Full wwPDB X-ray Structure Validation Report (i)

Apr 3, 2023 – 05:04 PM EDT

PDB ID	:	7FS7
Title	:	Structure of liver pyruvate kinase in complex with allosteric modulator 20
Authors	:	Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2022-12-18
Resolution	:	2.77 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:

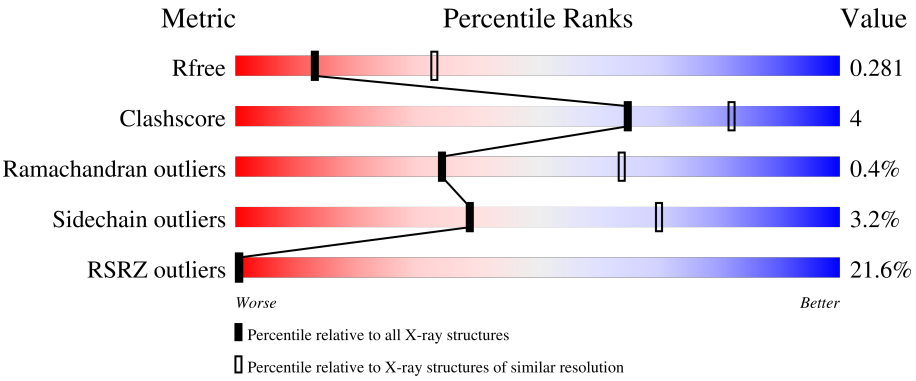
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	40% 84% 10% 6%
1	B	447	21% 85% 12% •
1	C	447	20% 80% 14% • 5%
1	D	447	5% 82% 12% • 5%
1	E	447	37% 82% 11% 6%

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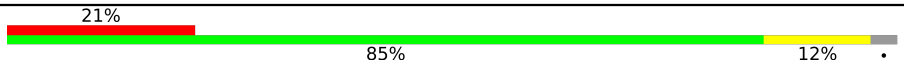
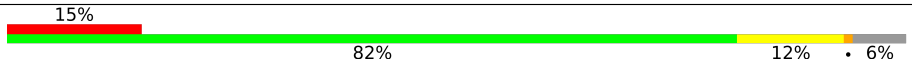
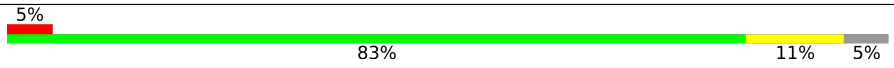
Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	602	-	-	-	X
3	OXL	F	602	-	X	-	-
5	K	E	604	-	-	-	X
6	OAT	G	605	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 26801 atoms, of which 63 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	419	Total	C	N	O	S	0	5	0
			3210	2018	579	593	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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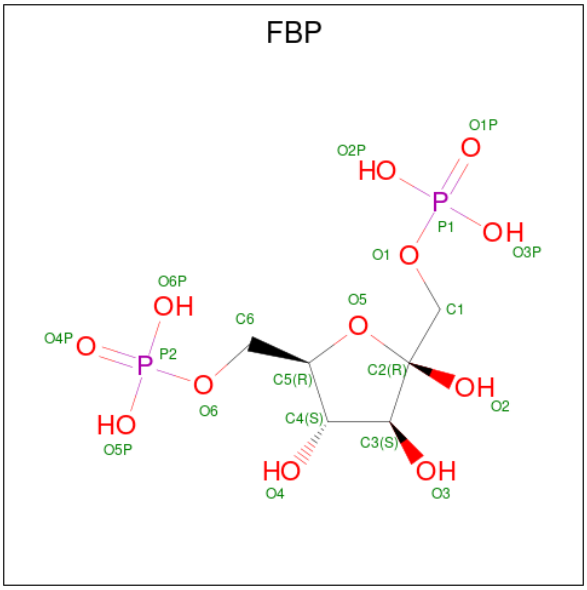
Chain	Residue	Modelled	Actual	Comment	Reference
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	130	GLY	-	linker	UNP P30613
H	131	SER	-	linker	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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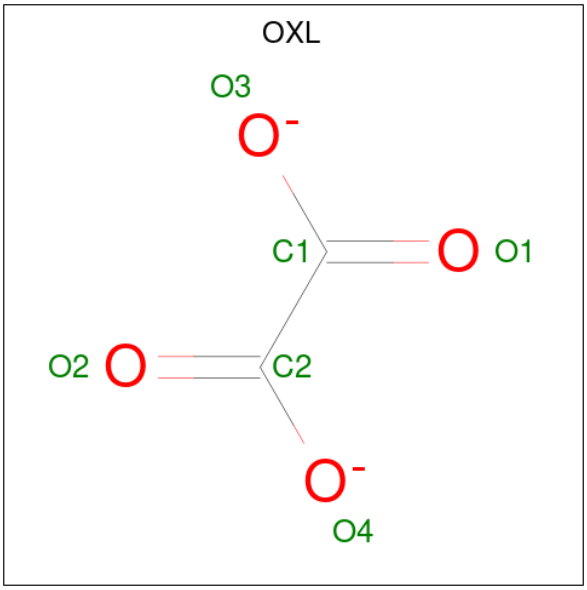
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O P 20 6 12 2	0	0
2	H	1	Total C O P 20 6 12 2	0	0

- 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

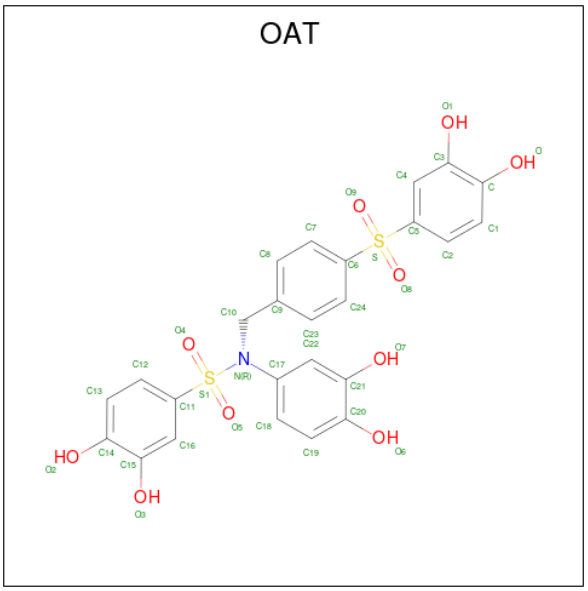
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 N-{[4-(3,4-dihydroxybenzene-1-sulfonyl)phenyl]methyl}-N-(3,4-dihydroxyphenyl)-3,4-dihydroxybenzene-1-sulfonamide (three-letter code: OAT) (formula: $C_{25}H_{21}NO_{10}S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	S	21	0
			59	25	21	1	10	2		
6	G	1	Total	C	H	N	O	S	21	0
			59	25	21	1	10	2		
6	H	1	Total	C	H	N	O	S	21	0
			59	25	21	1	10	2		

- Molecule 7 is water.

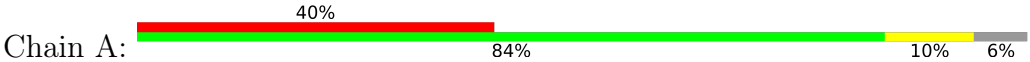
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	O	0	0
			5	5		
7	B	15	Total	O	0	0
			15	15		
7	C	45	Total	O	0	0
			45	45		
7	D	79	Total	O	0	0
			79	79		
7	E	9	Total	O	0	0
			9	9		
7	F	35	Total	O	0	0
			35	35		
7	G	48	Total	O	0	0
			48	48		
7	H	87	Total	O	0	0
			87	87		

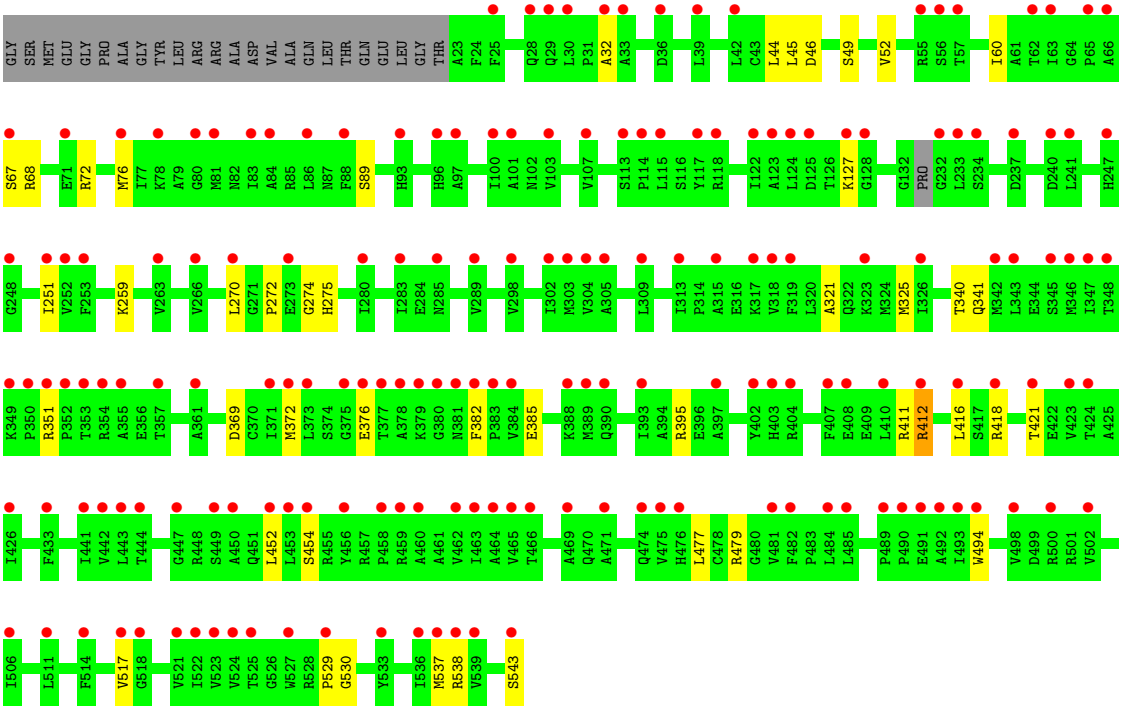
3 Residue-property plots (i)

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

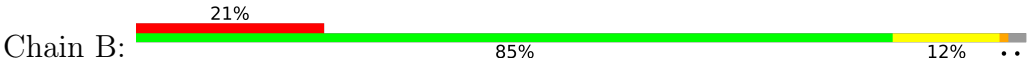
Chain A:

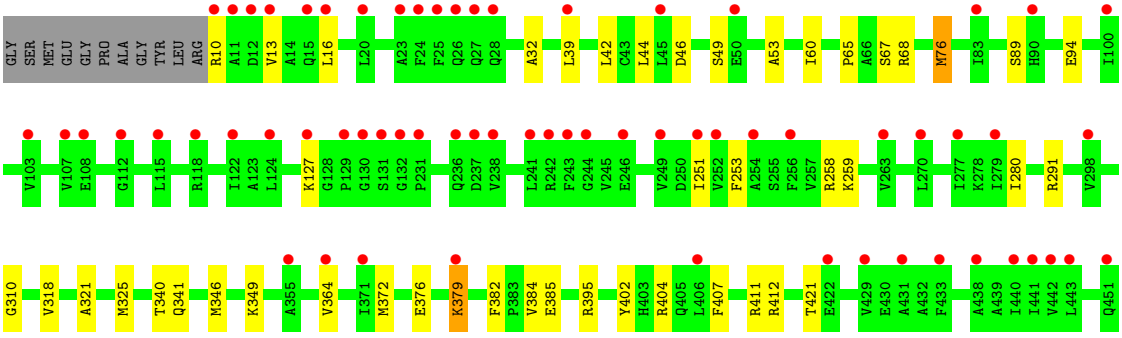




• Molecule 1: Pyruvate kinase PKLR

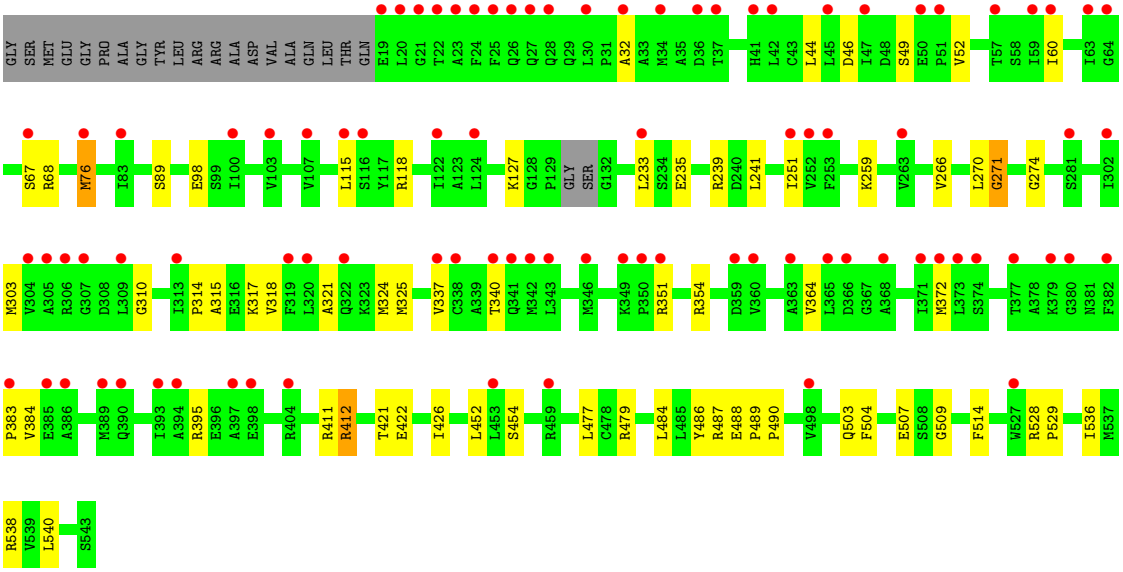
Chain B:





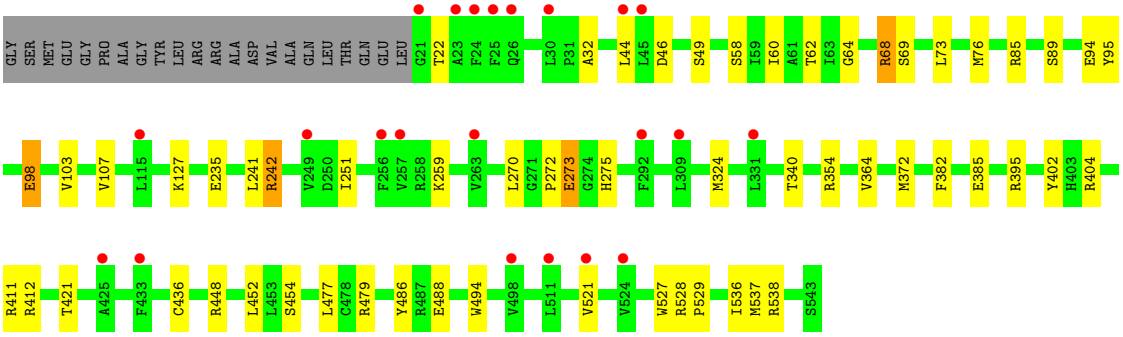
• Molecule 1: Pyruvate kinase PKLR

Chain C:



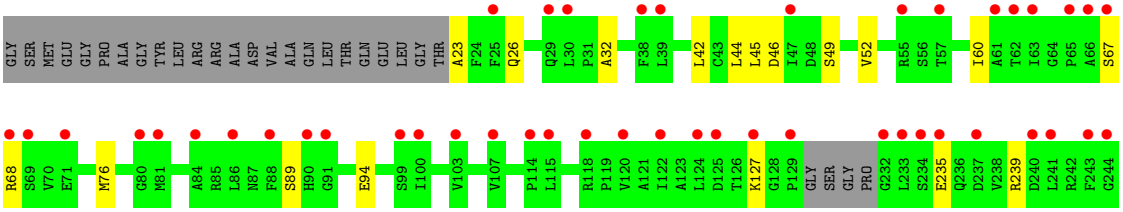
• Molecule 1: Pyruvate kinase PKLR

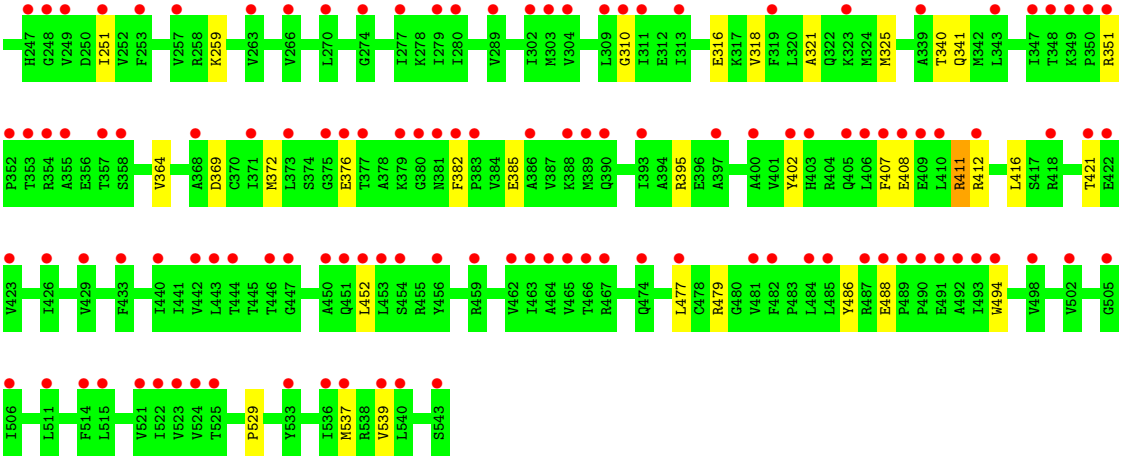
Chain D:



• Molecule 1: Pyruvate kinase PKLR

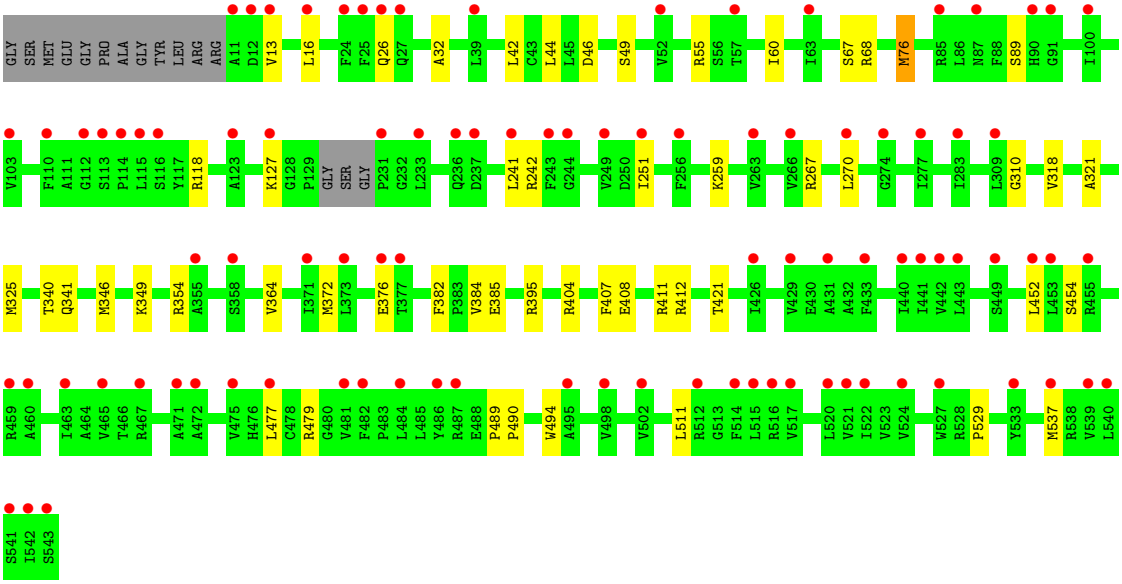
Chain E:





