

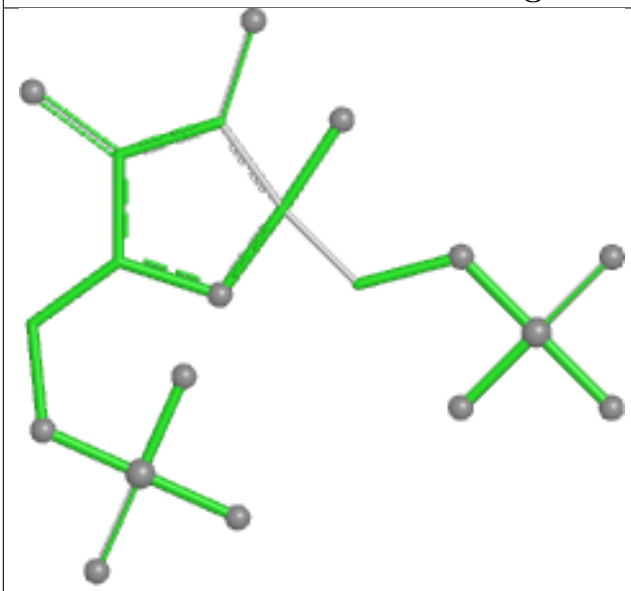


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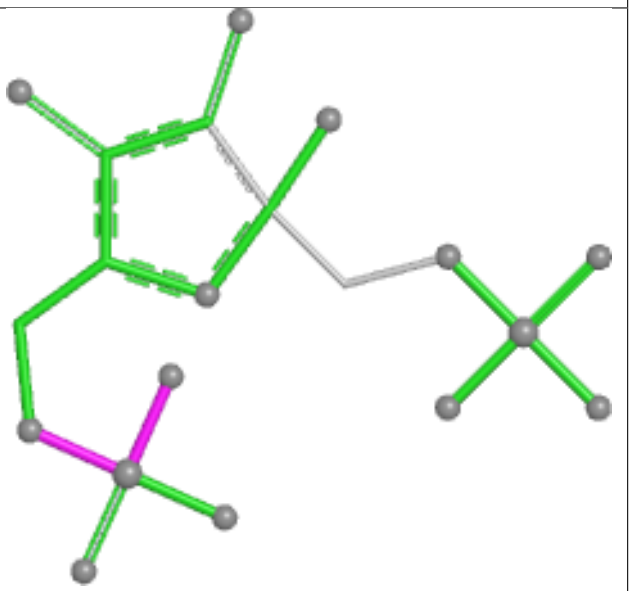


Rings

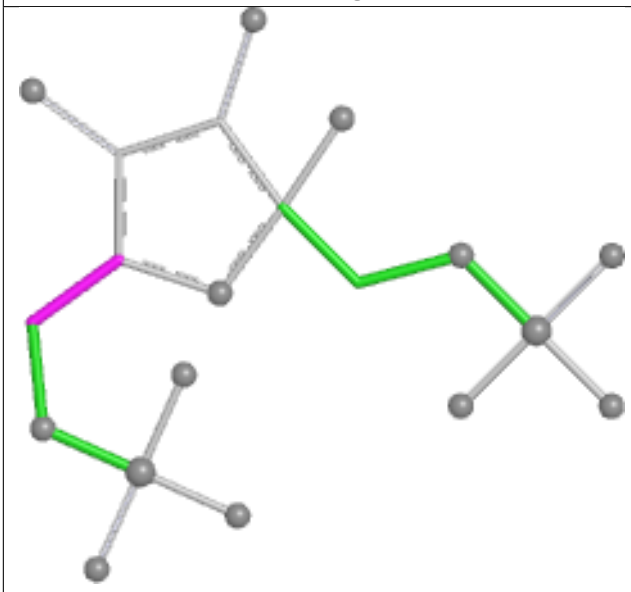
Ligand FBP D 601



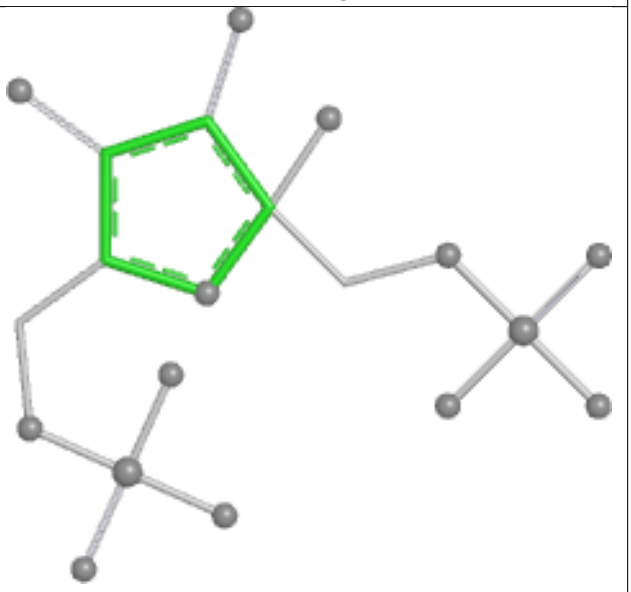
Bond lengths



Bond angles

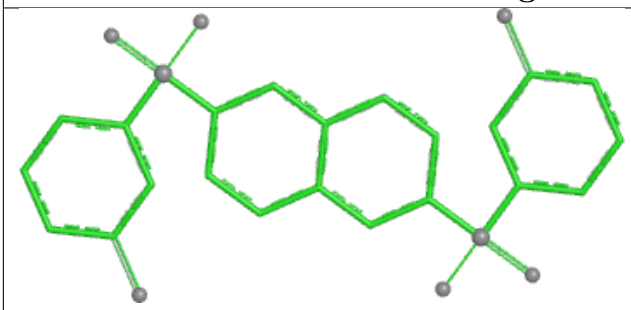


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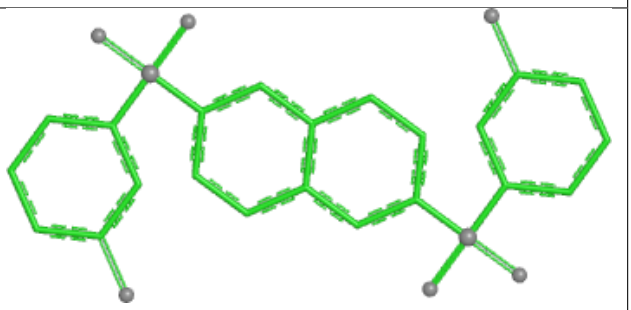


