Full wwPDB X-ray Structure Validation Report (i)

Apr 3, 2023 – 05:39 PM EDT

PDB ID	:	7FSB
Title	:	Structure of liver pyruvate kinase in complex with allosteric modulator 41
Authors	:	Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2022-12-18
Resolution	:	2.50 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:

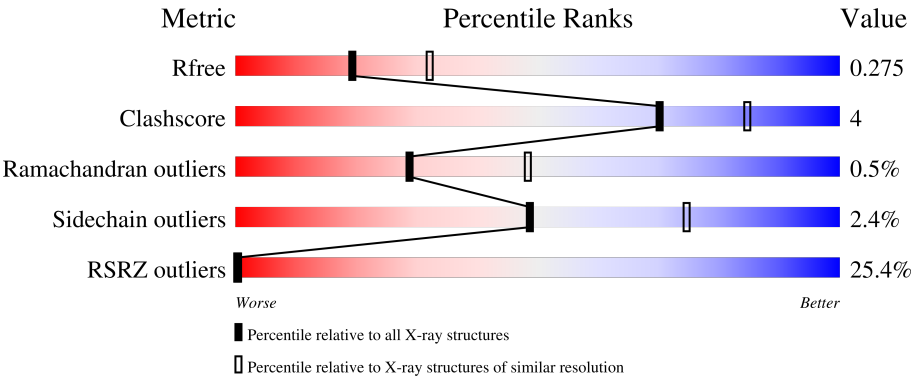
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	51% 84% 9% • 6%
1	B	447	31% 89% 8% •
1	C	447	22% 81% 13% • 5%
1	D	447	2% 85% 9% • 5%
1	E	447	45% 83% 9% • 6%

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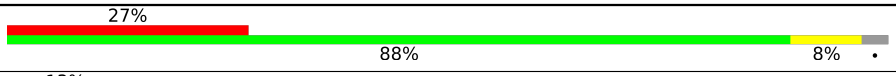
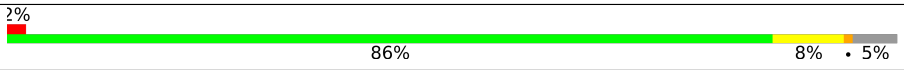
Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	

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	A	604	-	-	-	X
5	K	E	604	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 26926 atoms, of which 76 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	6	0
			3236	2034	585	597	20			
1	B	436	Total	C	N	O	S	0	4	0
			3329	2090	604	615	20			
1	C	425	Total	C	N	O	S	0	4	0
			3247	2040	585	603	19			
1	D	425	Total	C	N	O	S	0	6	0
			3252	2042	590	601	19			
1	E	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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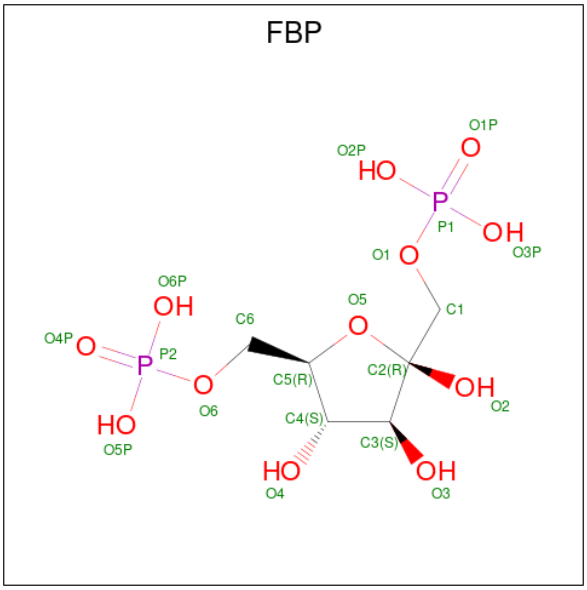
Chain	Residue	Modelled	Actual	Comment	Reference
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	130	GLY	-	linker	UNP P30613
H	131	SER	-	linker	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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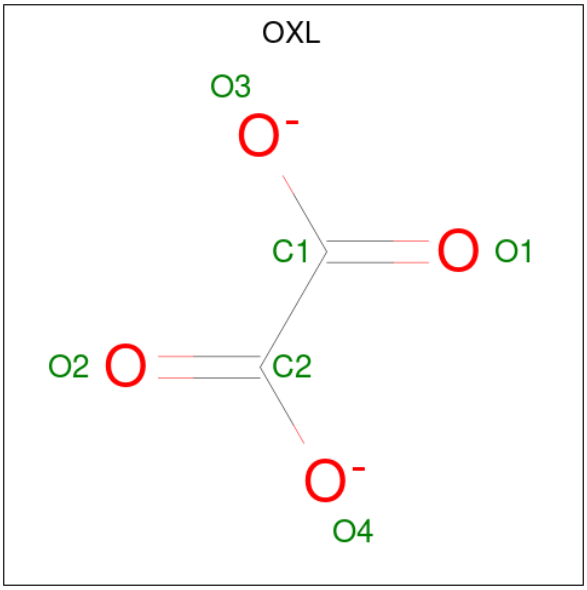
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O P 20 6 12 2	0	0
2	H	1	Total C O P 20 6 12 2	0	0

- 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

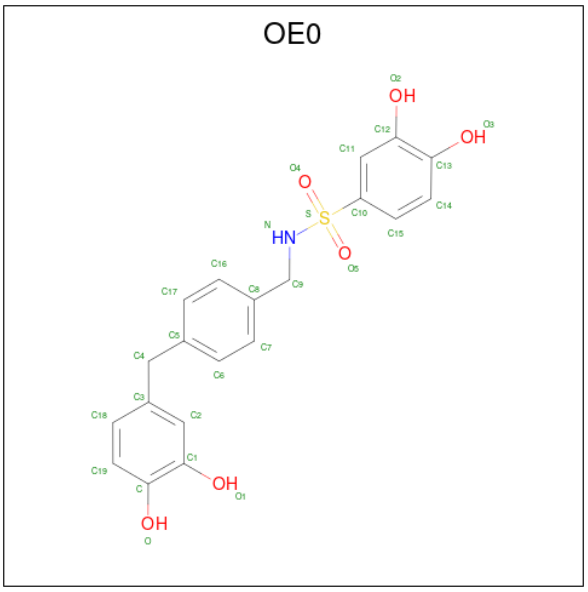
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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-dihydroxyphenyl)methyl]phenyl}methyl)-3,4-dihydroxybenzene-1-sulfonamide (three-letter code: OE0) (formula: $C_{20}H_{19}NO_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	19	0
			47	20	19	1	6	1		
6	B	1	Total	C	H	N	O	S	19	0
			47	20	19	1	6	1		
6	F	1	Total	C	H	N	O	S	19	0
			47	20	19	1	6	1		
6	G	1	Total	C	H	N	O	S	19	0
			47	20	19	1	6	1		

- Molecule 7 is water.

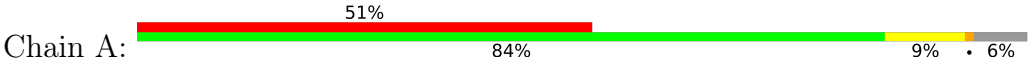
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		
7	B	18	Total	O	0	0
			18	18		
7	C	50	Total	O	0	0
			50	50		
7	D	123	Total	O	0	0
			123	123		
7	E	17	Total	O	0	0
			17	17		
7	F	30	Total	O	0	0
			30	30		
7	G	56	Total	O	0	0
			56	56		
7	H	131	Total	O	0	0
			131	131		

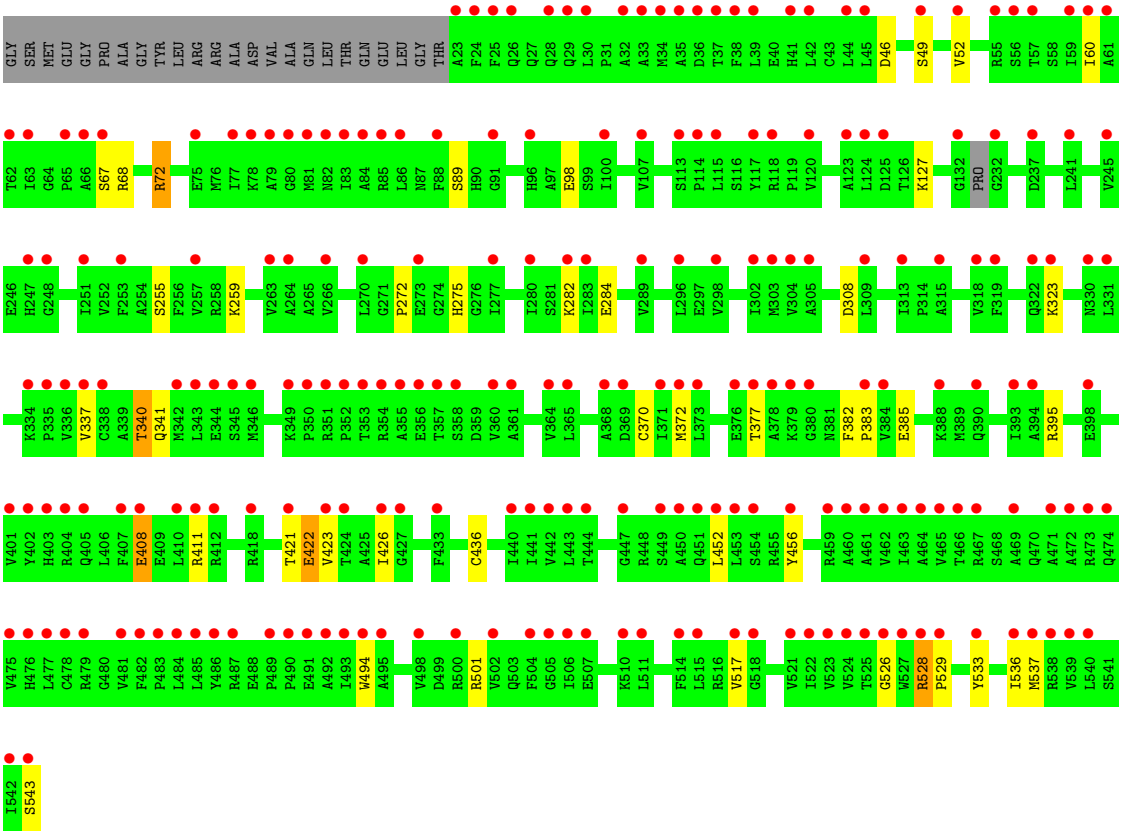
3 Residue-property plots (i)

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

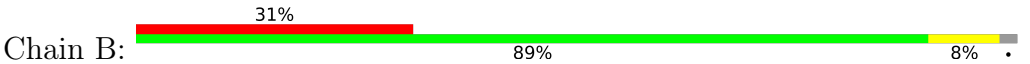
Chain A:

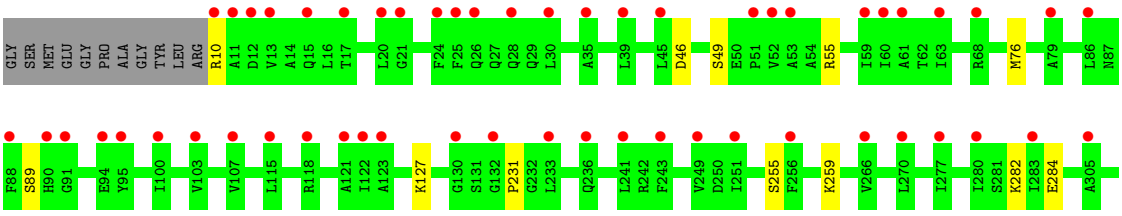


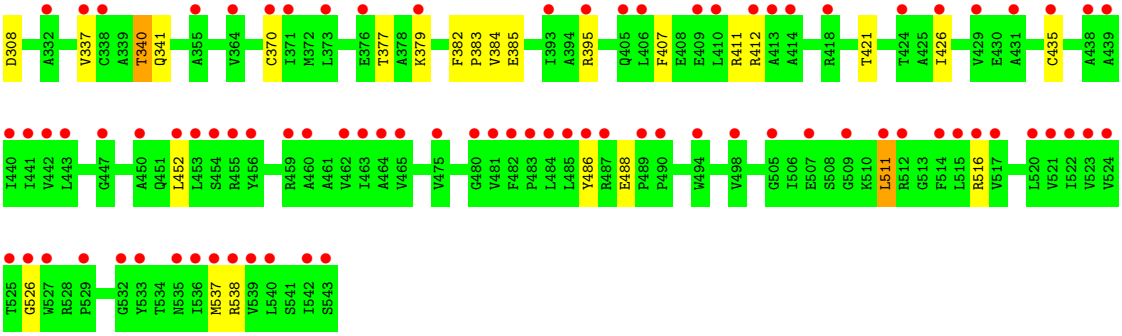


• Molecule 1: Pyruvate kinase PKLR

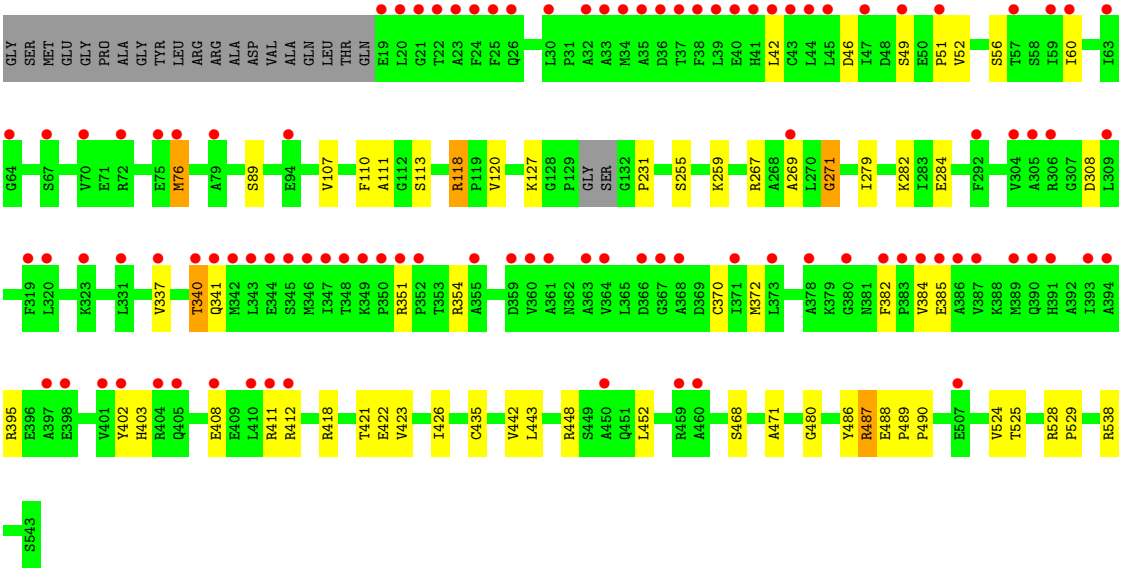
Chain B:



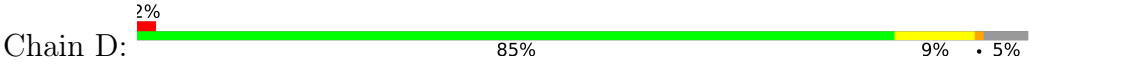


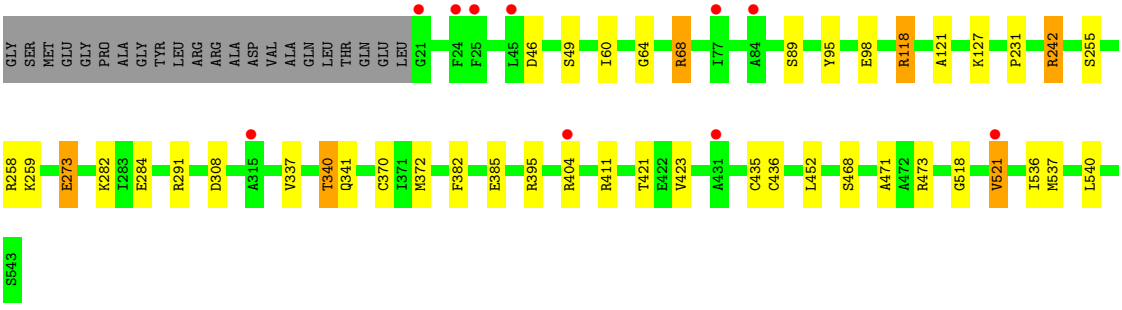


• Molecule 1: Pyruvate kinase PKLR

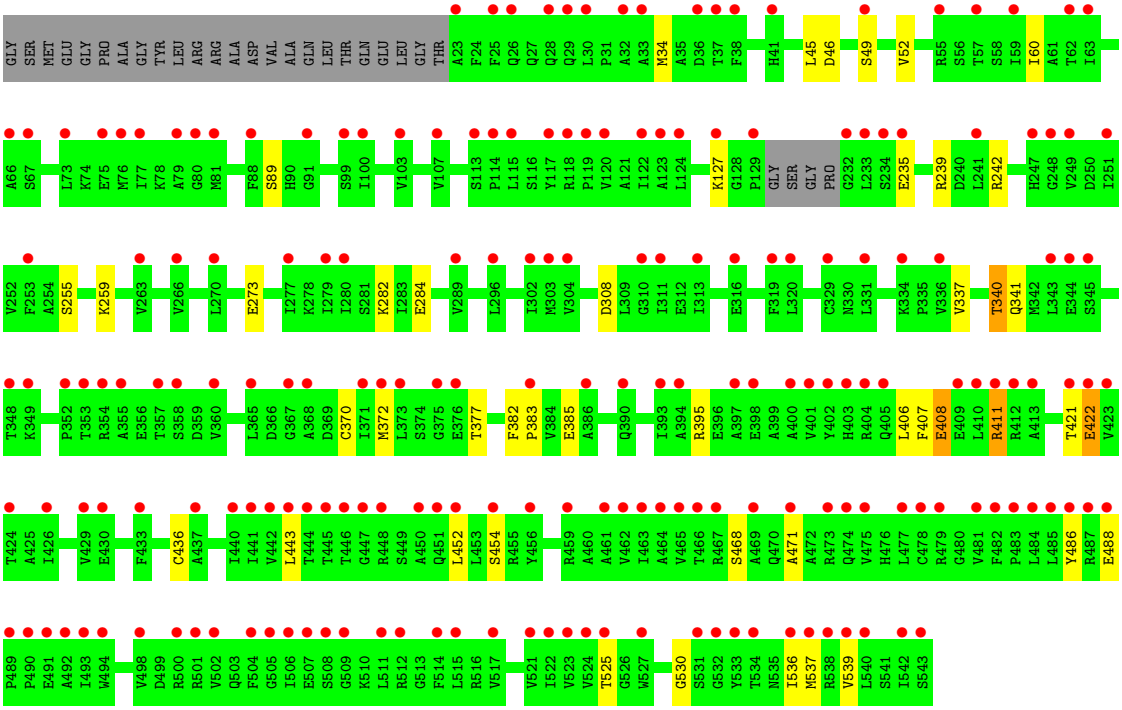


• Molecule 1: Pyruvate kinase PKLR



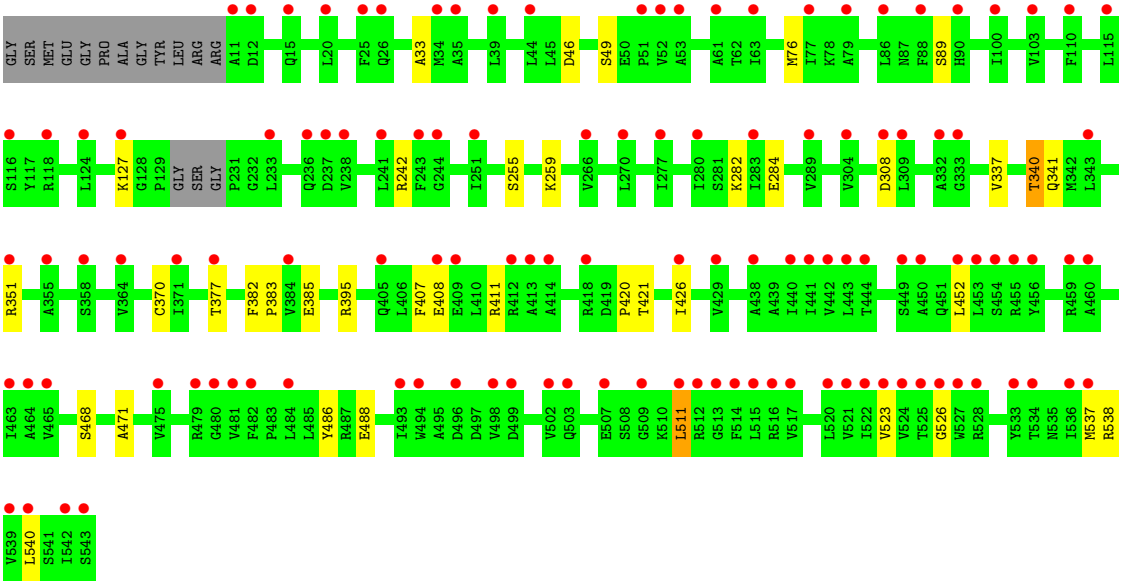


• Molecule 1: Pyruvate kinase PKLR



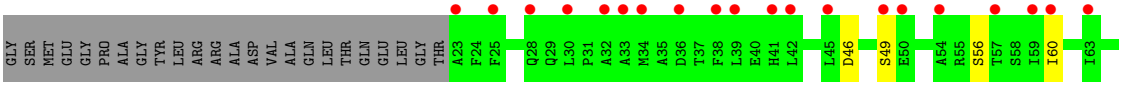
• Molecule 1: Pyruvate kinase PKLR

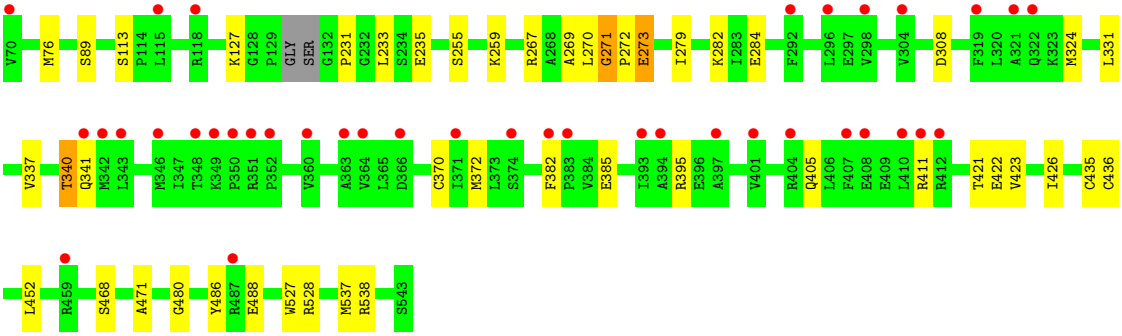
Chain F:



• Molecule 1: Pyruvate kinase PKLR

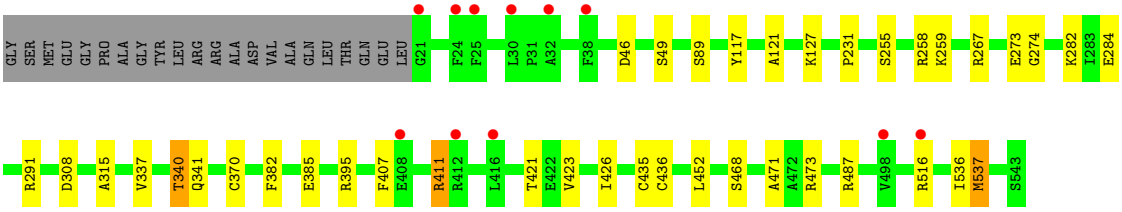
Chain G:





• 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	208.05Å 113.23Å 188.47Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	188.38 – 2.50 188.38 – 2.49	Depositor EDS
% Data completeness (in resolution range)	71.3 (188.38-2.50) 71.2 (188.38-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.267 , 0.292 0.258 , 0.275	Depositor DCC
R_{free} test set	5205 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26926	wwPDB-VP
Average B, all atoms (Å^2)	94.0	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 92.07 % 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 1.1067e-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, FBP, K, MG, OE0

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	0.33	0/3307	0.52	0/4469
1	B	0.36	0/3396	0.52	0/4592
1	C	0.46	0/3313	0.58	0/4479
1	D	0.50	0/3326	0.60	0/4497
1	E	0.34	0/3278	0.53	0/4430
1	F	0.38	0/3396	0.53	0/4591
1	G	0.46	0/3303	0.57	0/4465
1	H	0.49	0/3316	0.60	0/4483
All	All	0.42	0/26635	0.56	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	27	0
1	B	3329	0	3394	20	1
1	C	3247	0	3300	44	0
1	D	3252	0	3310	27	0
1	E	3210	0	3270	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3321	0	3393	22	1
1	G	3231	0	3285	30	0
1	H	3251	0	3306	24	0
2	A	20	0	10	2	0
2	B	20	0	10	1	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	1	0
2	F	20	0	10	1	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	28	19	0	1	0
6	B	28	19	0	0	0
6	F	28	19	0	0	0
6	G	28	19	0	2	0
7	A	12	0	0	0	0
7	B	18	0	0	0	0
7	C	50	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	123	0	0	1	0
7	E	17	0	0	1	0
7	F	30	0	0	1	0
7	G	56	0	0	0	0
7	H	131	0	0	0	0
All	All	26850	76	26637	190	2

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PRO:HA	1:A:275:HIS:NE2	1.84	0.92
1:C:528:ARG:NH2	1:G:233:LEU:O	2.06	0.89
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.63	0.81
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.62	0.79
1:F:411:ARG:HG3	1:F:426:ILE:HD11	1.62	0.79
1:C:351:ARG:HH22	1:C:354:ARG:HH22	1.36	0.73
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.72	0.71
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.57	0.69
1:E:235:GLU:O	1:E:239:ARG:HD3	1.93	0.69
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.75	0.69
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.75	0.68
1:B:89:SER:HA	1:B:127:LYS:HG3	1.76	0.68
1:F:89:SER:HA	1:F:127:LYS:HG3	1.75	0.67
1:D:89:SER:HA	1:D:127:LYS:HG3	1.76	0.67
1:E:89:SER:HA	1:E:127:LYS:HG3	1.76	0.67
1:H:89:SER:HA	1:H:127:LYS:HG3	1.76	0.67
1:G:89:SER:HA	1:G:127:LYS:HG3	1.77	0.66
1:C:411:ARG:HG2	1:C:426:ILE:HD11	1.76	0.66
1:G:411:ARG:HG2	1:G:426:ILE:HD11	1.77	0.66
1:F:351:ARG:HH21	1:H:315:ALA:HB2	1.60	0.66
1:A:89:SER:HA	1:A:127:LYS:HG3	1.75	0.65
1:C:89:SER:HA	1:C:127:LYS:HG3	1.78	0.64
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.81	0.63
1:C:340:THR:HG22	1:C:341:GLN:HG3	1.81	0.63
1:C:111:ALA:HB1	1:C:487:ARG:NH2	2.14	0.62
1:F:411:ARG:CG	1:F:426:ILE:HD11	2.30	0.62
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.82	0.62
1:A:422:GLU:HG2	1:A:452:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:GLU:HG2	1:E:452:LEU:HD13	1.82	0.61
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.83	0.61
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.35	0.60
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.84	0.60
1:A:408:GLU:OE2	1:B:411:ARG:NH2	2.34	0.60
1:F:340:THR:HG22	1:F:341:GLN:HG3	1.84	0.59
1:G:411:ARG:CG	1:G:426:ILE:HD11	2.33	0.59
1:B:526:GLY:HA3	2:B:601:FBP:O3	2.03	0.59
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.85	0.58
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.83	0.58
1:C:411:ARG:HH12	1:D:411:ARG:HH21	1.52	0.58
1:D:68:ARG:NH2	1:D:95:TYR:O	2.37	0.57
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.86	0.57
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.86	0.57
1:H:340:THR:HG22	1:H:341:GLN:HG3	1.86	0.57
1:E:408:GLU:OE2	1:F:411:ARG:NH2	2.38	0.56
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.87	0.56
1:H:421:THR:HG22	1:H:452:LEU:HD12	1.86	0.56
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.88	0.56
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.88	0.56
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.87	0.56
1:G:405:GLN:HB3	6:G:605:OE0:O5	2.05	0.56
1:B:411:ARG:CG	1:B:426:ILE:HD11	2.32	0.56
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.87	0.55
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.87	0.55
1:C:269:ALA:C	1:C:271:GLY:H	2.10	0.55
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.89	0.55
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.88	0.55
1:C:412:ARG:NH2	1:D:404:ARG:HH11	2.05	0.55
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.90	0.54
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.89	0.54
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.22	0.54
1:A:528:ARG:NH1	1:A:533:TYR:CE2	2.75	0.53
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.89	0.53
1:D:64:GLY:O	1:D:68:ARG:HG3	2.09	0.53
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.89	0.53
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.89	0.53
1:A:68:ARG:HH22	1:A:98:GLU:HB3	1.73	0.53
1:C:408:GLU:HG3	1:C:411:ARG:HH12	1.74	0.53
1:E:407:PHE:O	1:E:411:ARG:HB2	2.10	0.52
1:C:408:GLU:HG3	1:C:411:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:530:GLY:O	2:E:601:FBP:O4	2.24	0.52
1:H:382:PHE:HB3	1:H:385:GLU:HB2	1.92	0.52
1:C:411:ARG:NH1	1:D:411:ARG:HH21	2.09	0.51
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.76	0.51
1:A:517:VAL:HG22	1:A:543:SER:HB3	1.93	0.51
6:A:605:OE0:O5	1:C:402:TYR:HB3	2.11	0.51
1:C:448:ARG:HD3	7:C:710:HOH:O	2.10	0.51
1:G:269:ALA:C	1:G:271:GLY:H	2.13	0.51
1:B:407:PHE:CE2	1:B:411:ARG:NH1	2.77	0.51
1:D:382:PHE:HB3	1:D:385:GLU:HB2	1.92	0.50
1:E:406:LEU:HA	6:G:605:OE0:C18	2.41	0.50
1:C:403:HIS:HE1	7:C:708:HOH:O	1.93	0.49
1:C:107:VAL:HG21	1:C:120:VAL:HB	1.94	0.49
1:A:67:SER:HA	1:A:72:ARG:HG2	1.94	0.49
1:C:411:ARG:NH1	1:D:411:ARG:NH2	2.61	0.49
1:A:494:TRP:NE1	1:A:529:PRO:HG3	2.27	0.49
1:F:526:GLY:HA3	2:F:601:FBP:O3	2.13	0.49
1:H:468:SER:HB3	1:H:471:ALA:HB3	1.95	0.48
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.96	0.48
1:C:529:PRO:HG3	1:G:235:GLU:HG2	1.95	0.48
1:C:337:VAL:HG22	1:C:370:CYS:HB2	1.96	0.47
1:A:423:VAL:HG21	1:B:435:CYS:HB3	1.95	0.47
1:C:486:TYR:CE2	1:C:488:GLU:HB2	2.48	0.47
1:G:337:VAL:HG22	1:G:370:CYS:HB2	1.97	0.47
1:A:341:GLN:OE1	1:C:354:ARG:HG2	2.15	0.47
1:A:526:GLY:HA3	2:A:601:FBP:O3	2.15	0.47
1:H:411:ARG:HB3	1:H:426:ILE:HD11	1.97	0.47
1:D:521:VAL:HG12	1:D:540:LEU:HB3	1.97	0.47
1:G:537:MET:CE	1:H:537:MET:HG2	2.46	0.46
1:H:117:TYR:CD2	1:H:487:ARG:NH2	2.83	0.46
1:E:443:LEU:HD13	1:E:525:THR:HG22	1.98	0.46
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.51	0.46
1:B:46:ASP:HB3	1:B:49:SER:HB2	1.98	0.45
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.98	0.45
1:E:337:VAL:HG22	1:E:370:CYS:HB2	1.97	0.45
1:F:337:VAL:HG22	1:F:370:CYS:HB2	1.97	0.45
1:G:46:ASP:HB3	1:G:49:SER:HB2	1.97	0.45
1:F:46:ASP:HB3	1:F:49:SER:HB2	1.99	0.45
1:G:435:CYS:HB3	1:H:423:VAL:HG21	1.98	0.45
1:C:46:ASP:HB3	1:C:49:SER:HB2	1.99	0.45
1:D:468:SER:HB3	1:D:471:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ARG:HH11	1:C:118:ARG:H	1.64	0.45
1:G:255:SER:HA	1:G:282:LYS:HD3	1.99	0.45
1:C:435:CYS:HB3	1:D:423:VAL:HG21	1.98	0.44
1:E:46:ASP:HB3	1:E:49:SER:HB2	1.98	0.44
1:E:539:VAL:CG2	1:F:420:PRO:HB3	2.47	0.44
1:C:60:ILE:HB	1:C:372:MET:HG3	2.00	0.44
1:D:46:ASP:HB3	1:D:49:SER:HB2	2.00	0.44
1:D:337:VAL:HG22	1:D:370:CYS:HB2	2.00	0.44
1:E:45:LEU:HB2	1:G:324:MET:HB2	1.99	0.44
1:G:60:ILE:HB	1:G:372:MET:HG3	2.00	0.44
1:H:46:ASP:HB3	1:H:49:SER:HB2	2.00	0.44
1:A:46:ASP:HB3	1:A:49:SER:HB2	2.00	0.44
1:C:284:GLU:HB3	1:C:308:ASP:HB2	1.99	0.44
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.00	0.44
1:D:255:SER:HA	1:D:282:LYS:HD3	2.00	0.44
1:E:255:SER:HA	1:E:282:LYS:HD3	2.00	0.44
1:F:377:THR:HA	1:F:383:PRO:HB3	1.99	0.44
1:C:442:VAL:HG23	1:C:524:VAL:HB	2.00	0.43
1:E:377:THR:HA	1:E:383:PRO:HB3	2.00	0.43
1:A:255:SER:HA	1:A:282:LYS:HD3	1.99	0.43
1:D:284:GLU:HB3	1:D:308:ASP:HB2	2.00	0.43
1:H:255:SER:HA	1:H:282:LYS:HD3	2.00	0.43
1:F:255:SER:HA	1:F:282:LYS:HD3	2.00	0.43
1:C:255:SER:HA	1:C:282:LYS:HD3	2.01	0.43
1:F:468:SER:HB3	1:F:471:ALA:HB3	2.01	0.43
1:G:411:ARG:NH2	1:H:411:ARG:CZ	2.81	0.43
1:E:242:ARG:HA	7:E:701:HOH:O	2.19	0.43
1:A:377:THR:HA	1:A:383:PRO:HB3	2.00	0.43
1:G:527:TRP:CE2	1:G:528:ARG:HG2	2.54	0.43
1:B:284:GLU:HB3	1:B:308:ASP:HB2	2.01	0.43
1:D:118:ARG:HD2	7:D:776:HOH:O	2.19	0.43
1:G:537:MET:HE1	1:H:537:MET:HG2	2.01	0.43
1:G:284:GLU:HB3	1:G:308:ASP:HB2	2.00	0.42
1:H:407:PHE:O	1:H:411:ARG:HG3	2.19	0.42
1:F:523:VAL:HG21	1:F:540[A]:LEU:HD12	2.00	0.42
1:A:60:ILE:HB	1:A:372:MET:HG3	2.01	0.42
1:B:377:THR:HA	1:B:383:PRO:HB3	2.01	0.42
1:C:267:ARG:CZ	1:C:279:ILE:HD12	2.50	0.42
1:G:468:SER:HB3	1:G:471:ALA:HB3	2.02	0.42
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.20	0.42
1:H:284:GLU:HB3	1:H:308:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ARG:NH2	1:D:518:GLY:O	2.46	0.42
1:A:411:ARG:NH2	1:B:411:ARG:HH12	2.17	0.42
1:B:55:ARG:HB2	1:B:395:ARG:HG2	2.02	0.42
1:A:284:GLU:HB3	1:A:308:ASP:HB2	2.02	0.42
1:E:284:GLU:HB3	1:E:308:ASP:HB2	2.02	0.42
1:F:284:GLU:HB3	1:F:308:ASP:HB2	2.02	0.42
1:C:468:SER:HB3	1:C:471:ALA:HB3	2.01	0.42
1:E:60:ILE:HB	1:E:372:MET:HG3	2.01	0.42
1:A:528:ARG:NH1	1:A:533:TYR:CZ	2.88	0.42
1:G:56:SER:HB2	1:G:480:GLY:HA2	2.02	0.42
1:H:121:ALA:HA	1:H:473:ARG:HB3	2.02	0.42
1:E:468:SER:HB3	1:E:471:ALA:HB3	2.01	0.41
1:B:255:SER:HA	1:B:282:LYS:HD3	2.00	0.41
1:F:33:ALA:HB1	7:F:704:HOH:O	2.20	0.41
1:D:121:ALA:HA	1:D:473:ARG:HB3	2.02	0.41
1:G:423:VAL:HG21	1:H:435:CYS:HB3	2.03	0.41
1:A:426:ILE:HD13	1:A:456:TYR:CD1	2.55	0.41
1:G:267:ARG:HG2	1:G:279:ILE:CD1	2.51	0.41
1:H:258:ARG:O	1:H:291:ARG:HD3	2.21	0.41
1:A:501:ARG:NH1	2:A:601:FBP:O2P	2.44	0.41
1:H:267[B]:ARG:NH1	1:H:274:GLY:O	2.54	0.41
1:C:56:SER:HB2	1:C:480:GLY:HA2	2.03	0.41
1:C:423:VAL:HG21	1:D:435:CYS:HB3	2.03	0.41
1:C:489:PRO:HA	1:C:490:PRO:HD3	1.88	0.41
1:D:60:ILE:HB	1:D:372:MET:HG3	2.02	0.41
1:F:486:TYR:CE2	1:F:488:GLU:HB2	2.56	0.41
1:C:76[A]:MET:HG2	1:C:384:VAL:HG22	2.03	0.41
1:D:242[A]:ARG:NH2	1:D:273:GLU:OE1	2.45	0.40
1:E:486:TYR:CE2	1:E:488:GLU:HB2	2.55	0.40
1:E:486:TYR:CZ	1:E:488:GLU:HB2	2.56	0.40
1:C:118:ARG:H	1:C:118:ARG:NH1	2.19	0.40
1:G:411:ARG:NH2	1:H:411:ARG:NH2	2.70	0.40
1:H:407:PHE:CE2	1:H:411:ARG:HD3	2.57	0.40
1:C:443:LEU:HD22	1:C:525:THR:HG22	2.04	0.40
1:A:323:LYS:HB3	1:C:42:LEU:HD22	2.03	0.40
1:B:76[A]:MET:HG2	1:B:384:VAL:HG22	2.03	0.40
1:B:486:TYR:CE2	1:B:488:GLU:HB2	2.56	0.40
1:D:258:ARG:O	1:D:291:ARG:HD3	2.21	0.40
1:C:110:PHE:CB	1:C:118:ARG:HH12	2.35	0.40

All (2) 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]	1.98	0.22
1:F:511:LEU:O	1:F:511:LEU:O[2_656]	2.11	0.09

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%)	416 (98%)	7 (2%)	1 (0%)	47	68
1	B	438/447 (98%)	428 (98%)	8 (2%)	2 (0%)	29	48
1	C	425/447 (95%)	414 (97%)	8 (2%)	3 (1%)	22	39
1	D	429/447 (96%)	424 (99%)	3 (1%)	2 (0%)	29	48
1	E	420/447 (94%)	414 (99%)	5 (1%)	1 (0%)	47	68
1	F	435/447 (97%)	427 (98%)	7 (2%)	1 (0%)	47	68
1	G	423/447 (95%)	412 (97%)	7 (2%)	4 (1%)	17	31
1	H	427/447 (96%)	421 (99%)	4 (1%)	2 (0%)	29	48
All	All	3421/3576 (96%)	3356 (98%)	49 (1%)	16 (0%)	29	48

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	271	GLY
1	B	231	PRO
1	C	231	PRO
1	D	231	PRO
1	G	231	PRO
1	H	231	PRO
1	A	340	THR
1	G	270	LEU
1	B	340	THR
1	C	340	THR
1	D	340	THR

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Mol	Chain	Res	Type
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR
1	G	271	GLY

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%)	330 (97%)	10 (3%)	42	69
1	B	349/352 (99%)	341 (98%)	8 (2%)	50	76
1	C	341/352 (97%)	332 (97%)	9 (3%)	46	72
1	D	342/352 (97%)	332 (97%)	10 (3%)	42	69
1	E	338/352 (96%)	325 (96%)	13 (4%)	33	58
1	F	350/352 (99%)	341 (97%)	9 (3%)	46	72
1	G	340/352 (97%)	332 (98%)	8 (2%)	49	74
1	H	340/352 (97%)	333 (98%)	7 (2%)	53	78
All	All	2740/2816 (97%)	2666 (97%)	74 (3%)	49	71

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	72	ARG
1	A	259	LYS
1	A	395	ARG
1	A	408	GLU
1	A	422	GLU
1	A	436	CYS
1	A	528	ARG
1	A	537[A]	MET
1	A	537[B]	MET

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Mol	Chain	Res	Type
1	B	10	ARG
1	B	259	LYS
1	B	379	LYS
1	B	412	ARG
1	B	511	LEU
1	B	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	51	PRO
1	C	52	VAL
1	C	76[A]	MET
1	C	76[B]	MET
1	C	113	SER
1	C	118	ARG
1	C	259	LYS
1	C	395	ARG
1	C	487	ARG
1	D	68	ARG
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	259	LYS
1	D	273	GLU
1	D	395	ARG
1	D	436	CYS
1	D	521	VAL
1	D	537	MET
1	E	34	MET
1	E	52	VAL
1	E	259	LYS
1	E	273	GLU
1	E	395	ARG
1	E	408	GLU
1	E	411	ARG
1	E	422	GLU
1	E	436	CYS
1	E	454[A]	SER
1	E	454[B]	SER
1	E	537[A]	MET
1	E	537[B]	MET
1	F	76[A]	MET
1	F	76[B]	MET