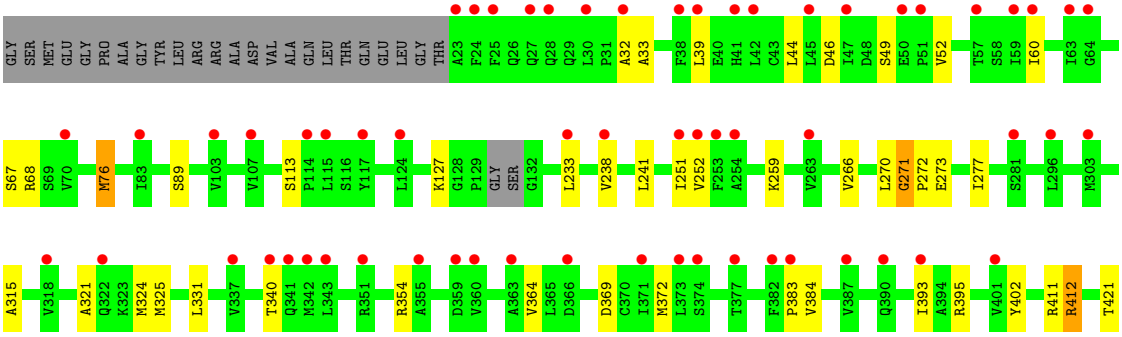
• Molecule 1: Pyruvate kinase PKLR

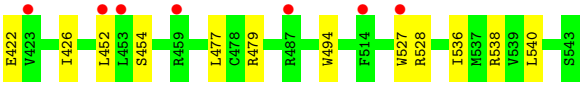
Chain F:



• Molecule 1: Pyruvate kinase PKLR

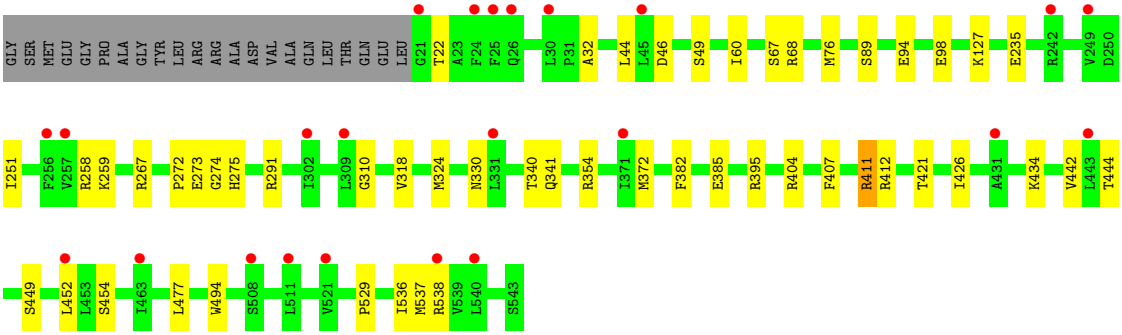
Chain G:





• Molecule 1: Pyruvate kinase PKLR

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.02Å 113.18Å 187.30Å 90.00° 92.90° 90.00°	Depositor
Resolution (Å)	187.06 – 2.77 187.06 – 2.77	Depositor EDS
% Data completeness (in resolution range)	69.5 (187.06-2.77) 69.5 (187.06-2.77)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.251 , 0.301 0.243 , 0.281	Depositor DCC
R_{free} test set	3781 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	80.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 82.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26801	wwPDB-VP
Average B, all atoms (Å^2)	102.0	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 91.37 % 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 1.5377e-08. 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: OXL, OAT, FBP, MG, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/3307	0.53	0/4469
1	B	0.38	0/3396	0.53	0/4592
1	C	0.46	0/3313	0.57	0/4479
1	D	0.50	0/3326	0.59	0/4497
1	E	0.36	0/3278	0.53	0/4430
1	F	0.39	0/3396	0.54	0/4591
1	G	0.45	0/3303	0.57	0/4465
1	H	0.49	0/3316	0.57	0/4483
All	All	0.43	0/26635	0.55	0/36006

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	3299	23	0
1	B	3329	0	3394	29	1
1	C	3247	0	3299	41	0
1	D	3252	0	3310	29	0
1	E	3210	0	3270	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3321	0	3393	30	0
1	G	3231	0	3284	44	0
1	H	3251	0	3306	33	0
2	A	20	0	10	1	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	B	38	21	0	4	0
6	G	38	21	0	3	0
6	H	38	21	0	0	0
7	A	5	0	0	0	0
7	B	15	0	0	0	0
7	C	45	0	0	0	0
7	D	79	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	9	0	0	0	0
7	F	35	0	0	0	0
7	G	48	0	0	1	0
7	H	87	0	0	3	0
All	All	26738	63	26635	215	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (215) 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:H:449:SER:HB2	7:H:737:HOH:O	1.65	0.95
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.57	0.86
1:H:442:VAL:HG22	7:H:737:HOH:O	1.76	0.86
1:H:444:THR:HB	7:H:737:HOH:O	1.75	0.85
1:C:528:ARG:HH22	1:G:233:LEU:HB3	1.48	0.79
1:E:402:TYR:HB3	6:G:605:OAT:O5	1.84	0.78
1:E:235:GLU:O	1:E:239:ARG:HD3	1.87	0.73
1:D:242[A]:ARG:NH2	1:D:273:GLU:OE1	2.22	0.72
1:A:517:VAL:HG22	1:A:543:SER:HB3	1.73	0.70
1:C:351:ARG:HH22	1:C:354:ARG:HH22	1.38	0.69
1:D:94:GLU:O	1:D:98:GLU:HG3	1.93	0.69
1:G:411:ARG:HH22	1:H:411:ARG:NH2	1.89	0.69
6:B:605:OAT:O5	1:D:402:TYR:HB3	1.92	0.68
1:H:94:GLU:O	1:H:98:GLU:HG3	1.94	0.67
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.30	0.67
1:D:89:SER:HA	1:D:127:LYS:HG3	1.78	0.66
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.31	0.65
1:C:270:LEU:O	1:C:271:GLY:O	2.14	0.65
1:A:89:SER:HA	1:A:127:LYS:HG3	1.78	0.64
1:H:89:SER:HA	1:H:127:LYS:HG3	1.79	0.64
1:G:270:LEU:O	1:G:271:GLY:O	2.14	0.64
1:E:89:SER:HA	1:E:127:LYS:HG3	1.78	0.64
1:C:89:SER:HA	1:C:127:LYS:HG3	1.79	0.64
1:D:64:GLY:O	1:D:68:ARG:HG3	1.98	0.63
1:F:89:SER:HA	1:F:127:LYS:HG3	1.79	0.63
1:C:411:ARG:HH12	1:D:411:ARG:NH2	1.97	0.62
1:B:89:SER:HA	1:B:127:LYS:HG3	1.80	0.62
1:G:89:SER:HA	1:G:127:LYS:HG3	1.80	0.62
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.82	0.61
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.82	0.61
1:D:251:ILE:HG12	1:D:477:LEU:HD11	1.83	0.61
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.81	0.61
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.84	0.59
1:A:412:ARG:NH1	1:B:404:ARG:HH11	2.00	0.59
1:C:528:ARG:NH2	1:G:233:LEU:HB3	2.17	0.59
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.84	0.59
1:A:270:LEU:HB3	1:A:274:GLY:HA3	1.85	0.58
1:G:241:LEU:HD22	1:G:270:LEU:HD21	1.86	0.58
1:C:235:GLU:CD	1:G:494:TRP:HB2	2.24	0.58
1:A:411:ARG:NH2	1:B:411:ARG:HH22	2.01	0.57
1:C:251:ILE:HG12	1:C:477:LEU:HD11	1.87	0.56
1:D:103:VAL:O	1:D:107:VAL:HG23	2.06	0.56
1:F:408:GLU:HG2	1:F:411:ARG:NH2	2.20	0.56
1:A:411:ARG:HH21	1:B:411:ARG:HH22	1.54	0.55
1:B:407:PHE:CE2	1:B:411:ARG:NH1	2.75	0.55
1:G:411:ARG:NH2	1:H:411:ARG:NH2	2.54	0.54
1:E:351:ARG:HH21	1:G:315:ALA:HB2	1.72	0.54
1:D:382:PHE:HB3	1:D:385:GLU:HB2	1.90	0.54
1:C:503:GLN:O	1:C:507:GLU:HG2	2.09	0.53
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.76	0.53
1:C:412:ARG:NH1	1:D:404:ARG:HD3	2.24	0.53
1:H:251:ILE:HG12	1:H:477:LEU:HD11	1.91	0.52
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.90	0.52
1:D:46:ASP:HB3	1:D:49:SER:HB2	1.92	0.52
1:B:341:GLN:OE1	1:D:354:ARG:HG2	2.10	0.52
1:C:239:ARG:HH21	1:G:494:TRP:HD1	1.57	0.52
1:C:115:LEU:O	1:C:118:ARG:NH1	2.43	0.52
1:D:241:LEU:HD22	1:D:270:LEU:HD21	1.92	0.51
1:H:267[B]:ARG:NH1	1:H:274:GLY:O	2.42	0.51
1:H:382:PHE:HB3	1:H:385:GLU:HB2	1.91	0.51
1:C:536:ILE:HG12	1:D:538:ARG:HG3	1.93	0.51
1:H:46:ASP:HB3	1:H:49:SER:HB2	1.93	0.51
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.26	0.51
1:G:251:ILE:HG12	1:G:477:LEU:HD11	1.92	0.50
1:H:411:ARG:HG2	1:H:426:ILE:HD11	1.91	0.50
1:B:258:ARG:O	1:B:291:ARG:HD3	2.11	0.50
1:E:67:SER:HB2	1:E:76[A]:MET:SD	2.52	0.50
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.94	0.50
1:C:46:ASP:HB3	1:C:49:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLN:OE1	1:C:354:ARG:HG2	2.11	0.50
1:E:251:ILE:HG12	1:E:477:LEU:HD11	1.93	0.49
1:A:67:SER:HB2	1:A:76[A]:MET:SD	2.52	0.49
1:C:233:LEU:O	1:G:528:ARG:NH2	2.32	0.49
1:G:46:ASP:HB3	1:G:49:SER:HB2	1.93	0.49
1:B:251:ILE:HG12	1:B:477:LEU:HD11	1.94	0.49
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.94	0.49
1:B:65:PRO:HG2	1:B:379:LYS:HG2	1.94	0.49
1:A:251:ILE:HG12	1:A:477:LEU:HD11	1.94	0.49
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.94	0.49
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.94	0.49
1:B:46:ASP:HB3	1:B:49:SER:HB2	1.95	0.48
1:D:68:ARG:NH2	1:D:95:TYR:O	2.46	0.48
1:F:251:ILE:HG12	1:F:477:LEU:HD11	1.94	0.48
1:F:46:ASP:HB3	1:F:49:SER:HB2	1.95	0.48
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.95	0.48
1:G:60:ILE:HB	1:G:372:MET:HG3	1.96	0.48
1:G:67:SER:HB2	1:G:76[B]:MET:SD	2.53	0.48
1:E:23:ALA:HB3	1:E:26:GLN:HG2	1.95	0.48
1:F:408:GLU:HG2	1:F:411:ARG:HH22	1.79	0.48
1:H:421:THR:HG22	1:H:452:LEU:HD12	1.96	0.48
1:C:241:LEU:HD22	1:C:270:LEU:HD21	1.95	0.48
1:G:538:ARG:CG	1:H:536:ILE:HG12	2.43	0.48
1:C:60:ILE:HB	1:C:372:MET:HG3	1.96	0.47
1:G:33:ALA:HB2	7:G:703:HOH:O	2.13	0.47
1:F:67:SER:HB2	1:F:76[B]:MET:SD	2.55	0.47
1:A:46:ASP:HB3	1:A:49:SER:HB2	1.97	0.47
1:B:67:SER:HB2	1:B:76[B]:MET:SD	2.55	0.47
1:C:67:SER:HB2	1:C:76[B]:MET:SD	2.55	0.47
1:E:408:GLU:OE1	1:F:411:ARG:NH2	2.44	0.47
1:E:412:ARG:HD3	1:F:404:ARG:NH1	2.30	0.47
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.97	0.47
1:B:402:TYR:HB3	6:B:605:OAT:O9	2.14	0.46
1:G:527:TRP:CD2	1:G:528:ARG:HG2	2.50	0.46
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.97	0.46
1:E:46:ASP:HB3	1:E:49:SER:HB2	1.96	0.46
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.97	0.46
1:F:32:ALA:HA	1:F:44:LEU:HB2	1.98	0.46
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.97	0.46
1:A:494:TRP:CD1	1:A:529:PRO:HG3	2.51	0.45
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HB	1:A:372:MET:HG3	1.98	0.45
1:C:68:ARG:NH2	1:C:98:GLU:HB3	2.30	0.45
1:B:60:ILE:HB	1:B:372:MET:HG3	1.98	0.45
1:G:536:ILE:HG23	1:H:538[A]:ARG:HG2	1.98	0.45
1:B:346:MET:HA	1:B:349:LYS:O	2.16	0.45
1:C:529:PRO:HB2	1:G:238:VAL:HG21	1.97	0.45
1:D:60:ILE:HB	1:D:372:MET:HG3	1.98	0.45
1:D:448:ARG:HD3	7:D:732:HOH:O	2.16	0.45
1:C:32:ALA:HA	1:C:44:LEU:HB2	1.98	0.45
1:H:68:ARG:NH1	1:H:98:GLU:OE1	2.45	0.45
1:G:39:LEU:HB2	6:G:605:OAT:O6	2.17	0.45
1:C:239:ARG:NH2	1:G:494:TRP:CD1	2.85	0.45
1:D:494:TRP:CD1	1:D:529:PRO:HG3	2.53	0.44
1:E:494:TRP:CD1	1:E:529:PRO:HG3	2.52	0.44
1:A:32:ALA:HA	1:A:44:LEU:HB2	1.99	0.44
1:C:364:VAL:O	1:C:479:ARG:NH1	2.48	0.44
1:F:241:LEU:HD22	1:F:270:LEU:HD21	2.00	0.44
1:G:32:ALA:HA	1:G:44:LEU:HB2	1.99	0.44
1:B:32:ALA:HA	1:B:44:LEU:HB2	1.99	0.44
1:C:509:GLY:HA2	1:C:514:PHE:HD2	1.82	0.44
1:D:62:THR:HA	1:D:85:ARG:HB3	1.99	0.44
1:A:351:ARG:HH21	1:C:315:ALA:HB2	1.82	0.44
1:H:60:ILE:HB	1:H:372:MET:HG3	1.98	0.44
1:E:407:PHE:O	1:E:411:ARG:HB2	2.18	0.44
1:H:494:TRP:CD1	1:H:529:PRO:HG3	2.52	0.44
1:B:76[A]:MET:HG2	1:B:384:VAL:HG22	1.99	0.44
1:F:494:TRP:CD1	1:F:529:PRO:HG3	2.53	0.44
1:G:321:ALA:O	1:G:325:MET:HG3	2.18	0.44
1:F:26:GLN:O	1:F:49:SER:OG	2.28	0.43
1:G:76[A]:MET:HG2	1:G:384:VAL:HG22	1.99	0.43
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.18	0.43
1:C:321:ALA:O	1:C:325:MET:HG3	2.17	0.43
1:E:341:GLN:OE1	1:G:354:ARG:HG2	2.19	0.43
1:E:416:LEU:HB2	1:F:16:LEU:HD22	2.00	0.43
1:F:364:VAL:O	1:F:479:ARG:NH1	2.48	0.43
1:G:411:ARG:NH2	1:H:411:ARG:CZ	2.81	0.43
1:C:76[A]:MET:HG2	1:C:384:VAL:HG22	1.99	0.43
1:F:76[A]:MET:HG2	1:F:384:VAL:HG22	2.00	0.43
1:B:494:TRP:CD1	1:B:529:PRO:HG3	2.53	0.43
1:C:484:LEU:HB3	1:C:504:PHE:CE2	2.53	0.43
1:H:258:ARG:O	1:H:291:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:412:ARG:NH2	1:H:404:ARG:HD3	2.34	0.43
1:D:527:TRP:CD2	1:D:528:ARG:HG2	2.54	0.43
1:F:341:GLN:OE1	1:H:354:ARG:HG2	2.19	0.43
1:G:266:VAL:O	1:G:270:LEU:HG	2.19	0.43
1:E:408:GLU:CD	1:F:411:ARG:HH21	2.21	0.43
1:F:42:LEU:O	1:H:324:MET:HA	2.19	0.43
1:E:26:GLN:O	1:E:49:SER:OG	2.29	0.43
1:E:32:ALA:HA	1:E:44:LEU:HB2	1.99	0.43
1:C:314:PRO:HG2	1:C:317:LYS:HD2	2.01	0.42
1:D:364:VAL:O	1:D:479:ARG:NH1	2.49	0.42
1:E:45:LEU:HB2	1:G:324:MET:HB2	2.01	0.42
1:E:364:VAL:O	1:E:479:ARG:NH1	2.47	0.42
1:F:55:ARG:HB2	1:F:395:ARG:HG3	2.02	0.42
1:F:60:ILE:HB	1:F:372:MET:HG3	1.99	0.42
1:F:267[B]:ARG:HH21	1:F:270:LEU:HD12	1.83	0.42
1:C:538:ARG:CG	1:D:536:ILE:HG12	2.50	0.42
1:E:60:ILE:HB	1:E:372:MET:HG3	2.00	0.42
1:C:351:ARG:HH22	1:C:354:ARG:NH2	2.12	0.42
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.50	0.42
1:H:310:GLY:HA2	1:H:318:VAL:HG21	2.01	0.42
1:B:53:ALA:O	1:B:395:ARG:NH2	2.52	0.42
1:B:364:VAL:O	1:B:479:ARG:NH1	2.51	0.42
1:F:310:GLY:HA2	1:F:318:VAL:HG21	2.02	0.42
1:H:67:SER:HB2	1:H:76[A]:MET:SD	2.60	0.42
1:D:73:LEU:HA	1:D:76[B]:MET:HG3	2.01	0.41
1:A:321:ALA:O	1:A:325:MET:HG3	2.20	0.41
1:G:411:ARG:HH22	1:H:411:ARG:HH21	1.65	0.41
1:A:530:GLY:O	2:A:601:FBP:O4	2.31	0.41
1:E:310:GLY:HA2	1:E:318:VAL:HG21	2.03	0.41
1:H:32:ALA:HA	1:H:44:LEU:HB2	2.02	0.41
1:A:369:ASP:HA	1:A:479:ARG:HB2	2.03	0.41
1:B:310:GLY:HA2	1:B:318:VAL:HG21	2.02	0.41
1:F:346:MET:HA	1:F:349:LYS:O	2.20	0.41
1:E:316:GLU:HB2	1:G:393:ILE:HA	2.02	0.41
1:E:321:ALA:O	1:E:325:MET:HG3	2.20	0.41
1:C:489:PRO:HA	1:C:490:PRO:HD3	1.92	0.41
1:E:486:TYR:CE2	1:E:488:GLU:HB2	2.56	0.41
1:F:321:ALA:O	1:F:325:MET:HG3	2.20	0.41
1:H:407:PHE:CE2	1:H:411:ARG:HD3	2.56	0.41
1:B:39:LEU:HB2	6:B:605:OAT:O6	2.20	0.41
1:B:321:ALA:O	1:B:325:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:VAL:O	1:C:270:LEU:HG	2.21	0.41
1:C:310:GLY:HA2	1:C:318:VAL:HG21	2.03	0.41
1:D:486:TYR:CE2	1:D:488:GLU:HB2	2.56	0.41
1:E:369:ASP:HA	1:E:479:ARG:HB2	2.03	0.41
1:G:402:TYR:HB3	6:G:605:OAT:O8	2.21	0.41
1:A:45:LEU:HB2	1:C:324:MET:HB2	2.02	0.41
6:B:605:OAT:C22	6:B:605:OAT:O4	2.68	0.41
1:G:364:VAL:O	1:G:479:ARG:NH1	2.50	0.41
1:G:422[B]:GLU:HG3	1:H:434:LYS:HE2	2.03	0.41
1:B:489:PRO:HA	1:B:490:PRO:HD3	1.98	0.41
1:F:354:ARG:HG2	1:H:341:GLN:OE1	2.21	0.41
1:G:252:VAL:HG23	1:G:277:ILE:HG21	2.03	0.41
1:G:369:ASP:HA	1:G:479:ARG:HB2	2.03	0.41
1:B:42:LEU:O	1:D:324:MET:HA	2.21	0.40
1:B:253:PHE:HD1	1:B:280:ILE:HB	1.86	0.40
1:A:416:LEU:CB	1:B:16:LEU:HD22	2.52	0.40
1:C:303:MET:HG3	1:C:337:VAL:HB	2.04	0.40
1:D:68:ARG:HD2	1:D:95:TYR:OH	2.21	0.40
1:F:489:PRO:HA	1:F:490:PRO:HD3	1.99	0.40
1:D:32:ALA:HA	1:D:44:LEU:HB2	2.02	0.40
1:E:42:LEU:O	1:G:324:MET:HA	2.21	0.40
1:E:416:LEU:CB	1:F:16:LEU:HD22	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:LEU:O	1:B:511:LEU:O[2_555]	2.07	0.13

