Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2022 – 05:15 PM EST

PDB ID	:	5SCK
Title	:	Structure of liver pyruvate kinase in complex with anthraquinone derivative 42
Authors	:	Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.
Deposited on	:	2021-12-01
Resolution	:	1.72 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

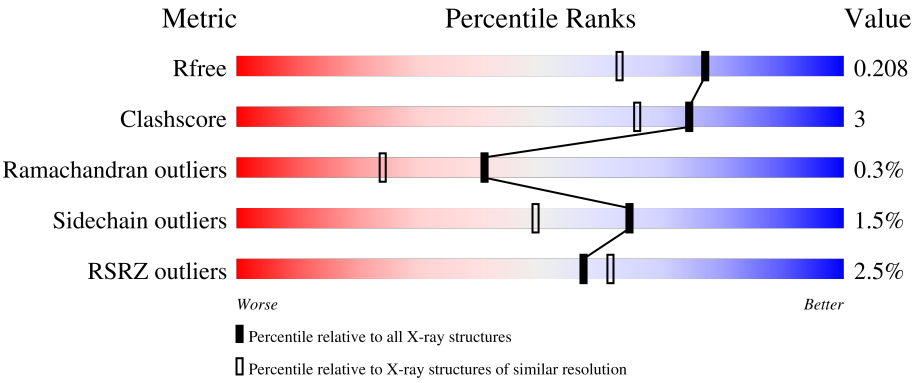
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	4% 85% 7% • 6%
1	B	447	2% 87% 10% •
1	C	447	3% 87% 8% 5%
1	D	447	2% 88% 7% 5%
1	E	447	3% 86% 7% 6%

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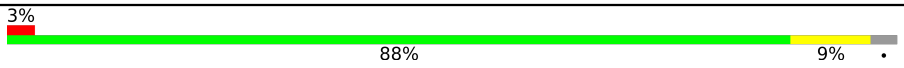
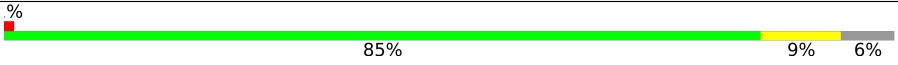
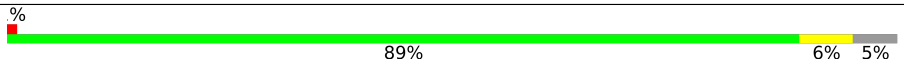
Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 29942 atoms, of which 80 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	13	0
			3238	2033	581	604	20			
1	B	436	Total	C	N	O	S	3	8	0
			3350	2104	604	622	20			
1	C	424	Total	C	N	O	S	0	7	0
			3260	2051	584	606	19			
1	D	425	Total	C	N	O	S	0	8	0
			3258	2045	590	604	19			
1	E	419	Total	C	N	O	S	0	13	0
			3257	2049	584	604	20			
1	F	432	Total	C	N	O	S	0	8	0
			3327	2094	597	616	20			
1	G	422	Total	C	N	O	S	0	9	0
			3257	2048	586	604	19			
1	H	425	Total	C	N	O	S	0	9	0
			3277	2057	597	604	19			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	230	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression tag	UNP Q16716
B	12	ASP	SER	conflict	UNP Q16716
B	130	GLY	-	linker	UNP Q16716
B	131	SER	-	linker	UNP Q16716
B	132	GLY	-	linker	UNP Q16716
C	-1	GLY	-	expression tag	UNP Q16716

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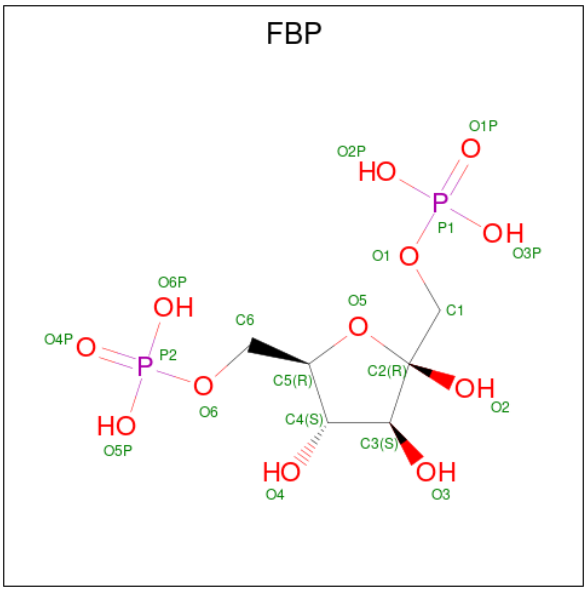
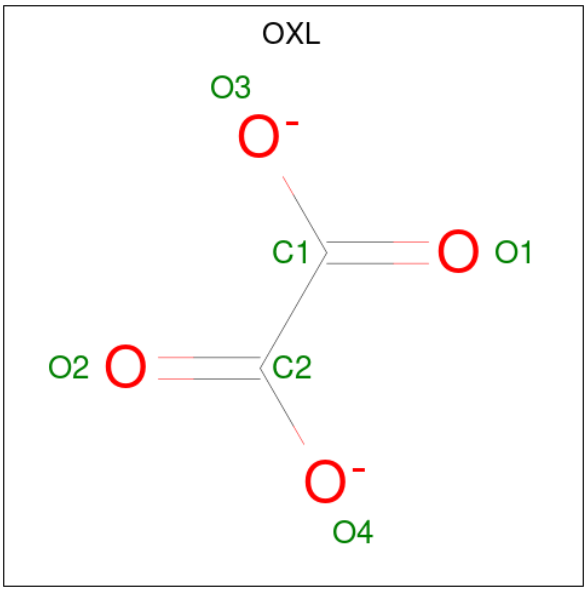
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	228	GLY	-	linker	UNP Q16716
C	229	SER	-	linker	UNP Q16716
C	230	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict	UNP Q16716
D	130	GLY	-	linker	UNP Q16716
D	131	SER	-	linker	UNP Q16716
D	132	GLY	-	linker	UNP Q16716
E	-1	GLY	-	expression tag	UNP Q16716
E	0	SER	-	expression tag	UNP Q16716
E	12	ASP	SER	conflict	UNP Q16716
E	228	GLY	-	linker	UNP Q16716
E	229	SER	-	linker	UNP Q16716
E	230	GLY	-	linker	UNP Q16716
F	-1	GLY	-	expression tag	UNP Q16716
F	0	SER	-	expression tag	UNP Q16716
F	12	ASP	SER	conflict	UNP Q16716
F	228	GLY	-	linker	UNP Q16716
F	229	SER	-	linker	UNP Q16716
F	230	GLY	-	linker	UNP Q16716
G	-1	GLY	-	expression tag	UNP Q16716
G	0	SER	-	expression tag	UNP Q16716
G	12	ASP	SER	conflict	UNP Q16716
G	228	GLY	-	linker	UNP Q16716
G	229	SER	-	linker	UNP Q16716
G	230	GLY	-	linker	UNP Q16716
H	-1	GLY	-	expression tag	UNP Q16716
H	0	SER	-	expression tag	UNP Q16716
H	12	ASP	SER	conflict	UNP Q16716
H	130	GLY	-	linker	UNP Q16716
H	131	SER	-	linker	UNP Q16716
H	132	GLY	-	linker	UNP Q16716