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Mol	Chain	Res	Type
1	F	242	ARG
1	F	259	LYS
1	F	395	ARG
1	F	408	GLU
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	76[A]	MET
1	G	76[B]	MET
1	G	113	SER
1	G	259	LYS
1	G	273	GLU
1	G	331	LEU
1	G	395	ARG
1	G	436	CYS
1	H	259	LYS
1	H	273	GLU
1	H	395	ARG
1	H	411	ARG
1	H	436	CYS
1	H	516	ARG
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	236	GLN
1	F	236	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OXL	G	602	4	5,5,5	1.97	2 (40%)	6,6,6	1.11	1 (16%)
3	OXL	H	602	4	5,5,5	1.76	2 (40%)	6,6,6	1.32	1 (16%)
3	OXL	F	602	4	5,5,5	2.64	4 (80%)	6,6,6	1.60	2 (33%)
3	OXL	D	602	4	5,5,5	2.08	2 (40%)	6,6,6	1.18	0
6	OE0	A	605	-	30,30,30	0.15	0	43,43,43	0.46	0
2	FBP	D	601	-	18,20,20	0.93	1 (5%)	23,32,32	1.09	2 (8%)
2	FBP	F	601	-	18,20,20	0.68	0	23,32,32	0.89	1 (4%)
2	FBP	E	601	-	18,20,20	0.46	0	23,32,32	0.96	1 (4%)
3	OXL	C	602	4	5,5,5	1.82	2 (40%)	6,6,6	1.19	1 (16%)
6	OE0	G	605	-	30,30,30	0.18	0	43,43,43	0.72	1 (2%)
2	FBP	C	601	-	18,20,20	0.66	0	23,32,32	1.06	2 (8%)
3	OXL	B	602	4	5,5,5	2.05	2 (40%)	6,6,6	0.94	0
3	OXL	A	602	4	5,5,5	1.91	2 (40%)	6,6,6	1.26	1 (16%)
2	FBP	A	601	-	18,20,20	0.62	0	23,32,32	0.94	1 (4%)
6	OE0	F	605	-	30,30,30	0.19	0	43,43,43	0.67	1 (2%)
2	FBP	G	601	-	18,20,20	0.64	0	23,32,32	1.00	1 (4%)
3	OXL	E	602	4	5,5,5	2.00	2 (40%)	6,6,6	1.03	0
6	OE0	B	605	-	30,30,30	0.22	0	43,43,43	0.65	1 (2%)
2	FBP	B	601	-	18,20,20	0.70	0	23,32,32	1.04	2 (8%)
2	FBP	H	601	-	18,20,20	0.71	0	23,32,32	1.24	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	G	602	4	-	1/4/4/4	-
3	OXL	H	602	4	-	0/4/4/4	-
3	OXL	F	602	4	-	0/4/4/4	-
3	OXL	D	602	4	-	1/4/4/4	-
6	OE0	A	605	-	-	3/16/16/16	0/3/3/3
2	FBP	D	601	-	-	1/13/32/32	0/1/1/1
2	FBP	F	601	-	-	6/13/32/32	0/1/1/1
2	FBP	E	601	-	-	3/13/32/32	0/1/1/1
3	OXL	C	602	4	-	0/4/4/4	-
6	OE0	G	605	-	-	0/16/16/16	0/3/3/3
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	0/4/4/4	-
3	OXL	A	602	4	-	1/4/4/4	-
2	FBP	A	601	-	-	4/13/32/32	0/1/1/1
6	OE0	F	605	-	-	3/16/16/16	0/3/3/3
2	FBP	G	601	-	-	7/13/32/32	0/1/1/1
3	OXL	E	602	4	-	1/4/4/4	-
6	OE0	B	605	-	-	0/16/16/16	0/3/3/3
2	FBP	B	601	-	-	7/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXL	O2-C2	3.92	1.33	1.22
3	D	602	OXL	O2-C2	3.57	1.32	1.22
3	E	602	OXL	O1-C1	3.53	1.32	1.22
3	F	602	OXL	O2-C2	3.41	1.31	1.22
3	A	602	OXL	O2-C2	3.26	1.31	1.22
3	G	602	OXL	O1-C1	3.22	1.31	1.22
2	D	601	FBP	P2-O5P	-3.01	1.43	1.54
3	H	602	OXL	O2-C2	2.99	1.30	1.22
3	C	602	OXL	O1-C1	2.98	1.30	1.22
3	F	602	OXL	O3-C1	-2.97	1.21	1.30
3	F	602	OXL	O1-C1	2.91	1.30	1.22
3	G	602	OXL	O3-C1	-2.91	1.22	1.30
3	D	602	OXL	O4-C2	-2.67	1.22	1.30
3	C	602	OXL	O3-C1	-2.63	1.22	1.30
3	E	602	OXL	O3-C1	-2.60	1.23	1.30
3	A	602	OXL	O4-C2	-2.47	1.23	1.30
3	F	602	OXL	O4-C2	-2.41	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	602	OXL	O4-C2	-2.39	1.23	1.30
3	B	602	OXL	O4-C2	-2.28	1.23	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	FBP	O5P-P2-O6	3.97	117.29	106.73
2	D	601	FBP	O5P-P2-O6	3.65	116.45	106.73
6	G	605	OE0	C8-C9-N	3.36	119.20	111.96
2	A	601	FBP	P1-O1-C1	3.35	127.53	118.30
2	B	601	FBP	P1-O1-C1	3.21	127.14	118.30
6	F	605	OE0	C8-C9-N	3.07	118.58	111.96
2	F	601	FBP	P1-O1-C1	2.93	126.36	118.30
2	C	601	FBP	O6-P2-O4P	2.90	114.60	106.47
2	E	601	FBP	P1-O1-C1	2.76	125.89	118.30
6	B	605	OE0	C8-C9-N	2.74	117.85	111.96
3	H	602	OXL	O4-C2-C1	2.62	120.94	113.16
3	F	602	OXL	O4-C2-C1	2.40	120.30	113.16
3	A	602	OXL	O4-C2-C1	2.38	120.23	113.16
3	C	602	OXL	O3-C1-C2	2.32	120.04	113.16
3	F	602	OXL	O3-C1-C2	2.32	120.04	113.16
2	B	601	FBP	O5P-P2-O6	2.22	112.64	106.73
2	D	601	FBP	P1-O1-C1	2.22	124.40	118.30
2	G	601	FBP	O5P-P2-O6	2.04	112.16	106.73
2	C	601	FBP	O3P-P1-O2P	2.03	115.40	107.64
3	G	602	OXL	O3-C1-C2	2.01	119.13	113.16

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	C1-O1-P1-O2P
2	B	601	FBP	C1-O1-P1-O3P
2	B	601	FBP	O1-C1-C2-O2
2	B	601	FBP	O1-C1-C2-O5
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C1-O1-P1-O1P
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	F	601	FBP	O1-C1-C2-O5
2	F	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C1-O1-P1-O2P
2	G	601	FBP	O1-C1-C2-O2
2	G	601	FBP	O1-C1-C2-O5
2	G	601	FBP	C4-C5-C6-O6
6	A	605	OE0	C9-N-S-C10
6	A	605	OE0	C9-N-S-O4
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
6	F	605	OE0	C9-N-S-O4
6	A	605	OE0	C9-N-S-O5
6	F	605	OE0	C9-N-S-O5
2	G	601	FBP	O5-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	F	605	OE0	C9-N-S-C10
2	B	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C4-C5-C6-O6
2	A	601	FBP	C1-O1-P1-O3P
2	F	601	FBP	C1-O1-P1-O3P
2	G	601	FBP	C1-O1-P1-O3P
2	A	601	FBP	C1-O1-P1-O1P
2	F	601	FBP	C1-O1-P1-O1P
2	G	601	FBP	C1-O1-P1-O1P
2	H	601	FBP	C6-O6-P2-O4P
3	A	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4

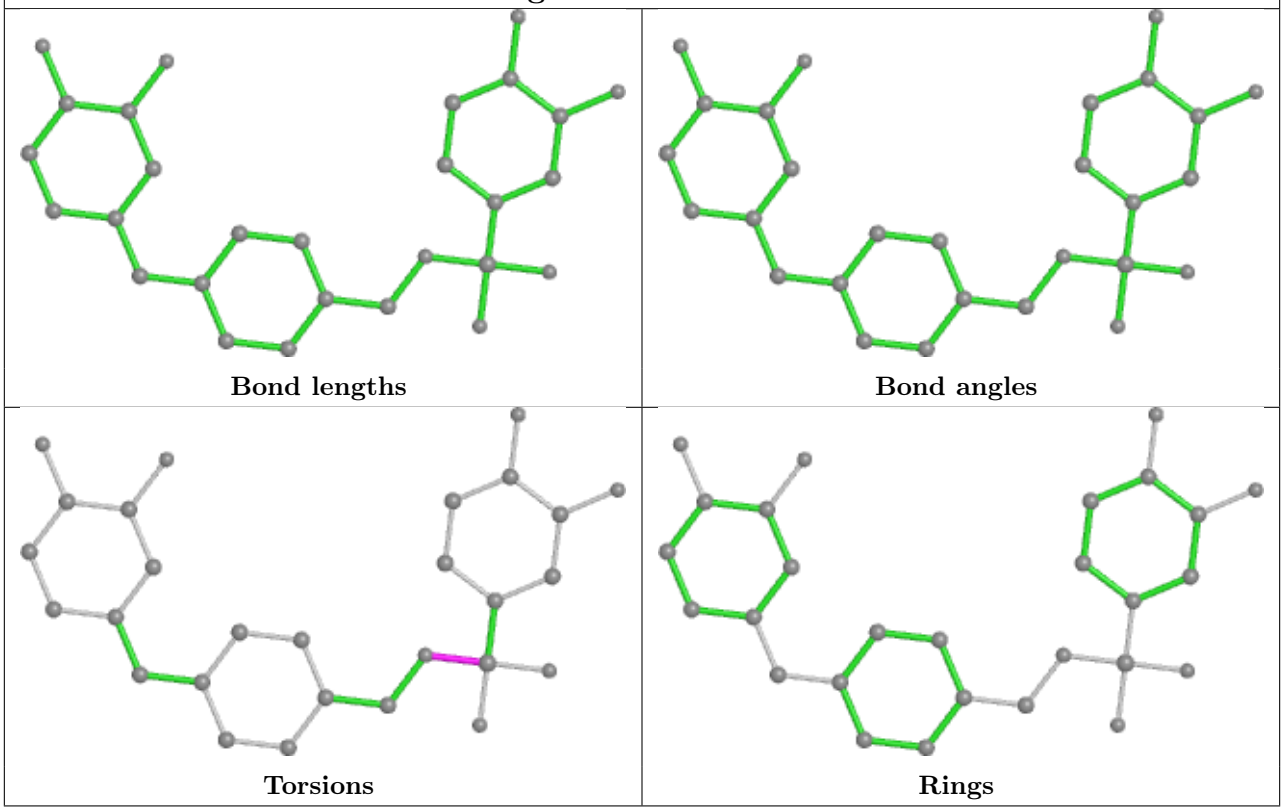
There are no ring outliers.

6 monomers are involved in 8 short contacts:

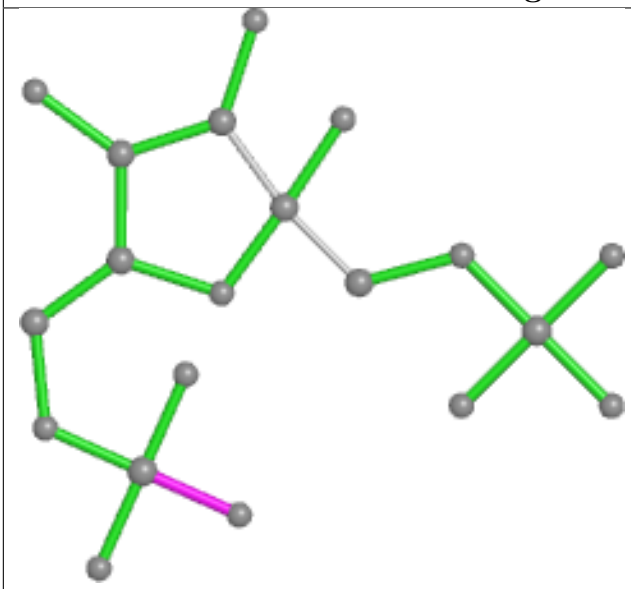
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	605	OE0	1	0
2	F	601	FBP	1	0
2	E	601	FBP	1	0
6	G	605	OE0	2	0
2	A	601	FBP	2	0
2	B	601	FBP	1	0

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.