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%)	415 (98%)	8 (2%)	1 (0%)	47 76
1	B	438/447 (98%)	427 (98%)	10 (2%)	1 (0%)	47 76
1	C	425/447 (95%)	412 (97%)	9 (2%)	4 (1%)	17 44
1	D	429/447 (96%)	421 (98%)	7 (2%)	1 (0%)	47 76
1	E	420/447 (94%)	412 (98%)	7 (2%)	1 (0%)	47 76
1	F	435/447 (97%)	424 (98%)	10 (2%)	1 (0%)	47 76
1	G	423/447 (95%)	412 (97%)	8 (2%)	3 (1%)	22 50
1	H	427/447 (96%)	416 (97%)	10 (2%)	1 (0%)	47 76
All	All	3421/3576 (96%)	3339 (98%)	69 (2%)	13 (0%)	34 64

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	271	GLY
1	G	271	GLY
1	A	340	THR
1	D	340	THR
1	B	340	THR
1	C	274	GLY
1	C	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR
1	C	383	PRO
1	G	383	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%)	329 (97%)	11 (3%)	39 70
1	B	349/352 (99%)	335 (96%)	14 (4%)	31 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	341/352 (97%)	332 (97%)	9 (3%)	46 76
1	D	342/352 (97%)	325 (95%)	17 (5%)	24 53
1	E	338/352 (96%)	328 (97%)	10 (3%)	41 72
1	F	350/352 (99%)	337 (96%)	13 (4%)	34 65
1	G	340/352 (97%)	329 (97%)	11 (3%)	39 70
1	H	340/352 (97%)	330 (97%)	10 (3%)	42 73
All	All	2740/2816 (97%)	2645 (96%)	95 (4%)	39 67

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	68	ARG
1	A	72	ARG
1	A	259	LYS
1	A	376	GLU
1	A	395	ARG
1	A	412	ARG
1	A	454	SER
1	A	537[A]	MET
1	A	537[B]	MET
1	A	538	ARG
1	B	10	ARG
1	B	13	VAL
1	B	68	ARG
1	B	76[A]	MET
1	B	76[B]	MET
1	B	94	GLU
1	B	259	LYS
1	B	376	GLU
1	B	379	LYS
1	B	412	ARG
1	B	454	SER
1	B	511	LEU
1	B	537[A]	MET
1	B	537[B]	MET
1	C	52	VAL
1	C	76[A]	MET
1	C	76[B]	MET
1	C	259	LYS

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Mol	Chain	Res	Type
1	C	395	ARG
1	C	412	ARG
1	C	454	SER
1	C	487	ARG
1	C	540	LEU
1	D	22	THR
1	D	58[A]	SER
1	D	58[B]	SER
1	D	68	ARG
1	D	69	SER
1	D	98	GLU
1	D	235	GLU
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	259	LYS
1	D	273	GLU
1	D	395	ARG
1	D	412	ARG
1	D	436	CYS
1	D	454	SER
1	D	521	VAL
1	D	537	MET
1	E	52	VAL
1	E	68	ARG
1	E	94	GLU
1	E	259	LYS
1	E	376	GLU
1	E	395	ARG
1	E	411	ARG
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	13	VAL
1	F	68	ARG
1	F	76[A]	MET
1	F	76[B]	MET
1	F	118	ARG
1	F	242	ARG
1	F	259	LYS
1	F	376	GLU
1	F	412	ARG
1	F	454	SER

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Mol	Chain	Res	Type
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	52	VAL
1	G	68	ARG
1	G	76[A]	MET
1	G	76[B]	MET
1	G	113	SER
1	G	259	LYS
1	G	331	LEU
1	G	395	ARG
1	G	412	ARG
1	G	454	SER
1	G	540	LEU
1	H	22	THR
1	H	235	GLU
1	H	259	LYS
1	H	273	GLU
1	H	330	ASN
1	H	395	ARG
1	H	411	ARG
1	H	412	ARG
1	H	454	SER
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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 16 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
6	OAT	H	605	-	41,41,41	0.30	0	62,62,62	0.62	2 (3%)
3	OXL	E	602	4	5,5,5	2.06	2 (40%)	6,6,6	1.15	1 (16%)
2	FBP	B	601	-	18,20,20	0.71	1 (5%)	23,32,32	1.08	1 (4%)
3	OXL	H	602	4	5,5,5	2.01	2 (40%)	6,6,6	1.07	1 (16%)
6	OAT	B	605	-	41,41,41	0.37	0	62,62,62	0.66	2 (3%)
3	OXL	D	602	4	5,5,5	2.07	2 (40%)	6,6,6	1.13	0
3	OXL	F	602	4	5,5,5	2.63	4 (80%)	6,6,6	1.38	1 (16%)
2	FBP	F	601	-	18,20,20	0.56	0	23,32,32	1.04	1 (4%)
6	OAT	G	605	-	41,41,41	0.33	0	62,62,62	0.71	2 (3%)
2	FBP	G	601	-	18,20,20	0.63	0	23,32,32	1.24	2 (8%)
3	OXL	C	602	4	5,5,5	1.87	2 (40%)	6,6,6	1.21	1 (16%)
2	FBP	D	601	-	18,20,20	0.76	1 (5%)	23,32,32	1.15	1 (4%)
2	FBP	E	601	-	18,20,20	0.49	0	23,32,32	1.01	1 (4%)
2	FBP	A	601	-	18,20,20	0.58	0	23,32,32	1.06	1 (4%)
2	FBP	H	601	-	18,20,20	0.54	0	23,32,32	1.45	3 (13%)
2	FBP	C	601	-	18,20,20	0.82	1 (5%)	23,32,32	1.27	2 (8%)
3	OXL	G	602	4	5,5,5	1.97	2 (40%)	6,6,6	1.12	1 (16%)
3	OXL	B	602	4	5,5,5	1.95	2 (40%)	6,6,6	1.02	0
3	OXL	A	602	4	5,5,5	1.91	2 (40%)	6,6,6	1.14	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OAT	H	605	-	-	3/32/32/32	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	E	602	4	-	1/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	0/4/4/4	-
6	OAT	B	605	-	-	10/32/32/32	0/4/4/4
3	OXL	D	602	4	-	1/4/4/4	-
3	OXL	F	602	4	-	1/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
6	OAT	G	605	-	-	11/32/32/32	0/4/4/4
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	C	602	4	-	1/4/4/4	-
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
2	FBP	E	601	-	-	3/13/32/32	0/1/1/1
2	FBP	A	601	-	-	3/13/32/32	0/1/1/1
2	FBP	H	601	-	-	3/13/32/32	0/1/1/1
2	FBP	C	601	-	-	7/13/32/32	0/1/1/1
3	OXL	G	602	4	-	1/4/4/4	-
3	OXL	B	602	4	-	0/4/4/4	-
3	OXL	A	602	4	-	1/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	OXL	O2-C2	3.62	1.32	1.22
3	E	602	OXL	O1-C1	3.54	1.32	1.22
3	H	602	OXL	O2-C2	3.52	1.32	1.22
3	B	602	OXL	O2-C2	3.44	1.31	1.22
3	A	602	OXL	O2-C2	3.32	1.31	1.22
3	F	602	OXL	O2-C2	3.24	1.31	1.22
3	F	602	OXL	O3-C1	-3.08	1.21	1.30
3	G	602	OXL	O1-C1	3.05	1.30	1.22
3	C	602	OXL	O1-C1	3.04	1.30	1.22
3	G	602	OXL	O3-C1	-2.98	1.21	1.30
3	F	602	OXL	O1-C1	2.95	1.30	1.22
2	C	601	FBP	P1-O3P	-2.86	1.43	1.54
2	D	601	FBP	P2-O5P	-2.72	1.44	1.54
3	C	602	OXL	O3-C1	-2.69	1.22	1.30
3	D	602	OXL	O4-C2	-2.60	1.23	1.30
3	B	602	OXL	O4-C2	-2.59	1.23	1.30
3	E	602	OXL	O3-C1	-2.58	1.23	1.30
3	A	602	OXL	O4-C2	-2.46	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	OXL	O4-C2	-2.41	1.23	1.30
3	H	602	OXL	O4-C2	-2.35	1.23	1.30
2	B	601	FBP	P2-O5P	-2.03	1.47	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	FBP	O5P-P2-O6	4.28	118.11	106.73
2	A	601	FBP	P1-O1-C1	4.07	129.50	118.30
2	F	601	FBP	P1-O1-C1	4.01	129.35	118.30
2	C	601	FBP	O6-P2-O4P	3.81	117.15	106.47
2	B	601	FBP	P1-O1-C1	3.58	128.15	118.30
2	E	601	FBP	P1-O1-C1	3.43	127.74	118.30
6	G	605	OAT	C9-C10-N	3.37	118.80	111.85
2	H	601	FBP	P1-O1-C1	3.09	126.81	118.30
2	D	601	FBP	P1-O1-C1	2.98	126.50	118.30
2	G	601	FBP	P1-O1-C1	2.79	125.98	118.30
6	B	605	OAT	C9-C10-N	2.68	117.38	111.85
2	G	601	FBP	O6P-P2-O6	2.65	113.77	106.73
2	H	601	FBP	O6P-P2-O6	-2.58	99.88	106.73
2	C	601	FBP	P1-O1-C1	2.55	125.32	118.30
6	G	605	OAT	C17-N-S1	-2.52	112.68	117.73
3	F	602	OXL	O4-C2-C1	2.27	119.92	113.16
3	A	602	OXL	O4-C2-C1	2.26	119.87	113.16
3	C	602	OXL	O3-C1-C2	2.24	119.82	113.16
6	H	605	OAT	C9-C10-N	2.19	116.36	111.85
3	H	602	OXL	O4-C2-C1	2.11	119.42	113.16
3	G	602	OXL	O3-C1-C2	2.07	119.30	113.16
6	B	605	OAT	C10-N-S1	2.06	122.54	117.94
6	H	605	OAT	C17-N-S1	-2.02	113.68	117.73
3	E	602	OXL	O3-C1-C2	2.01	119.14	113.16

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	FBP	C1-O1-P1-O2P
2	C	601	FBP	C1-O1-P1-O3P
2	C	601	FBP	O1-C1-C2-O2
2	C	601	FBP	O1-C1-C2-C3
2	C	601	FBP	O1-C1-C2-O5
2	D	601	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	G	605	OAT	C16-C11-S1-N
6	G	605	OAT	C17-N-S1-O4
6	G	605	OAT	C12-C11-S1-N
2	H	601	FBP	C4-C5-C6-O6
6	B	605	OAT	C22-C17-N-S1
6	H	605	OAT	C10-N-S1-O5
6	B	605	OAT	C17-N-S1-O4
6	B	605	OAT	C17-N-S1-O5
6	G	605	OAT	C17-N-S1-O5
6	G	605	OAT	C17-N-S1-C11
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	D	601	FBP	O5-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
6	G	605	OAT	C12-C11-S1-O4
6	G	605	OAT	C16-C11-S1-O4
6	G	605	OAT	C10-N-S1-O4
2	C	601	FBP	C1-O1-P1-O1P
2	E	601	FBP	C6-O6-P2-O4P
6	B	605	OAT	C12-C11-S1-O4
6	H	605	OAT	C10-N-S1-C11
6	B	605	OAT	C17-N-S1-C11
6	B	605	OAT	C16-C11-S1-O4
6	B	605	OAT	C12-C11-S1-N
6	B	605	OAT	C16-C11-S1-N
2	H	601	FBP	O5-C5-C6-O6
6	G	605	OAT	C10-N-S1-O5
6	H	605	OAT	C10-N-S1-O4
6	G	605	OAT	C9-C10-N-C17
2	A	601	FBP	O5-C5-C6-O6
2	C	601	FBP	C6-O6-P2-O4P
6	G	605	OAT	C10-N-S1-C11
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	B	601	FBP	O5-C5-C6-O6
2	A	601	FBP	C6-O6-P2-O5P
2	H	601	FBP	C6-O6-P2-O4P
6	B	605	OAT	C22-C17-N-C10
6	B	605	OAT	C18-C17-N-S1

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Mol	Chain	Res	Type	Atoms
3	A	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4

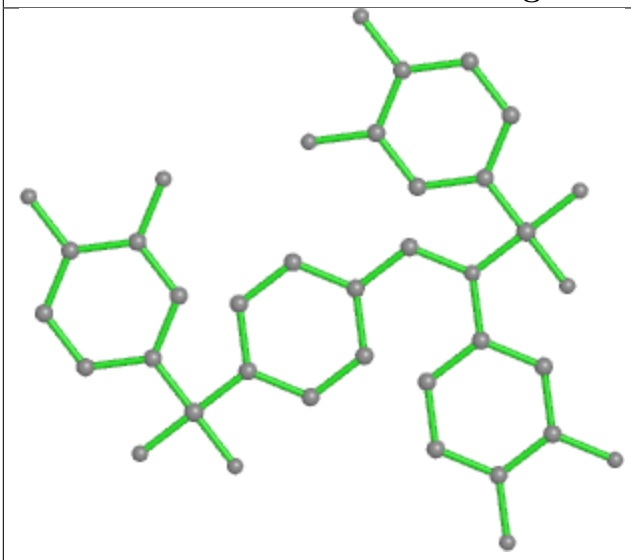
There are no ring outliers.

3 monomers are involved in 8 short contacts:

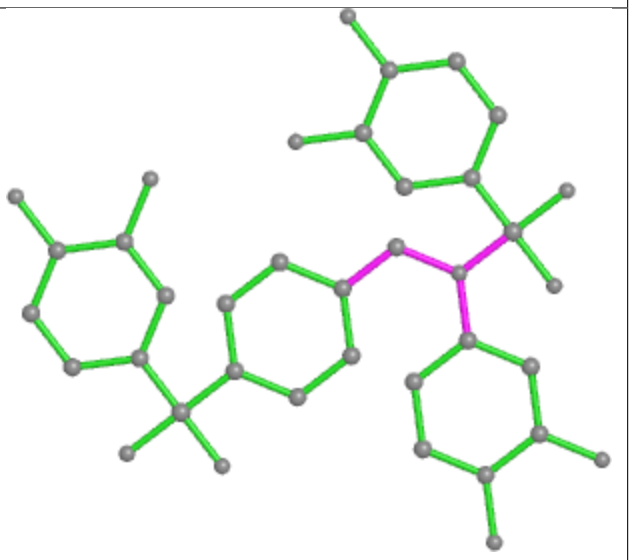
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	605	OAT	4	0
6	G	605	OAT	3	0
2	A	601	FBP	1	0

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.