- 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		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
2	H	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is OXALATE ION (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

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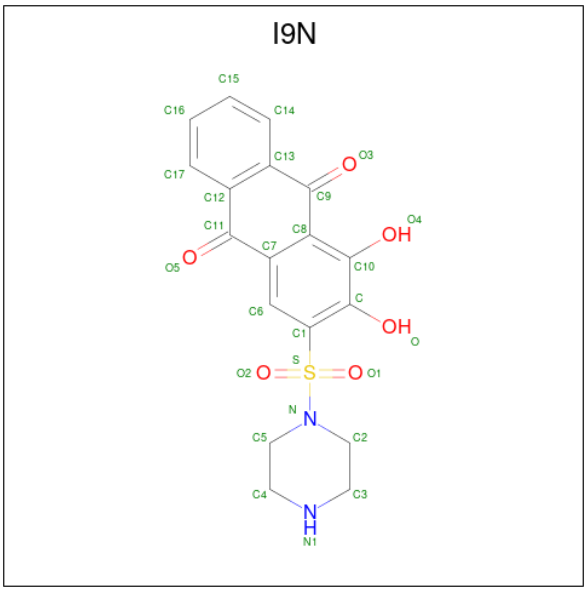
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

- 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 1,2-dihydroxy-3-(piperazine-1-sulfonyl)anthracene-9,10-dione (three-letter code: I9N) (formula: $C_{18}H_{16}N_2O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	S	16	0
			43	18	16	2	6	1		
6	C	1	Total	C	H	N	O	S	16	0
			43	18	16	2	6	1		
6	E	1	Total	C	H	N	O	S	16	0
			43	18	16	2	6	1		
6	F	1	Total	C	H	N	O	S	16	0
			43	18	16	2	6	1		
6	G	1	Total	C	H	N	O	S	16	0
			43	18	16	2	6	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	288	Total	O	0	0
			288	288		
7	B	371	Total	O	0	0
			371	371		
7	C	427	Total	O	0	0
			427	427		
7	D	478	Total	O	0	0
			478	478		
7	E	336	Total	O	0	0
			336	336		
7	F	425	Total	O	0	0
			425	425		
7	G	462	Total	O	0	0
			462	462		

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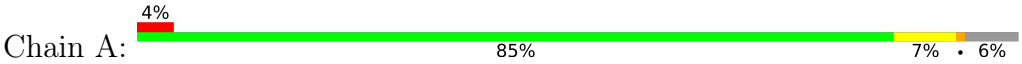
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	492	Total 492	O 492	0	0

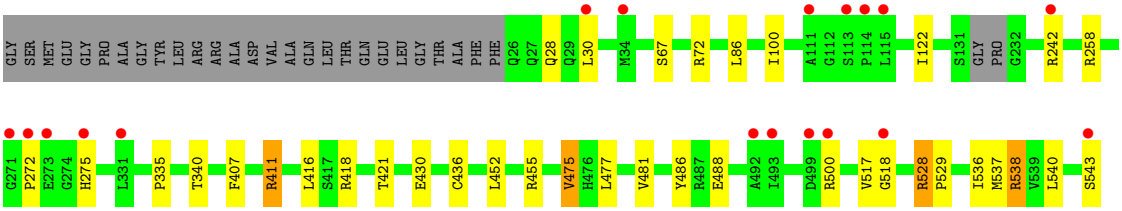
3 Residue-property plots (i)

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

• Molecule 1: Pyruvate kinase

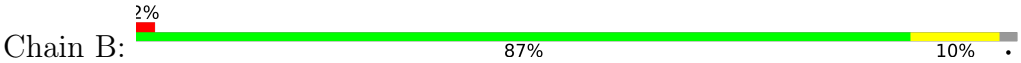
Chain A:

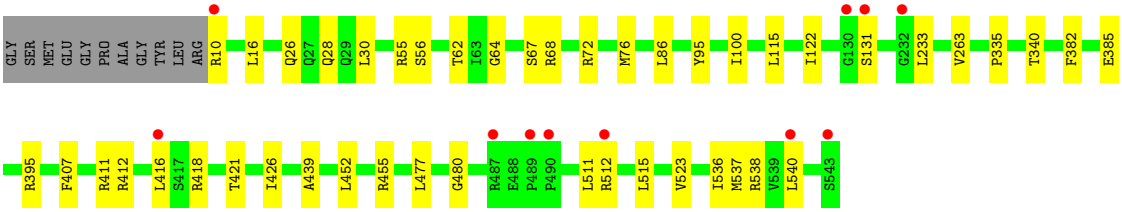




• Molecule 1: Pyruvate kinase

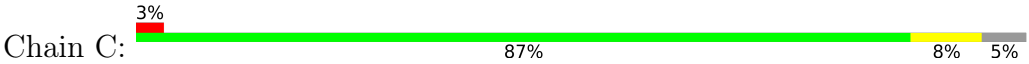
Chain B:

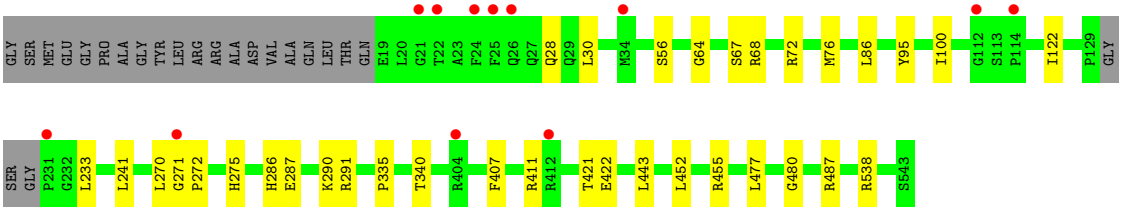




• Molecule 1: Pyruvate kinase

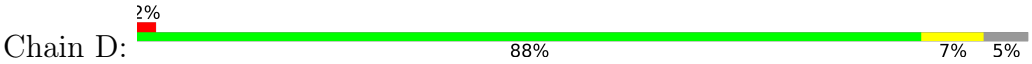
Chain C:

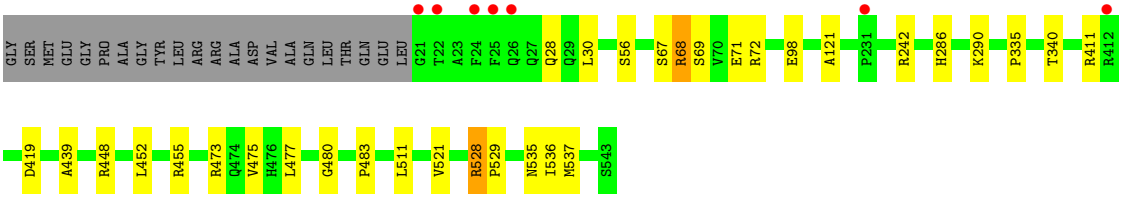




• Molecule 1: Pyruvate kinase

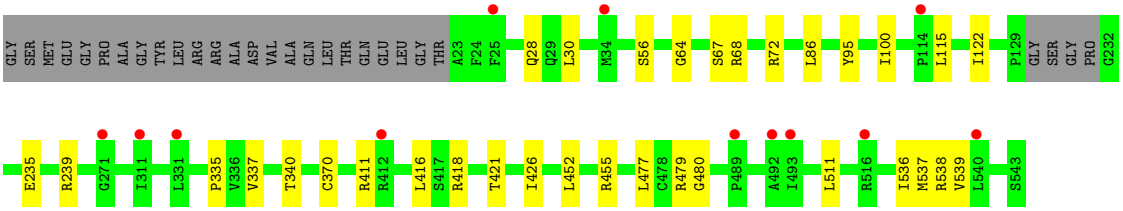
Chain D:





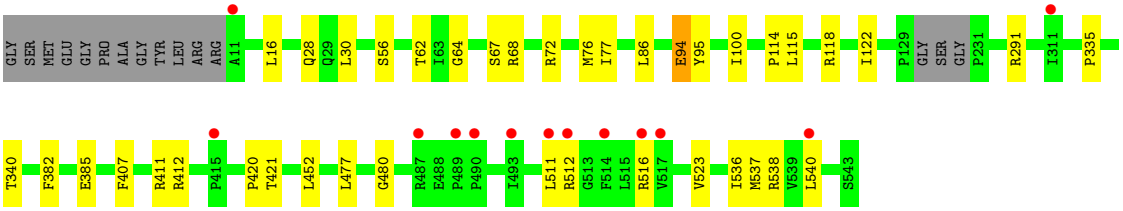
• Molecule 1: Pyruvate kinase

Chain E:



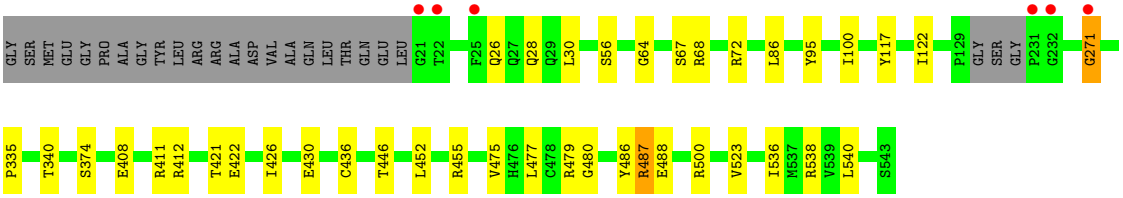
• Molecule 1: Pyruvate kinase

Chain F:



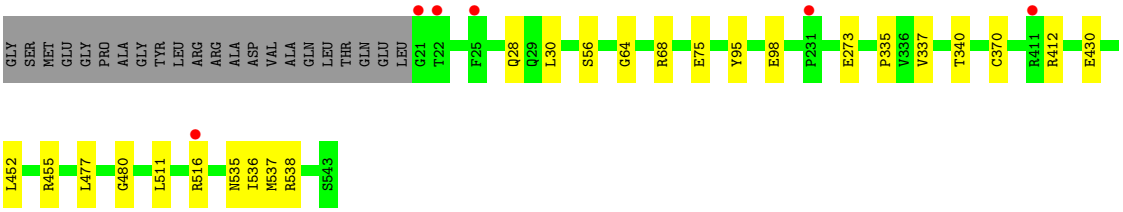
• Molecule 1: Pyruvate kinase

Chain G:



• Molecule 1: Pyruvate kinase

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	207.55Å 112.03Å 188.18Å 90.00° 91.21° 90.00°	Depositor
Resolution (Å)	188.14 – 1.72 188.14 – 1.72	Depositor EDS
% Data completeness (in resolution range)	71.4 (188.14-1.72) 71.3 (188.14-1.72)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.72Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.194 , 0.217 0.188 , 0.208	Depositor DCC
R_{free} test set	16591 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29942	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 38.27 % 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 3.7788e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, I9N, K, FBP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/3328	0.55	0/4497
1	B	0.41	0/3429	0.56	0/4636
1	C	0.43	0/3335	0.58	0/4508
1	D	0.46	0/3337	0.58	0/4510
1	E	0.37	0/3350	0.53	0/4527
1	F	0.41	0/3405	0.55	0/4603
1	G	0.44	0/3335	0.58	0/4507
1	H	0.46	0/3357	0.58	0/4537
All	All	0.42	0/26876	0.56	0/36325

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	3238	0	3312	24	0
1	B	3350	0	3417	29	0
1	C	3260	0	3320	27	0
1	D	3258	0	3314	23	0
1	E	3257	0	3323	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3327	0	3399	24	0
1	G	3257	0	3320	24	0
1	H	3277	0	3341	16	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	B	27	16	0	1	0
6	C	27	16	0	0	0
6	E	27	16	0	0	0
6	F	27	16	0	1	0
6	G	27	16	0	1	0
7	A	288	0	0	0	0
7	B	371	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	427	0	0	4	0
7	D	478	0	0	0	0
7	E	336	0	0	0	0
7	F	425	0	0	0	0
7	G	462	0	0	1	0
7	H	492	0	0	2	0
All	All	29862	80	26826	168	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:GLY:HA3	7:C:941:HOH:O	1.29	1.26
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.57	0.85
1:D:528:ARG:HD2	1:D:529:PRO:O	1.80	0.81
1:H:68:ARG:NH2	1:H:95:TYR:O	2.16	0.79
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.64	0.78
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.66	0.77
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.66	0.77
1:A:528:ARG:HD2	1:A:529:PRO:O	1.87	0.75
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.69	0.75
1:A:418[B]:ARG:HG3	1:B:16:LEU:HD11	1.71	0.72
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.71	0.71
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.72	0.71
1:E:418[B]:ARG:HG3	1:F:16:LEU:HD11	1.72	0.70
1:A:538:ARG:HG3	1:B:536:ILE:HG12	1.71	0.70
1:D:71[B]:GLU:H	1:D:71[B]:GLU:CD	1.97	0.68
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.78	0.65
1:C:407:PHE:CE2	1:C:411:ARG:NH1	2.64	0.65
1:B:26:GLN:NE2	7:B:701:HOH:O	2.23	0.65
1:C:272:PRO:HD2	7:C:941:HOH:O	1.96	0.65
1:B:407:PHE:CE2	1:B:411:ARG:NH1	2.65	0.64
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.64	0.64
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.13	0.64
1:C:411:ARG:NH2	1:D:411:ARG:NH2	2.46	0.63
1:B:115:LEU:HA	1:B:512:ARG:HD2	1.81	0.63
1:G:64:GLY:O	1:G:68:ARG:HG3	1.98	0.62
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.81	0.62
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.84	0.60
1:C:64:GLY:O	1:C:68:ARG:HG3	2.01	0.60
1:E:64:GLY:O	1:E:68:ARG:HG3	2.02	0.59
1:F:67:SER:HA	1:F:72:ARG:HG2	1.84	0.59
1:B:407:PHE:CD2	1:B:411:ARG:NH1	2.71	0.58
1:C:67:SER:HA	1:C:72:ARG:HG2	1.85	0.58
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.85	0.58
1:D:528:ARG:CD	1:D:529:PRO:O	2.52	0.58
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.86	0.58
1:H:68:ARG:HH22	1:H:98:GLU:HB2	1.70	0.57