Rings

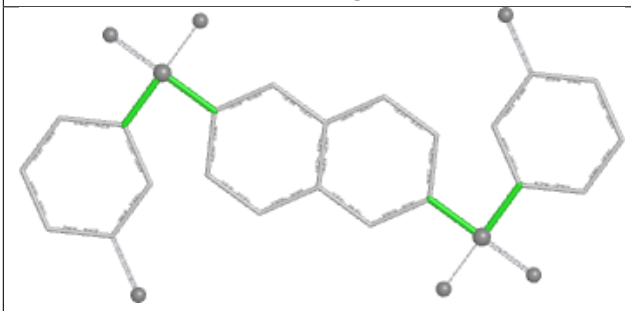
Ligand WVF B 604



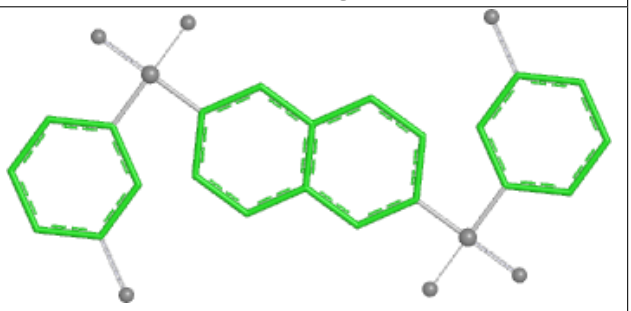
Bond lengths



Bond angles

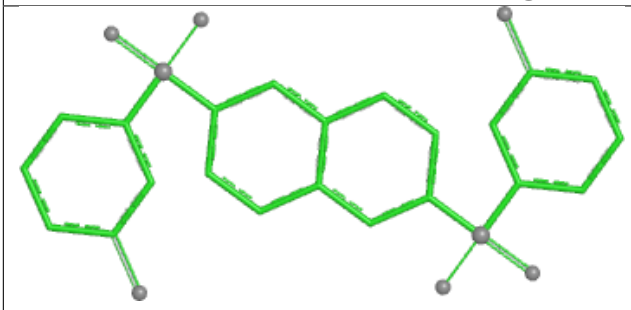


Torsions

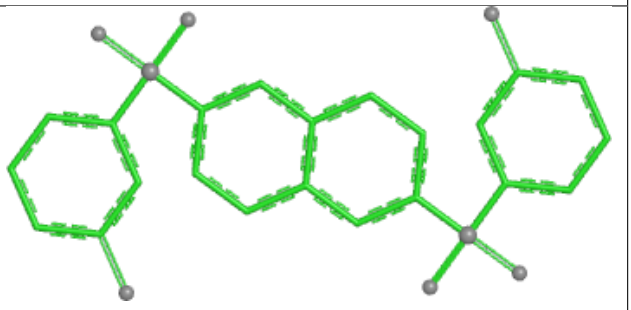


Rings

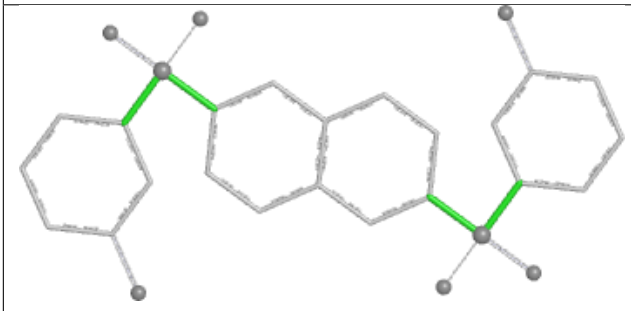
Ligand WVF F 603



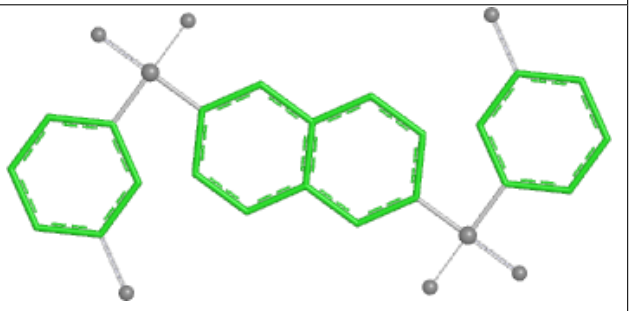
Bond lengths



Bond angles

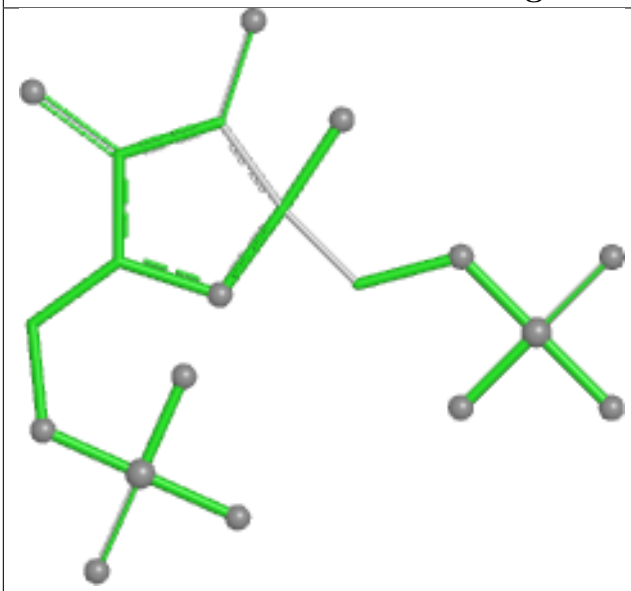


Torsions

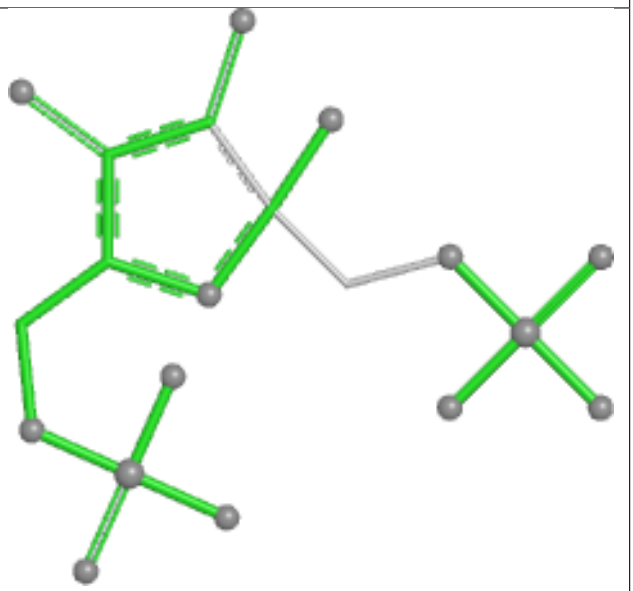


Rings

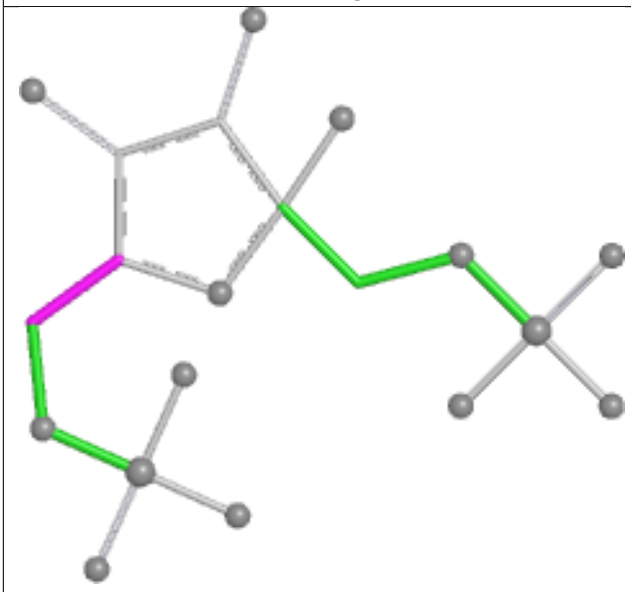
Ligand FBP C 601



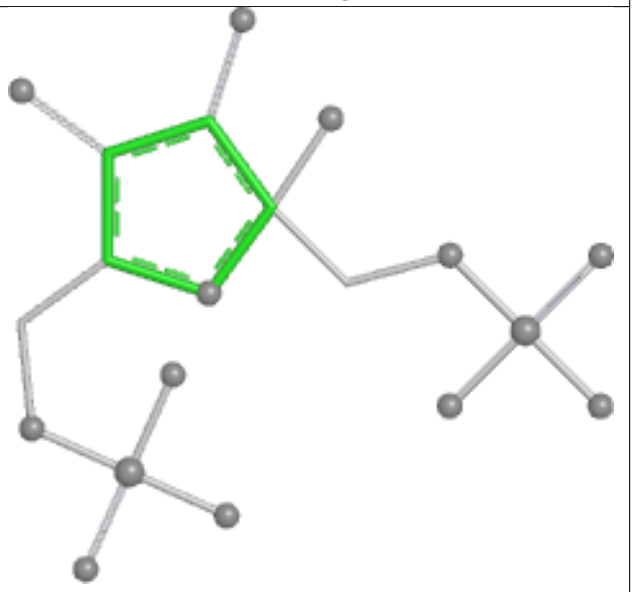
Bond lengths



Bond angles

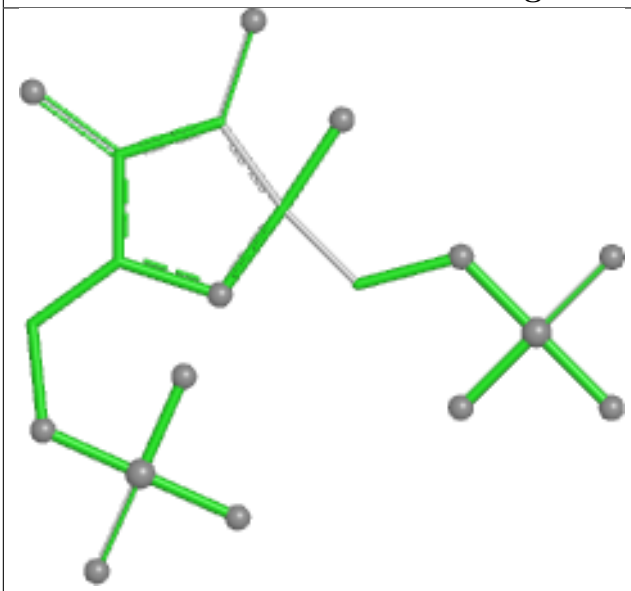