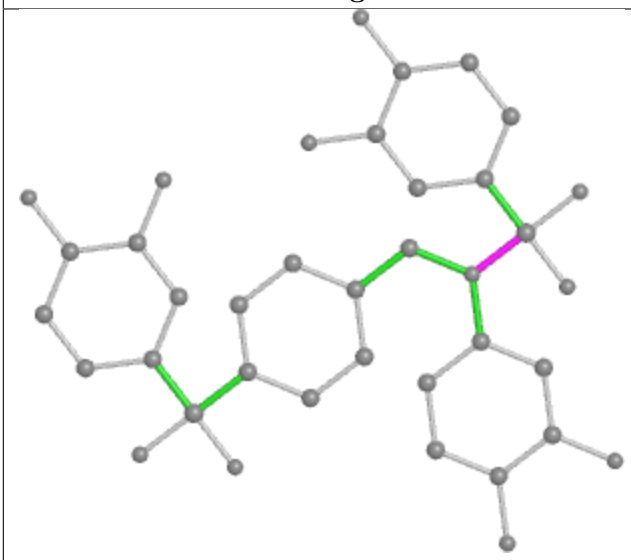
Ligand OAT H 605



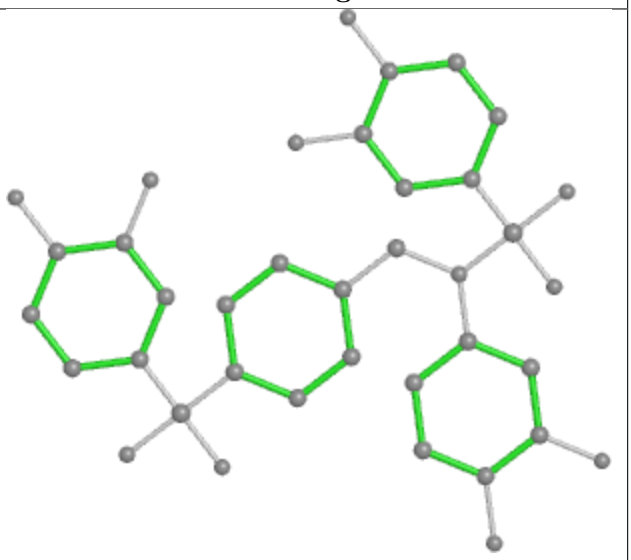
Bond lengths



Bond angles

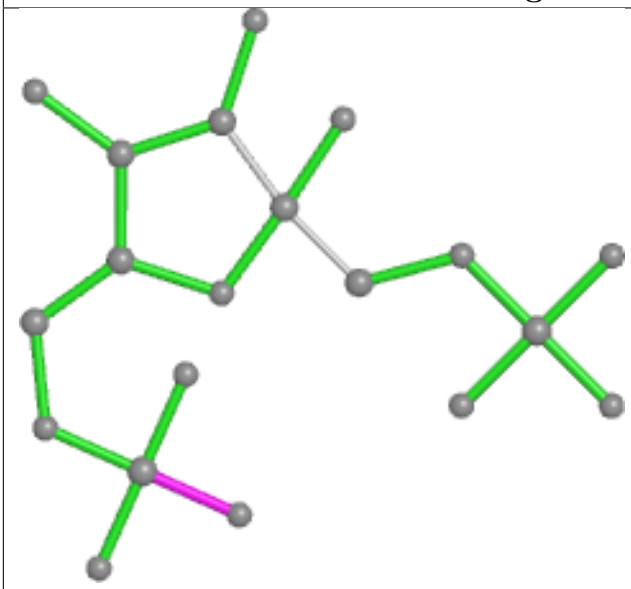


Torsions

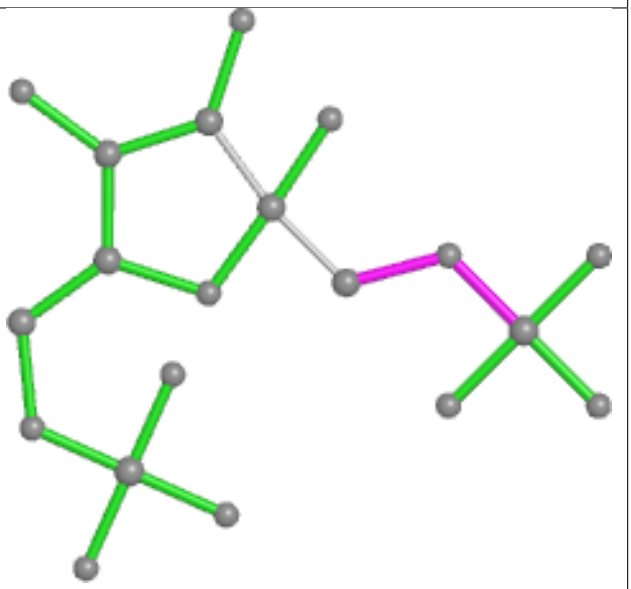


Rings

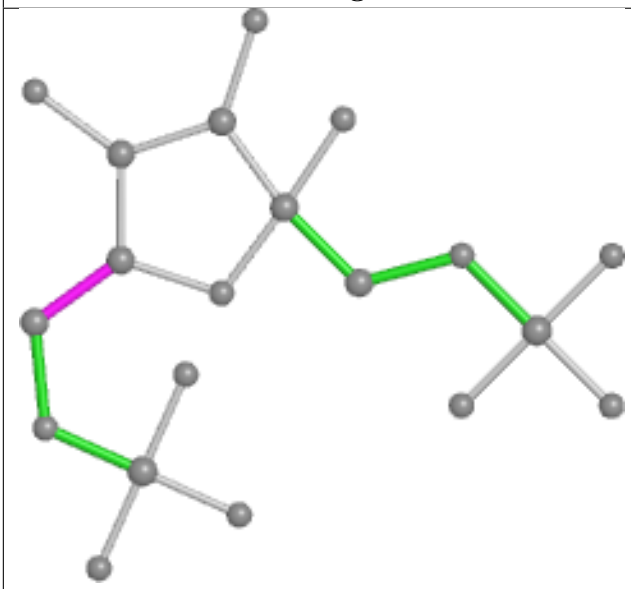
Ligand FBP B 601



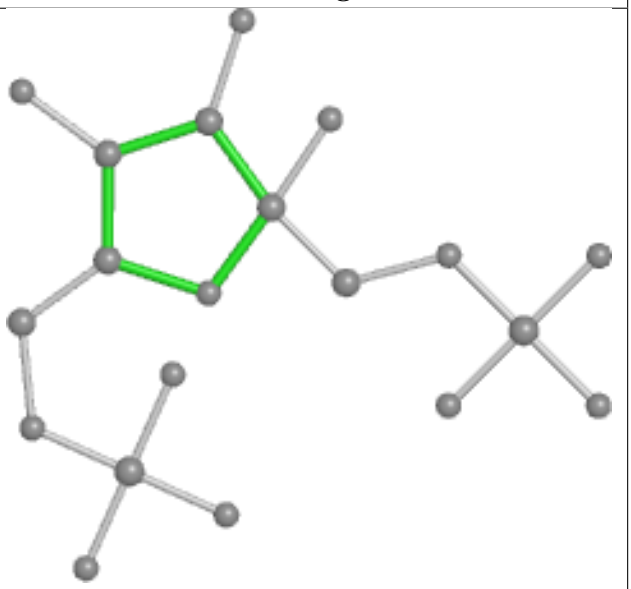
Bond lengths



Bond angles

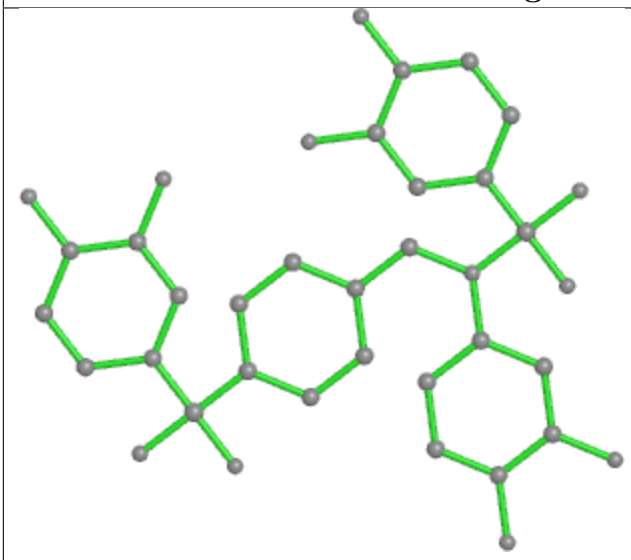


Torsions

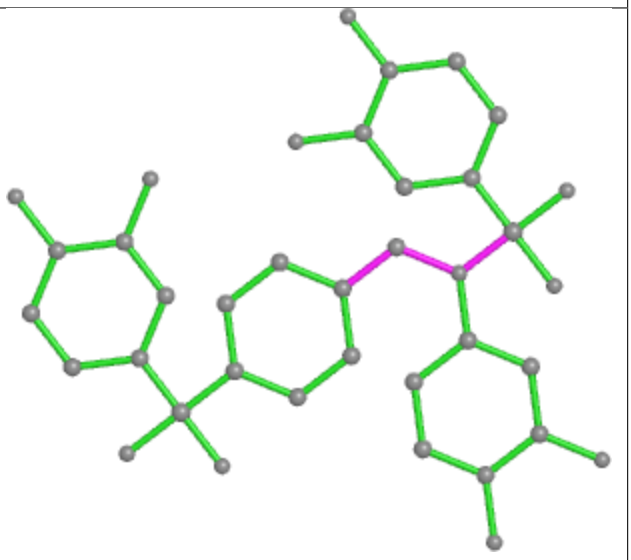


Rings

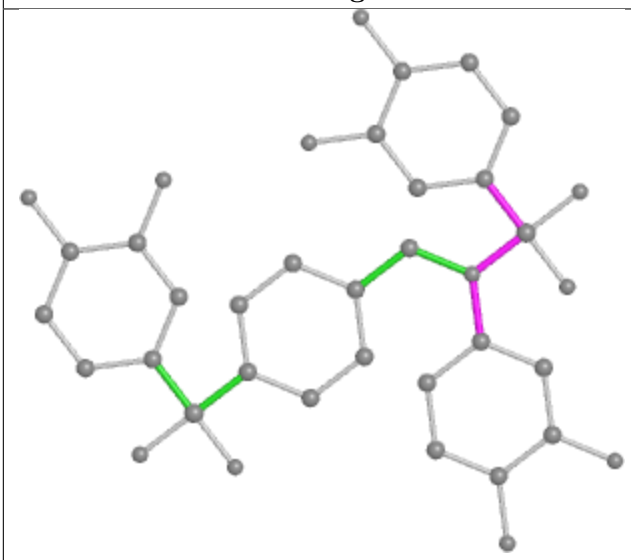
Ligand OAT B 605



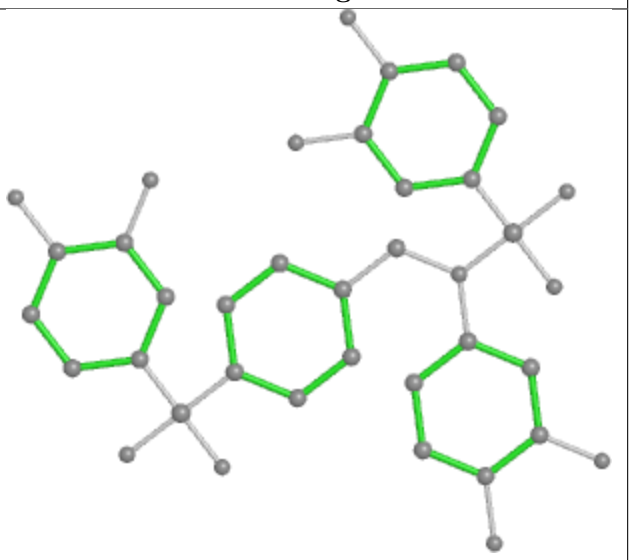
Bond lengths



Bond angles

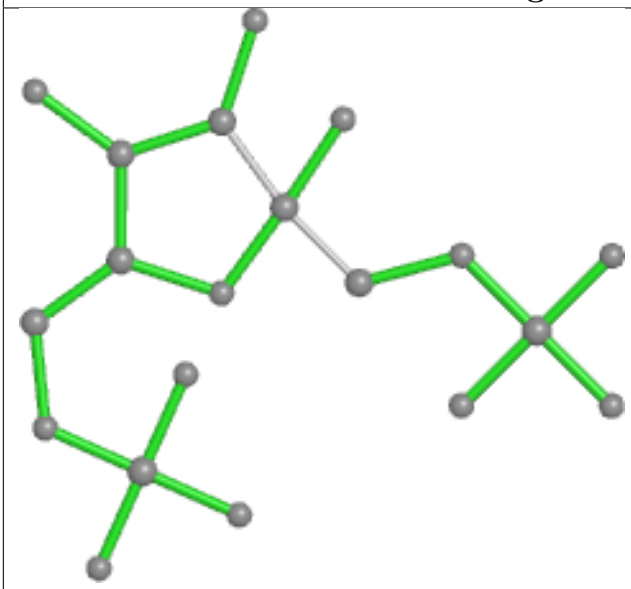


Torsions

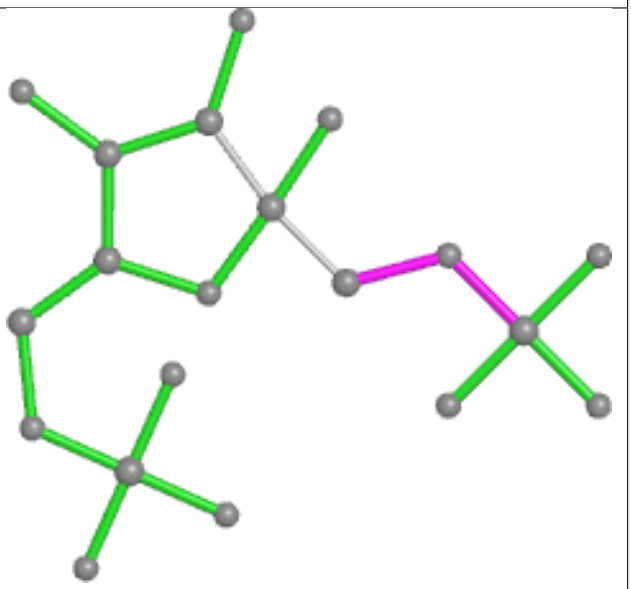


Rings

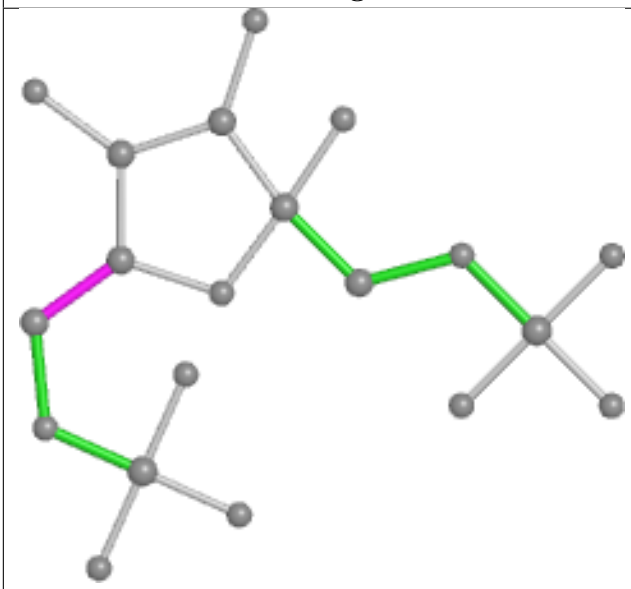
Ligand FBP F 601



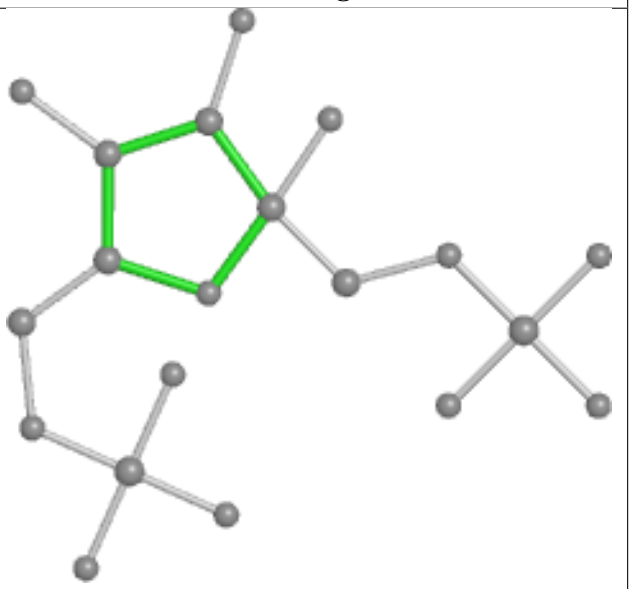
Bond lengths



Bond angles

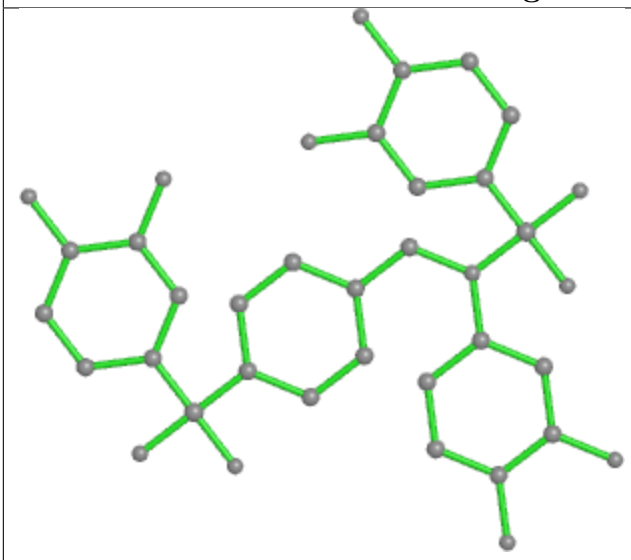


Torsions

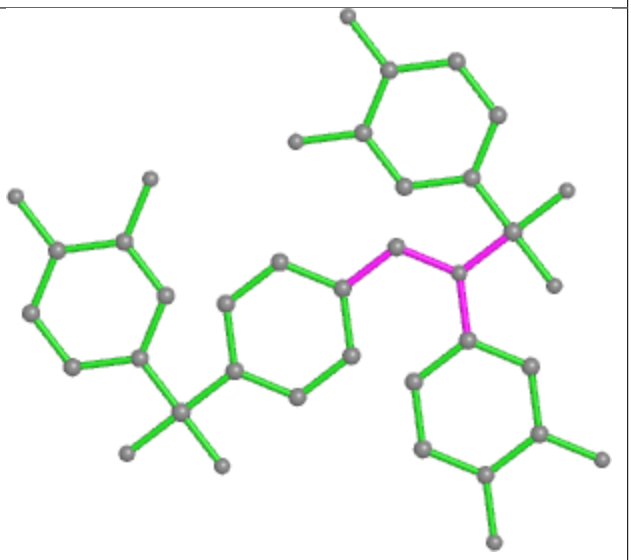


Rings

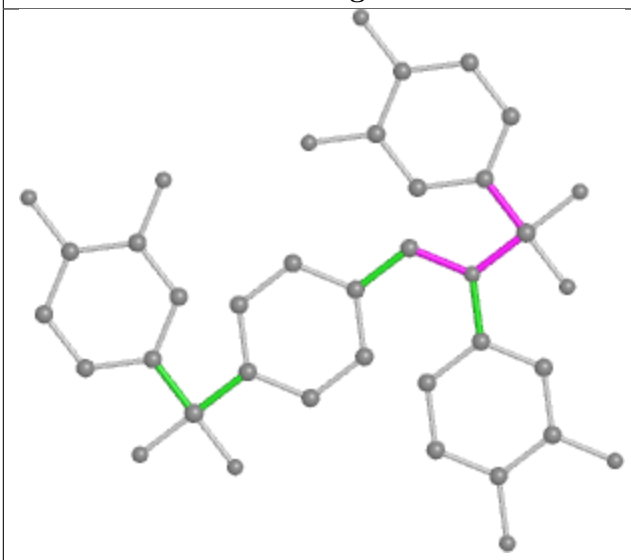
Ligand OAT G 605



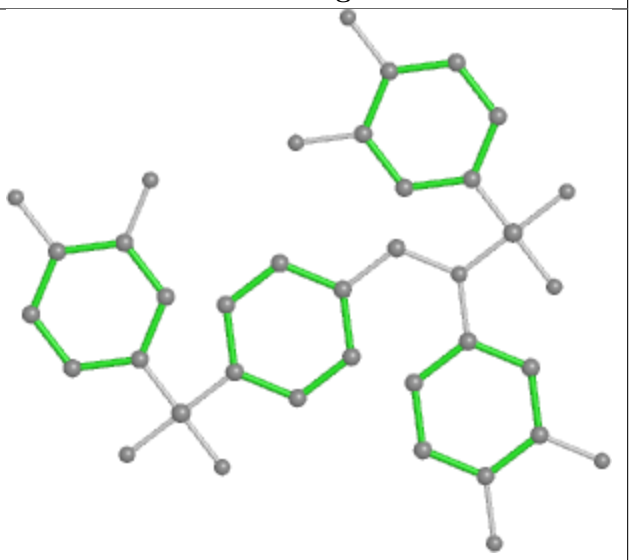
Bond lengths



Bond angles