1:A:67:SER:HA	1:A:72:ARG:HG2	1.86	0.57
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.85	0.57
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.86	0.57
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.86	0.57
1:F:64:GLY:O	1:F:68:ARG:HG3	2.06	0.56
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.88	0.56
1:G:374[B]:SER:OG	6:G:603:I9N:O2	2.24	0.56
1:D:535:ASN:OD1	1:D:536:ILE:HG13	2.06	0.56
1:B:67:SER:HA	1:B:72:ARG:HG2	1.88	0.55
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.88	0.55
1:C:271:GLY:O	1:C:275:HIS:CE1	2.58	0.55
1:B:64:GLY:O	1:B:68:ARG:HG3	2.06	0.55
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.88	0.55
1:A:407:PHE:CE2	1:A:411:ARG:NH1	2.75	0.55
1:C:100:ILE:HG23	1:C:122:ILE:HD13	1.88	0.55
1:G:67:SER:HA	1:G:72:ARG:HG2	1.89	0.55
1:D:69:SER:OG	1:D:71[B]:GLU:HG2	2.07	0.54
1:G:523:VAL:HG21	1:G:540[A]:LEU:HD12	1.88	0.54
1:E:67:SER:HA	1:E:72:ARG:HG2	1.90	0.53
1:G:271:GLY:HA2	7:G:853:HOH:O	2.09	0.52
1:A:100:ILE:HG23	1:A:122:ILE:HD13	1.92	0.52
1:B:62:THR:HG21	6:B:603:I9N:O1	2.10	0.52
1:F:28:GLN:HG3	1:F:30:LEU:HG	1.91	0.52
1:G:86:LEU:HD11	1:G:100:ILE:HG12	1.91	0.52
1:H:56:SER:HB2	1:H:480:GLY:CA	2.39	0.52
1:B:86:LEU:HD11	1:B:100:ILE:HG12	1.92	0.52
1:A:416:LEU:HB3	1:B:16:LEU:HD22	1.92	0.52
1:C:538:ARG:HD3	7:C:792:HOH:O	2.10	0.52
1:C:86:LEU:HD11	1:C:100:ILE:HG12	1.92	0.51
1:F:62:THR:HG21	6:F:603:I9N:O1	2.10	0.51
1:F:100:ILE:HG23	1:F:122:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:PRO:HD3	1:G:446:THR:HG22	1.92	0.51
1:G:56:SER:HB2	1:G:480:GLY:CA	2.40	0.50
1:A:28:GLN:HG3	1:A:30:LEU:HG	1.94	0.50
1:F:86:LEU:HD11	1:F:100:ILE:HG12	1.93	0.50
1:C:28:GLN:HG3	1:C:30:LEU:HG	1.94	0.49
1:D:28:GLN:HG3	1:D:30:LEU:HG	1.94	0.49
1:E:100:ILE:HG23	1:E:122:ILE:HD13	1.94	0.49
1:E:28:GLN:HG3	1:E:30:LEU:HG	1.95	0.49
1:B:100:ILE:HG23	1:B:122:ILE:HD13	1.93	0.49
1:G:430[A]:GLU:OE1	1:H:430[A]:GLU:OE1	2.31	0.49
1:E:86:LEU:HD11	1:E:100:ILE:HG12	1.95	0.49
1:H:28:GLN:HG3	1:H:30:LEU:HG	1.95	0.49
1:G:100:ILE:HG23	1:G:122:ILE:HD13	1.95	0.48
1:B:68:ARG:HD2	1:B:95:TYR:OH	2.14	0.48
1:A:517:VAL:HG22	1:A:543:SER:HB3	1.94	0.48
1:G:28:GLN:HG3	1:G:30:LEU:HG	1.95	0.48
1:A:411:ARG:NH1	1:A:430:GLU:OE2	2.46	0.48
1:A:517:VAL:HG22	1:A:543:SER:CB	2.44	0.48
1:F:67:SER:HB2	1:F:76[B]:MET:SD	2.54	0.48
1:F:94:GLU:H	1:F:94:GLU:CD	2.17	0.48
1:B:28:GLN:HG3	1:B:30:LEU:HG	1.94	0.47
1:E:68:ARG:HD2	1:E:95:TYR:OH	2.15	0.47
1:F:68:ARG:HD2	1:F:95:TYR:OH	2.14	0.47
1:B:56:SER:HB2	1:B:480:GLY:CA	2.44	0.47
1:A:518:GLY:O	1:B:418:ARG:NH2	2.47	0.47
1:E:235:GLU:O	1:E:239:ARG:HD3	2.14	0.47
1:G:68:ARG:HD2	1:G:95:TYR:OH	2.16	0.46
1:C:411:ARG:HH22	1:D:411:ARG:NH2	2.13	0.46
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.79	0.46
1:F:56:SER:HB2	1:F:480:GLY:CA	2.45	0.46
1:A:86:LEU:HD11	1:A:100:ILE:HG12	1.97	0.46
1:C:68:ARG:HD2	1:C:95:TYR:OH	2.16	0.46
1:E:56:SER:HB2	1:E:480:GLY:CA	2.45	0.46
1:H:516:ARG:HD3	7:H:948:HOH:O	2.14	0.46
1:D:67:SER:HA	1:D:72:ARG:HG2	1.98	0.45
1:C:411:ARG:NH2	1:D:411:ARG:HH21	2.12	0.45
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.51	0.45
1:D:439:ALA:O	1:D:521:VAL:HG23	2.15	0.45
1:C:452:LEU:O	1:C:455:ARG:HG2	2.16	0.45
1:C:56:SER:HB2	1:C:480:GLY:CA	2.46	0.45
1:C:272:PRO:CD	7:C:941:HOH:O	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:335:PRO:HB3	1:F:477:LEU:O	2.18	0.45
1:B:439:ALA:HB3	1:B:515:LEU:HD21	1.99	0.44
1:E:335:PRO:HB3	1:E:477:LEU:O	2.17	0.44
1:G:335:PRO:HB3	1:G:477:LEU:O	2.17	0.44
1:B:523:VAL:HG21	1:B:540[A]:LEU:HD12	2.00	0.44