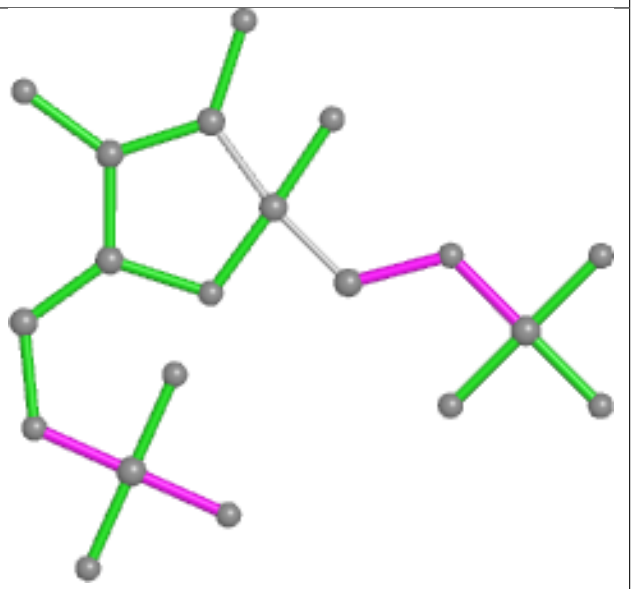
Ligand OE0 A 605



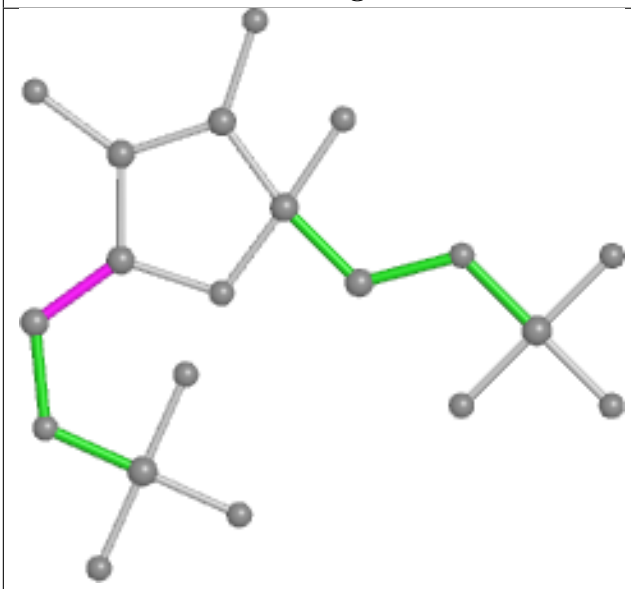
Ligand FBP D 601



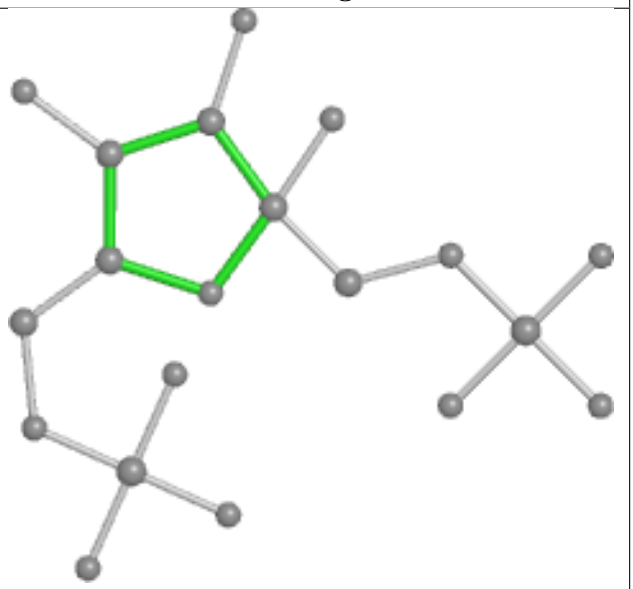
Bond lengths



Bond angles

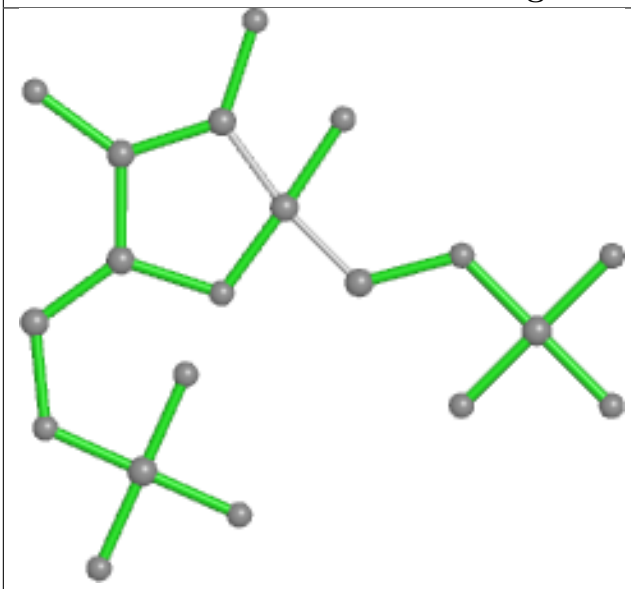


Torsions

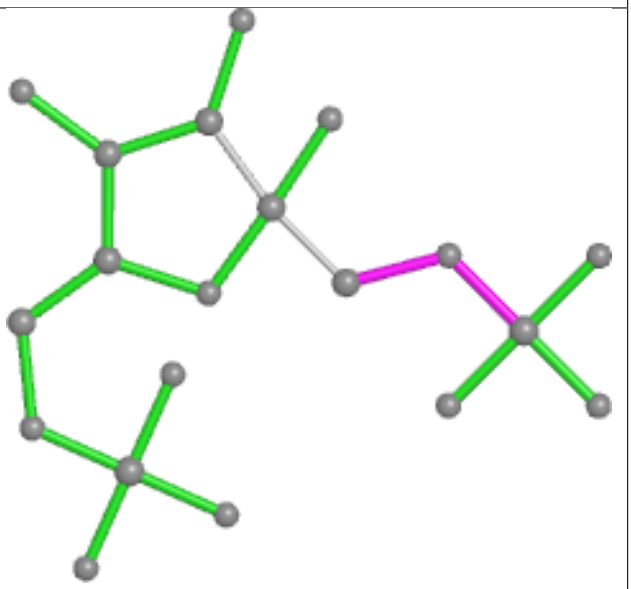


Rings

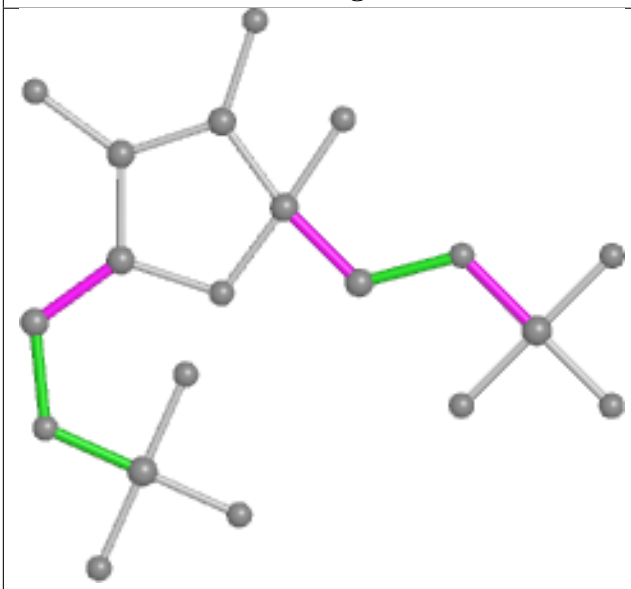
Ligand FBP F 601



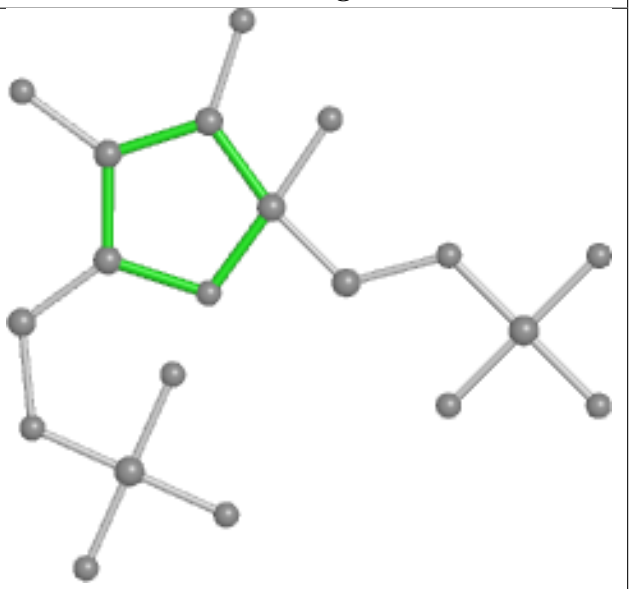
Bond lengths



Bond angles

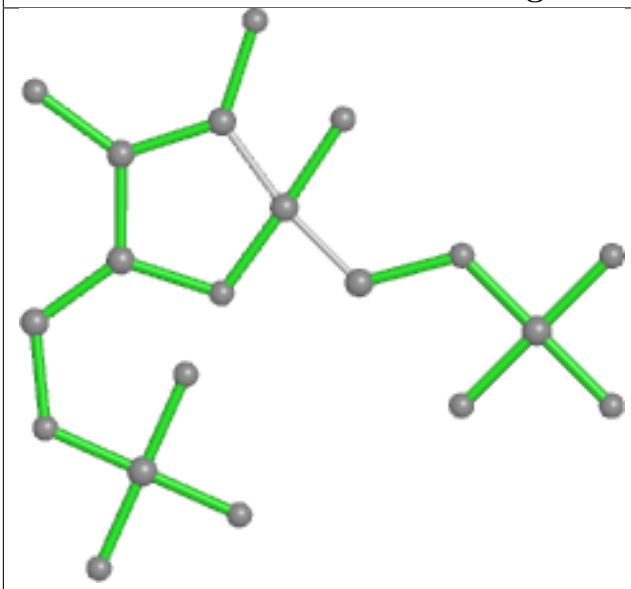


Torsions

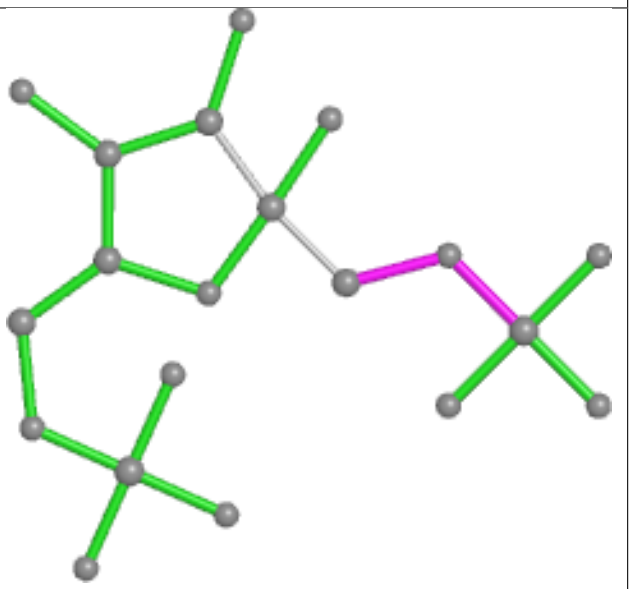


Rings

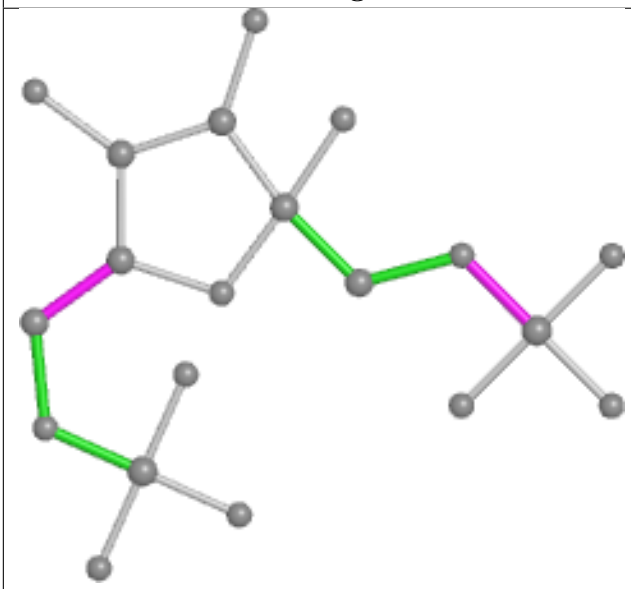
Ligand FBP E 601



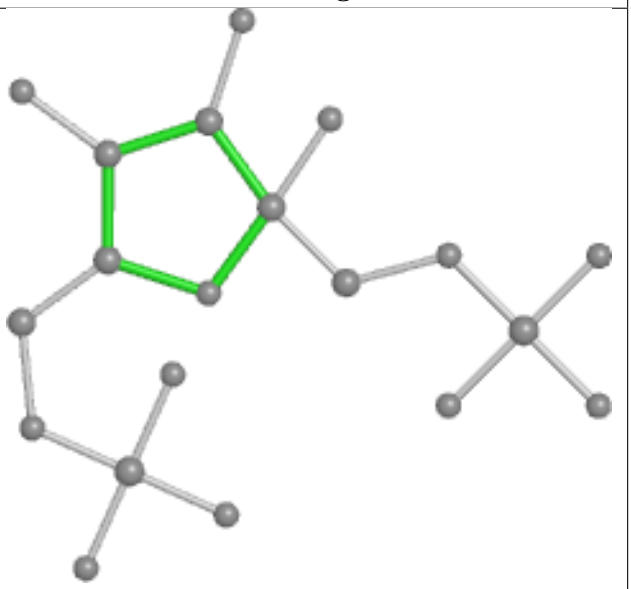
Bond lengths



Bond angles

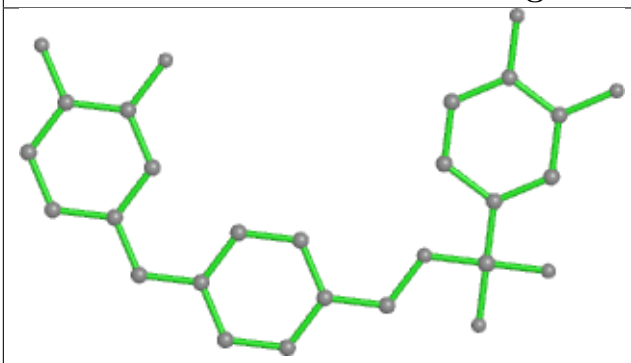


Torsions

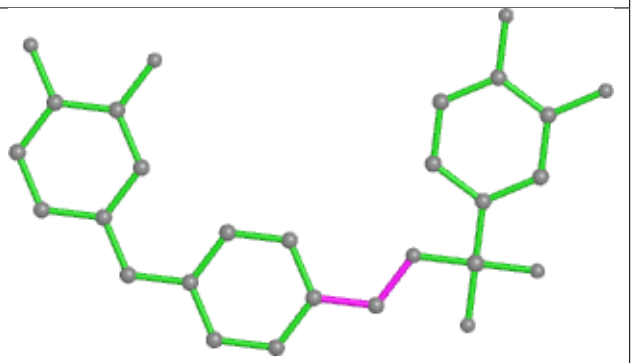


Rings

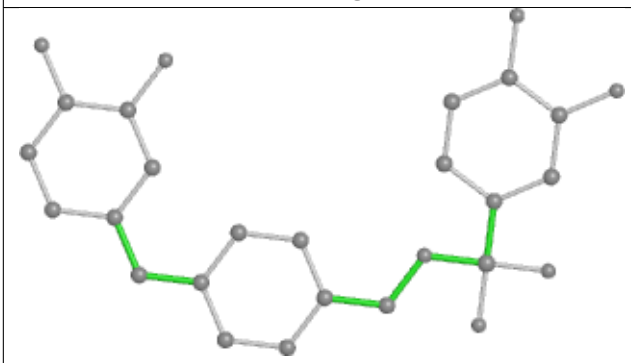
Ligand OE0 G 605



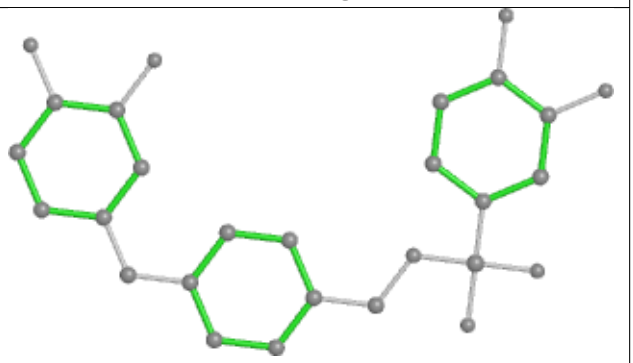
Bond lengths



Bond angles

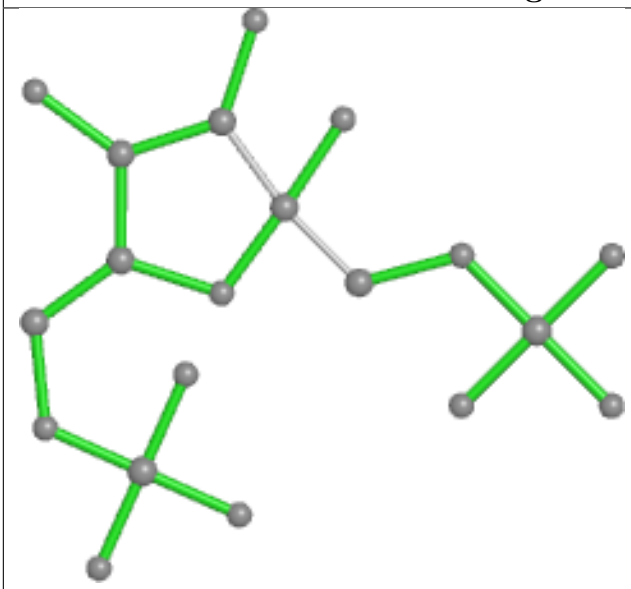


Torsions

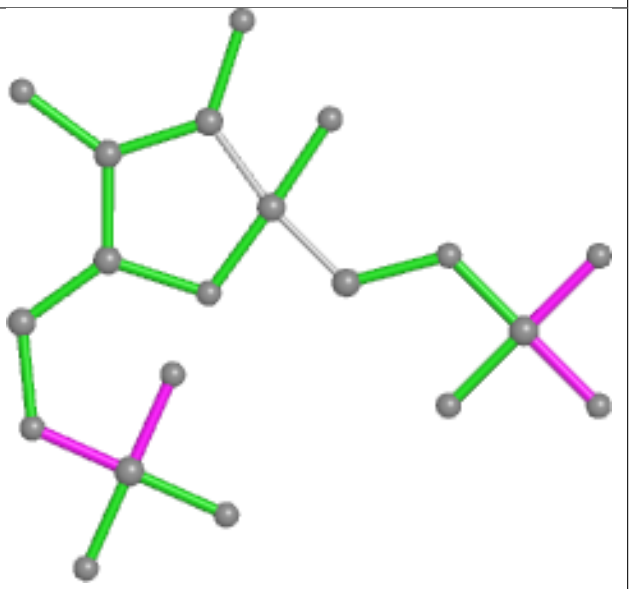


Rings

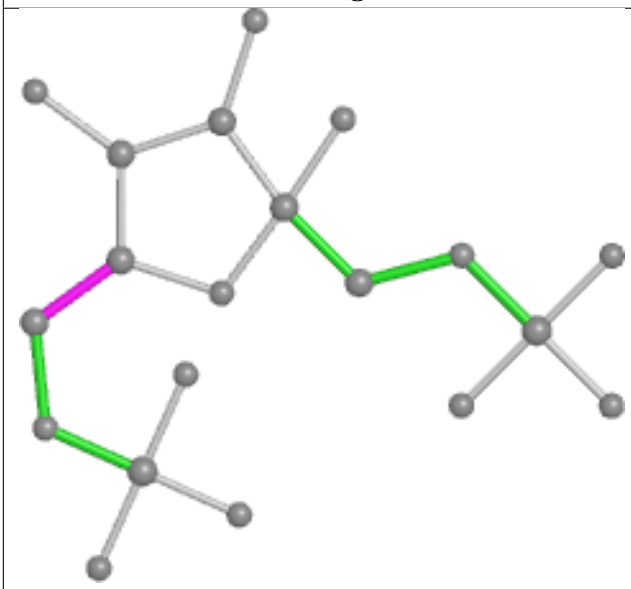
Ligand FBP C 601



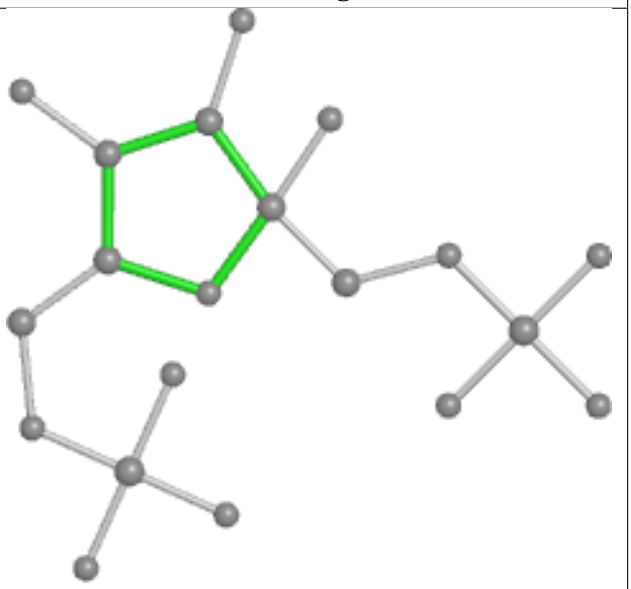
Bond lengths



Bond angles



Torsions



Rings

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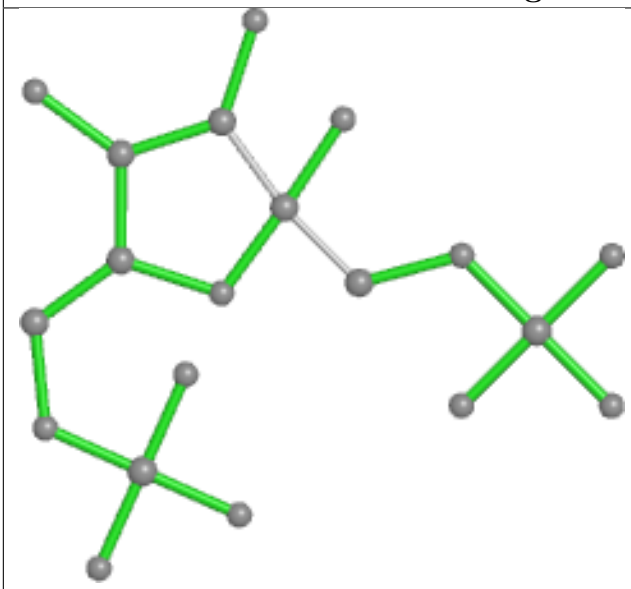
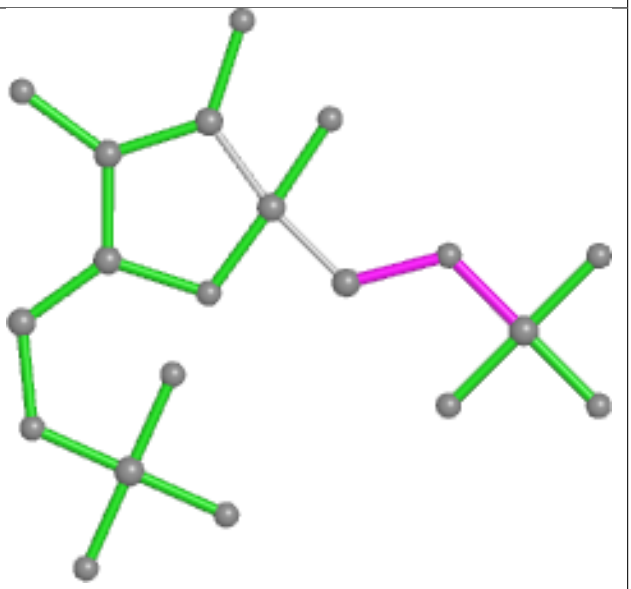
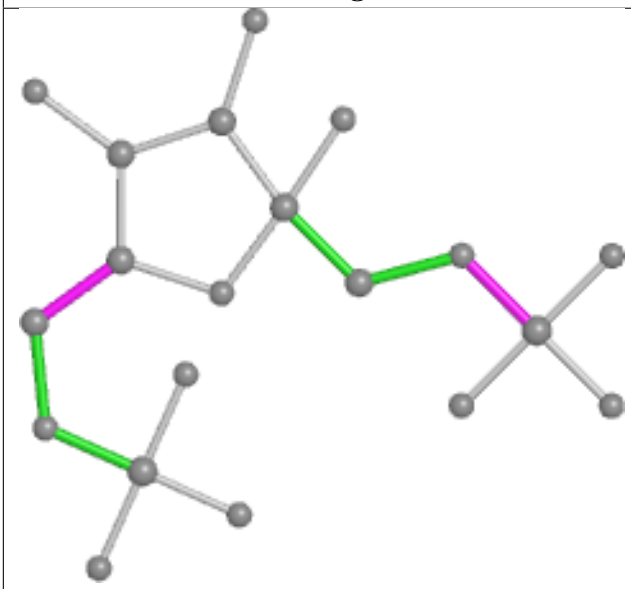