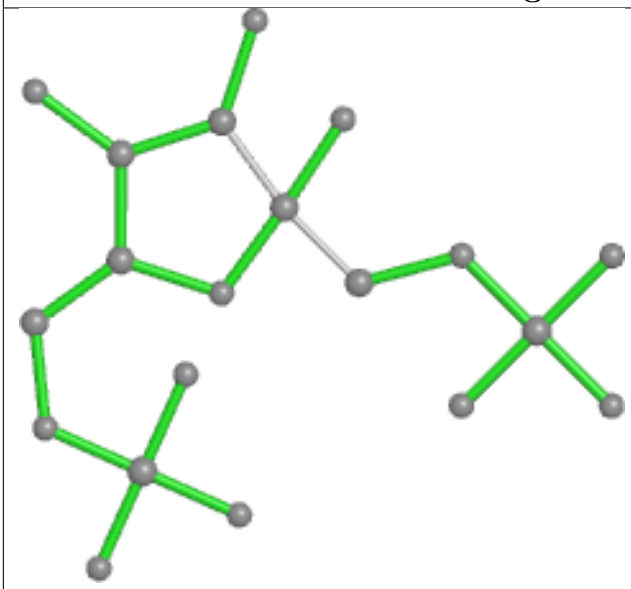


Torsions

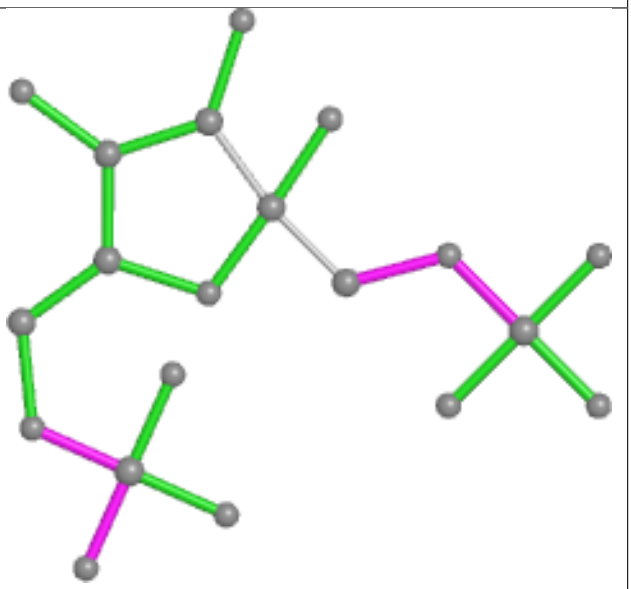


Rings

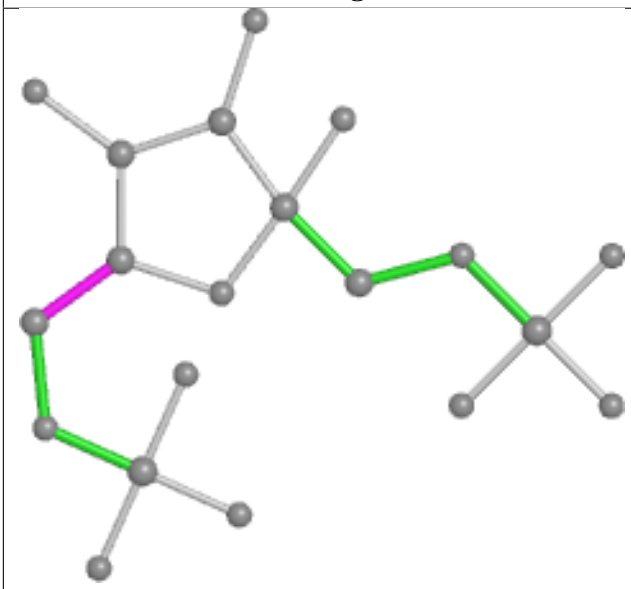
Ligand FBP G 601



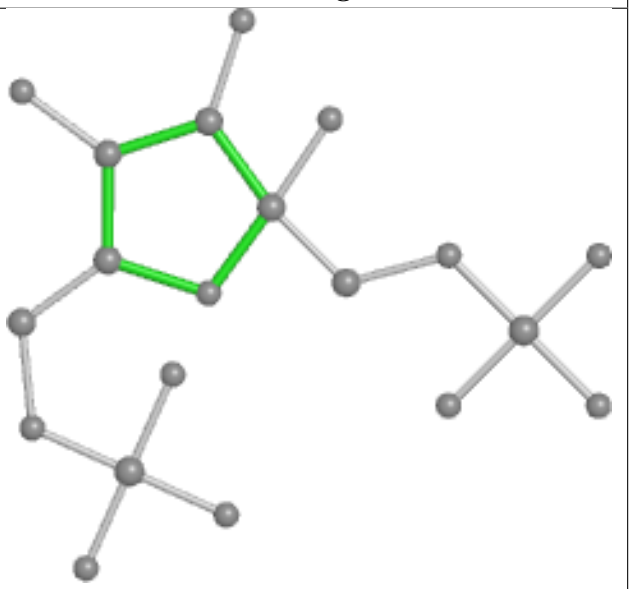
Bond lengths



Bond angles

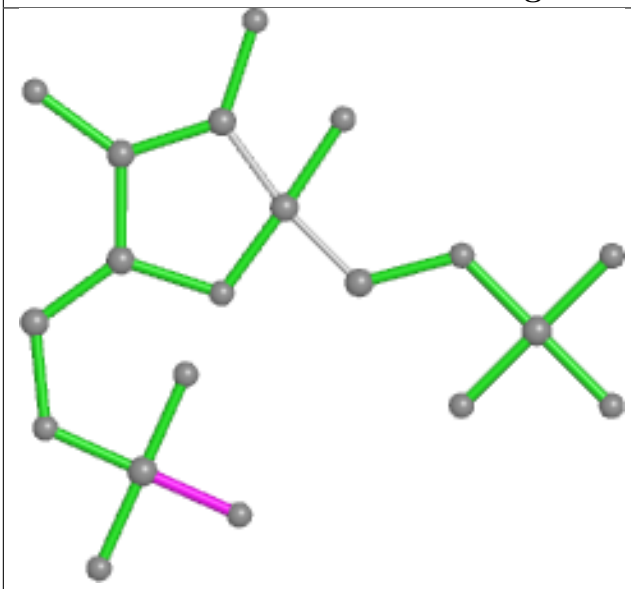


Torsions

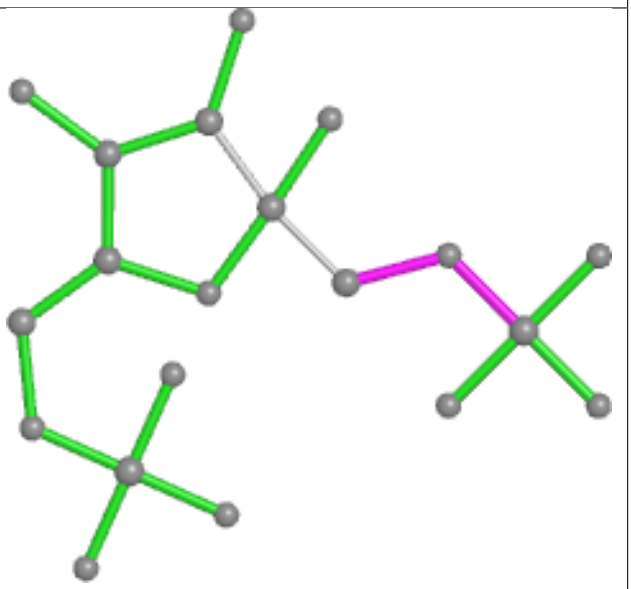


Rings

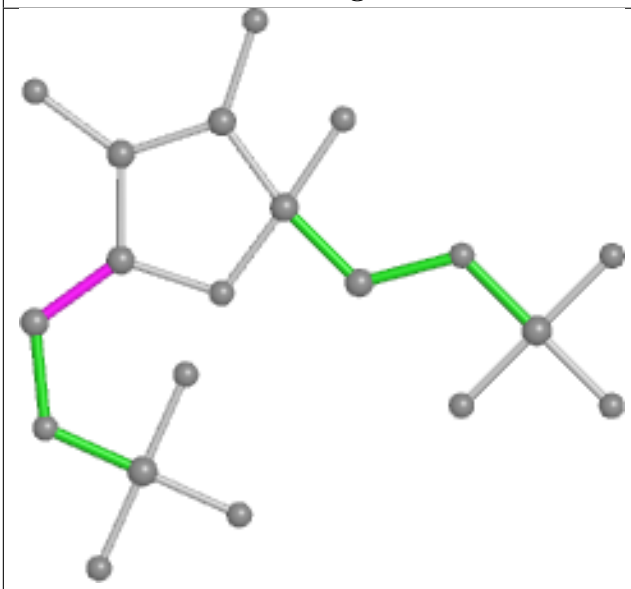
Ligand FBP D 601



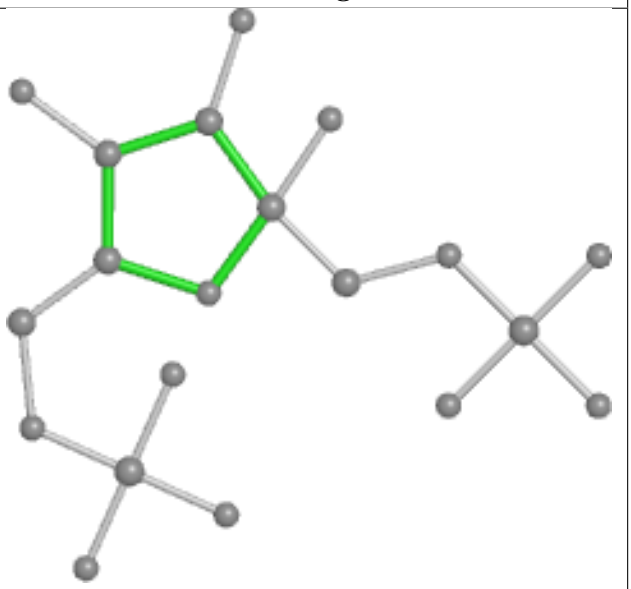
Bond lengths



Bond angles

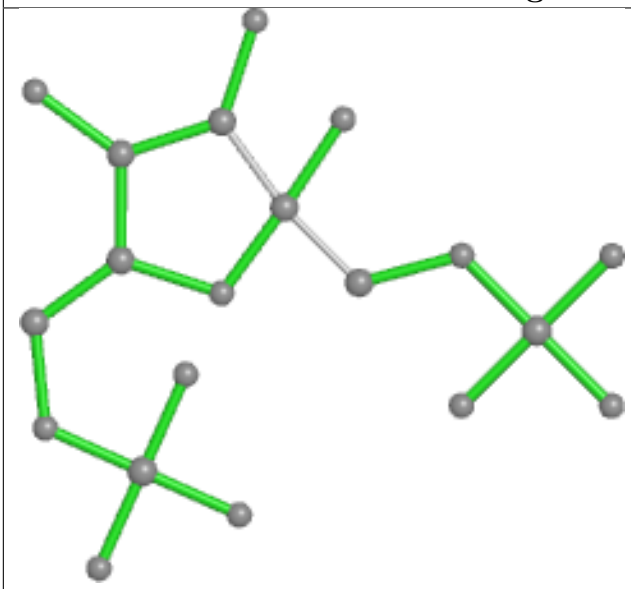


Torsions

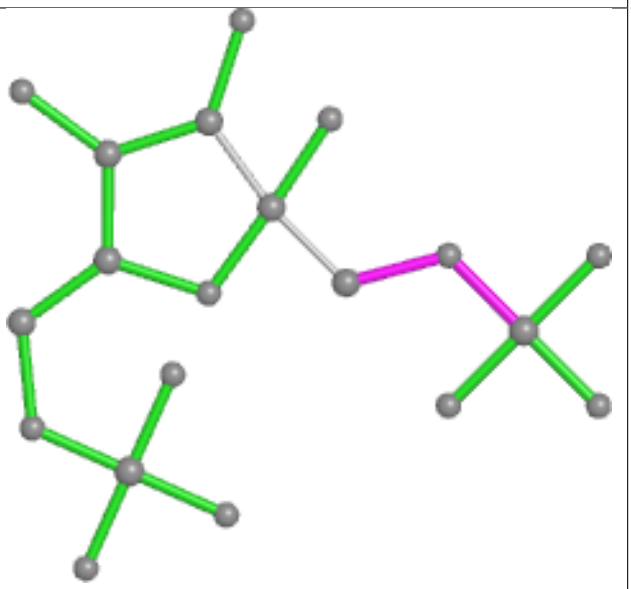


Rings

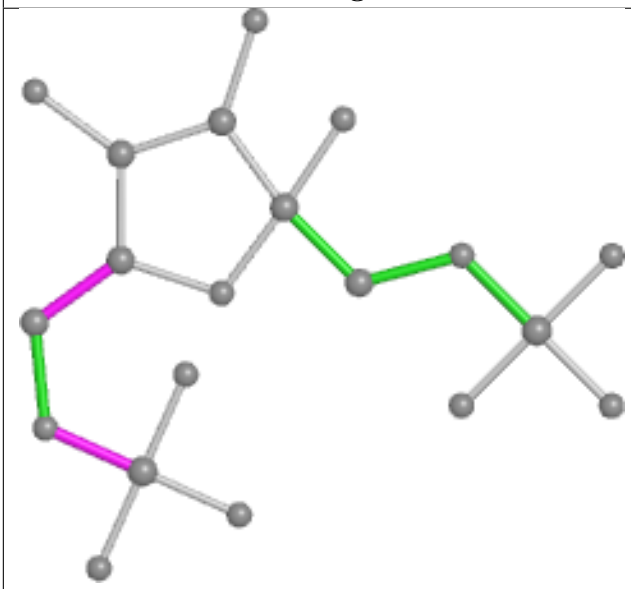
Ligand FBP E 601



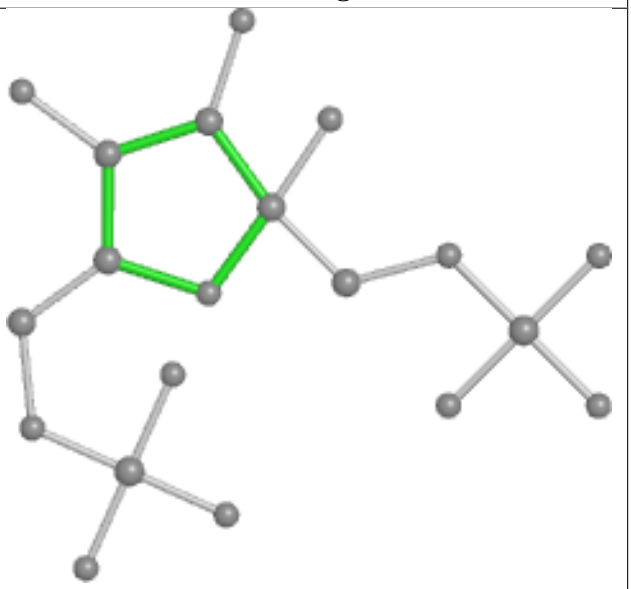
Bond lengths



Bond angles

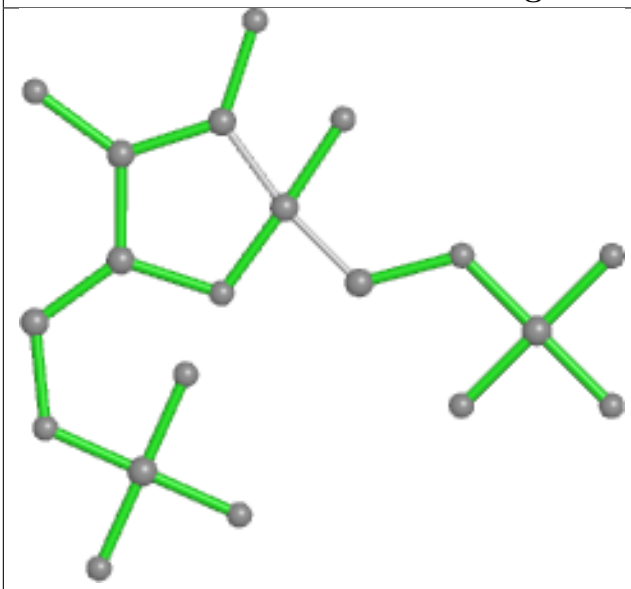


Torsions

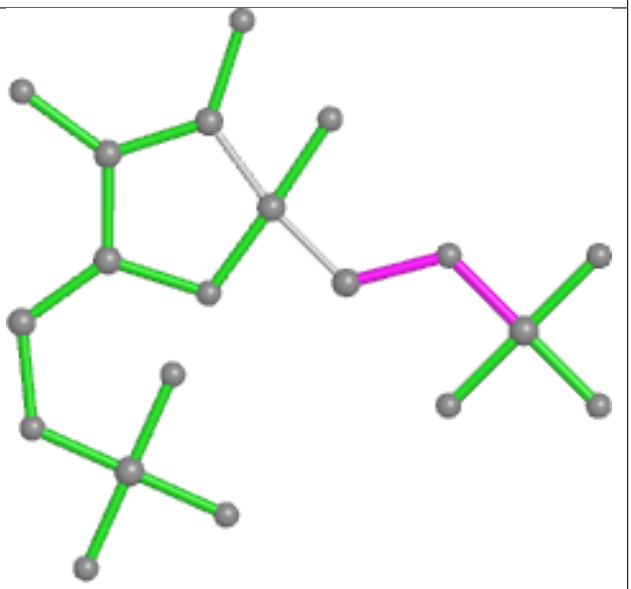


Rings

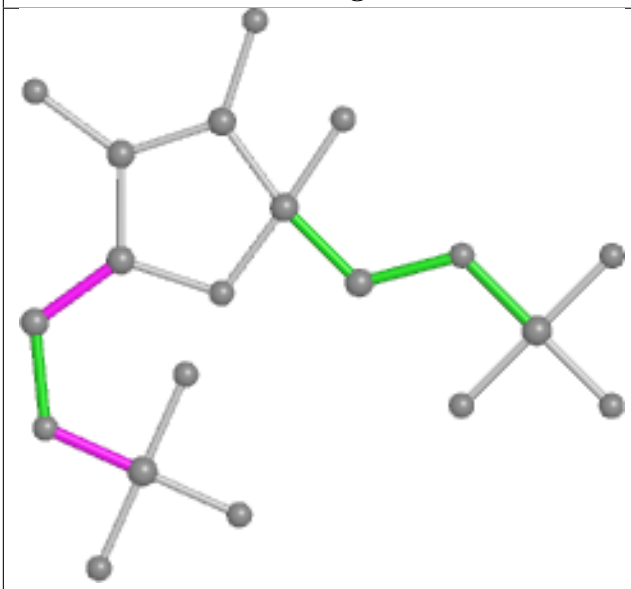
Ligand FBP A 601



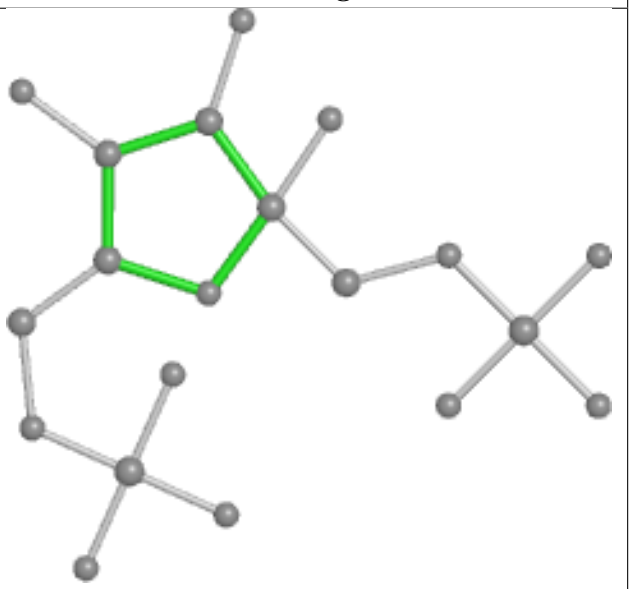
Bond lengths



Bond angles

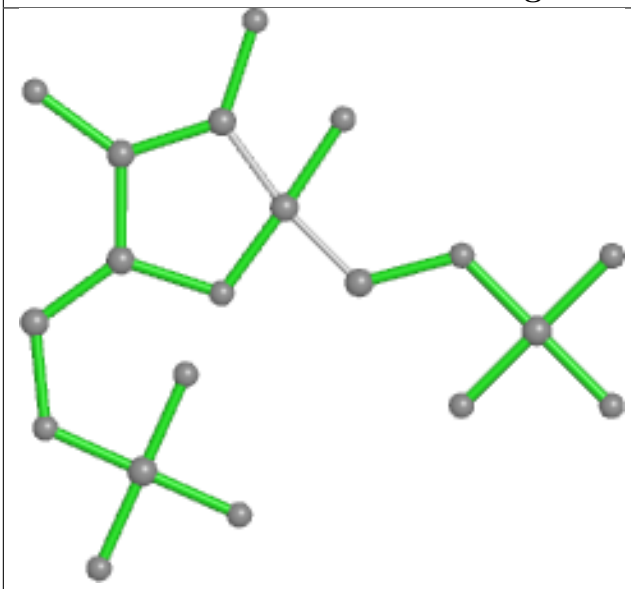


Torsions

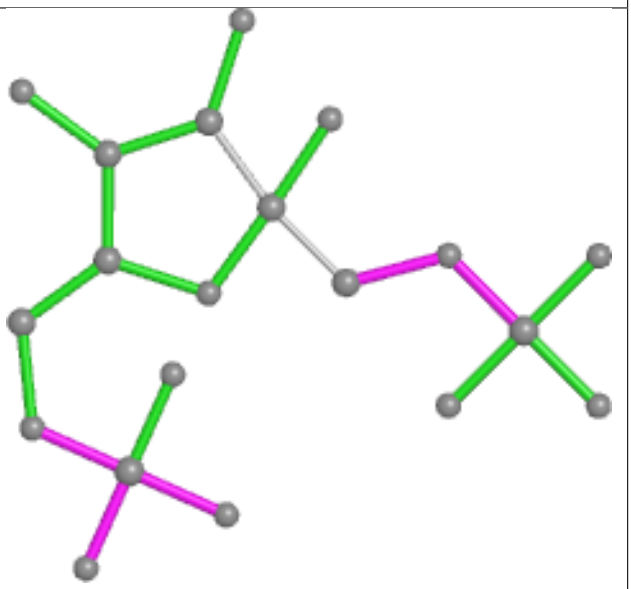


Rings