1:D:56:SER:HB2	1:D:480:GLY:CA	2.47	0.44
1:A:452:LEU:O	1:A:455:ARG:HG2	2.17	0.44
1:C:67:SER:HB2	1:C:76[B]:MET:SD	2.58	0.44
1:B:67:SER:HB2	1:B:76[B]:MET:SD	2.57	0.44
1:G:452:LEU:O	1:G:455:ARG:HG2	2.18	0.44
1:E:416:LEU:HB3	1:F:16:LEU:HD22	1.99	0.44
1:F:523:VAL:HG21	1:F:540[A]:LEU:HD12	1.99	0.44
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.99	0.44
1:A:475:VAL:HG22	1:A:481:VAL:HG11	2.00	0.43
1:D:419:ASP:OD2	1:D:448:ARG:NH2	2.50	0.43
1:A:421:THR:HG22	1:A:452:LEU:HD12	2.00	0.43
1:F:77:ILE:HG22	1:F:118:ARG:HD3	1.98	0.43
1:F:115:LEU:HD21	1:F:511:LEU:HD12	2.00	0.43
1:G:117:TYR:CD2	1:G:487:ARG:NH2	2.87	0.43
1:H:68:ARG:NH2	1:H:98:GLU:HB2	2.32	0.43
1:C:335:PRO:HB3	1:C:477:LEU:O	2.18	0.43
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.53	0.43
1:A:335:PRO:HB3	1:A:477:LEU:O	2.19	0.43
1:B:452:LEU:O	1:B:455:ARG:HG2	2.19	0.43
1:B:335:PRO:HB3	1:B:477:LEU:O	2.18	0.42
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.02	0.42
1:G:408:GLU:HG3	1:G:411:ARG:HH22	1.84	0.42
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.35	0.42
1:B:55:ARG:HB2	1:B:395:ARG:HG2	2.00	0.42
1:E:421:THR:HG22	1:E:452:LEU:HD12	2.01	0.42
1:E:452:LEU:O	1:E:455:ARG:HG2	2.19	0.42
1:F:421:THR:HG22	1:F:452:LEU:HD12	2.02	0.42
1:H:64:GLY:O	1:H:68:ARG:HG3	2.20	0.42
1:H:335:PRO:HB3	1:H:477:LEU:O	2.20	0.42
1:C:233:LEU:HD21	1:C:241:LEU:HD12	2.02	0.41
1:H:535:ASN:OD1	1:H:536:ILE:HG13	2.20	0.41
1:C:287:GLU:HG2	1:C:291:ARG:HD2	2.02	0.41
1:D:335:PRO:HB3	1:D:477:LEU:O	2.20	0.41
1:B:421:THR:HG22	1:B:452:LEU:HD12	2.02	0.41
1:C:286:HIS:CE1	1:C:290:LYS:HG3	2.56	0.41
1:D:286:HIS:CE1	1:D:290:LYS:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:VAL:HG13	1:A:543:SER:HB3	2.03	0.41
1:C:421:THR:HG22	1:C:452:LEU:HD12	2.03	0.41
1:D:121:ALA:HA	1:D:473:ARG:HB3	2.03	0.41
1:E:337:VAL:HG22	1:E:370:CYS:HB2	2.03	0.41
1:F:114:PRO:O	1:F:512:ARG:NH2	2.50	0.41
1:G:479:ARG:HG2	1:G:480:GLY:N	2.36	0.41
1:H:452:LEU:O	1:H:455:ARG:HG2	2.21	0.41
1:F:382:PHE:HB3	1:F:385:GLU:HB2	2.02	0.41
1:A:242:ARG:HD3	1:A:242:ARG:HA	1.95	0.40
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.93	0.40
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.55	0.40
1:E:479:ARG:HG2	1:E:480:GLY:N	2.36	0.40
1:D:452:LEU:O	1:D:455:ARG:HG2	2.21	0.40
1:G:421:THR:HG22	1:G:452:LEU:HD12	2.03	0.40
1:H:75:GLU:HG3	7:H:1148:HOH:O	2.21	0.40
1:A:436:CYS:SG	1:B:416:LEU:HD13	2.62	0.40
1:D:475:VAL:CG2	1:D:483:PRO:HB3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/447 (96%)	422 (99%)	4 (1%)	1 (0%)	47	30
1	B	442/447 (99%)	437 (99%)	4 (1%)	1 (0%)	47	30
1	C	427/447 (96%)	422 (99%)	4 (1%)	1 (0%)	47	30
1	D	431/447 (96%)	428 (99%)	2 (0%)	1 (0%)	47	30
1	E	428/447 (96%)	424 (99%)	3 (1%)	1 (0%)	47	30
1	F	436/447 (98%)	432 (99%)	3 (1%)	1 (0%)	47	30
1	G	427/447 (96%)	421 (99%)	4 (1%)	2 (0%)	29	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	432/447 (97%)	428 (99%)	3 (1%)	1 (0%)	47 30
All	All	3450/3576 (96%)	3414 (99%)	27 (1%)	9 (0%)	41 24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR
1	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	345/352 (98%)	336 (97%)	9 (3%)	46 26
1	B	353/352 (100%)	346 (98%)	7 (2%)	55 37
1	C	344/352 (98%)	340 (99%)	4 (1%)	71 58
1	D	343/352 (97%)	337 (98%)	6 (2%)	60 44
1	E	346/352 (98%)	342 (99%)	4 (1%)	71 58
1	F	351/352 (100%)	345 (98%)	6 (2%)	60 44
1	G	344/352 (98%)	337 (98%)	7 (2%)	55 37
1	H	345/352 (98%)	341 (99%)	4 (1%)	71 58
All	All	2771/2816 (98%)	2724 (98%)	47 (2%)	65 44