Torsions

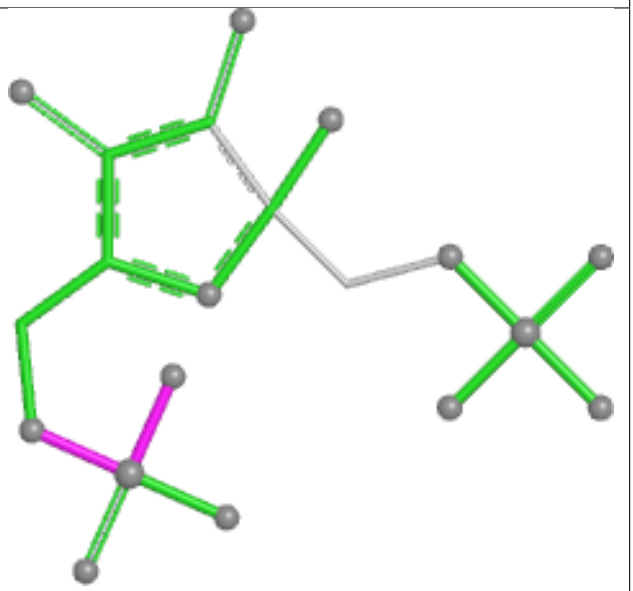


Rings

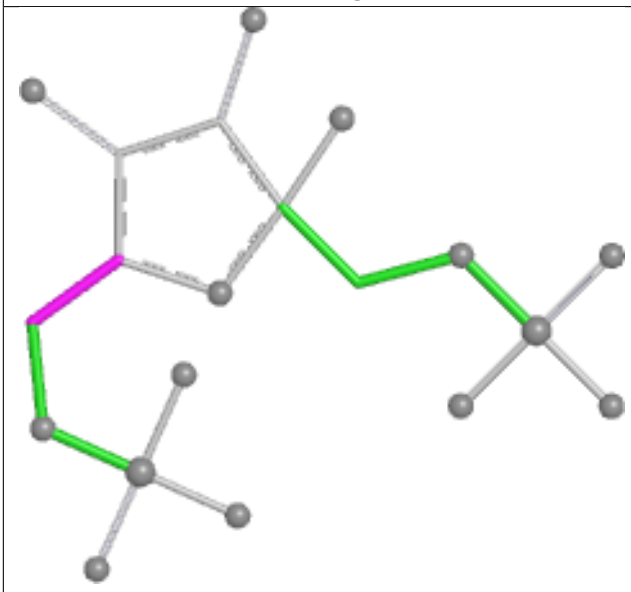
Ligand FBP H 601



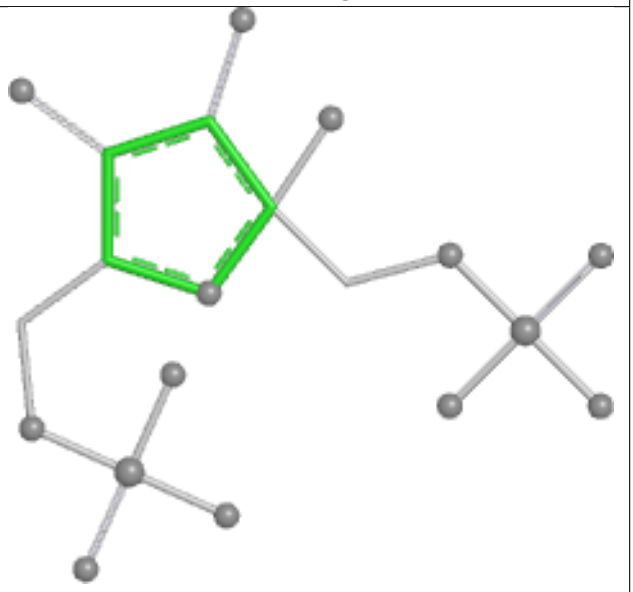
Bond lengths



Bond angles

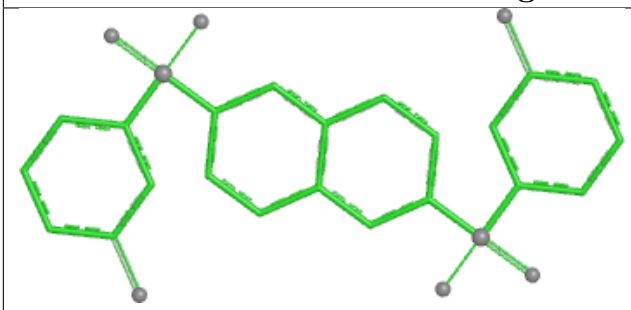


Torsions

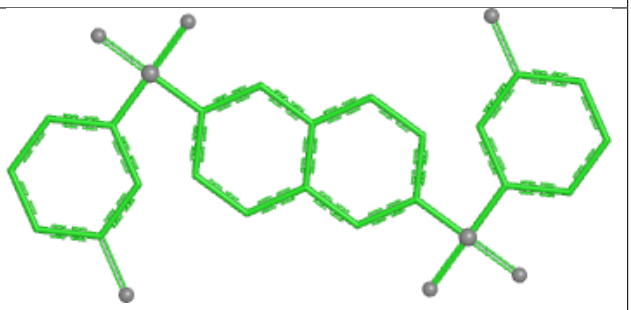


Rings

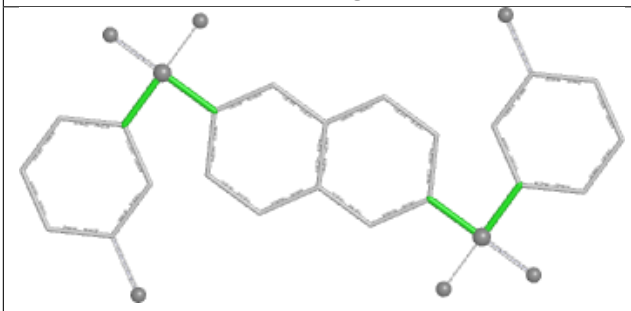
Ligand WVF A 603



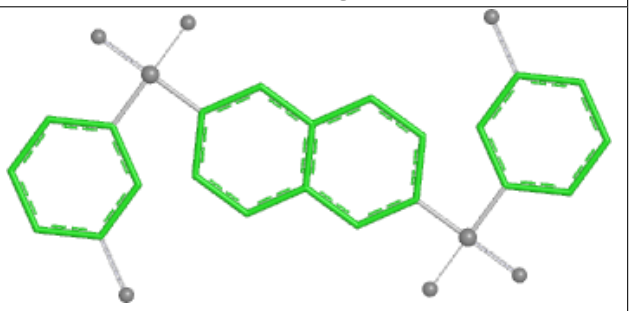
Bond lengths



Bond angles

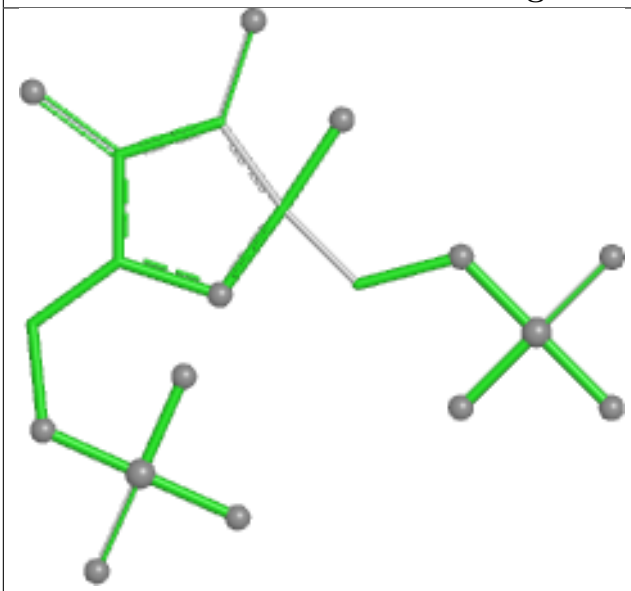


Torsions

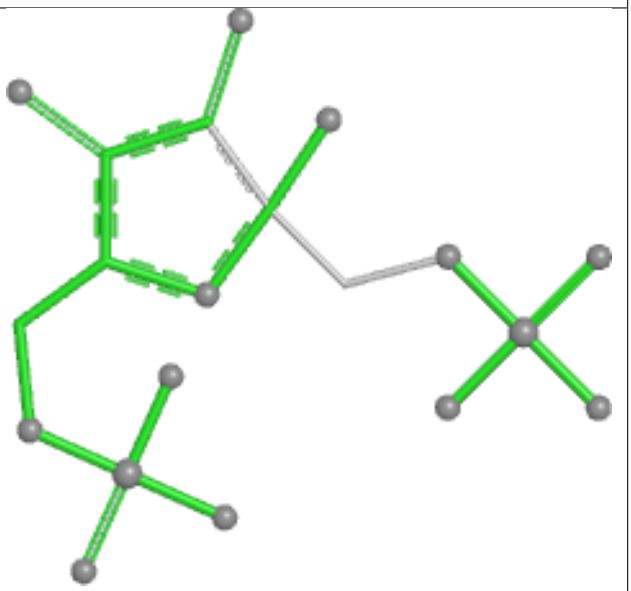


Rings

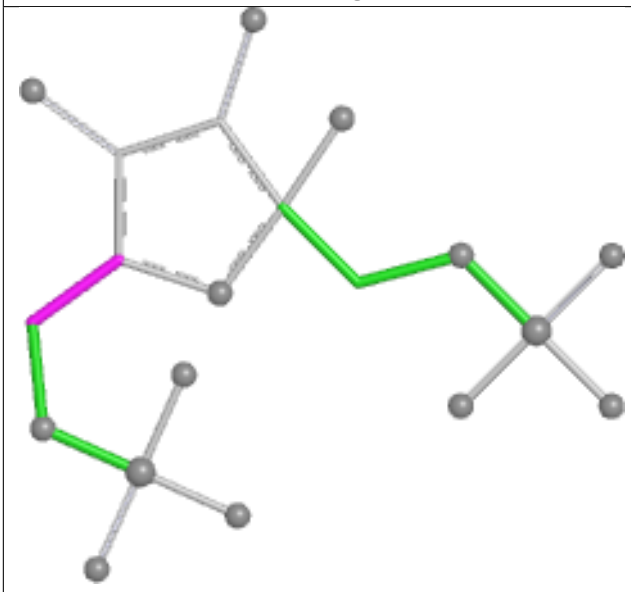
Ligand FBP F 601



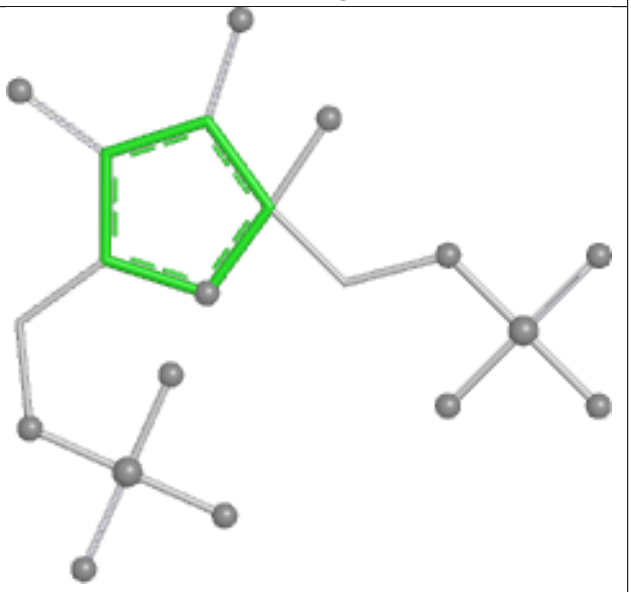
Bond lengths



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	421/447 (94%)	0.74	43 (10%)	12	14	20, 42, 68, 84	13 (3%)
1	B	436/447 (97%)	0.80	58 (13%)	7	7	19, 42, 72, 82	8 (1%)
1	C	425/447 (95%)	0.16	20 (4%)	36	38	19, 34, 53, 85	10 (2%)
1	D	425/447 (95%)	-0.07	12 (2%)	55	59	17, 30, 50, 82	8 (1%)
1	E	419/447 (93%)	0.50	27 (6%)	25	28	20, 39, 65, 80	14 (3%)
1	F	433/447 (96%)	0.40	28 (6%)	25	27	19, 37, 60, 79	8 (1%)
1	G	430/447 (96%)	0.08	19 (4%)	39	42	18, 32, 51, 87	11 (2%)
1	H	425/447 (95%)	-0.15	15 (3%)	47	52	15, 28, 49, 72	9 (2%)
All	All	3414/3576 (95%)	0.31	222 (6%)	25	27	15, 35, 63, 87	81 (2%)