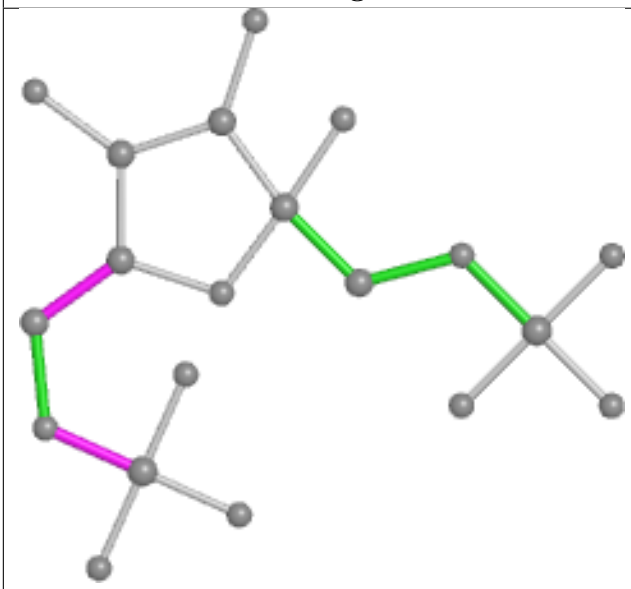
Ligand FBP H 601



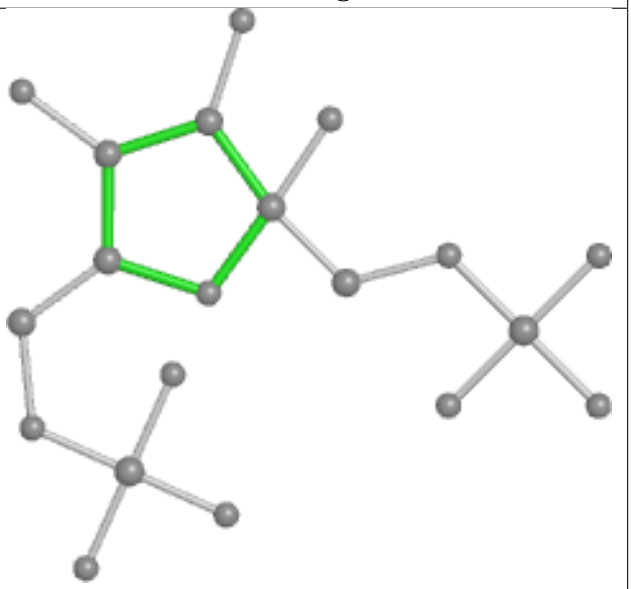
Bond lengths



Bond angles

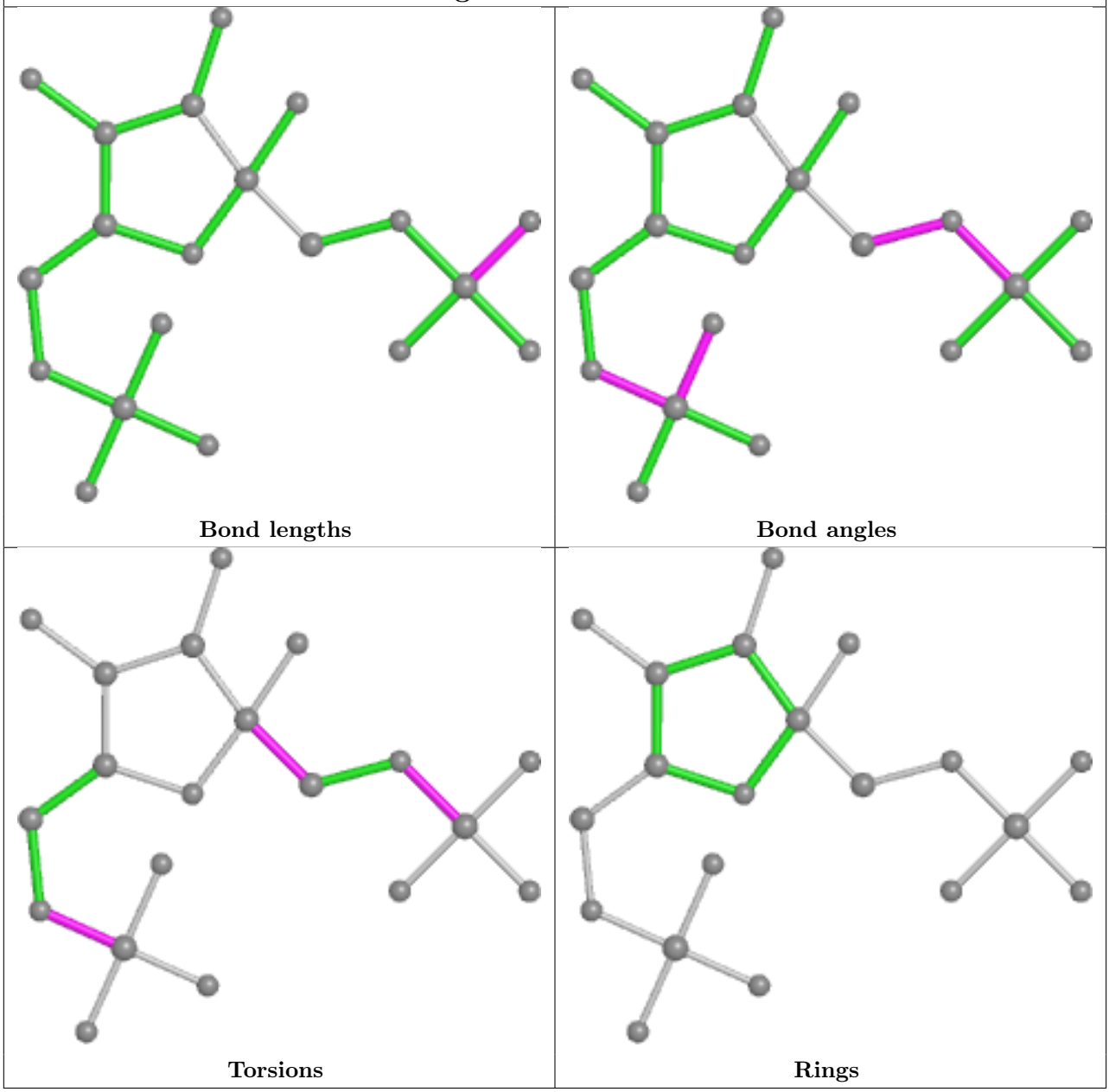


Torsions



Rings

Ligand FBP C 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%)	2.02	178 (42%) 0 0	99, 142, 183, 196	0
1	B	436/447 (97%)	1.28	92 (21%) 1 0	69, 107, 146, 160	0
1	C	425/447 (95%)	1.36	90 (21%) 0 0	51, 98, 143, 171	0
1	D	425/447 (95%)	0.85	22 (5%) 27 22	45, 65, 104, 157	0
1	E	419/447 (93%)	1.80	167 (39%) 0 0	90, 133, 172, 183	0
1	F	432/447 (96%)	1.23	95 (21%) 0 0	67, 103, 141, 156	0
1	G	421/447 (94%)	1.09	68 (16%) 1 1	50, 86, 121, 146	1 (0%)
1	H	425/447 (95%)	0.86	23 (5%) 25 20	43, 63, 101, 155	0
All	All	3405/3576 (95%)	1.31	735 (21%) 0 0	43, 100, 163, 196	1 (0%)

All (735) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22	THR	17.7
1	A	115	LEU	13.6
1	B	12	ASP	13.0
1	E	115	LEU	10.9
1	A	63	ILE	10.9
1	E	442	VAL	10.6
1	A	241	LEU	10.4
1	C	21	GLY	10.0
1	A	492	ALA	9.6
1	B	13	VAL	9.0
1	E	447	GLY	9.0
1	B	543	SER	8.8
1	B	542	ILE	8.6
1	A	484	LEU	8.5
1	F	12	ASP	8.3
1	A	465	VAL	8.2