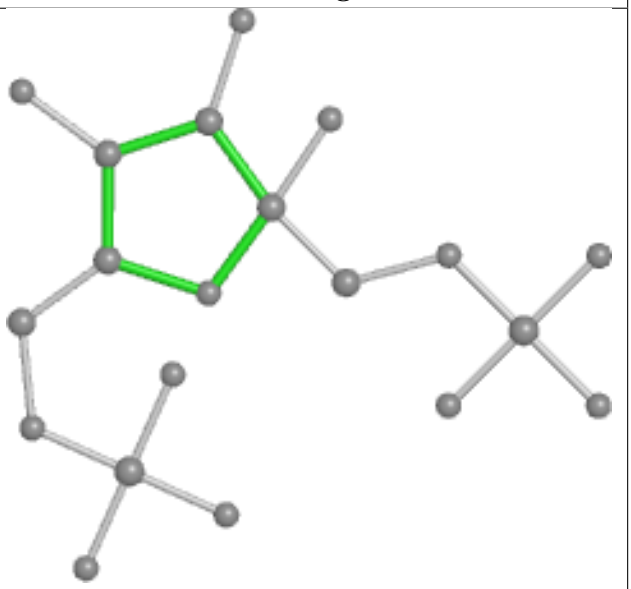
Bond lengths



Bond angles

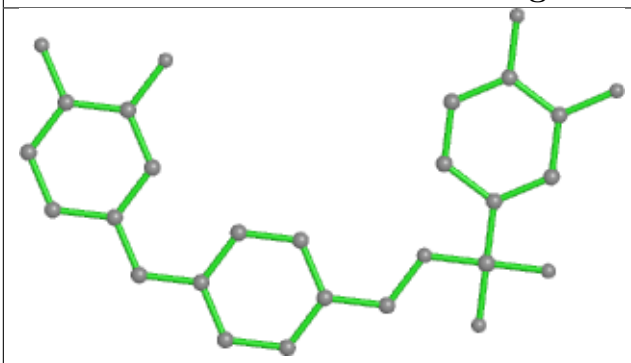


Torsions

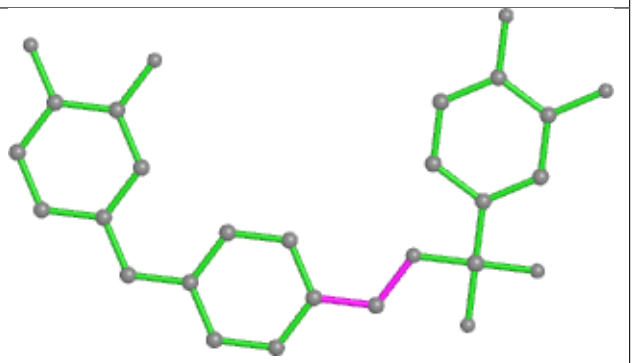


Rings

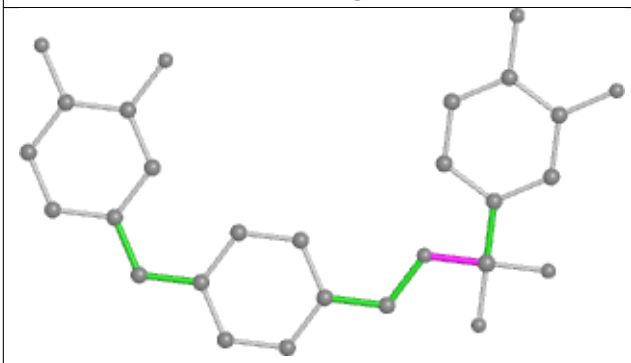
Ligand OE0 F 605



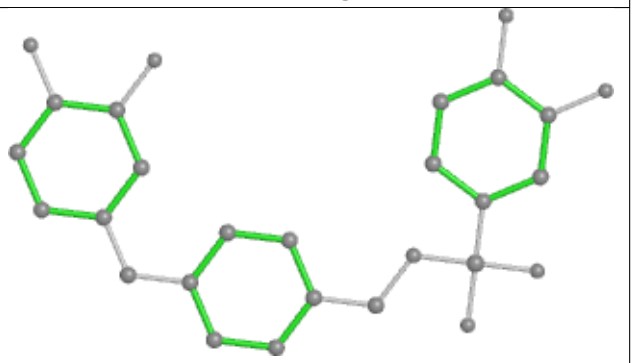
Bond lengths



Bond angles

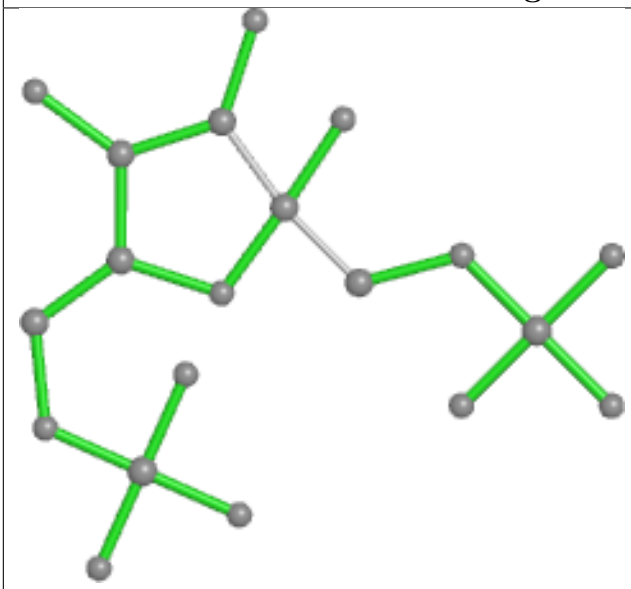


Torsions

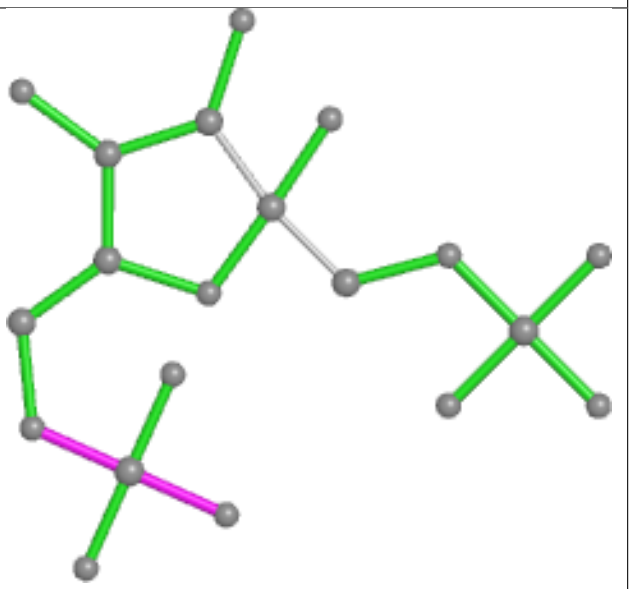


Rings

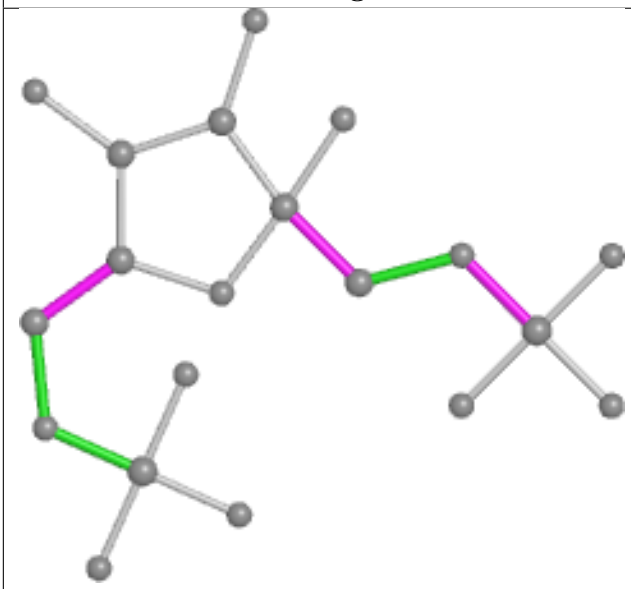
Ligand FBP G 601



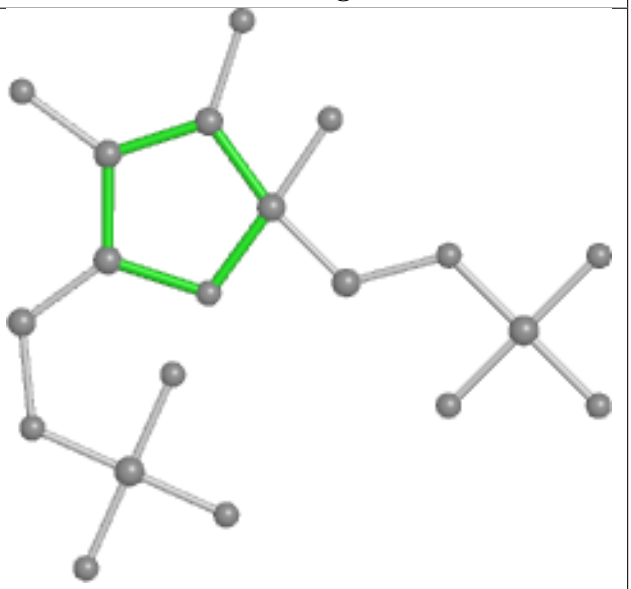
Bond lengths



Bond angles

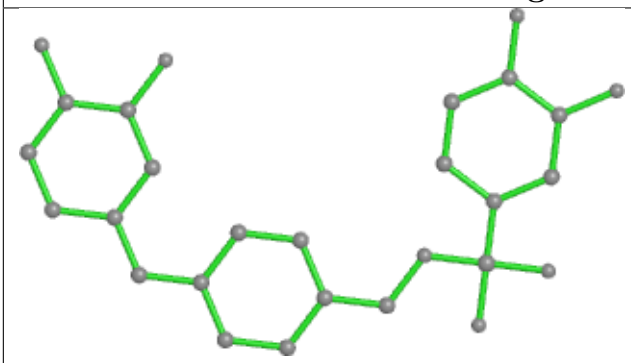


Torsions

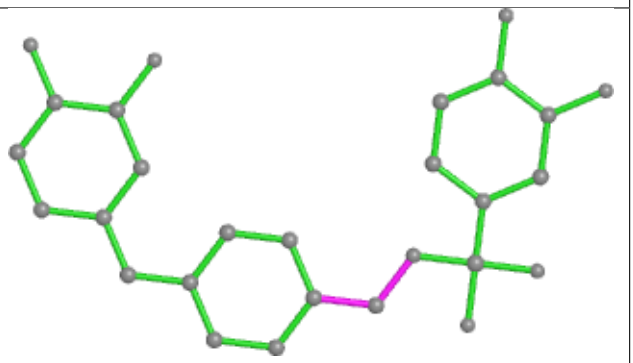


Rings

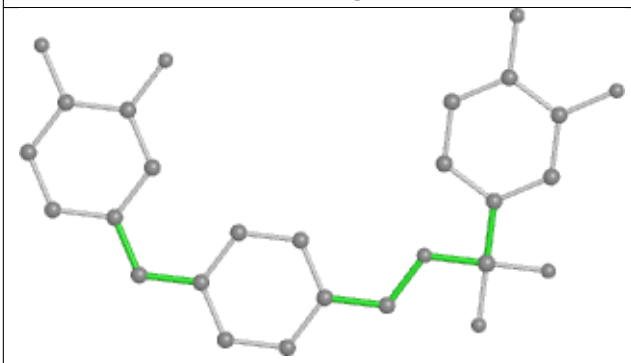
Ligand OE0 B 605



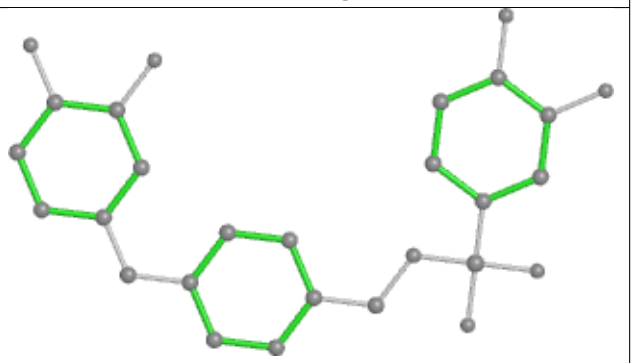
Bond lengths



Bond angles

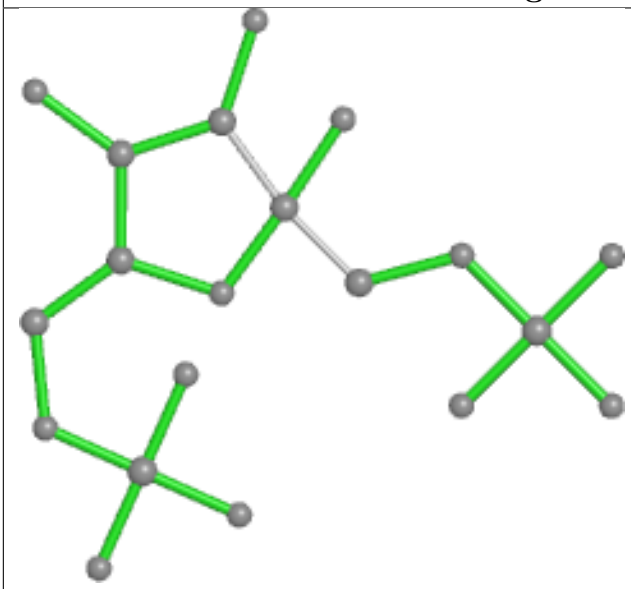


Torsions

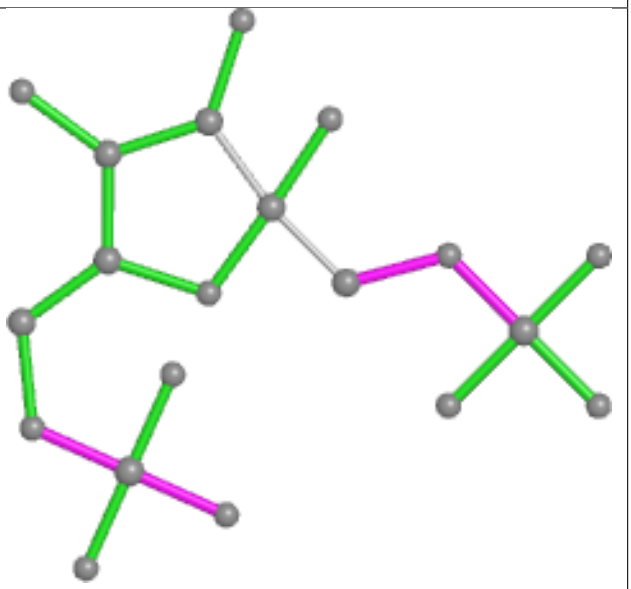


Rings

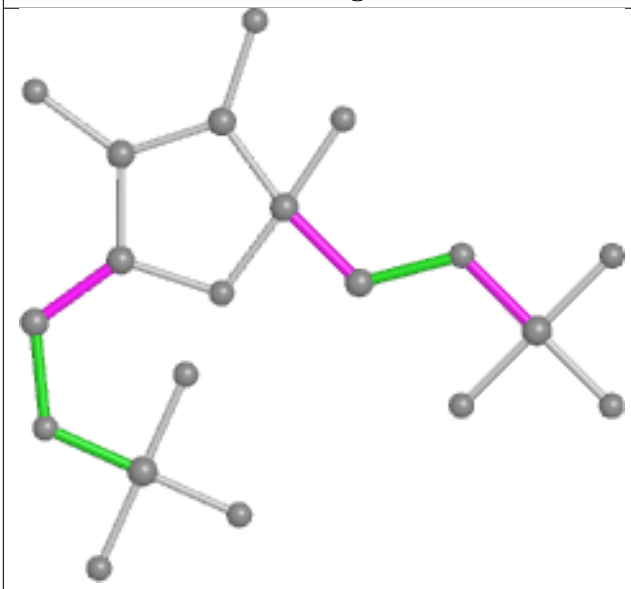
Ligand FBP B 601



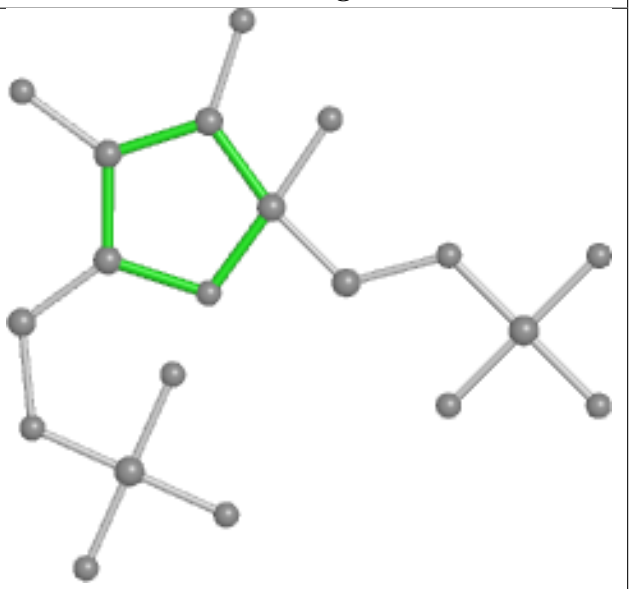
Bond lengths



Bond angles

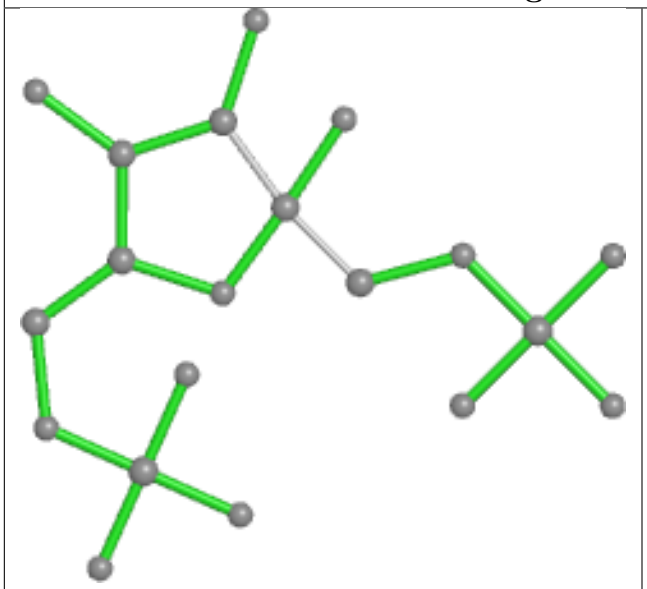


Torsions

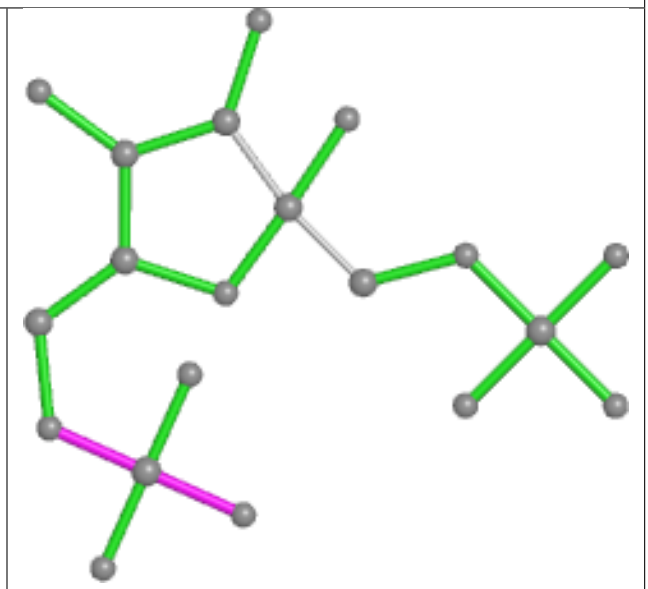


Rings

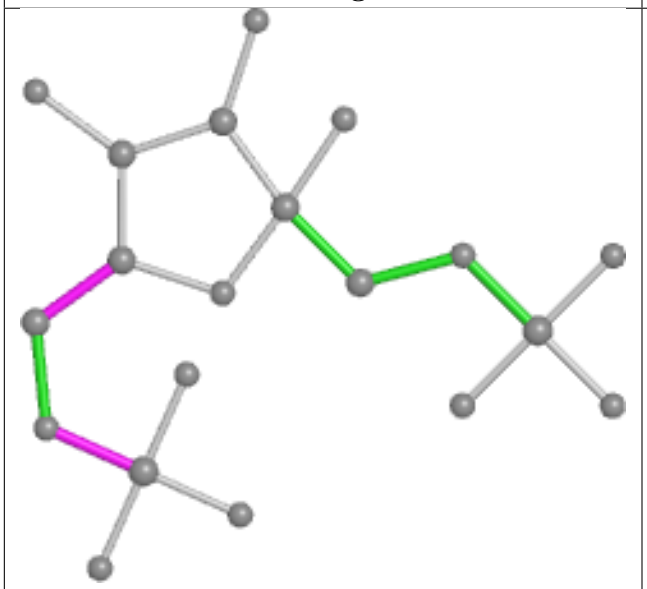
Ligand FBP H 601



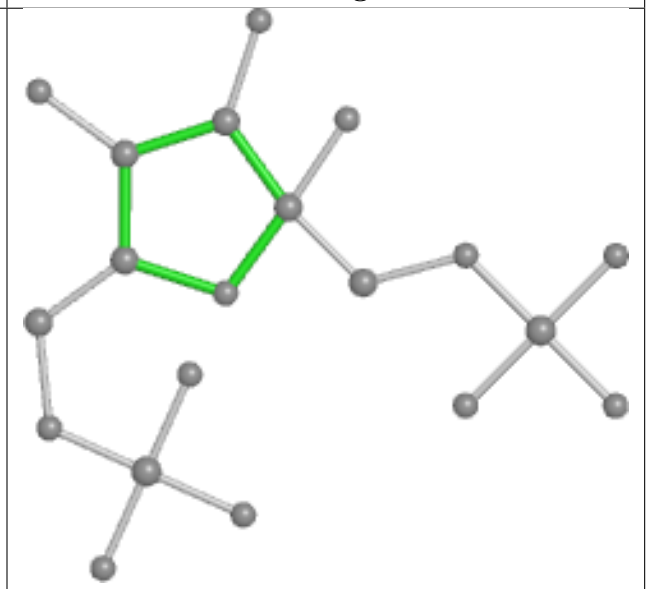
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	422/447 (94%)	2.71	226 (53%)	0	0	96, 139, 177, 191	0
1	B	436/447 (97%)	1.65	139 (31%)	0	0	61, 107, 148, 159	0
1	C	425/447 (95%)	1.39	100 (23%)	0	0	39, 82, 131, 163	0
1	D	425/447 (95%)	0.80	10 (2%)	59	62	35, 55, 90, 143	0
1	E	419/447 (93%)	2.45	199 (47%)	0	0	84, 129, 164, 188	0
1	F	432/447 (96%)	1.44	121 (28%)	0	0	59, 97, 138, 153	0
1	G	421/447 (94%)	1.03	59 (14%)	2	2	39, 73, 110, 133	1 (0%)
1	H	425/447 (95%)	0.77	11 (2%)	56	59	37, 54, 90, 139	0
All	All	3405/3576 (95%)	1.53	865 (25%)	0	0	35, 91, 158, 191	1 (0%)

All (865) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	SER	18.0
1	A	484	LEU	13.5
1	E	442	VAL	13.0
1	A	114	PRO	12.6
1	A	482	PHE	12.3
1	E	464	ALA	11.6
1	E	487	ARG	11.5
1	E	114	PRO	11.4
1	E	502	VAL	10.9
1	A	465	VAL	10.7
1	A	464	ALA	10.6
1	E	539	VAL	10.4
1	E	543	SER	10.3
1	C	22	THR	10.3
1	B	540[A]	LEU	10.3
1	B	10	ARG	10.0