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	273	GLY	6.5
1	C	273	GLY	6.1
1	A	25	PHE	5.9
1	F	233	PRO	5.8
1	C	233	PRO	5.7
1	B	545	SER	5.4
1	G	16	LEU	5.3
1	E	277[A]	HIS	5.1
1	B	513	LEU	5.0
1	H	21	GLY	4.9
1	A	132	GLY	4.5
1	E	25	PHE	4.4
1	D	25	PHE	4.3
1	G	277[A]	HIS	4.2
1	B	115	LEU	4.2
1	D	21	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	515	GLY	4.1
1	A	545	SER	4.0
1	A	269[A]	ARG	4.0
1	E	114	PRO	4.0
1	C	20	LEU	4.0
1	A	112	GLY	3.9
1	C	277[A]	HIS	3.8
1	B	269[A]	ARG	3.8
1	F	518	ARG	3.8
1	D	23	ALA	3.8
1	A	502	ARG	3.8
1	D	34	MET	3.7
1	A	34	MET	3.7
1	A	113	SER	3.7
1	D	24	PHE	3.7
1	A	115	LEU	3.6
1	D	277[A]	HIS	3.6
1	B	491	PRO	3.6
1	C	234	GLY	3.5
1	B	492	PRO	3.5
1	G	20	LEU	3.5
1	E	234	GLY	3.4
1	A	413	ARG	3.3
1	E	115	LEU	3.3
1	F	269[A]	ARG	3.3
1	G	131	SER	3.3
1	A	240	VAL	3.3
1	H	25	PHE	3.3
1	B	519	VAL	3.3
1	D	22	THR	3.3
1	F	491	PRO	3.3
1	F	492	PRO	3.3
1	H	22	THR	3.2
1	A	516	PHE	3.2
1	G	17	THR	3.2
1	B	418	LEU	3.2
1	G	25	PHE	3.2
1	B	114	PRO	3.1
1	B	70	VAL	3.1
1	B	518	ARG	3.1
1	F	514	ARG	3.1
1	A	235	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	70	VAL	3.0
1	E	516	PHE	3.0
1	B	416	ALA	3.0
1	B	413	ARG	3.0
1	E	112	GLY	3.0
1	E	129	PRO	3.0
1	B	514	ARG	3.0
1	G	34	MET	3.0
1	B	235	LEU	2.9
1	A	95	TYR	2.9
1	B	95	TYR	2.9
1	E	116	SER	2.9
1	C	22	THR	2.9
1	C	25	PHE	2.9
1	A	23	ALA	2.9
1	A	272	LEU	2.9
1	H	34	MET	2.9
1	B	506	PHE	2.9
1	B	512	LYS	2.9
1	C	21	GLY	2.9
1	B	508	ILE	2.9
1	A	116	SER	2.8
1	C	34	MET	2.8
1	H	518	ARG	2.8
1	F	353	ARG	2.8
1	G	130	GLY	2.8
1	F	115	LEU	2.8
1	E	23	ALA	2.7
1	E	26	GLN	2.7
1	H	23	ALA	2.7
1	B	511	GLY	2.7
1	F	418	LEU	2.7
1	A	313	ILE	2.7
1	F	234	GLY	2.7
1	F	235	LEU	2.7
1	E	111	ALA	2.7
1	G	116[A]	SER	2.7
1	E	544	ILE	2.7
1	B	380	ALA	2.6
1	B	90	HIS	2.6
1	B	118	ARG	2.6
1	A	24	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	274	PRO	2.6
1	E	34	MET	2.6
1	F	490	GLU	2.6
1	B	277	HIS	2.6
1	A	414	ARG	2.6
1	D	414	ARG	2.6
1	A	428	ILE	2.6
1	A	251	VAL	2.6
1	E	269[A]	ARG	2.5
1	F	414	ARG	2.5
1	H	244[A]	ARG	2.5
1	C	272[A]	LEU	2.5
1	B	130	GLY	2.5
1	H	545	SER	2.5
1	B	350	THR	2.5
1	B	233	PRO	2.5
1	F	129	PRO	2.5
1	G	129	PRO	2.5
1	B	486	LEU	2.5
1	A	277	HIS	2.5
1	E	113	SER	2.5
1	G	22	THR	2.5
1	B	244	ARG	2.5
1	B	544	ILE	2.5
1	C	274	PRO	2.5
1	E	492	PRO	2.5
1	B	128	GLY	2.4
1	C	413	ARG	2.4
1	C	414	ARG	2.4
1	D	233	PRO	2.4
1	E	244	ARG	2.4
1	H	414	ARG	2.4
1	F	509	GLU	2.4
1	E	258	PHE	2.4
1	F	381	LYS	2.4
1	A	498	ASP	2.4
1	A	265	VAL	2.4
1	E	235	LEU	2.4
1	A	88	PHE	2.4
1	B	245	PHE	2.4
1	A	406	ARG	2.4
1	E	353	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	494	ALA	2.4
1	C	18	GLN	2.4
1	B	510	SER	2.4
1	F	486	LEU	2.3
1	A	245	PHE	2.3
1	B	106	ALA	2.3
1	E	128	GLY	2.3
1	A	244	ARG	2.3
1	A	73	LEU	2.3
1	B	487	LEU	2.3
1	F	277	HIS	2.3
1	B	238	GLN	2.3
1	A	517	LEU	2.3
1	C	117	TYR	2.3
1	A	111	ALA	2.3
1	C	114	PRO	2.3
1	H	233	PRO	2.3
1	A	128	GLY	2.3
1	F	112	GLY	2.3
1	F	489	ARG	2.3
1	A	26	GLN	2.3
1	A	118	ARG	2.2
1	B	119	PRO	2.2
1	F	417	PRO	2.2
1	H	516	PHE	2.2
1	B	268	VAL	2.2
1	G	414	ARG	2.2
1	B	86	LEU	2.2
1	B	417	PRO	2.2
1	D	131	SER	2.2
1	D	234	GLY	2.2
1	F	501	ASP	2.2
1	B	97	ALA	2.2
1	B	415	ALA	2.2
1	A	30	LEU	2.2
1	G	21	GLY	2.2
1	A	473	ALA	2.2
1	B	270	ALA	2.2
1	E	271	ALA	2.2
1	B	10	ARG	2.2
1	H	277[A]	HIS	2.1
1	B	110	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	24	PHE	2.1
1	F	410	GLU	2.1
1	B	107	VAL	2.1
1	B	259	VAL	2.1
1	E	240	VAL	2.1
1	E	543[A]	SER	2.1
1	F	413	ARG	2.1
1	B	497	ALA	2.1
1	F	506	PHE	2.1
1	G	26	GLN	2.1
1	B	495	ILE	2.1
1	B	504	VAL	2.1
1	C	353	ARG	2.1
1	D	244[A]	ARG	2.1
1	E	247	VAL	2.1
1	F	118	ARG	2.1
1	A	410	GLU	2.1
1	H	275	GLU	2.1
1	A	274	PRO	2.1
1	B	100	ILE	2.1
1	C	113	SER	2.1
1	G	413	ARG	2.1
1	G	518	ARG	2.1
1	H	417	PRO	2.1
1	B	66	ALA	2.1
1	B	494	ALA	2.1
1	B	77	ILE	2.0
1	B	258	PHE	2.0
1	B	99	SER	2.0
1	G	313	ILE	2.0
1	A	117	TYR	2.0
1	C	129	PRO	2.0
1	A	496	TRP	2.0
1	C	115	LEU	2.0
1	F	244	ARG	2.0
1	H	33	ALA	2.0
1	B	113	SER	2.0
1	A	273	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 oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OXL	E	602	6/6	0.88	0.11	48,49,49,49	0
5	MG	B	605	1/1	0.89	0.12	50,50,50,50	0
3	OXL	F	602	6/6	0.91	0.10	43,44,46,47	0
7	EDO	E	603	4/4	0.91	0.12	44,45,45,45	6
3	OXL	A	602	6/6	0.93	0.08	48,49,49,50	0
7	EDO	H	603	4/4	0.93	0.13	35,35,36,36	6
3	OXL	D	602	6/6	0.94	0.07	35,36,38,38	0
6	K	A	605	1/1	0.94	0.09	72,72,72,72	0
7	EDO	B	603	4/4	0.94	0.10	35,36,38,38	6
7	EDO	D	603	4/4	0.94	0.11	39,39,40,40	6
3	OXL	B	602	6/6	0.94	0.08	41,43,45,46	0
7	EDO	G	603	4/4	0.94	0.10	38,38,40,40	6
3	OXL	C	602	6/6	0.94	0.08	42,43,44,45	0
3	OXL	H	602	6/6	0.95	0.07	35,36,36,37	0
3	OXL	G	602	6/6	0.95	0.07	39,40,41,42	0
4	WVF	A	603	30/30	0.96	0.08	27,31,35,35	16
6	K	C	605	1/1	0.96	0.12	57,57,57,57	0
7	EDO	F	604	4/4	0.96	0.09	37,37,38,38	6
2	FBP	B	601	20/20	0.96	0.07	39,40,44,45	0
7	EDO	C	603	4/4	0.96	0.07	33,33,34,34	6
6	K	F	606	1/1	0.97	0.10	72,72,72,72	0
6	K	G	605	1/1	0.97	0.12	57,57,57,57	0
4	WVF	E	604	30/30	0.97	0.07	30,33,35,36	16
4	WVF	F	603	30/30	0.97	0.07	28,32,35,35	16
2	FBP	F	601	20/20	0.97	0.06	34,39,44,44	0
2	FBP	A	601	20/20	0.97	0.06	37,39,40,40	0
6	K	B	606	1/1	0.97	0.09	58,58,58,58	0
4	WVF	B	604	30/30	0.97	0.07	27,31,33,33	16
6	K	E	606	1/1	0.97	0.15	71,71,71,71	0
2	FBP	E	601	20/20	0.98	0.05	33,35,37,37	0
6	K	H	605	1/1	0.98	0.11	47,47,47,47	0
2	FBP	G	601	20/20	0.98	0.04	23,26,28,29	0

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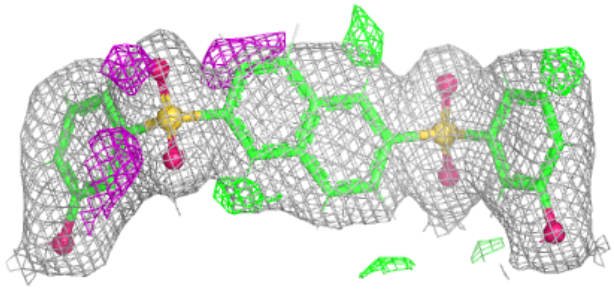
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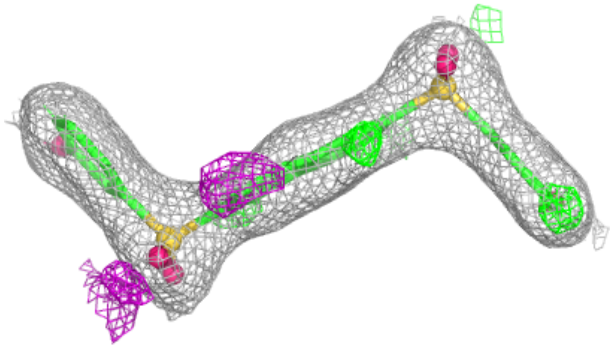
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	E	605	1/1	0.99	0.03	40,40,40,40	0
5	MG	F	605	1/1	0.99	0.03	36,36,36,36	0
5	MG	G	604	1/1	0.99	0.03	33,33,33,33	0
2	FBP	C	601	20/20	0.99	0.04	25,26,31,33	0
2	FBP	H	601	20/20	0.99	0.04	22,24,26,27	0
5	MG	A	604	1/1	0.99	0.04	50,50,50,50	0
6	K	D	605	1/1	0.99	0.10	43,43,43,43	0
2	FBP	D	601	20/20	0.99	0.04	23,25,29,29	0
5	MG	C	604	1/1	0.99	0.03	37,37,37,37	0
5	MG	H	604	1/1	1.00	0.03	31,31,31,31	0
5	MG	D	604	1/1	1.00	0.02	35,35,35,35	0

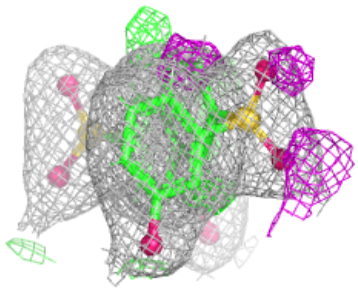
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WVF A 603:

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

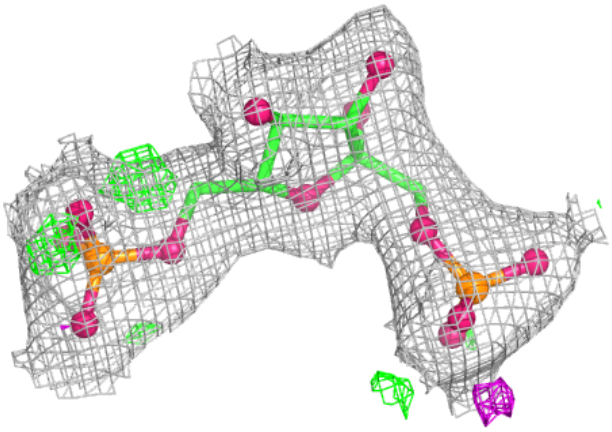


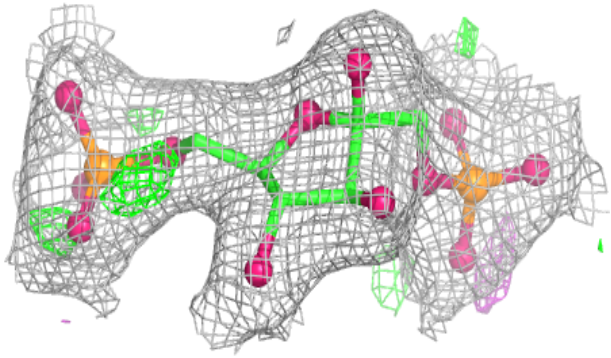


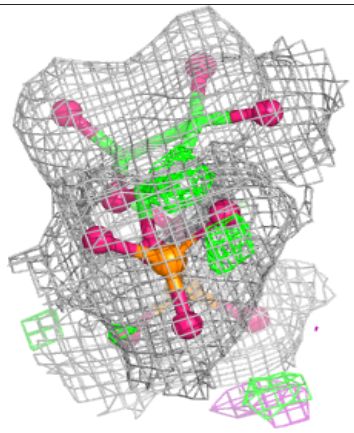


Electron density around FBP B 601:

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

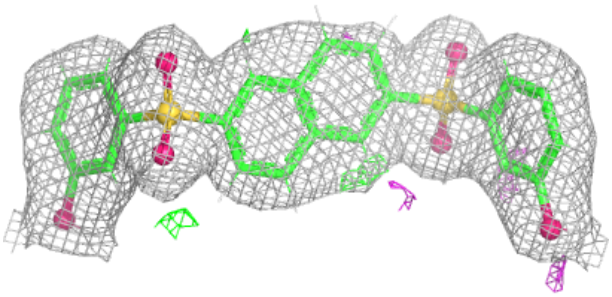


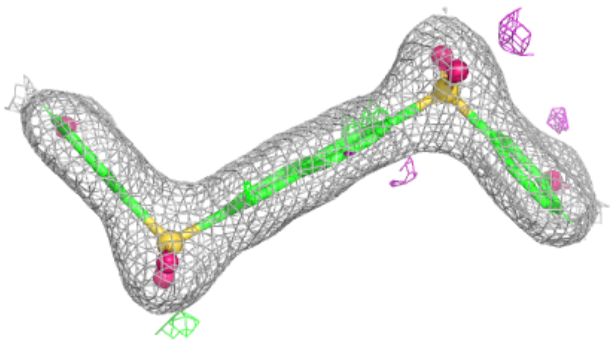


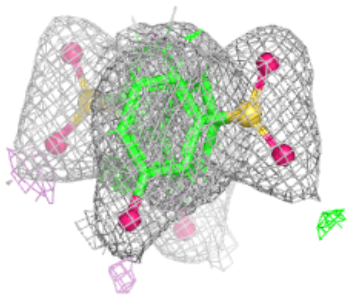


Electron density around WVF E 604:

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

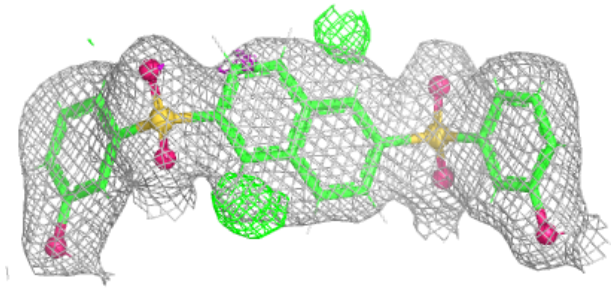


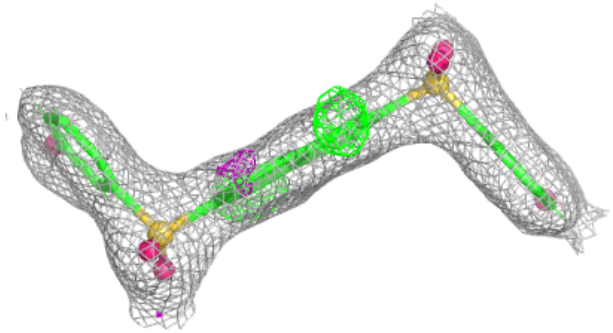


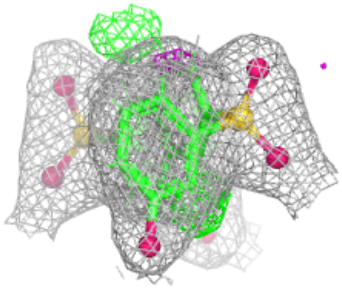


Electron density around WVF F 603:

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

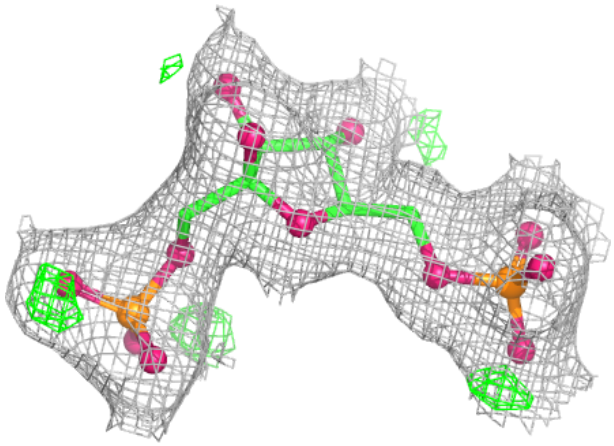


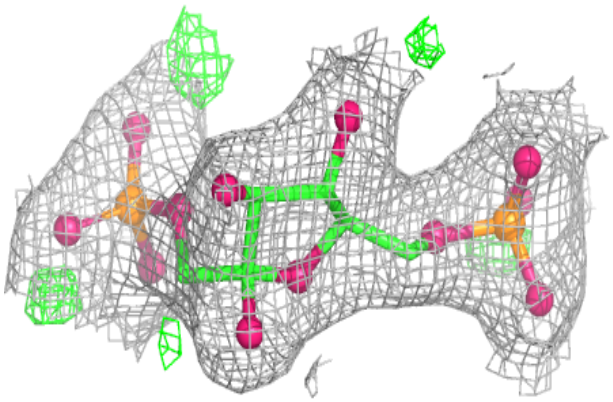


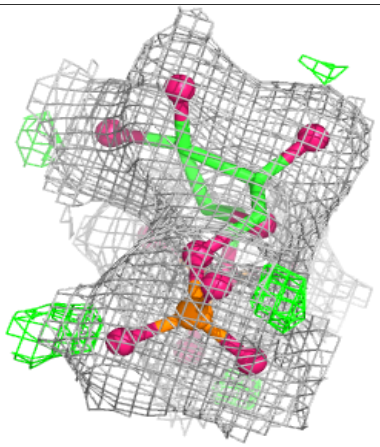


Electron density around FBP F 601:

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

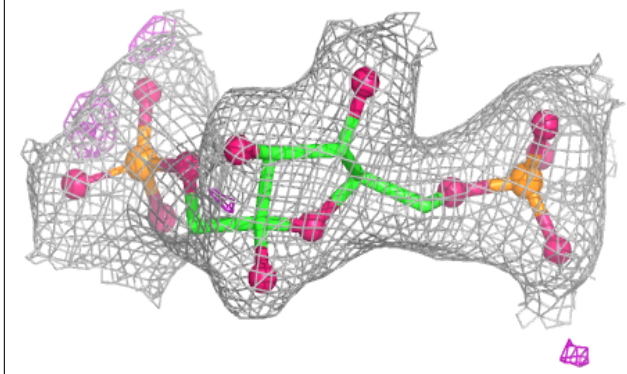


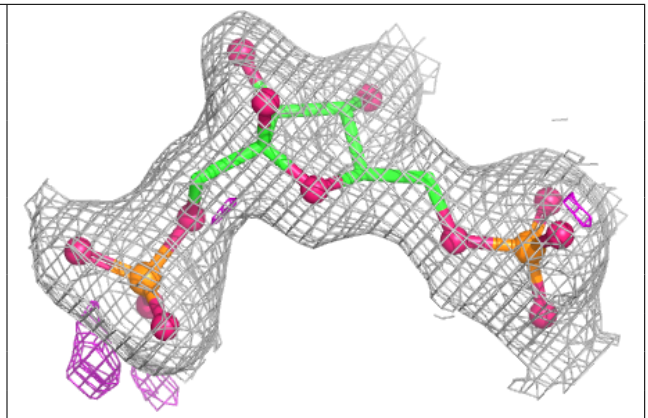


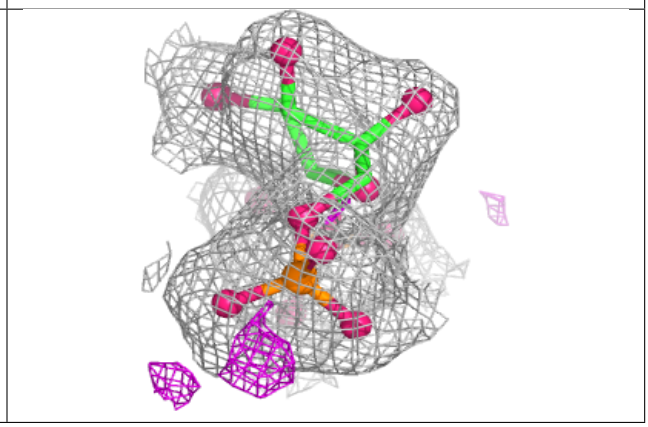


Electron density around FBP A 601:

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

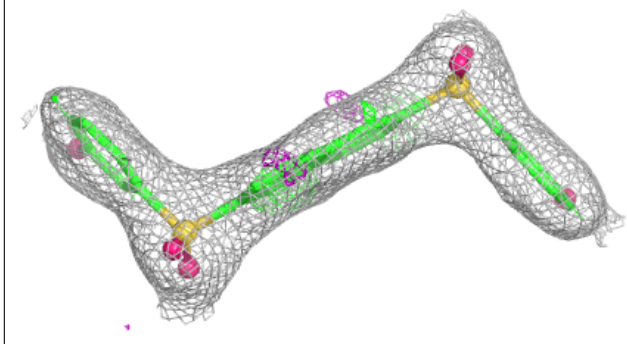


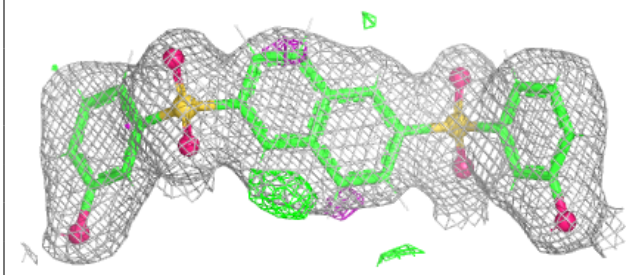


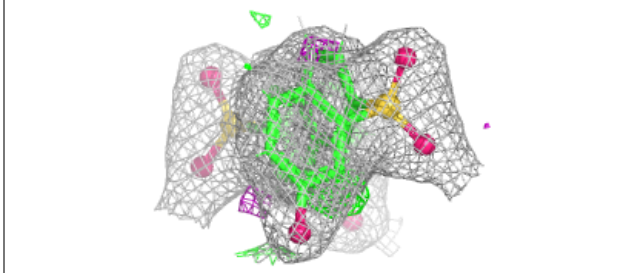


Electron density around WVF B 604:

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

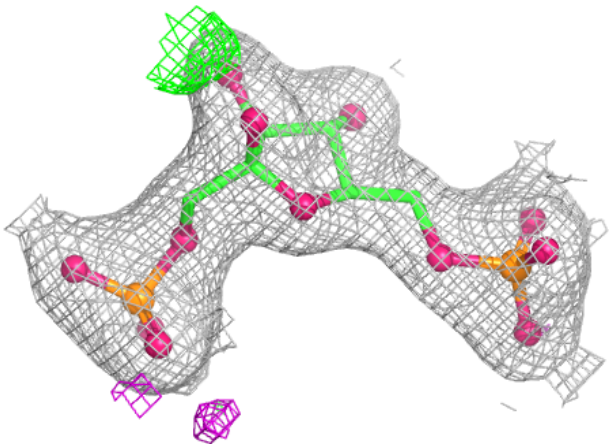


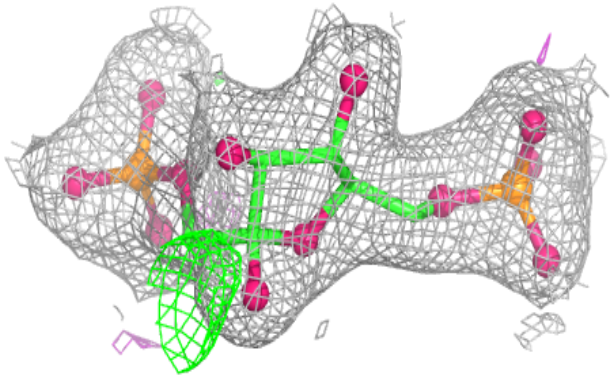


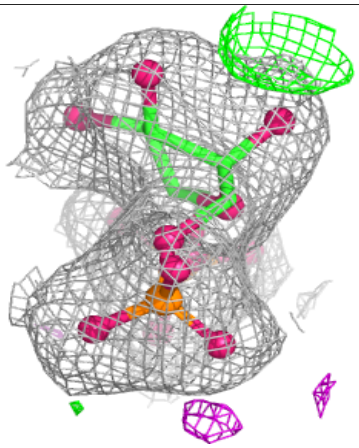


Electron density around FBP E 601:

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

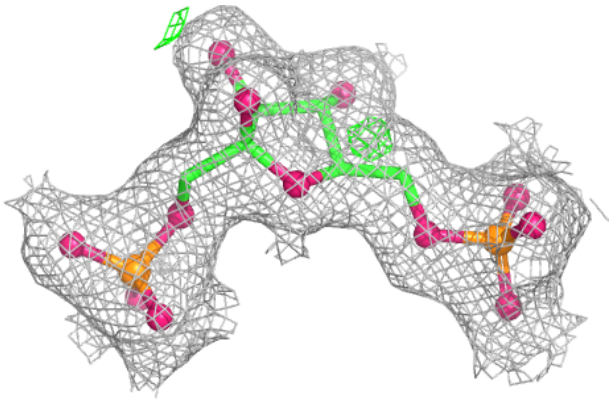


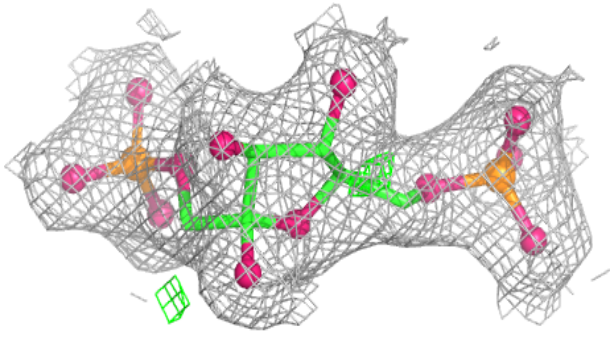


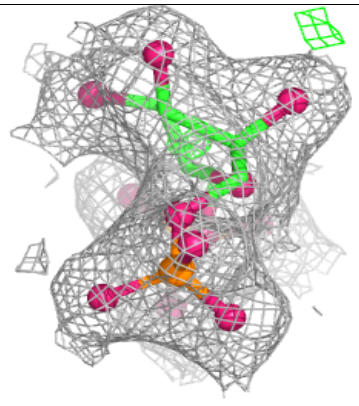


Electron density around FBP G 601:

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

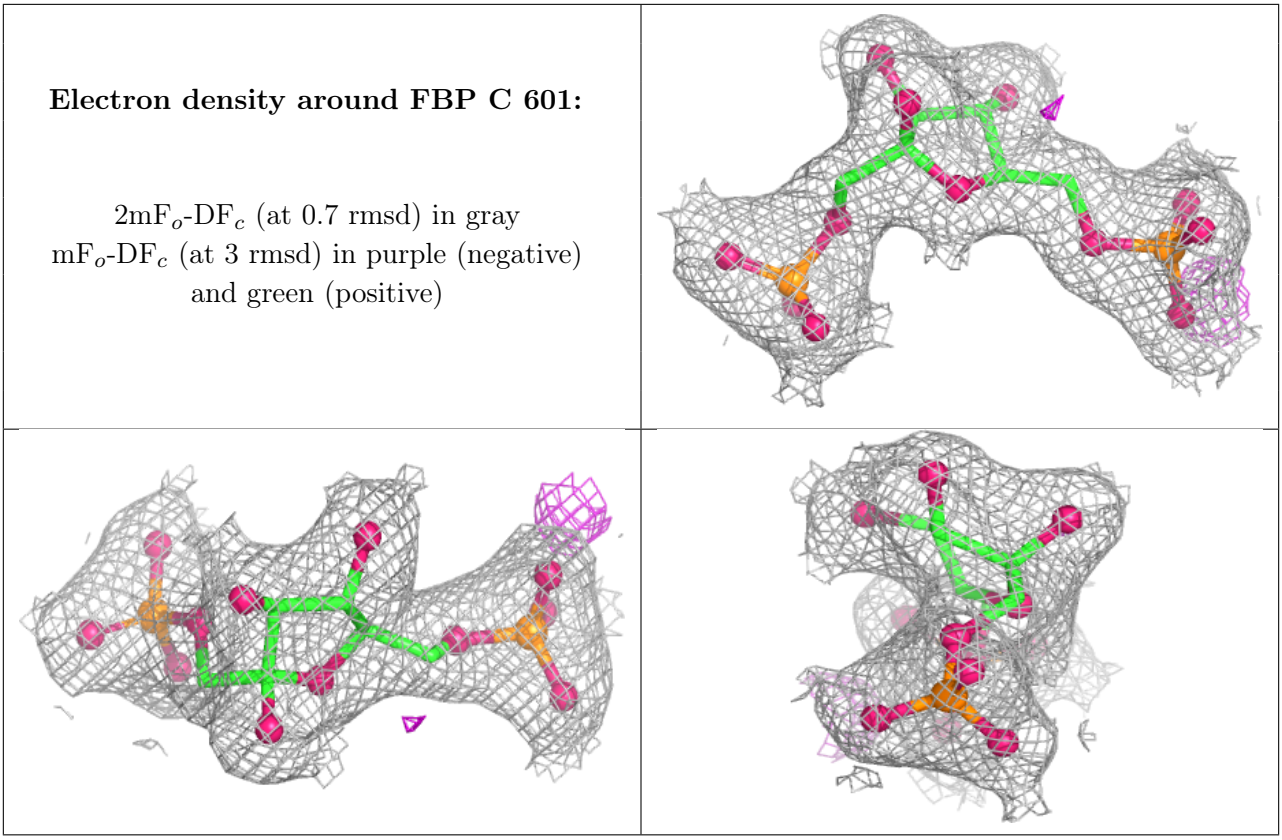






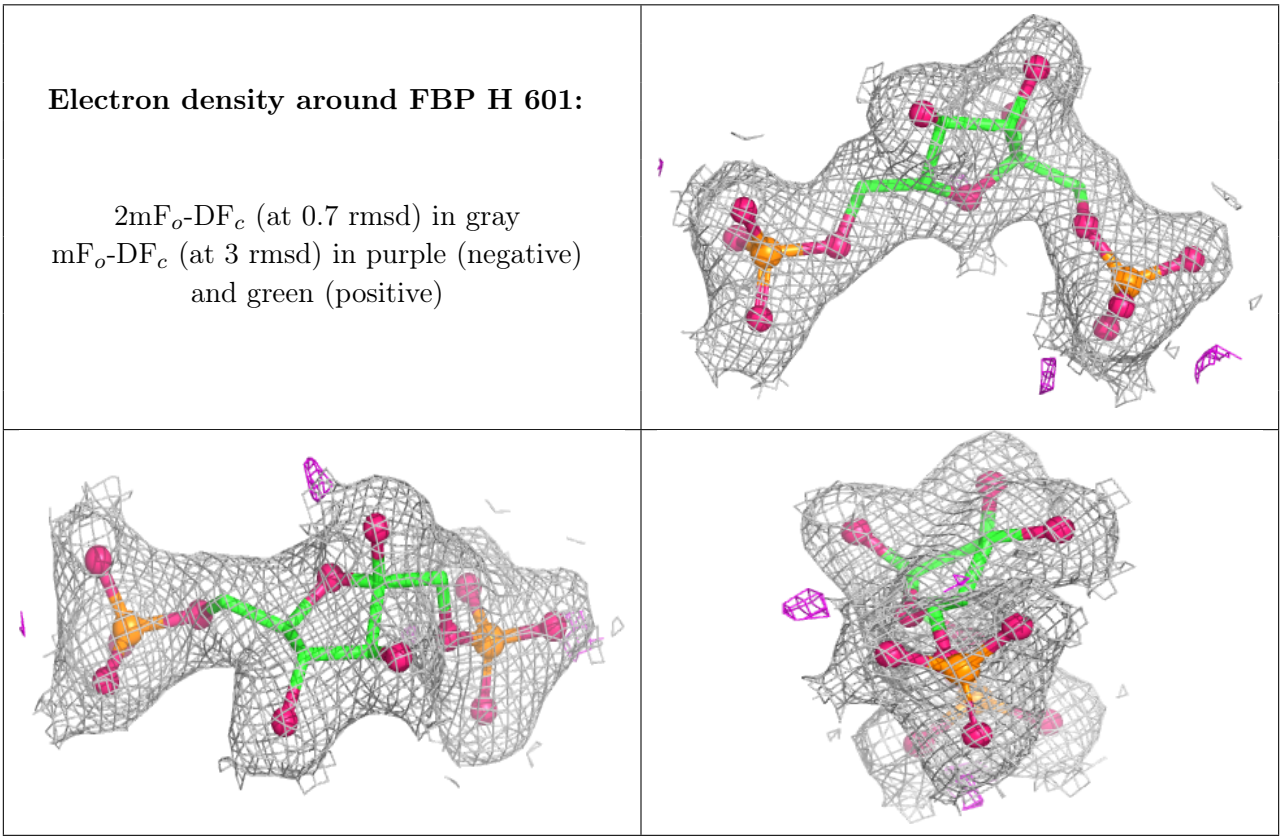
Electron density around FBP C 601:

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



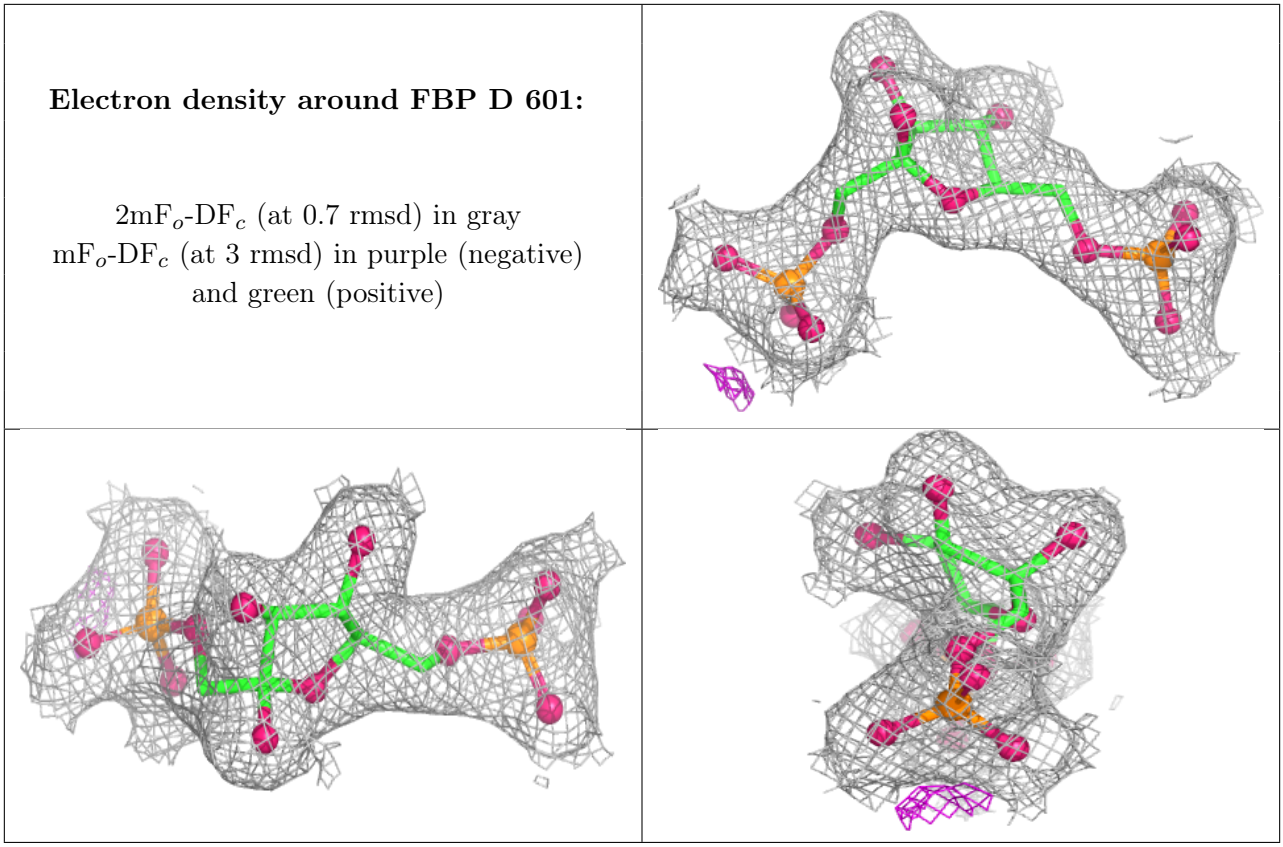
Electron density around FBP H 601:

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



Electron density around FBP 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

There are no such residues in this entry.