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Mol	Chain	Res	Type	RSRZ
1	B	540[A]	LEU	8.1
1	B	132	GLY	8.1
1	E	493	ILE	8.1
1	A	353	THR	8.1
1	F	540[A]	LEU	8.0
1	A	482	PHE	8.0
1	B	16	LEU	8.0
1	B	517	VAL	7.9
1	B	249	VAL	7.7
1	A	493	ILE	7.6
1	C	19	GLU	7.5
1	A	86	LEU	7.4
1	H	25	PHE	7.4
1	E	270	LEU	7.2
1	A	543	SER	7.2
1	C	51	PRO	7.2
1	A	114	PRO	7.0
1	A	350	PRO	7.0
1	E	484	LEU	6.9
1	F	517	VAL	6.8
1	C	23	ALA	6.7
1	A	403	HIS	6.6
1	A	313	ILE	6.6
1	E	319	PHE	6.6
1	F	527	TRP	6.6
1	B	11	ALA	6.4
1	C	42	LEU	6.4
1	D	25	PHE	6.4
1	A	319	PHE	6.4
1	A	66	ALA	6.3
1	B	25	PHE	6.2
1	E	241	LEU	6.2
1	A	343	LEU	6.2
1	A	380	GLY	6.2
1	B	115	LEU	6.2
1	A	453	LEU	6.2
1	E	373	LEU	6.0
1	F	543	SER	6.0
1	A	463	ILE	5.9
1	E	304	VAL	5.9
1	A	263	VAL	5.9
1	E	459	ARG	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	485	LEU	5.7
1	A	373	LEU	5.6
1	E	251	ILE	5.6
1	C	306	ARG	5.6
1	A	383	PRO	5.5
1	C	366	ASP	5.5
1	E	403	HIS	5.5
1	A	352	PRO	5.4
1	F	115	LEU	5.4
1	A	382	PHE	5.4
1	C	309	LEU	5.4
1	E	66	ALA	5.3
1	C	343	LEU	5.3
1	E	465	VAL	5.3
1	B	527	TRP	5.3
1	F	237	ASP	5.2
1	B	241	LEU	5.2
1	A	536	ILE	5.1
1	C	393	ILE	5.1
1	G	115	LEU	5.1
1	A	357	THR	5.1
1	A	96	HIS	5.0
1	E	382	PHE	5.0
1	B	20	LEU	5.0
1	A	489	PRO	5.0
1	A	100	ILE	4.9
1	B	277	ILE	4.9
1	A	459	ARG	4.9
1	G	63	ILE	4.9
1	E	349	LYS	4.9
1	A	88	PHE	4.9
1	A	304	VAL	4.9
1	E	103	VAL	4.9
1	C	390	GLN	4.8
1	A	253	PHE	4.8
1	C	322	GLN	4.8
1	H	21	GLY	4.7
1	A	527	TRP	4.7
1	E	463	ILE	4.7
1	G	28	GLN	4.7
1	A	25	PHE	4.7
1	A	30	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	81	MET	4.7
1	A	407	PHE	4.7
1	A	494	TRP	4.7
1	G	322	GLN	4.7
1	B	231	PRO	4.6
1	D	24	PHE	4.6
1	G	50	GLU	4.6
1	F	475	VAL	4.6
1	F	25	PHE	4.5
1	E	379	LYS	4.5
1	D	26	GLN	4.5
1	G	45	LEU	4.5
1	E	348	THR	4.5
1	A	481	VAL	4.4
1	F	516	ARG	4.4
1	G	363	ALA	4.4
1	E	354	ARG	4.4
1	E	492	ALA	4.4
1	E	234	SER	4.4
1	F	113	SER	4.4
1	E	57	THR	4.4
1	A	442	VAL	4.4
1	A	464	ALA	4.4
1	F	542[A]	ILE	4.4
1	E	487	ARG	4.3
1	E	393	ILE	4.3
1	E	402	TYR	4.3
1	F	241	LEU	4.3
1	C	37	THR	4.3
1	A	361	ALA	4.3
1	E	114	PRO	4.2
1	C	382	PHE	4.2
1	A	537[A]	MET	4.2
1	C	32	ALA	4.2
1	A	67	SER	4.2
1	E	421	THR	4.2
1	F	251	ILE	4.2
1	F	521	VAL	4.2
1	A	379	LYS	4.2
1	B	521	VAL	4.2
1	C	304	VAL	4.2
1	E	381	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	539	VAL	4.2
1	H	24	PHE	4.2
1	E	244	GLY	4.1
1	B	524	VAL	4.1
1	A	393	ILE	4.1
1	C	59	ILE	4.1
1	C	389	MET	4.1
1	E	247	HIS	4.1
1	A	443	LEU	4.1
1	E	397	ALA	4.1
1	A	347	ILE	4.1
1	A	447	GLY	4.1
1	A	55	ARG	4.1
1	G	51	PRO	4.1
1	A	237	ASP	4.1
1	E	118	ARG	4.0
1	A	349	LYS	4.0
1	A	397	ALA	4.0
1	A	491	GLU	4.0
1	E	63	ILE	4.0
1	E	522	ILE	4.0
1	B	103	VAL	4.0
1	E	350	PRO	4.0
1	F	103	VAL	4.0
1	C	363	ALA	4.0
1	A	522	ILE	4.0
1	C	45	LEU	3.9
1	E	537[A]	MET	3.9
1	E	248	GLY	3.9
1	E	355	ALA	3.9
1	E	464	ALA	3.9
1	C	373	LEU	3.9
1	B	520	LEU	3.9
1	A	485	LEU	3.9
1	F	270	LEU	3.9
1	A	280	ILE	3.9
1	F	277	ILE	3.9
1	E	539	VAL	3.9
1	F	26	GLN	3.9
1	A	506	ILE	3.9
1	C	24	PHE	3.9
1	A	354	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	10	ARG	3.9
1	E	380	GLY	3.9
1	A	127	LYS	3.8
1	E	536	ILE	3.8
1	C	341	GLN	3.8
1	E	422	GLU	3.8
1	A	283	ILE	3.8
1	B	485	LEU	3.8
1	F	274	GLY	3.7
1	F	16	LEU	3.7
1	C	47	ILE	3.7
1	G	42	LEU	3.7
1	E	65	PRO	3.7
1	B	507	GLU	3.7
1	B	477	LEU	3.7
1	A	247	HIS	3.7
1	A	124	LEU	3.7
1	G	38	PHE	3.7
1	A	355	ALA	3.7
1	E	482	PHE	3.7
1	A	402	TYR	3.7
1	F	39	LEU	3.6
1	F	371	ILE	3.6
1	F	520	LEU	3.6
1	A	441	ILE	3.6
1	G	32	ALA	3.6
1	A	251	ILE	3.6
1	E	456	TYR	3.6
1	E	489	PRO	3.6
1	F	487	ARG	3.6
1	A	418[A]	ARG	3.6
1	C	371	ILE	3.6
1	A	377	THR	3.6
1	E	353	THR	3.6
1	C	349	LYS	3.6
1	A	65	PRO	3.5
1	B	24	PHE	3.5
1	E	122	ILE	3.5
1	B	237	ASP	3.5
1	B	438	ALA	3.5
1	E	543	SER	3.5
1	H	30	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	68	ARG	3.5
1	F	524	VAL	3.5
1	C	20	LEU	3.5
1	F	112	GLY	3.5
1	E	502	VAL	3.5
1	F	233	LEU	3.5
1	A	474	GLN	3.5
1	B	355	ALA	3.5
1	G	114	PRO	3.5
1	G	337	VAL	3.5
1	B	122	ILE	3.5
1	B	127	LYS	3.4
1	F	539	VAL	3.4
1	E	347	ILE	3.4
1	E	443	LEU	3.4
1	A	101	ALA	3.4
1	C	386	ALA	3.4
1	C	263	VAL	3.4
1	E	263	VAL	3.4
1	E	453	LEU	3.4
1	A	232	GLY	3.4
1	B	463	ILE	3.4
1	E	289	VAL	3.4
1	E	100	ILE	3.4
1	C	28	GLN	3.4
1	C	103	VAL	3.4
1	B	90	HIS	3.4
1	B	27	GLN	3.4
1	E	444	THR	3.3
1	F	114	PRO	3.3
1	A	289	VAL	3.3
1	C	63	ILE	3.3
1	F	522	ILE	3.3
1	G	359	ASP	3.3
1	E	61	ALA	3.3
1	A	351	ARG	3.3
1	F	533	TYR	3.3
1	G	390	GLN	3.3
1	E	490	PRO	3.3
1	E	67	SER	3.3
1	C	397	ALA	3.3
1	G	374[A]	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	426	ILE	3.3
1	A	346	MET	3.3
1	F	27	GLN	3.3
1	E	440	ILE	3.3
1	G	527	TRP	3.3
1	B	39	LEU	3.3
1	C	342	MET	3.3
1	B	431	ALA	3.3
1	F	463	ILE	3.2
1	E	477	LEU	3.2
1	A	423	VAL	3.2
1	G	253	PHE	3.2
1	A	450	ALA	3.2
1	C	359	ASP	3.2
1	E	452	LEU	3.2
1	A	388	LYS	3.2
1	F	449	SER	3.2
1	B	112	GLY	3.2
1	E	514	PHE	3.2
1	F	263	VAL	3.2
1	F	502	VAL	3.2
1	F	11	ALA	3.2
1	G	27	GLN	3.2
1	C	340	THR	3.2
1	E	25	PHE	3.2
1	A	302	ILE	3.2
1	A	378	ALA	3.2
1	E	375	GLY	3.2
1	F	90	HIS	3.2
1	A	318	VAL	3.2
1	B	539	VAL	3.2
1	G	360	VAL	3.2
1	B	486	TYR	3.2
1	C	394	ALA	3.2
1	E	524	VAL	3.2
1	C	368	ALA	3.2
1	C	307	GLY	3.2
1	B	433	PHE	3.1
1	G	340	THR	3.1
1	A	248	GLY	3.1
1	F	453	LEU	3.1
1	E	389	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	47	ILE	3.1
1	A	490	PRO	3.1
1	E	390	GLN	3.1
1	A	233	LEU	3.1
1	E	237	ASP	3.1
1	E	418	ARG	3.1
1	F	266	VAL	3.1
1	E	540	LEU	3.1
1	C	351	ARG	3.1
1	E	433	PHE	3.1
1	F	443	LEU	3.1
1	B	533	TYR	3.1
1	B	236	GLN	3.1
1	E	491	GLU	3.1
1	A	348	THR	3.1
1	C	116	SER	3.1
1	A	240	ASP	3.1
1	C	50	GLU	3.1
1	A	62	THR	3.1
1	E	498	VAL	3.1
1	A	456	TYR	3.0
1	A	375	GLY	3.0
1	G	24	PHE	3.0
1	F	465	VAL	3.0
1	A	460	ALA	3.0
1	E	410	LEU	3.0
1	E	253	PHE	3.0
1	A	524	VAL	3.0
1	A	412	ARG	3.0
1	C	383	PRO	3.0
1	F	52	VAL	3.0
1	F	249	VAL	3.0
1	F	431	ALA	3.0
1	B	481	VAL	3.0
1	G	254	ALA	3.0
1	C	41	HIS	3.0
1	C	60	ILE	3.0
1	E	277	ILE	3.0
1	B	487	ARG	3.0
1	A	390	GLN	3.0
1	A	444	THR	3.0
1	G	318	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	469	ALA	3.0
1	E	29	GLN	3.0
1	A	514	PHE	3.0
1	B	118	ARG	3.0
1	B	254	ALA	3.0
1	F	471	ALA	3.0
1	D	21	GLY	2.9
1	E	310	GLY	2.9
1	B	242	ARG	2.9
1	C	374	SER	2.9
1	C	27	GLN	2.9
1	E	120	VAL	2.9
1	C	302	ILE	2.9
1	F	426	ILE	2.9
1	A	500	ARG	2.9
1	B	443	LEU	2.9
1	G	39	LEU	2.9
1	F	13	VAL	2.9
1	E	232	GLY	2.9
1	E	249	VAL	2.9
1	B	531	SER	2.9
1	C	281	SER	2.9
1	G	453	LEU	2.9
1	A	107	VAL	2.9
1	E	86	LEU	2.9
1	C	346	MET	2.9
1	A	33	ALA	2.9
1	F	91	GLY	2.9
1	A	122	ILE	2.9
1	A	305	ALA	2.9
1	A	371	ILE	2.8
1	A	511	LEU	2.8
1	A	421	THR	2.8
1	A	458	PRO	2.8
1	A	389	MET	2.8
1	E	412	ARG	2.8
1	C	76[A]	MET	2.8
1	C	337	VAL	2.8
1	D	23	ALA	2.8
1	E	481	VAL	2.8
1	E	99	SER	2.8
1	F	440	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	460	ALA	2.8
1	E	405	GLN	2.8
1	B	482	PHE	2.8
1	B	475	VAL	2.8
1	F	537[A]	MET	2.8
1	A	517	VAL	2.7
1	A	523	VAL	2.7
1	E	352	PRO	2.7
1	E	521	VAL	2.7
1	A	426	ILE	2.7
1	E	55	ARG	2.7
1	B	129	PRO	2.7
1	C	360	VAL	2.7
1	E	80	GLY	2.7
1	E	233	LEU	2.7
1	E	474	GLN	2.7
1	A	97	ALA	2.7
1	G	263	VAL	2.7
1	G	387	VAL	2.7
1	A	410	LEU	2.7
1	G	30	LEU	2.7
1	C	26	GLN	2.7
1	A	466	THR	2.7
1	C	377	THR	2.7
1	A	84	ALA	2.7
1	E	450	ALA	2.7
1	C	25	PHE	2.7
1	E	129	PRO	2.7
1	E	409	GLU	2.7
1	B	484	LEU	2.7
1	E	39	LEU	2.7
1	F	373	LEU	2.7
1	F	514	PHE	2.7
1	F	377	THR	2.7
1	G	459	ARG	2.7
1	B	429	VAL	2.7
1	B	442	VAL	2.7
1	B	537[A]	MET	2.7
1	F	355	ALA	2.7
1	G	233	LEU	2.7
1	A	533	TYR	2.7
1	C	338	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	251	ILE	2.7
1	E	313	ILE	2.7
1	F	123	ALA	2.6
1	E	30	LEU	2.6
1	E	376	GLU	2.6
1	A	285	ASN	2.6
1	B	514	PHE	2.6
1	B	371	ILE	2.6
1	A	416	LEU	2.6
1	C	365	LEU	2.6
1	E	451	GLN	2.6
1	A	408	GLU	2.6
1	C	379	LYS	2.6
1	E	84	ALA	2.6
1	E	90	HIS	2.6
1	A	298	VAL	2.6
1	A	381	ASN	2.6
1	A	326	ILE	2.6
1	F	495	ALA	2.6
1	A	475	VAL	2.6
1	D	263	VAL	2.6
1	A	309	LEU	2.6
1	D	30	LEU	2.6
1	C	64	GLY	2.6
1	E	127	LYS	2.6
1	A	103	VAL	2.6
1	B	263	VAL	2.6
1	A	452	LEU	2.6
1	G	373	LEU	2.6
1	C	253	PHE	2.6
1	E	62	THR	2.6
1	A	270	LEU	2.6
1	A	273	GLU	2.6
1	D	309	LEU	2.6
1	G	366	ASP	2.6
1	A	252	VAL	2.5
1	D	249	VAL	2.5
1	E	125	ASP	2.5
1	F	459	ARG	2.5
1	D	331	LEU	2.5
1	A	454	SER	2.5
1	D	292	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	525	THR	2.5
1	E	280	ILE	2.5
1	F	100	ILE	2.5
1	A	56	SER	2.5
1	C	36	ASP	2.5
1	A	323	LYS	2.5
1	C	453	LEU	2.5
1	F	515	LEU	2.5
1	B	15	GLN	2.5
1	A	76[A]	MET	2.5
1	E	243	PHE	2.5
1	G	383	PRO	2.5
1	C	100	ILE	2.5
1	B	107	VAL	2.5
1	F	486	TYR	2.5
1	G	401	VAL	2.5
1	C	372	MET	2.5
1	F	127	LYS	2.5
1	A	78	LYS	2.5
1	A	234	SER	2.5
1	G	342	MET	2.5
1	G	351	ARG	2.5
1	B	522	ILE	2.5
1	E	339	ALA	2.5
1	F	283	ILE	2.5
1	G	23	ALA	2.5
1	D	115	LEU	2.5
1	E	69	SER	2.5
1	A	538	ARG	2.5
1	A	28	GLN	2.4
1	F	231	PRO	2.4
1	A	123	ALA	2.4
1	E	357	THR	2.4
1	E	377	THR	2.4
1	G	343	LEU	2.4
1	H	538[A]	ARG	2.4
1	C	380	GLY	2.4
1	G	60	ILE	2.4
1	E	71	GLU	2.4
1	F	482	PHE	2.4
1	G	355	ALA	2.4
1	F	442	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	433	PHE	2.4
1	A	518	GLY	2.4
1	G	251	ILE	2.4
1	F	87	ASN	2.4
1	G	252	VAL	2.4
1	B	100	ILE	2.4
1	A	498	VAL	2.4
1	E	91	GLY	2.4
1	E	266	VAL	2.4
1	C	404	ARG	2.4
1	B	26	GLN	2.4
1	B	28	GLN	2.4
1	B	440	ILE	2.4
1	E	371	ILE	2.4
1	E	88	PHE	2.4
1	E	358	SER	2.4
1	E	368	ALA	2.4
1	E	406	LEU	2.4
1	A	384	VAL	2.4
1	A	404	ARG	2.4
1	E	408	GLU	2.4
1	H	242	ARG	2.4
1	A	345	SER	2.3
1	C	30	LEU	2.3
1	E	511	LEU	2.3
1	B	251	ILE	2.3
1	E	351	ARG	2.3
1	E	488	GLU	2.3
1	G	117	TYR	2.3
1	C	124	LEU	2.3
1	F	244	GLY	2.3
1	F	541	SER	2.3
1	G	41	HIS	2.3
1	F	309	LEU	2.3
1	F	481	VAL	2.3
1	A	372	MET	2.3
1	F	484	LEU	2.3
1	G	124	LEU	2.3
1	E	523	VAL	2.3
1	F	24	PHE	2.3
1	G	25	PHE	2.3
1	A	376	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	80	GLY	2.3
1	H	540	LEU	2.3
1	G	59	ILE	2.3
1	B	422	GLU	2.3
1	E	462	VAL	2.3
1	C	527	TRP	2.3
1	H	443	LEU	2.3
1	A	32	ALA	2.3
1	E	525	THR	2.3
1	G	57	THR	2.3
1	H	431	ALA	2.3
1	G	83	ILE	2.3
1	H	249	VAL	2.3
1	B	244	GLY	2.3
1	C	34	MET	2.3
1	B	256	PHE	2.3
1	C	459	ARG	2.3
1	B	279	ILE	2.3
1	C	122	ILE	2.3
1	F	110	PHE	2.3
1	G	70	VAL	2.3
1	B	50	GLU	2.2
1	D	425	ALA	2.2
1	A	36	ASP	2.2
1	G	452	LEU	2.2
1	A	118	ARG	2.2
1	A	315	ALA	2.2
1	H	257	VAL	2.2
1	B	108	GLU	2.2
1	A	449	SER	2.2
1	E	124	LEU	2.2
1	E	515	LEU	2.2
1	A	342	MET	2.2
1	G	303	MET	2.2
1	F	433	PHE	2.2
1	A	462	VAL	2.2
1	B	252	VAL	2.2
1	B	298	VAL	2.2
1	E	429	VAL	2.2
1	G	107	VAL	2.2
1	G	281	SER	2.2
1	B	270	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	406	LEU	2.2
1	B	467	ARG	2.2
1	D	44	LEU	2.2
1	A	471	ALA	2.2
1	C	305	ALA	2.2
1	A	125	ASP	2.2
1	E	240	ASP	2.2
1	E	235	GLU	2.2
1	E	274	GLY	2.2
1	A	266	VAL	2.2
1	B	238	VAL	2.2
1	B	441	ILE	2.2
1	F	63	ILE	2.2
1	B	131	SER	2.2
1	F	85	ARG	2.2
1	A	42	LEU	2.2
1	E	81	MET	2.2
1	F	472	ALA	2.2
1	A	317	LYS	2.2
1	G	64	GLY	2.2
1	G	514	PHE	2.2
1	A	83	ILE	2.2
1	G	103	VAL	2.2
1	A	39	LEU	2.2
1	C	350	PRO	2.2
1	H	45	LEU	2.2
1	H	511	LEU	2.2
1	A	29	GLN	2.2
1	F	376	GLU	2.2
1	B	130	GLY	2.2
1	F	512	ARG	2.2
1	A	113	SER	2.2
1	E	302	ILE	2.2
1	E	506	ILE	2.2
1	B	246	GLU	2.2
1	G	296	LEU	2.2
1	E	407	PHE	2.2
1	E	257	VAL	2.1
1	F	441	ILE	2.1
1	G	371	ILE	2.1
1	H	371	ILE	2.1
1	D	45	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	57	THR	2.1
1	E	467	ARG	2.1
1	E	494	TRP	2.1
1	E	323	LYS	2.1
1	B	243	PHE	2.1
1	A	521	VAL	2.1
1	C	83	ILE	2.1
1	C	313	ILE	2.1
1	E	309	LEU	2.1
1	F	477	LEU	2.1
1	H	331	LEU	2.1
1	E	505	GLY	2.1
1	F	57	THR	2.1
1	E	38	PHE	2.1
1	F	243	PHE	2.1
1	A	502	VAL	2.1
1	H	302	ILE	2.1
1	A	529	PRO	2.1
1	E	388	LYS	2.1
1	E	303	MET	2.1
1	G	382	PHE	2.1
1	H	256	PHE	2.1
1	B	45	LEU	2.1
1	D	498	VAL	2.1
1	D	511	LEU	2.1
1	E	533	TYR	2.1
1	G	238	VAL	2.1
1	A	303	MET	2.1
1	E	446	THR	2.1
1	E	466	THR	2.1
1	F	236	GLN	2.1
1	H	26	GLN	2.1
1	C	67	SER	2.1
1	A	128	GLY	2.1
1	F	455	ARG	2.1
1	F	467	ARG	2.1
1	D	521	VAL	2.1
1	A	117	TYR	2.1
1	A	476	HIS	2.1
1	E	343	LEU	2.1
1	F	429	VAL	2.1
1	G	393	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	93	HIS	2.1
1	C	107	VAL	2.1
1	C	115	LEU	2.1
1	F	452	LEU	2.1
1	E	383	PRO	2.1
1	H	463	ILE	2.1
1	E	400	ALA	2.1
1	E	454[A]	SER	2.1
1	A	71	GLU	2.1
1	B	83	ILE	2.1
1	D	524	VAL	2.1
1	E	423	VAL	2.1
1	H	452	LEU	2.1
1	E	386	ALA	2.1
1	G	487	ARG	2.1
1	C	57	THR	2.1
1	H	508	SER	2.1
1	C	498	VAL	2.0
1	G	341	GLN	2.0
1	G	423	VAL	2.0
1	C	385	GLU	2.0
1	B	515	LEU	2.0
1	C	233	LEU	2.0
1	B	364	VAL	2.0
1	E	107	VAL	2.0
1	H	521	VAL	2.0
1	E	279	ILE	2.0
1	C	398	GLU	2.0
1	B	23	ALA	2.0
1	G	377	THR	2.0
1	B	451	GLN	2.0
1	C	319	PHE	2.0
1	D	433	PHE	2.0
1	F	256	PHE	2.0
1	B	124	LEU	2.0
1	C	320	LEU	2.0
1	H	309	LEU	2.0
1	D	257	VAL	2.0
1	E	47	ILE	2.0
1	E	311	ILE	2.0
1	F	116	SER	2.0
1	F	358	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	424	THR	2.0
1	D	256	PHE	2.0
1	B	379	LYS	2.0
1	C	252	VAL	2.0
1	F	498	VAL	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
5	K	B	604	1/1	0.58	0.13	138,138,138,138	0
6	OAT	G	605	38/38	0.69	0.74	156,159,164,164	21
3	OXL	A	602	6/6	0.73	0.41	178,178,178,178	0
3	OXL	E	602	6/6	0.77	0.38	167,167,167,167	0
2	FBP	A	601	20/20	0.78	0.22	150,151,151,152	0
2	FBP	E	601	20/20	0.79	0.17	139,140,142,142	0
5	K	E	604	1/1	0.80	0.85	228,228,228,228	0
5	K	H	604	1/1	0.81	0.10	98,98,98,98	0
6	OAT	B	605	38/38	0.82	0.51	120,126,130,130	21
2	FBP	F	601	20/20	0.82	0.19	127,128,130,131	0
5	K	F	604	1/1	0.83	0.15	142,142,142,142	0
5	K	D	604	1/1	0.84	0.09	100,100,100,100	0
5	K	A	604	1/1	0.84	0.25	201,201,201,201	0
4	MG	G	603	1/1	0.84	0.13	67,67,67,67	0
4	MG	C	603	1/1	0.85	0.15	88,88,88,88	0
3	OXL	C	602	6/6	0.85	0.28	156,156,156,156	0
6	OAT	H	605	38/38	0.85	0.41	118,123,125,126	21
3	OXL	H	602	6/6	0.87	0.29	126,127,127,127	0

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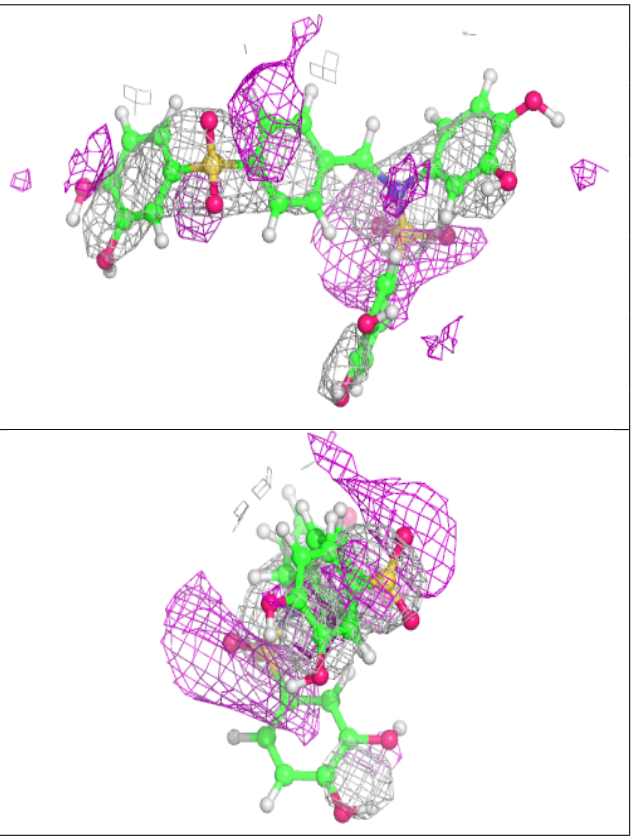
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	K	C	604	1/1	0.89	0.09	125,125,125,125	0
3	OXL	D	602	6/6	0.89	0.39	138,138,138,138	0
2	FBP	B	601	20/20	0.90	0.17	120,121,125,125	0
4	MG	A	603	1/1	0.91	0.06	141,141,141,141	0
3	OXL	G	602	6/6	0.93	0.22	123,123,123,124	0
5	K	G	604	1/1	0.93	0.07	104,104,104,104	0
4	MG	H	603	1/1	0.94	0.15	64,64,64,64	0
3	OXL	F	602	6/6	0.95	0.46	172,172,172,172	0
3	OXL	B	602	6/6	0.95	0.38	150,150,151,151	0
4	MG	F	603	1/1	0.96	0.17	71,71,71,71	0
4	MG	D	603	1/1	0.96	0.16	60,60,60,60	0
2	FBP	C	601	20/20	0.97	0.22	70,71,71,71	0
4	MG	B	603	1/1	0.97	0.09	79,79,79,79	0
2	FBP	H	601	20/20	0.98	0.23	43,52,53,54	0
4	MG	E	603	1/1	0.98	0.07	111,111,111,111	0
2	FBP	D	601	20/20	0.98	0.23	49,51,53,53	0
2	FBP	G	601	20/20	0.98	0.20	66,69,72,73	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.