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Mol	Chain	Res	Type	RSRZ
1	E	485	LEU	9.9
1	A	63	ILE	9.7
1	A	492	ALA	9.6
1	E	484	LEU	9.4
1	A	241	LEU	9.3
1	A	115	LEU	9.3
1	F	540[A]	LEU	9.3
1	A	502	VAL	9.2
1	A	353	THR	9.0
1	A	357	THR	8.9
1	C	23	ALA	8.7
1	A	527	TRP	8.6
1	C	382	PHE	8.5
1	A	377	THR	8.4
1	B	543	SER	8.4
1	A	522	ILE	8.1
1	A	517	VAL	8.1
1	E	249	VAL	8.1
1	B	542	ILE	8.0
1	A	485	LEU	8.0
1	A	494	TRP	8.0
1	E	452	LEU	8.0
1	C	42	LEU	7.9
1	E	304	VAL	7.8
1	F	443	LEU	7.7
1	A	80	GLY	7.6
1	E	477	LEU	7.5
1	A	539	VAL	7.4
1	A	373	LEU	7.3
1	E	447	GLY	7.3
1	E	450	ALA	7.2
1	E	514	PHE	7.2
1	B	539	VAL	7.2
1	A	452	LEU	7.1
1	E	80	GLY	7.1
1	E	505	GLY	7.1
1	A	500	ARG	7.1
1	A	304	VAL	7.1
1	A	489	PRO	7.0
1	A	498	VAL	7.0
1	E	482	PHE	7.0
1	E	489	PRO	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	475	VAL	6.9
1	F	480	GLY	6.9
1	E	115	LEU	6.9
1	E	465	VAL	6.9
1	E	522	ILE	6.8
1	E	540	LEU	6.7
1	B	443	LEU	6.7
1	A	67	SER	6.7
1	C	393	ILE	6.7
1	E	353	THR	6.6
1	C	19	GLU	6.6
1	A	113	SER	6.5
1	F	516	ARG	6.5
1	C	36	ASP	6.5
1	A	402	TYR	6.5
1	B	517	VAL	6.4
1	E	118	ARG	6.4
1	A	447	GLY	6.4
1	A	343	LEU	6.4
1	A	507	GLU	6.4
1	C	32	ALA	6.4
1	F	453	LEU	6.4
1	G	363	ALA	6.4
1	A	124	LEU	6.3
1	C	349	LYS	6.3
1	E	542	ILE	6.3
1	E	466	THR	6.3
1	B	12	ASP	6.3
1	A	86	LEU	6.2
1	E	402	TYR	6.2
1	A	33	ALA	6.2
1	E	81	MET	6.2
1	E	336	VAL	6.2
1	A	361	ALA	6.2
1	A	81	MET	6.1
1	E	494	TRP	6.1
1	C	366	ASP	6.1
1	E	498	VAL	6.1
1	E	537[A]	MET	6.1
1	A	469	ALA	6.1
1	G	42	LEU	6.1
1	A	342	MET	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	481	VAL	6.0
1	A	466	THR	6.0
1	B	463	ILE	5.9
1	E	57	THR	5.9
1	A	423	VAL	5.9
1	E	120	VAL	5.8
1	F	543	SER	5.8
1	A	376	GLU	5.7
1	E	29	GLN	5.7
1	G	32	ALA	5.7
1	E	524	VAL	5.7
1	A	88	PHE	5.7
1	A	450	ALA	5.6
1	A	383	PRO	5.6
1	C	59	ILE	5.6
1	F	527	TRP	5.5
1	A	515	LEU	5.5
1	E	319	PHE	5.5
1	B	525	THR	5.5
1	A	352	PRO	5.5
1	E	103	VAL	5.5
1	E	67	SER	5.4
1	A	536	ILE	5.4
1	B	130	GLY	5.4
1	F	456	TYR	5.4
1	B	25	PHE	5.4
1	A	453	LEU	5.4
1	A	540	LEU	5.4
1	A	459	ARG	5.4
1	F	542[A]	ILE	5.4
1	E	376	GLU	5.3
1	A	355	ALA	5.3
1	E	500	ARG	5.3
1	A	493	ILE	5.3
1	E	509	GLY	5.3
1	D	24	PHE	5.3
1	A	490	PRO	5.3
1	A	443	LEU	5.3
1	E	493	ILE	5.3
1	B	20	LEU	5.2
1	C	390	GLN	5.2
1	E	33	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	313	ILE	5.2
1	B	91	GLY	5.1
1	A	36	ASP	5.1
1	A	253	PHE	5.1
1	E	474	GLN	5.1
1	C	343	LEU	5.1
1	E	59	ILE	5.1
1	A	525	THR	5.1
1	A	66	ALA	5.1
1	G	33	ALA	5.1
1	E	440	ILE	5.1
1	F	539	VAL	5.0
1	E	270	LEU	5.0
1	A	486	TYR	5.0
1	E	527	TRP	5.0
1	G	63	ILE	5.0
1	A	471	ALA	5.0
1	B	523	VAL	5.0
1	E	122	ILE	5.0
1	B	438	ALA	5.0
1	A	426	ILE	5.0
1	A	524	VAL	5.0
1	D	25	PHE	5.0
1	E	412	ARG	5.0
1	B	355	ALA	4.9
1	E	504	PHE	4.9
1	E	117	TYR	4.9
1	H	21	GLY	4.8
1	B	453	LEU	4.8
1	A	481	VAL	4.8
1	F	465	VAL	4.8
1	B	393	ILE	4.8
1	F	460	ALA	4.8
1	A	442	VAL	4.8
1	E	538	ARG	4.8
1	B	277	ILE	4.8
1	A	514	PHE	4.7
1	A	280	ILE	4.7
1	A	463	ILE	4.7
1	A	91	GLY	4.7
1	E	368	ALA	4.7
1	E	251	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	410	LEU	4.6
1	A	251	ILE	4.6
1	A	117	TYR	4.6
1	A	401	VAL	4.6
1	B	249	VAL	4.6
1	G	34	MET	4.6
1	E	421	THR	4.6
1	E	451	GLN	4.6
1	E	511	LEU	4.6
1	F	371	ILE	4.6
1	A	537[A]	MET	4.6
1	C	352	PRO	4.5
1	F	522	ILE	4.5
1	C	35	ALA	4.5
1	A	441	ILE	4.5
1	F	116	SER	4.5
1	A	75	GLU	4.5
1	A	319	PHE	4.5
1	C	63	ILE	4.5
1	C	386	ALA	4.5
1	A	30	LEU	4.4
1	E	515	LEU	4.4
1	E	483	PRO	4.4
1	E	372	MET	4.4
1	A	277	ILE	4.4
1	E	393	ILE	4.4
1	E	32	ALA	4.4
1	B	426	ILE	4.4
1	E	426	ILE	4.4
1	E	400	ALA	4.3
1	E	373	LEU	4.3
1	A	479	ARG	4.3
1	E	358	SER	4.3
1	B	13	VAL	4.3
1	A	302	ILE	4.3
1	E	486	TYR	4.3
1	B	521	VAL	4.3
1	F	533	TYR	4.3
1	B	439	ALA	4.3
1	E	463	ILE	4.3
1	F	459	ARG	4.3
1	E	345	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	107	VAL	4.3
1	A	506	ILE	4.2
1	B	15	GLN	4.2
1	B	412	ARG	4.2
1	A	263	VAL	4.2
1	C	34	MET	4.2
1	E	390	GLN	4.2
1	E	536	ILE	4.2
1	A	384	VAL	4.2
1	B	413	ALA	4.2
1	E	277	ILE	4.2
1	E	401	VAL	4.2
1	A	477	LEU	4.2
1	E	446	THR	4.2
1	E	525	THR	4.2
1	B	452	LEU	4.1
1	F	270	LEU	4.1
1	G	343	LEU	4.1
1	E	490	PRO	4.1
1	H	24	PHE	4.1
1	E	488	GLU	4.1
1	F	426	ILE	4.1
1	F	450	ALA	4.1
1	E	448	ARG	4.1
1	A	523	VAL	4.1
1	F	15	GLN	4.1
1	F	494	TRP	4.1
1	A	394	ALA	4.1
1	F	355	ALA	4.1
1	C	341	GLN	4.1
1	B	450	ALA	4.1
1	E	517	VAL	4.1
1	F	524	VAL	4.1
1	C	20	LEU	4.0
1	C	363	ALA	4.0
1	C	397	ALA	4.0
1	B	442	VAL	4.0
1	H	25	PHE	4.0
1	F	115	LEU	4.0
1	C	37	THR	4.0
1	A	29	GLN	4.0
1	F	63	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	521	VAL	4.0
1	B	537[A]	MET	4.0
1	B	465	VAL	4.0
1	F	475	VAL	4.0
1	A	487	ARG	4.0
1	C	346	MET	4.0
1	C	348	THR	4.0
1	A	334	LYS	4.0
1	E	266	VAL	4.0
1	F	481	VAL	4.0
1	F	412	ARG	3.9
1	A	444	THR	3.9
1	A	460	ALA	3.9
1	E	507	GLU	3.9
1	F	526	GLY	3.9
1	A	25	PHE	3.9
1	A	38	PHE	3.9
1	G	382	PHE	3.9
1	G	411	ARG	3.9
1	E	289	VAL	3.9
1	A	388	LYS	3.9
1	B	456	TYR	3.9
1	E	454[A]	SER	3.9
1	C	401	VAL	3.9
1	F	482	PHE	3.9
1	E	386	ALA	3.9
1	A	56	SER	3.9
1	A	454	SER	3.9
1	B	429	VAL	3.9
1	F	484	LEU	3.9
1	E	456	TYR	3.8
1	F	511	LEU	3.8
1	E	302	ILE	3.8
1	E	394	ALA	3.8
1	B	520	LEU	3.8
1	A	57	THR	3.8
1	A	511	LEU	3.8
1	G	28	GLN	3.8
1	A	462	VAL	3.8
1	F	241	LEU	3.8
1	E	508	SER	3.8
1	F	452	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	371	ILE	3.7
1	B	236	GLN	3.7
1	F	496	ASP	3.7
1	A	528	ARG	3.7
1	E	124	LEU	3.7
1	B	505	GLY	3.7
1	A	473	ARG	3.7
1	C	21	GLY	3.7
1	B	527	TRP	3.7
1	C	305	ALA	3.7
1	E	76[A]	MET	3.7
1	F	35	ALA	3.7
1	A	456	TYR	3.7
1	C	359	ASP	3.7
1	C	373	LEU	3.7
1	C	389	MET	3.7
1	E	253	PHE	3.7
1	E	405	GLN	3.7
1	A	358	SER	3.7
1	E	403	HIS	3.7
1	B	414	ALA	3.7
1	F	463	ILE	3.6
1	F	537[A]	MET	3.6
1	A	390	GLN	3.6
1	B	431	ALA	3.6
1	A	283	ILE	3.6
1	B	440	ILE	3.6
1	A	449	SER	3.6
1	B	45	LEU	3.6
1	A	380	GLY	3.6
1	G	39	LEU	3.6
1	B	418	ARG	3.6
1	F	377	THR	3.6
1	F	266	VAL	3.6
1	F	493	ILE	3.6
1	B	516	ARG	3.6
1	E	127	LYS	3.6
1	A	23	ALA	3.6
1	E	397	ALA	3.6
1	E	375	GLY	3.6
1	A	237	ASP	3.6
1	F	236	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	316	GLU	3.6
1	A	424	THR	3.6
1	B	132	GLY	3.6
1	A	118	ARG	3.5
1	B	515	LEU	3.5
1	E	444	THR	3.5
1	A	404	ARG	3.5
1	E	459	ARG	3.5
1	A	476	HIS	3.5
1	F	100	ILE	3.5
1	C	39	LEU	3.5
1	G	352	PRO	3.5
1	A	467	ARG	3.5
1	A	346	MET	3.5
1	C	364	VAL	3.5
1	A	78	LYS	3.5
1	F	26	GLN	3.5
1	E	469	ALA	3.5
1	E	534	THR	3.5
1	B	507	GLU	3.5
1	C	45	LEU	3.5
1	A	82	ASN	3.5
1	E	343	LEU	3.5
1	F	525	THR	3.5
1	A	440	ILE	3.4
1	C	60	ILE	3.4
1	C	371	ILE	3.4
1	E	443	LEU	3.4
1	B	524	VAL	3.4
1	C	40	GLU	3.4
1	F	86	LEU	3.4
1	F	429	VAL	3.4
1	B	514	PHE	3.4
1	F	39	LEU	3.4
1	F	515	LEU	3.4
1	B	454	SER	3.4
1	D	21	GLY	3.4
1	E	523	VAL	3.4
1	F	498	VAL	3.4
1	E	478	CYS	3.4
1	A	32	ALA	3.4
1	A	282	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	404	ARG	3.4
1	A	247	HIS	3.4
1	A	403	HIS	3.4
1	E	371	ILE	3.4
1	A	533	TYR	3.4
1	F	438	ALA	3.4
1	C	304	VAL	3.4
1	G	401	VAL	3.4
1	C	404	ARG	3.4
1	A	232	GLY	3.3
1	A	107	VAL	3.3
1	C	344	GLU	3.3
1	A	472	ALA	3.3
1	C	412	ARG	3.3
1	B	266	VAL	3.3
1	E	280	ILE	3.3
1	A	61	ALA	3.3
1	G	412	ARG	3.3
1	A	474	GLN	3.3
1	C	41	HIS	3.3
1	E	303	MET	3.3
1	C	405	GLN	3.3
1	F	454	SER	3.3
1	A	365	LEU	3.3
1	B	39	LEU	3.3
1	B	371	ILE	3.3
1	B	511	LEU	3.3
1	F	233	LEU	3.3
1	G	393	ILE	3.3
1	A	303	MET	3.3
1	A	125	ASP	3.3
1	B	482	PHE	3.3
1	E	355	ALA	3.3
1	E	433	PHE	3.3
1	F	536	ILE	3.3
1	C	394	ALA	3.3
1	A	521	VAL	3.3
1	G	350	PRO	3.2
1	A	123	ALA	3.2
1	C	385	GLU	3.2
1	B	459	ARG	3.2
1	F	103	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	407	PHE	3.2
1	C	342	MET	3.2
1	E	26	GLN	3.2
1	C	350	PRO	3.2
1	F	51	PRO	3.2
1	E	66	ALA	3.2
1	E	313	ILE	3.2
1	F	512	ARG	3.2
1	B	462	VAL	3.2
1	E	481	VAL	3.2
1	C	79	ALA	3.2
1	C	383	PRO	3.2
1	E	352	PRO	3.2
1	B	61	ALA	3.2
1	B	464	ALA	3.2
1	E	501	ARG	3.2
1	B	486	TYR	3.1
1	E	75	GLU	3.1
1	F	52	VAL	3.1
1	G	36	ASP	3.1
1	G	59	ILE	3.1
1	E	383	PRO	3.1
1	F	118	ARG	3.1
1	A	289	VAL	3.1
1	C	340	THR	3.1
1	E	349	LYS	3.1
1	C	25	PHE	3.1
1	A	55	ARG	3.1
1	F	351	ARG	3.1
1	C	408	GLU	3.1
1	F	507	GLU	3.1
1	A	60	ILE	3.1
1	C	319	PHE	3.1
1	A	62	THR	3.1
1	B	460	ALA	3.1
1	E	531	SER	3.1
1	F	521	VAL	3.1
1	E	473	ARG	3.1
1	A	305	ALA	3.1
1	B	52	VAL	3.1
1	F	238	VAL	3.1
1	C	38	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	424	THR	3.0
1	B	484	LEU	3.0
1	E	357	THR	3.0
1	A	248	GLY	3.0
1	A	331[A]	LEU	3.0
1	H	30	LEU	3.0
1	A	412	ARG	3.0
1	H	32	ALA	3.0
1	F	517	VAL	3.0
1	E	63	ILE	3.0
1	E	91	GLY	3.0
1	A	411	ARG	3.0
1	E	23	ALA	3.0
1	A	542	ILE	3.0
1	A	369	ASP	3.0
1	A	378	ALA	3.0
1	E	296	LEU	3.0
1	E	437	ALA	3.0
1	A	273	GLU	3.0
1	E	36	ASP	3.0
1	E	100	ILE	3.0
1	A	478	CYS	2.9
1	A	296	LEU	2.9
1	B	533	TYR	2.9
1	A	52	VAL	2.9
1	G	70	VAL	2.9
1	C	43	CYS	2.9
1	A	344	GLU	2.9
1	B	94	GLU	2.9
1	A	245	VAL	2.9
1	F	514	PHE	2.9
1	A	37	THR	2.9
1	B	241	LEU	2.9
1	B	512	ARG	2.9
1	E	55	ARG	2.9
1	E	462	VAL	2.9
1	F	440	ILE	2.9
1	E	41	HIS	2.9
1	C	380	GLY	2.9
1	A	354	ARG	2.9
1	E	320	LEU	2.9
1	F	413	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	321	ALA	2.9
1	E	429	VAL	2.9
1	A	59	ILE	2.9
1	A	393	ILE	2.9
1	A	418[A]	ARG	2.9
1	C	44	LEU	2.9
1	A	266	VAL	2.8
1	A	336	VAL	2.8
1	H	408	GLU	2.8
1	F	88	PHE	2.8
1	A	84	ALA	2.8
1	B	406	LEU	2.8
1	E	30	LEU	2.8
1	E	38	PHE	2.8
1	A	96	HIS	2.8
1	C	306	ARG	2.8
1	E	467	ARG	2.8
1	B	441	ILE	2.8
1	F	277	ILE	2.8
1	B	30	LEU	2.8
1	F	455	ARG	2.8
1	F	244	GLY	2.8
1	E	28	GLN	2.8
1	A	491	GLU	2.8
1	F	442	VAL	2.8
1	G	364	VAL	2.8
1	E	533	TYR	2.8
1	G	349	LYS	2.8
1	E	354	ARG	2.8
1	F	414	ALA	2.8
1	F	333	GLY	2.8
1	B	529	PRO	2.8
1	B	522	ILE	2.8
1	A	315	ALA	2.8
1	A	44	LEU	2.8
1	A	330	ASN	2.8
1	A	408	GLU	2.8
1	B	86	LEU	2.8
1	E	334	LYS	2.8
1	B	498	VAL	2.8
1	F	523	VAL	2.8
1	B	79	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	298	VAL	2.7
1	E	398	GLU	2.7
1	B	11	ALA	2.7
1	E	311	ILE	2.7
1	A	39	LEU	2.7
1	E	241	LEU	2.7
1	A	538	ARG	2.7
1	C	459	ARG	2.7
1	B	370	CYS	2.7
1	C	57	THR	2.7
1	E	445	THR	2.7
1	G	322	GLN	2.7
1	E	475	VAL	2.7
1	G	360	VAL	2.7
1	B	63	ILE	2.7
1	B	121	ALA	2.7
1	B	480	GLY	2.7
1	B	532	GLY	2.7
1	E	471	ALA	2.7
1	A	270	LEU	2.7
1	G	115	LEU	2.7
1	G	383	PRO	2.7
1	G	404	ARG	2.7
1	F	309	LEU	2.7
1	C	269	ALA	2.7
1	E	62	THR	2.7
1	B	536	ILE	2.7
1	B	538	ARG	2.7
1	A	49	SER	2.6
1	A	410	LEU	2.6
1	A	26	GLN	2.6
1	C	351	ARG	2.6
1	F	418	ARG	2.6
1	B	123	ALA	2.6
1	E	532	GLY	2.6
1	A	398	GLU	2.6
1	F	499	ASP	2.6
1	B	107	VAL	2.6
1	E	263	VAL	2.6
1	A	421	THR	2.6
1	A	349	LYS	2.6
1	F	479	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	49	SER	2.6
1	B	35	ALA	2.6
1	C	367	GLY	2.6
1	B	270	LEU	2.6
1	B	51	PRO	2.6
1	E	441	ILE	2.6
1	C	26	GLN	2.6
1	C	361	ALA	2.6
1	A	42	LEU	2.6
1	E	365	LEU	2.6
1	C	75	GLU	2.6
1	C	345	SER	2.6
1	E	248	GLY	2.6
1	F	12	ASP	2.6
1	G	351	ARG	2.6
1	B	103	VAL	2.6
1	B	337	VAL	2.6
1	A	356	GLU	2.6
1	B	373	LEU	2.6
1	B	28	GLN	2.6
1	B	447	GLY	2.6
1	A	368	ALA	2.5
1	B	332	ALA	2.5
1	C	33	ALA	2.5
1	G	50	GLU	2.6
1	A	77	ILE	2.5
1	B	487	ARG	2.5
1	A	495	ALA	2.5
1	B	233	LEU	2.5
1	B	24	PHE	2.5
1	A	483	PRO	2.5
1	A	504	PHE	2.5
1	F	90	HIS	2.5
1	A	451	GLN	2.5
1	B	118	ARG	2.5
1	E	79	ALA	2.5
1	E	409	GLU	2.5
1	F	384	VAL	2.5
1	G	346	MET	2.5
1	C	72	ARG	2.5
1	A	364	VAL	2.5
1	B	509	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	502	VAL	2.5
1	G	304	VAL	2.5
1	A	405	GLN	2.5
1	B	251	ILE	2.5
1	A	132	GLY	2.5
1	A	427	GLY	2.5
1	A	526	GLY	2.5
1	B	535	ASN	2.5
1	F	534	THR	2.5
1	G	348	THR	2.5
1	A	257	VAL	2.5
1	E	88	PHE	2.5
1	G	342	MET	2.5
1	A	529	PRO	2.5
1	A	28	GLN	2.4
1	C	331	LEU	2.4
1	C	337	VAL	2.4
1	C	47	ILE	2.4
1	B	305	ALA	2.4
1	E	348	THR	2.4
1	E	233	LEU	2.4
1	F	358	SER	2.4
1	A	372	MET	2.4
1	B	90	HIS	2.4
1	C	368	ALA	2.4
1	A	34	MET	2.4
1	E	512	ARG	2.4
1	E	232	GLY	2.4
1	E	413	ALA	2.4
1	G	394	ALA	2.4
1	E	422	GLU	2.4
1	C	67	SER	2.4
1	E	331	LEU	2.4
1	F	449	SER	2.4
1	A	360	VAL	2.4
1	A	83	ILE	2.4
1	F	34	MET	2.4
1	F	513	GLY	2.4
1	G	60	ILE	2.4
1	A	338	CYS	2.4
1	F	409	GLU	2.4
1	F	20	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	520	LEU	2.4
1	C	70	VAL	2.4
1	E	367	GLY	2.4
1	B	100	ILE	2.4
1	G	319	PHE	2.4
1	B	435	CYS	2.4
1	F	79	ALA	2.4
1	G	45	LEU	2.4
1	H	416	LEU	2.4
1	C	384	VAL	2.4
1	C	76[A]	MET	2.4
1	C	378	ALA	2.4
1	F	464	ALA	2.4
1	C	460	ALA	2.3
1	E	344	GLU	2.3
1	E	25	PHE	2.3
1	B	379	LYS	2.3
1	C	355	ALA	2.3
1	E	461	ALA	2.3
1	E	113	SER	2.3
1	E	234	SER	2.3
1	G	41	HIS	2.3
1	A	337	VAL	2.3
1	C	360	VAL	2.3
1	C	450	ALA	2.3
1	D	315	ALA	2.3
1	B	526	GLY	2.3
1	B	490	PRO	2.3
1	G	371	ILE	2.3
1	E	123	ALA	2.3
1	G	49	SER	2.3
1	G	341	GLN	2.3
1	B	494	TRP	2.3
1	B	395	ARG	2.3
1	C	347	ILE	2.3
1	A	264	ALA	2.3
1	E	247	HIS	2.3
1	E	235	GLU	2.3
1	B	280	ILE	2.3
1	C	292	PHE	2.3
1	G	366	ASP	2.3
1	G	57	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	343	LEU	2.3
1	H	412	ARG	2.2
1	E	99	SER	2.2
1	A	433	PHE	2.2
1	E	37	THR	2.2
1	A	41	HIS	2.2
1	E	479	ARG	2.2
1	A	335	PRO	2.2
1	A	518	GLY	2.2
1	B	364	VAL	2.2
1	E	77	ILE	2.2
1	A	379	LYS	2.2
1	F	332	ALA	2.2
1	C	411	ARG	2.2
1	A	350	PRO	2.2
1	C	387	VAL	2.2
1	H	498	VAL	2.2
1	A	35	ALA	2.2
1	C	391	HIS	2.2
1	E	492	ALA	2.2
1	B	410	LEU	2.2
1	E	491	GLU	2.2
1	G	408	GLU	2.2
1	B	475	VAL	2.2
1	E	423	VAL	2.2
1	A	100	ILE	2.2
1	B	53	ALA	2.2
1	D	77	ILE	2.2
1	F	251	ILE	2.2
1	B	256	PHE	2.2
1	F	503	GLN	2.2
1	G	292	PHE	2.2
1	B	489	PRO	2.2
1	E	119	PRO	2.2
1	F	509	GLY	2.2
1	A	85	ARG	2.2
1	A	345	SER	2.2
1	E	430	GLU	2.2
1	C	24	PHE	2.2
1	F	25	PHE	2.2
1	A	505	GLY	2.2
1	E	129	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	329	CYS	2.2
1	F	408	GLU	2.2
1	A	120	VAL	2.2
1	A	323	LYS	2.2
1	B	26	GLN	2.2
1	B	59	ILE	2.2
1	F	237	ASP	2.2
1	F	444	THR	2.2
1	A	24	PHE	2.2
1	G	25	PHE	2.2
1	G	459	ARG	2.2
1	A	322	GLN	2.1
1	A	510	LYS	2.1
1	A	318	VAL	2.1
1	A	79	ALA	2.1
1	B	60	ILE	2.1
1	G	38	PHE	2.1
1	A	45	LEU	2.1
1	B	485	LEU	2.1
1	C	410	LEU	2.1
1	F	127	LYS	2.1
1	B	338	CYS	2.1
1	H	516	ARG	2.1
1	A	461	ALA	2.1
1	C	94	GLU	2.1
1	B	17	THR	2.1
1	B	405	GLN	2.1
1	E	49	SER	2.1
1	E	411	ARG	2.1
1	B	95	TYR	2.1
1	D	84	ALA	2.1
1	A	65	PRO	2.1
1	B	243	PHE	2.1
1	F	243	PHE	2.1
1	D	45	LEU	2.1
1	B	68	ARG	2.1
1	B	455	ARG	2.1
1	D	431	ALA	2.1
1	C	51	PRO	2.1
1	E	424	THR	2.1
1	B	88	PHE	2.1
1	F	124	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	528	ARG	2.1
1	G	118	ARG	2.1
1	B	21	GLY	2.1
1	F	11	ALA	2.1
1	G	54	ALA	2.1
1	B	376	GLU	2.1
1	C	402	TYR	2.1
1	G	487	ARG	2.1
1	F	280	ILE	2.1
1	F	283	ILE	2.1
1	C	320	LEU	2.1
1	F	44	LEU	2.1
1	G	407	PHE	2.1
1	B	483	PRO	2.1
1	G	23	ALA	2.1
1	E	360	VAL	2.1
1	G	298	VAL	2.1
1	E	279	ILE	2.1
1	E	73	LEU	2.1
1	F	110	PHE	2.1
1	G	30	LEU	2.1
1	C	507	GLU	2.1
1	D	404	ARG	2.1
1	F	53	ALA	2.0
1	F	61	ALA	2.0
1	F	308	ASP	2.0
1	G	397	ALA	2.0
1	F	289	VAL	2.0
1	F	304	VAL	2.0
1	F	364	VAL	2.0
1	E	506	ILE	2.0
1	F	77	ILE	2.0
1	G	410	LEU	2.0
1	H	38	PHE	2.0
1	B	409	GLU	2.0
1	D	521	VAL	2.0
1	B	122	ILE	2.0
1	C	323	LYS	2.0
1	G	374[A]	SER	2.0
1	C	64	GLY	2.0
1	C	309	LEU	2.0
1	E	310	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	441	ILE	2.0
1	C	398	GLU	2.0
1	F	405	GLN	2.0
1	A	351	ARG	2.0
1	A	309	LEU	2.0
1	B	115	LEU	2.0
1	B	283	ILE	2.0
1	C	30	LEU	2.0
1	G	296	LEU	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	E	604	1/1	-0.40	5.99	299,299,299,299	0
5	K	B	604	1/1	0.44	0.10	144,144,144,144	0
5	K	F	604	1/1	0.64	0.12	152,152,152,152	0
5	K	A	604	1/1	0.68	1.02	289,289,289,289	0
2	FBP	A	601	20/20	0.69	0.26	148,149,152,152	0
3	OXL	A	602	6/6	0.71	0.60	195,196,196,196	0
2	FBP	F	601	20/20	0.72	0.20	128,131,136,136	0
5	K	G	604	1/1	0.72	0.12	117,117,117,117	0
2	FBP	B	601	20/20	0.74	0.19	126,126,128,128	0
2	FBP	E	601	20/20	0.75	0.21	136,136,138,138	0
6	OE0	A	605	28/28	0.76	0.40	116,117,118,119	19
3	OXL	C	602	6/6	0.77	0.22	129,129,129,129	0
5	K	C	604	1/1	0.79	0.12	117,117,117,117	0
6	OE0	F	605	28/28	0.80	0.39	99,101,103,106	19