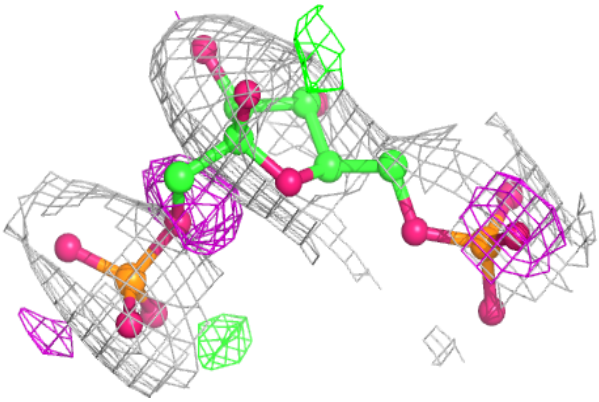
Electron density around OAT G 605:

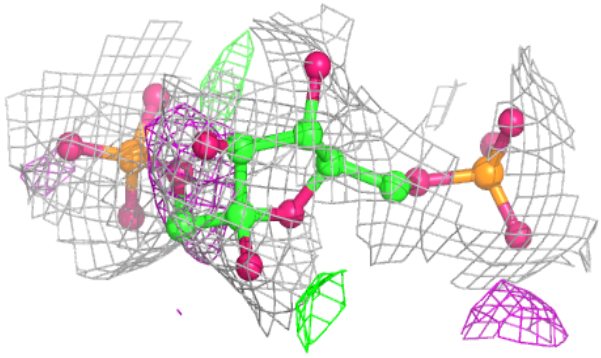
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

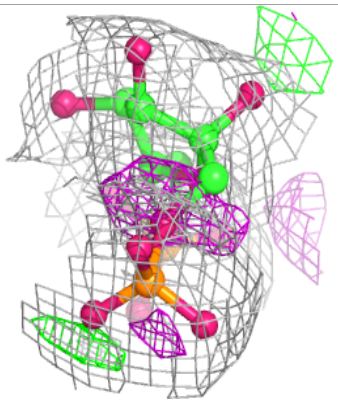


Electron density around FBP A 601:

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

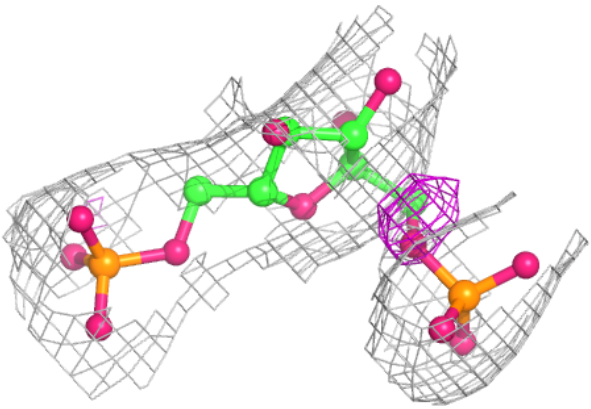


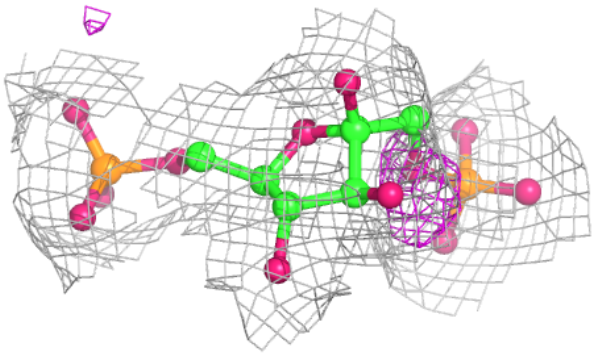


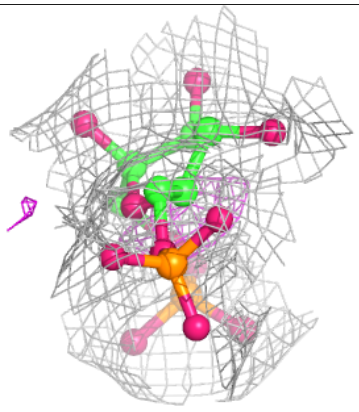


Electron density around FBP E 601:

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

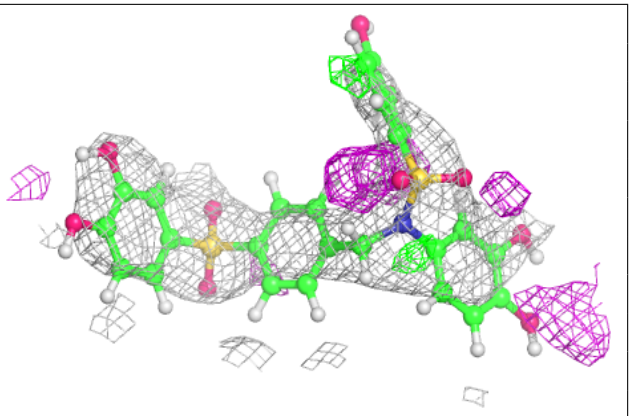


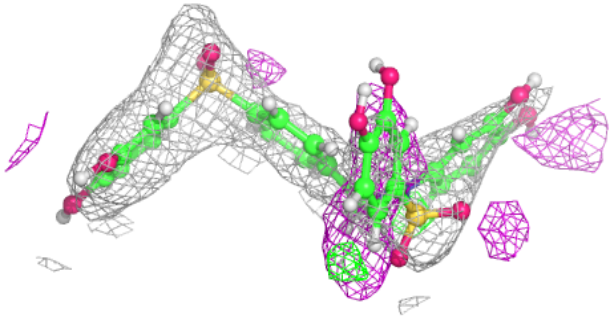


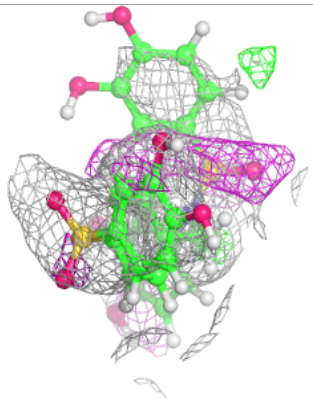


Electron density around OAT B 605:

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

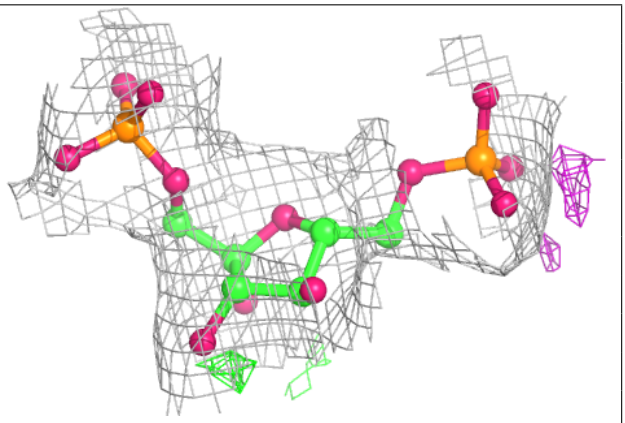


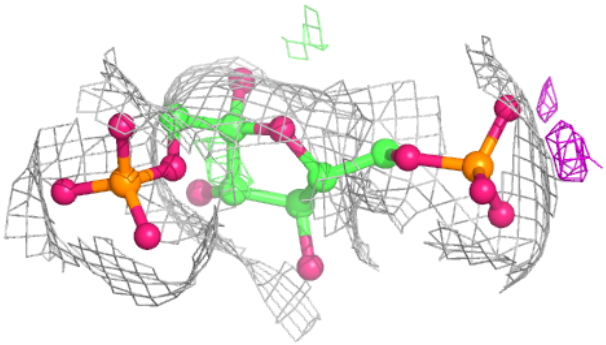


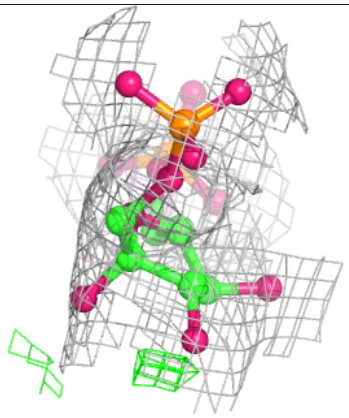


Electron density around FBP F 601:

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

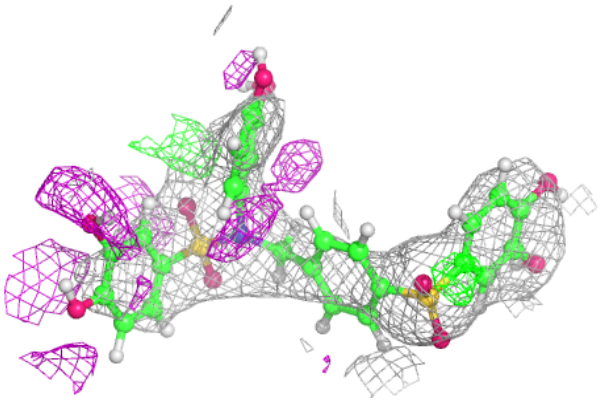


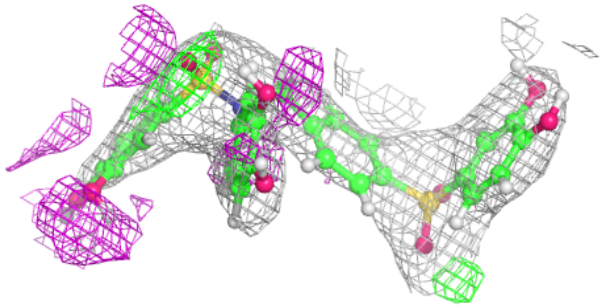


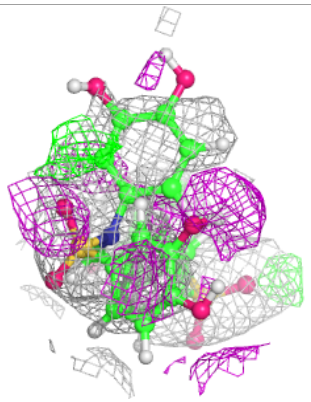


Electron density around OAT H 605:

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

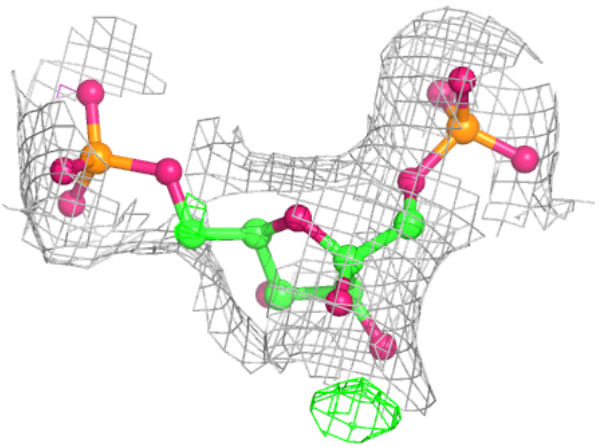


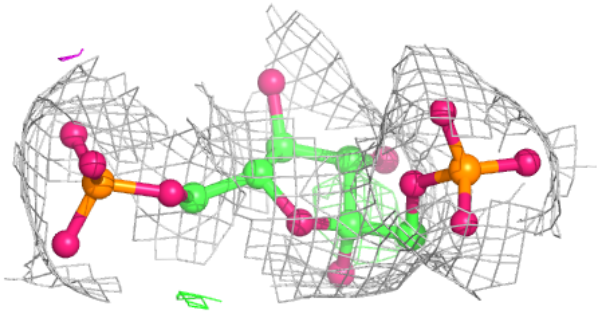


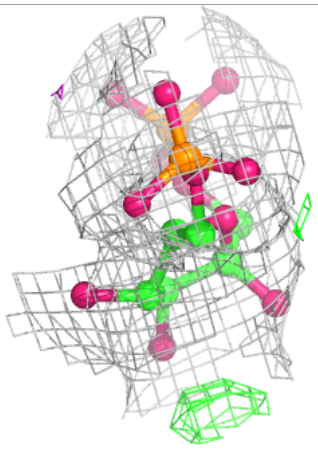


Electron density around FBP B 601:

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

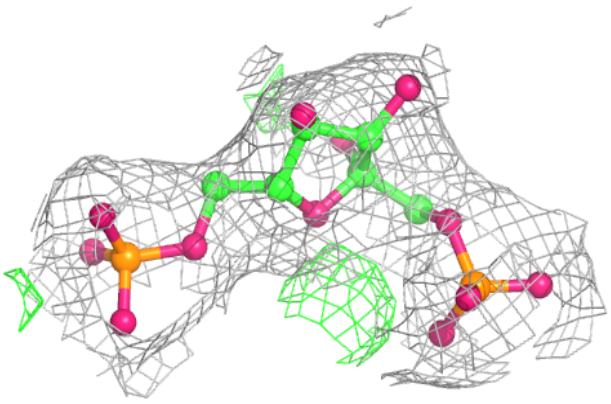


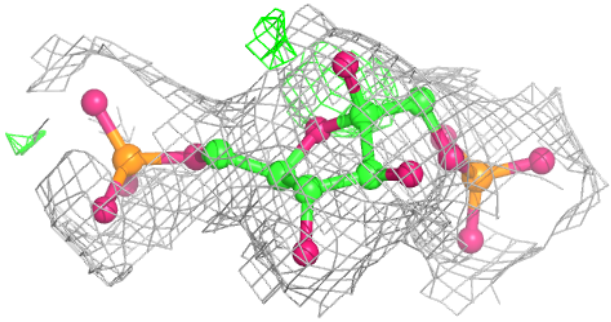


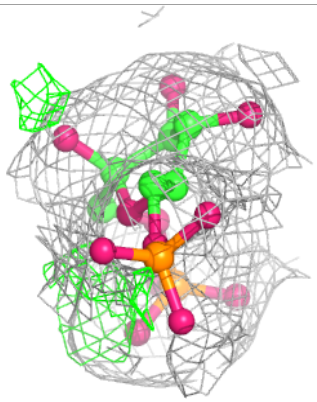


Electron density around FBP C 601:

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

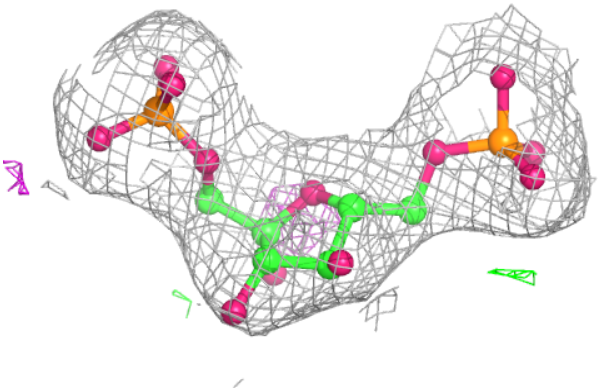


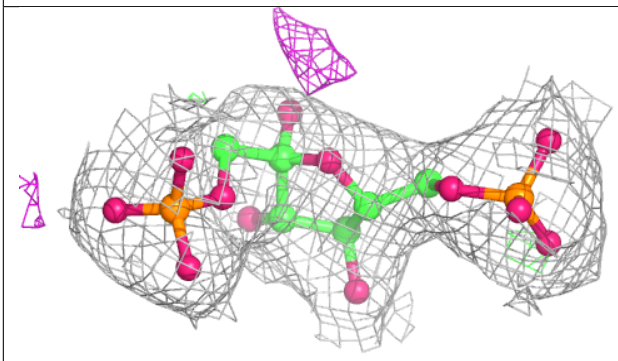




Electron density around FBP H 601:

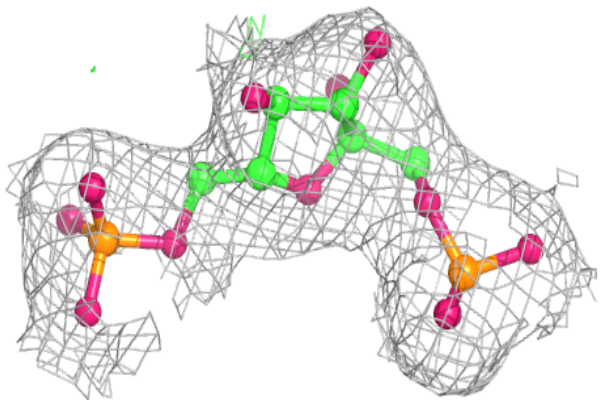
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

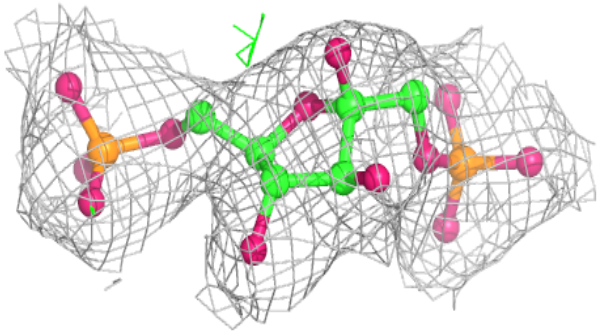


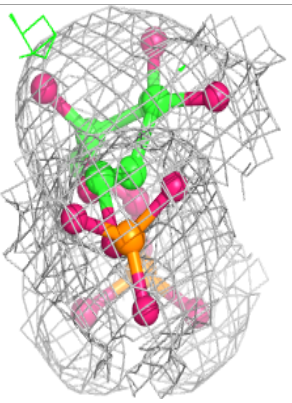


Electron density around FBP D 601:

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

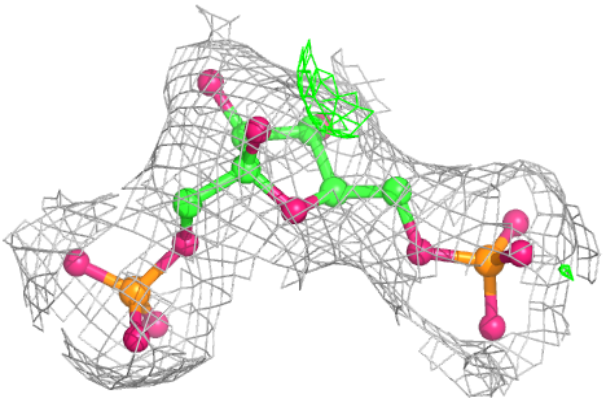


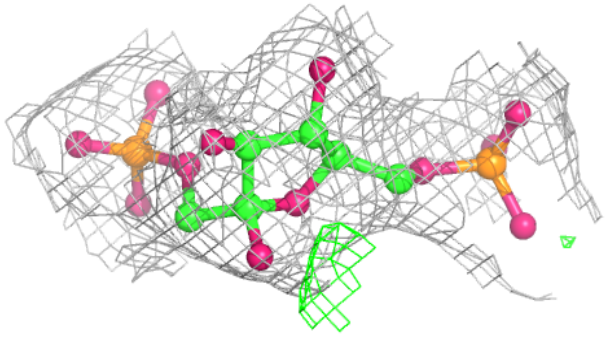


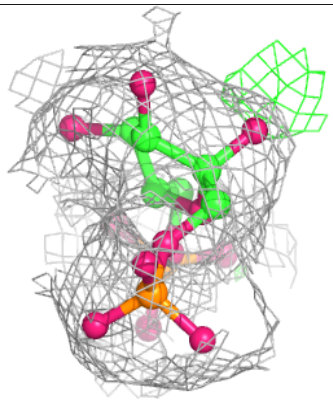


Electron density around FBP G 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.