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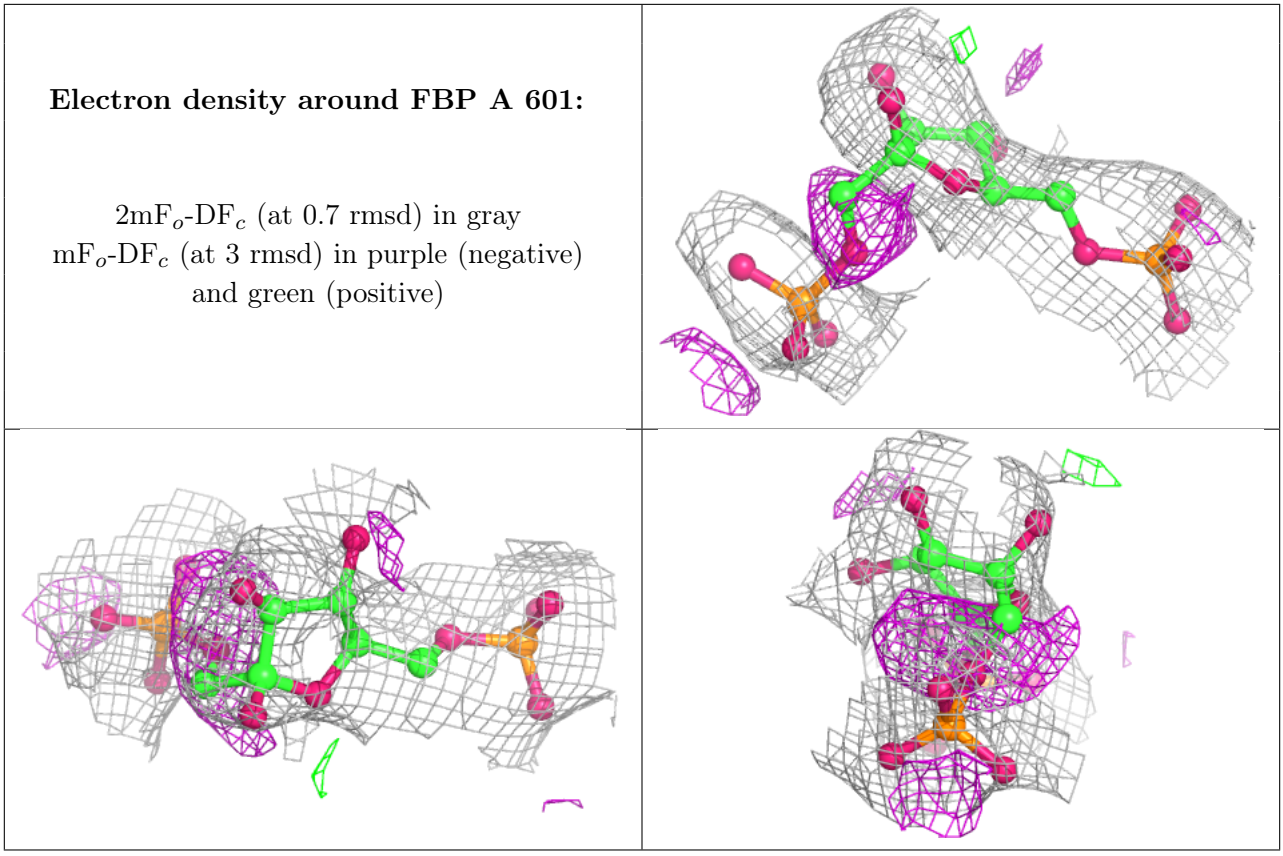
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OE0	G	605	28/28	0.82	0.37	104,105,106,106	19
3	OXL	E	602	6/6	0.84	0.36	156,156,156,156	0
6	OE0	B	605	28/28	0.86	0.35	90,92,96,97	19
3	OXL	F	602	6/6	0.88	0.34	128,128,128,128	0
4	MG	A	603	1/1	0.88	0.06	140,140,140,140	0
3	OXL	D	602	6/6	0.88	0.27	95,95,96,96	0
4	MG	E	603	1/1	0.89	0.05	137,137,137,137	0
3	OXL	G	602	6/6	0.91	0.21	114,115,115,115	0
3	OXL	B	602	6/6	0.92	0.30	108,108,109,109	0
3	OXL	H	602	6/6	0.93	0.25	85,86,87,87	0
5	K	H	604	1/1	0.93	0.12	94,94,94,94	0
5	K	D	604	1/1	0.95	0.09	91,91,91,91	0
4	MG	F	603	1/1	0.95	0.12	73,73,73,73	0
4	MG	B	603	1/1	0.95	0.15	88,88,88,88	0
4	MG	G	603	1/1	0.96	0.12	73,73,73,73	0
4	MG	C	603	1/1	0.97	0.14	90,90,90,90	0
4	MG	H	603	1/1	0.97	0.23	63,63,63,63	0
2	FBP	C	601	20/20	0.98	0.20	46,48,53,53	0
2	FBP	D	601	20/20	0.98	0.22	41,43,45,46	0
2	FBP	G	601	20/20	0.98	0.18	45,47,55,55	0
4	MG	D	603	1/1	0.98	0.22	75,75,75,75	0
2	FBP	H	601	20/20	0.98	0.20	37,40,42,43	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.

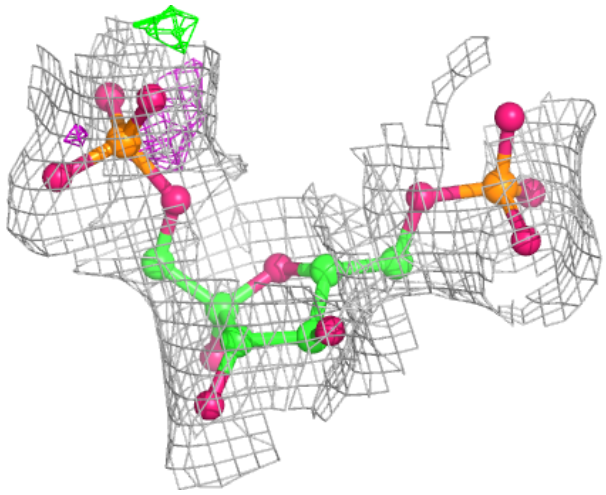
Electron density around FBP A 601:

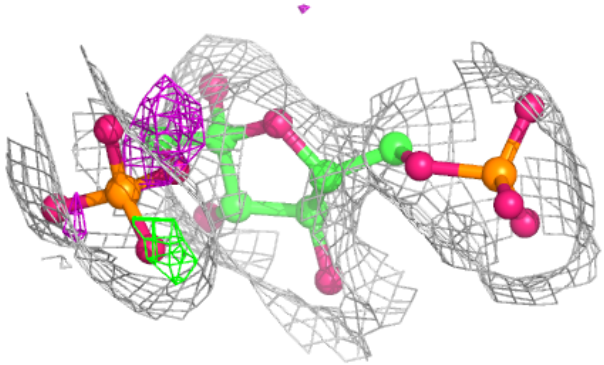
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

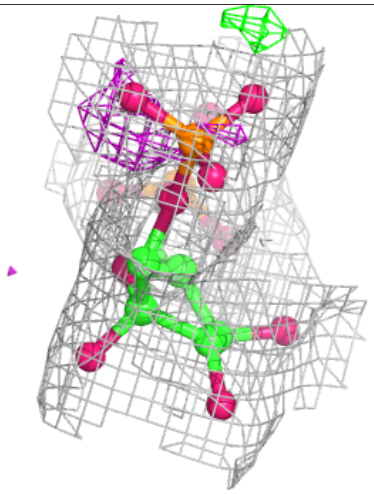


Electron density around FBP F 601:

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

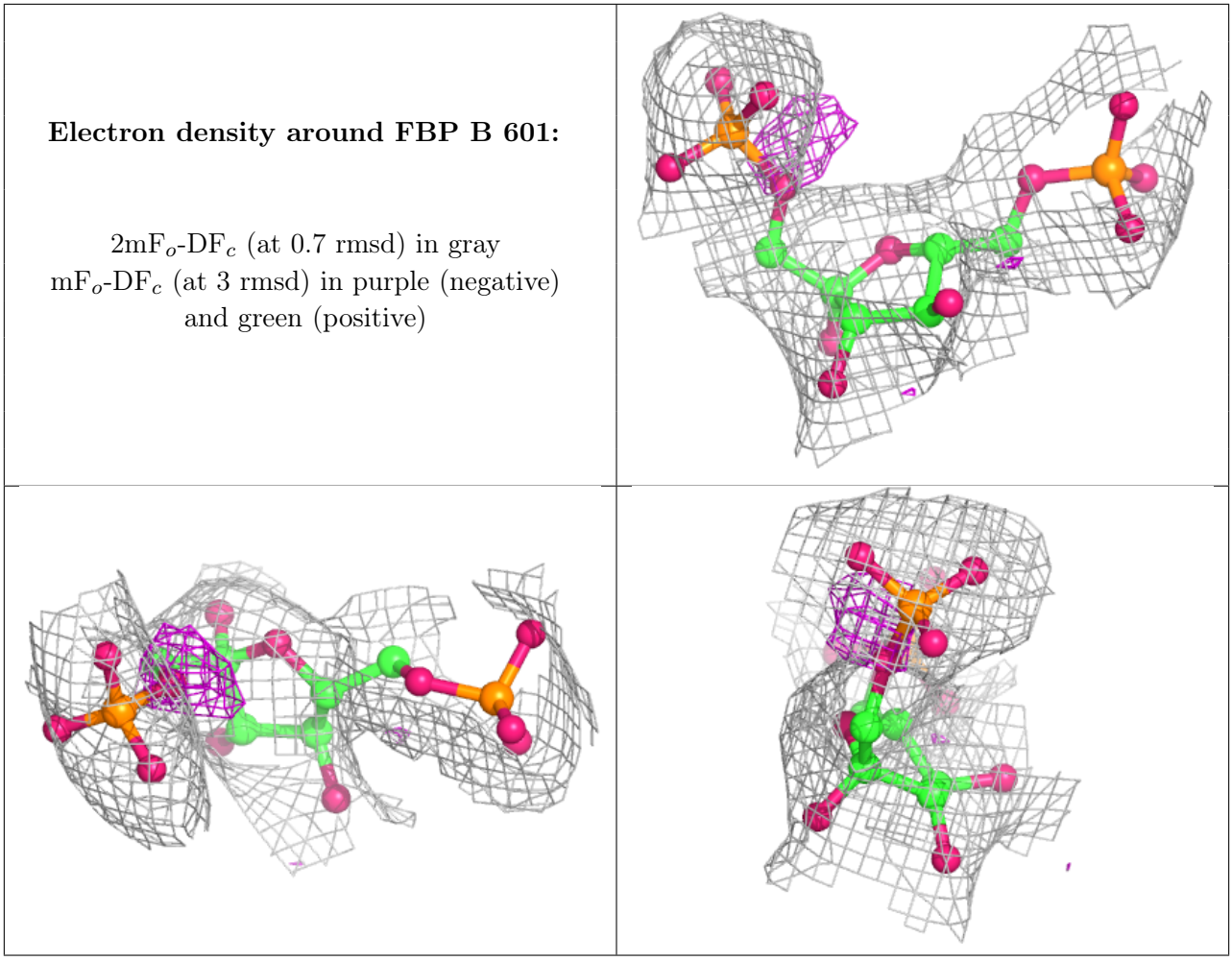






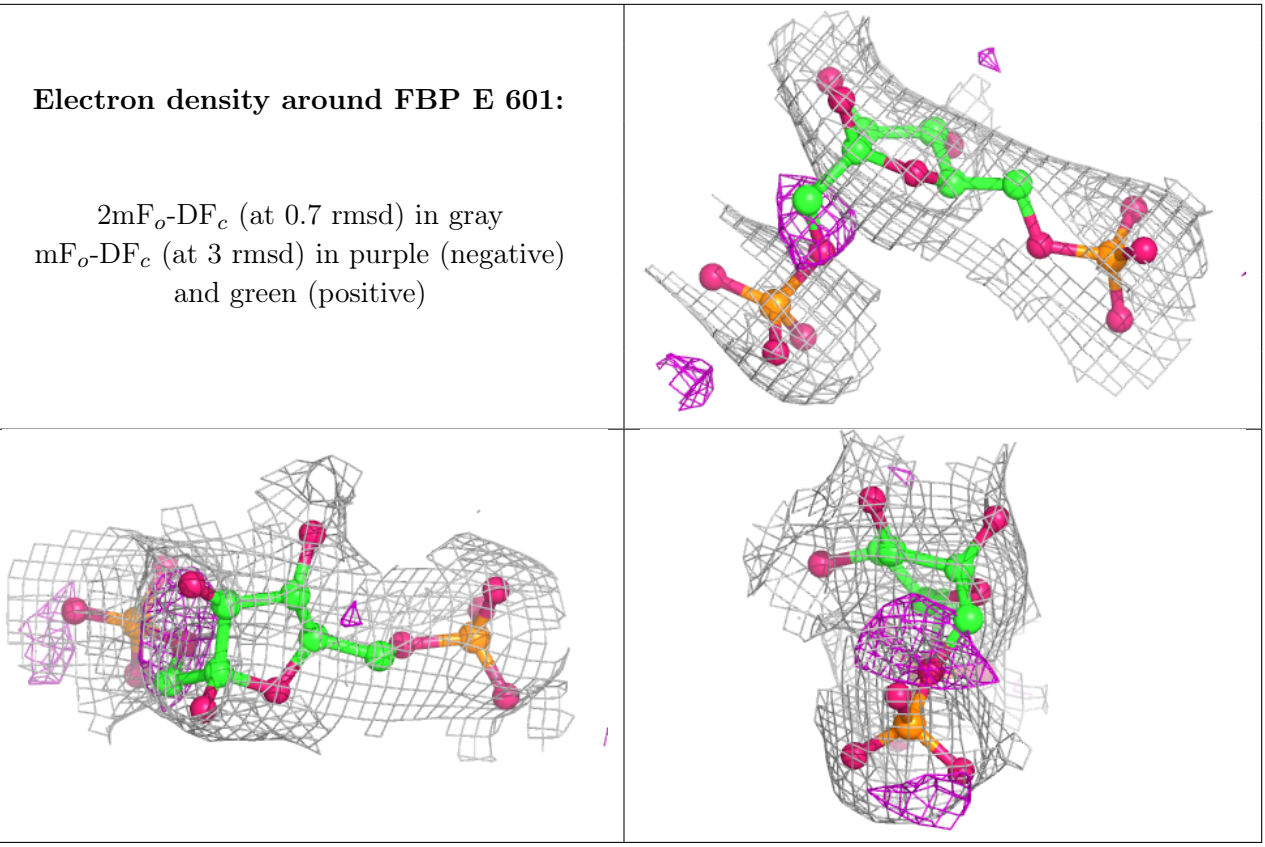
Electron density around FBP B 601:

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



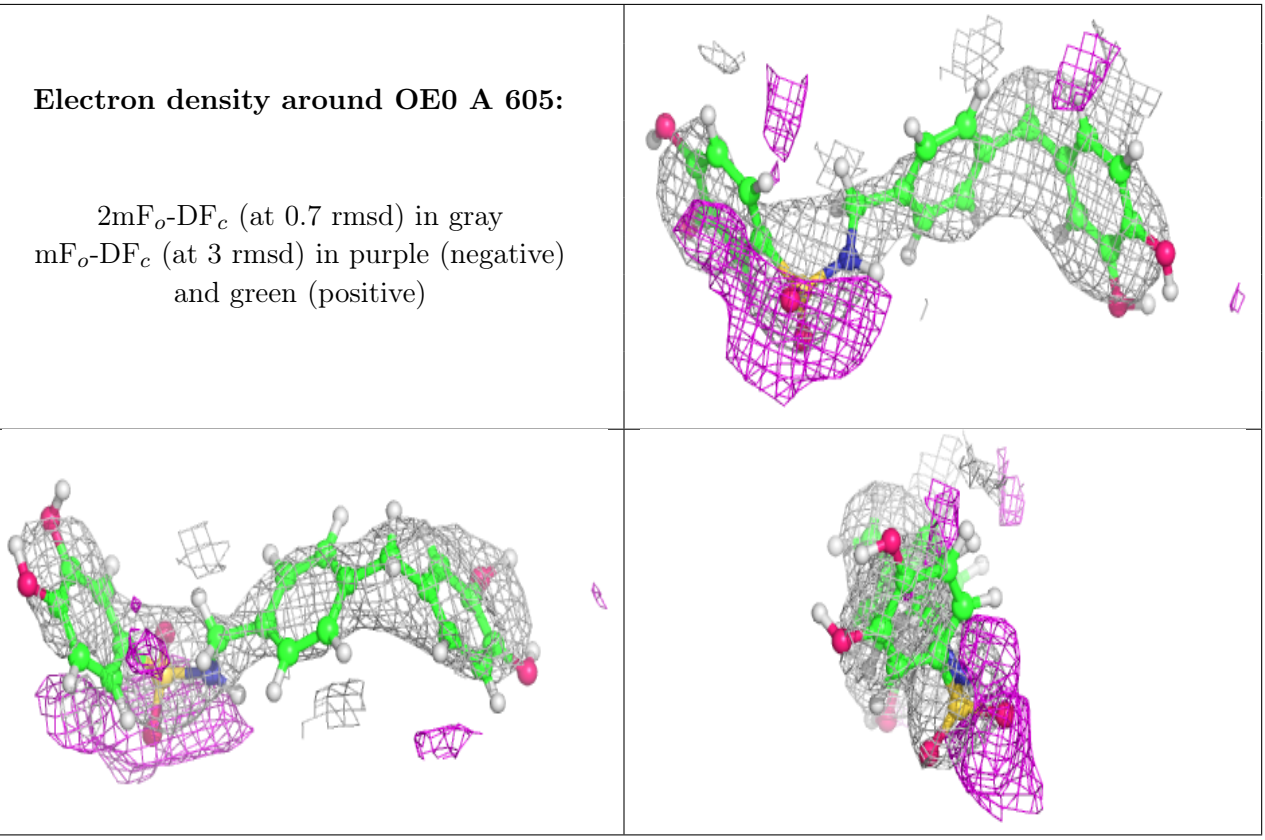
Electron density around FBP E 601:

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



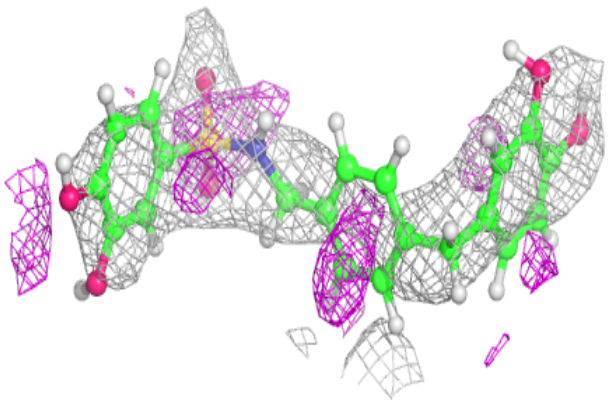
Electron density around OE0 A 605:

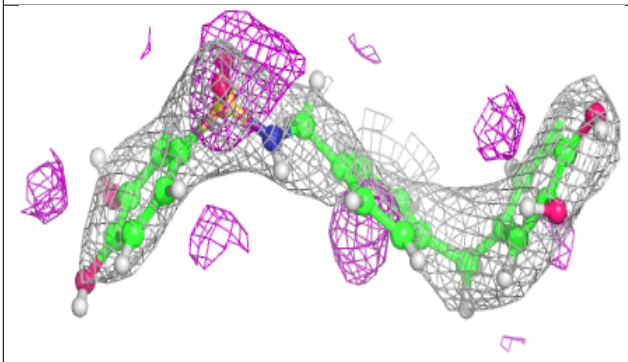
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

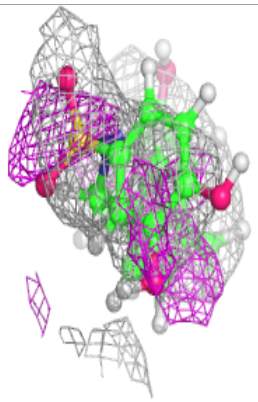


Electron density around OE0 F 605:

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

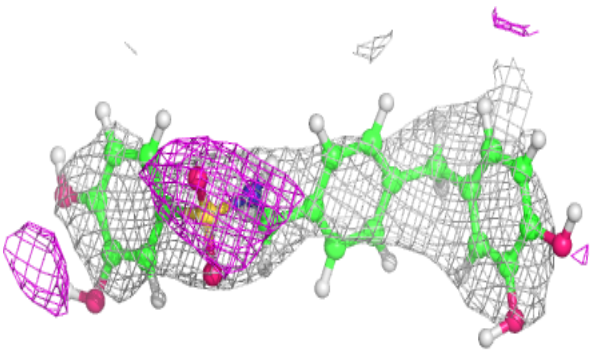


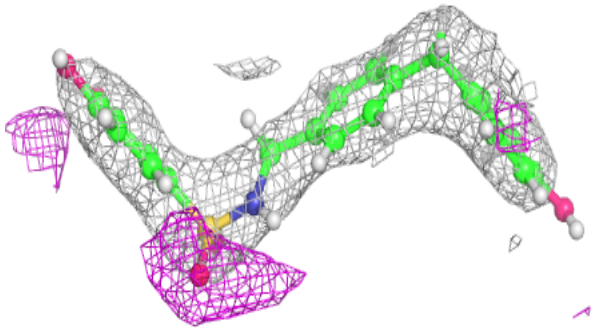


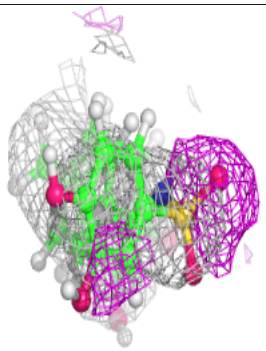


Electron density around OE0 G 605:

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

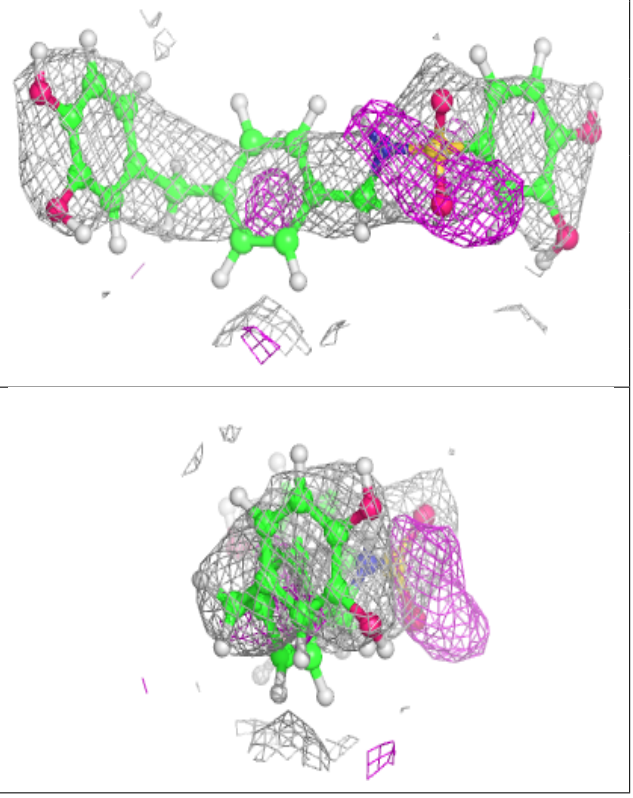


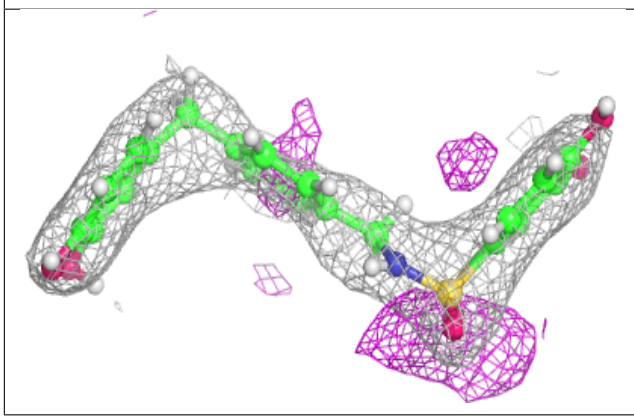




Electron density around OE0 B 605:

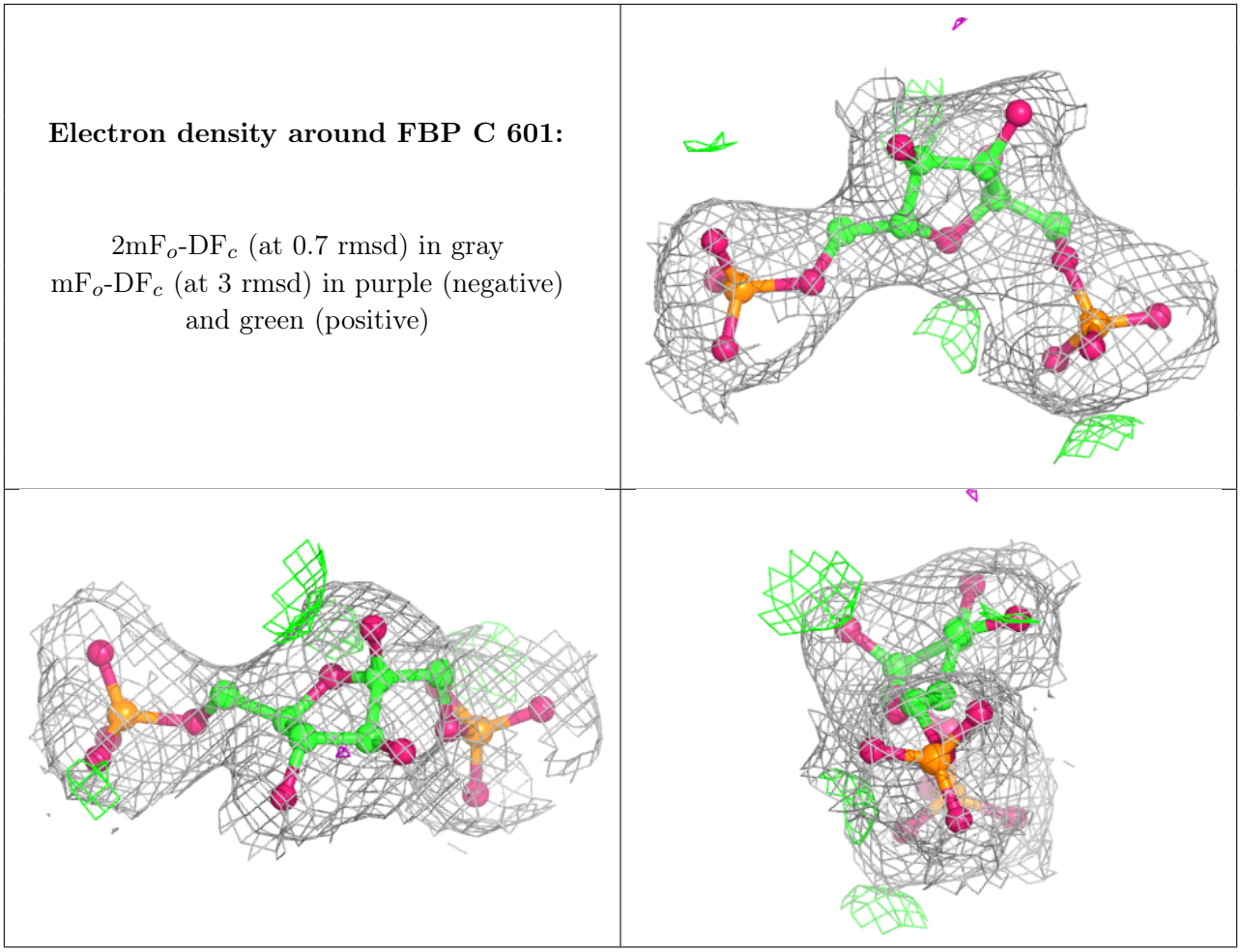
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





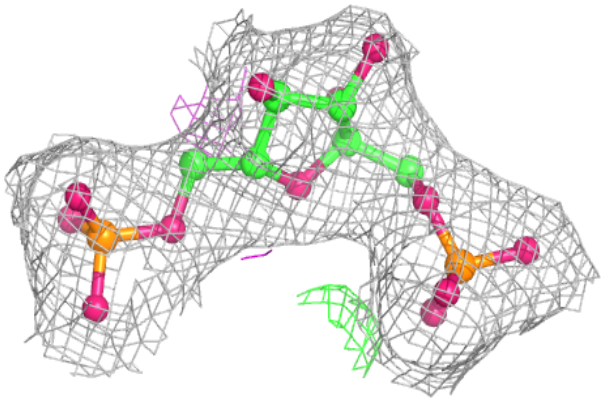
Electron density around FBP C 601:

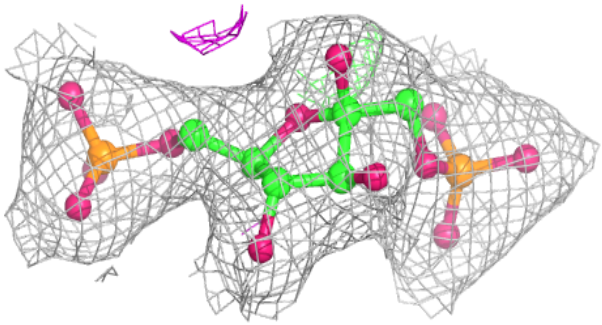
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

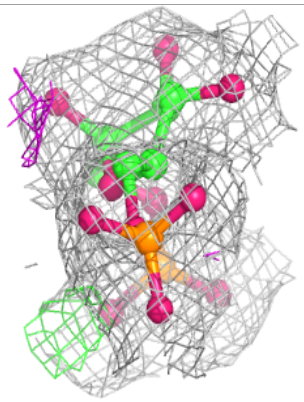


Electron density around FBP D 601:

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

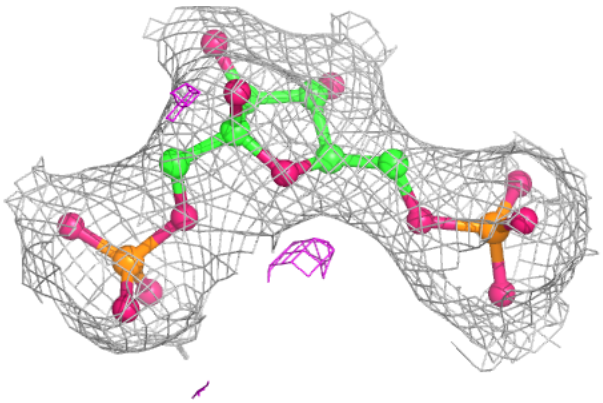


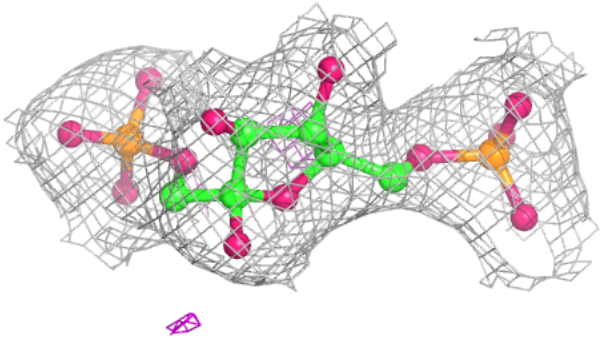


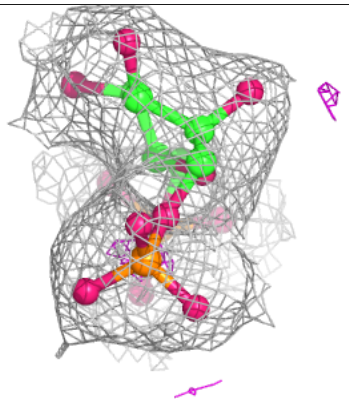


Electron density around FBP G 601:

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

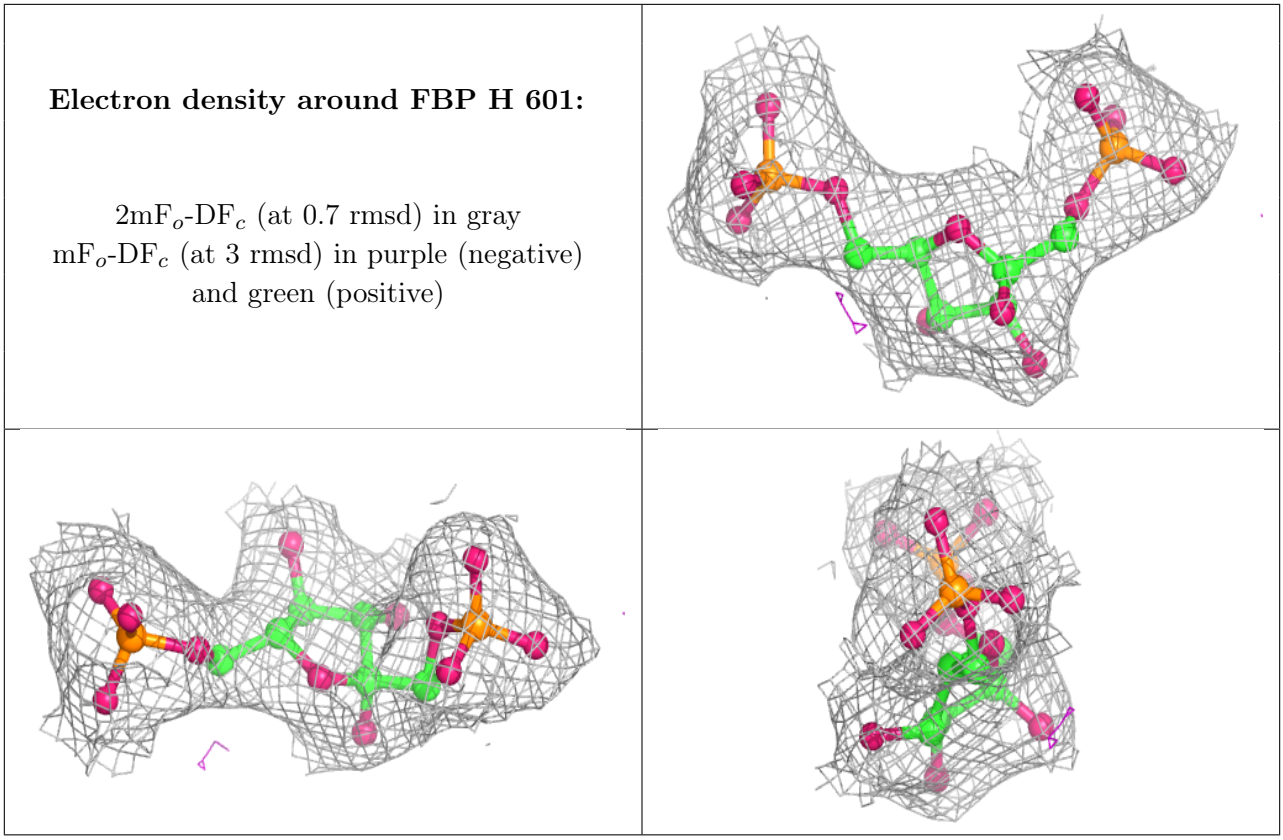






Electron density around FBP H 601:

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



6.5 Other polymers

There are no such residues in this entry.