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	ARG
1	A	411	ARG
1	A	475	VAL
1	A	500	ARG
1	A	528	ARG
1	A	537[A]	MET
1	A	537[B]	MET
1	A	538	ARG
1	A	540	LEU
1	B	10	ARG
1	B	131	SER
1	B	263	VAL
1	B	412	ARG
1	B	511	LEU
1	B	537[A]	MET
1	B	537[B]	MET
1	C	270[A]	LEU
1	C	270[B]	LEU
1	C	443	LEU
1	C	487	ARG
1	D	68	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	511	LEU
1	D	528	ARG
1	D	537	MET
1	E	115	LEU
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	F	94	GLU
1	F	291	ARG
1	F	412	ARG
1	F	516	ARG
1	F	537[A]	MET
1	F	537[B]	MET
1	G	26	GLN
1	G	412	ARG
1	G	436	CYS
1	G	475	VAL
1	G	487	ARG
1	G	500[A]	ARG
1	G	500[B]	ARG

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Mol	Chain	Res	Type
1	H	273	GLU
1	H	412	ARG
1	H	511	LEU
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	G	26	GLN
1	G	470	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 37 ligands modelled in this entry, 16 are monoatomic - leaving 21 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	F	602	4	0,5,5	-	-	0,6,6	-	-
3	OXL	B	602	4	0,5,5	-	-	0,6,6	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FBP	H	601	-	18,20,20	0.80	0	23,32,32	0.76	1 (4%)
2	FBP	G	601	-	18,20,20	0.42	0	23,32,32	0.73	0
6	I9N	G	603	-	30,30,30	0.33	0	44,46,46	0.59	1 (2%)
6	I9N	C	603	-	30,30,30	0.28	0	44,46,46	0.79	1 (2%)
6	I9N	E	603	-	30,30,30	0.30	0	44,46,46	0.66	1 (2%)
3	OXL	C	602	4	0,5,5	-	-	0,6,6	-	-
2	FBP	E	601	-	18,20,20	0.78	1 (5%)	23,32,32	0.82	1 (4%)
2	FBP	D	601	-	18,20,20	0.62	0	23,32,32	0.74	1 (4%)
3	OXL	H	602	4	0,5,5	-	-	0,6,6	-	-
6	I9N	B	603	-	30,30,30	0.32	0	44,46,46	0.57	1 (2%)
2	FBP	F	601	-	18,20,20	0.47	0	23,32,32	0.62	0
3	OXL	D	602	4	0,5,5	-	-	0,6,6	-	-
2	FBP	A	601	-	18,20,20	0.53	0	23,32,32	0.76	1 (4%)
2	FBP	C	601	-	18,20,20	0.76	0	23,32,32	0.89	0
2	FBP	B	601	-	18,20,20	0.86	1 (5%)	23,32,32	0.83	1 (4%)
3	OXL	G	602	4	0,5,5	-	-	0,6,6	-	-
6	I9N	F	603	-	30,30,30	0.27	0	44,46,46	0.58	1 (2%)
3	OXL	E	602	4	0,5,5	-	-	0,6,6	-	-
3	OXL	A	602	4	0,5,5	-	-	0,6,6	-	-

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	F	602	4	-	0/0/4/4	-
3	OXL	B	602	4	-	0/0/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
6	I9N	G	603	-	-	3/12/36/36	1/4/4/4
6	I9N	C	603	-	-	3/12/36/36	1/4/4/4
6	I9N	E	603	-	-	4/12/36/36	0/4/4/4
3	OXL	C	602	4	-	0/0/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	0/0/4/4	-
6	I9N	B	603	-	-	4/12/36/36	1/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	4	-	0/0/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	G	602	4	-	0/0/4/4	-
6	I9N	F	603	-	-	4/12/36/36	0/4/4/4
3	OXL	E	602	4	-	0/0/4/4	-
3	OXL	A	602	4	-	0/0/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FBP	P2-O5P	-2.27	1.46	1.54
2	E	601	FBP	P1-O3P	-2.21	1.46	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	603	I9N	C1-S-N	3.83	113.88	106.81
6	G	603	I9N	C2-N-S	2.72	121.99	117.05
6	E	603	I9N	C5-N-S	2.64	121.84	117.05
2	E	601	FBP	O3P-P1-O2P	2.60	117.59	107.64
2	D	601	FBP	O5P-P2-O6	2.44	113.22	106.73
2	H	601	FBP	O5P-P2-O6	2.37	113.03	106.73
6	F	603	I9N	C1-S-N	2.36	111.17	106.81
2	B	601	FBP	O3P-P1-O2P	2.11	115.72	107.64
6	B	603	I9N	C2-N-S	2.05	120.78	117.05
2	A	601	FBP	O3P-P1-O1P	2.02	118.58	110.68

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
6	C	603	I9N	C5-N-S-O2
6	E	603	I9N	C2-N-S-O2
6	G	603	I9N	C5-N-S-O2
6	B	603	I9N	C5-N-S-O2

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Mol	Chain	Res	Type	Atoms
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	E	603	I9N	C5-N-S-C1
6	F	603	I9N	C5-N-S-C1
6	E	603	I9N	C5-N-S-O2
6	F	603	I9N	C2-N-S-O2
6	B	603	I9N	C5-N-S-C1
6	C	603	I9N	C5-N-S-C1
6	F	603	I9N	C2-N-S-C1
6	E	603	I9N	C2-N-S-C1
6	G	603	I9N	C5-N-S-C1
6	B	603	I9N	C2-N-S-O2
6	F	603	I9N	C5-N-S-O2
6	B	603	I9N	C2-N-S-C1
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	G	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
6	C	603	I9N	C6-C1-S-O2
6	G	603	I9N	C2-N-S-O2

All (3) ring outliers are listed below:

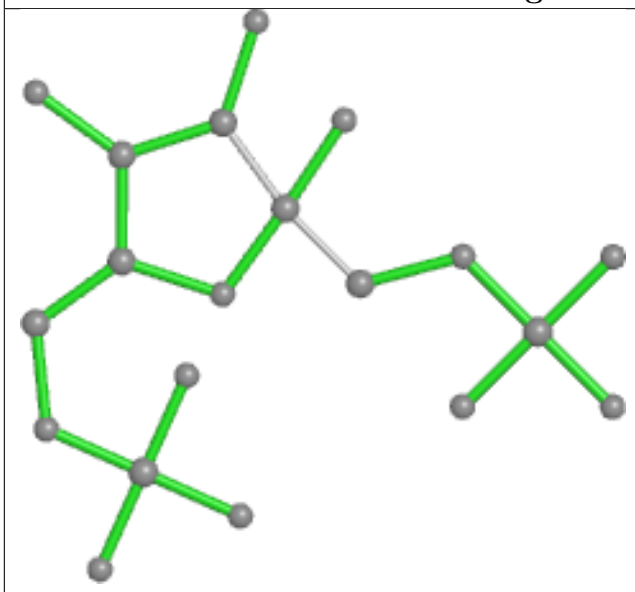
Mol	Chain	Res	Type	Atoms
6	B	603	I9N	C2-C3-C4-C5-N-N1
6	G	603	I9N	C2-C3-C4-C5-N-N1
6	C	603	I9N	C2-C3-C4-C5-N-N1

3 monomers are involved in 3 short contacts:

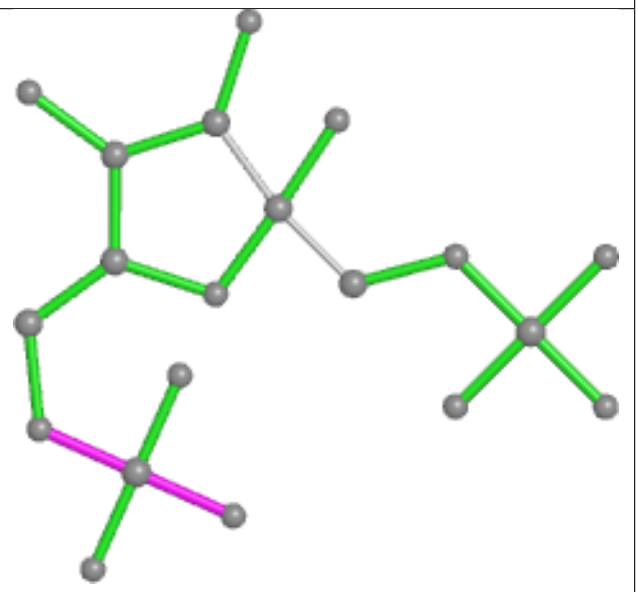
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	603	I9N	1	0
6	B	603	I9N	1	0
6	F	603	I9N	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

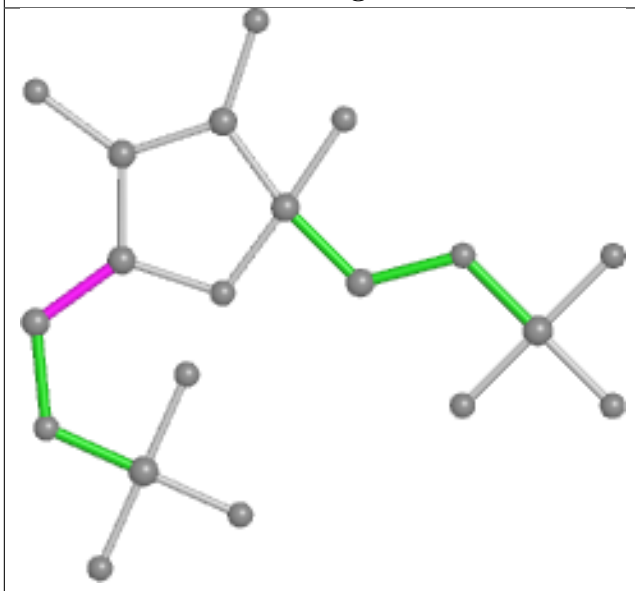
Ligand FBP H 601



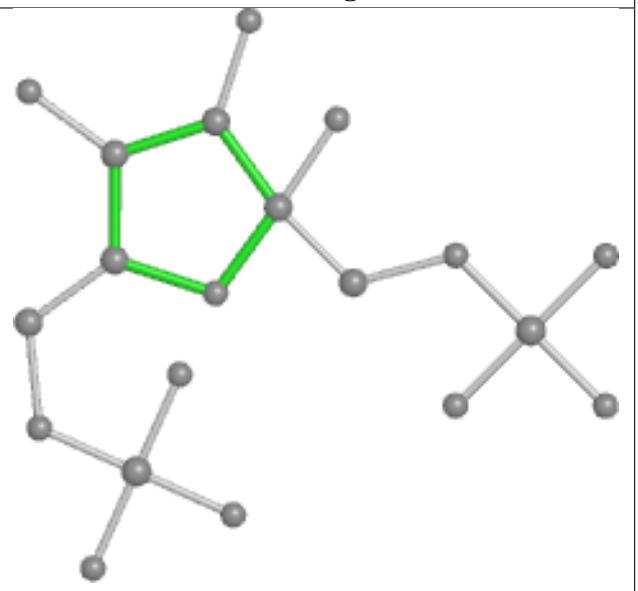
Bond lengths



Bond angles

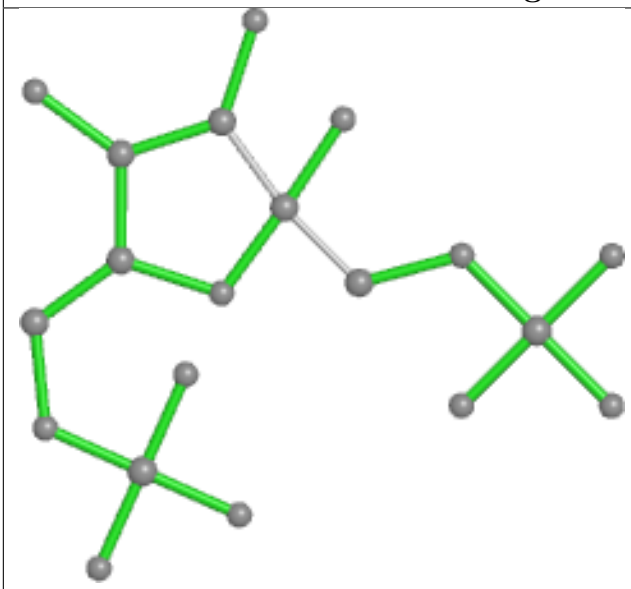


Torsions

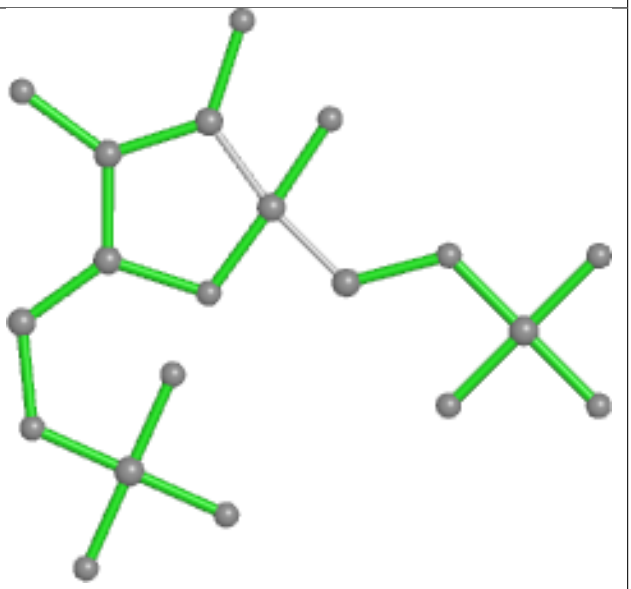


Rings

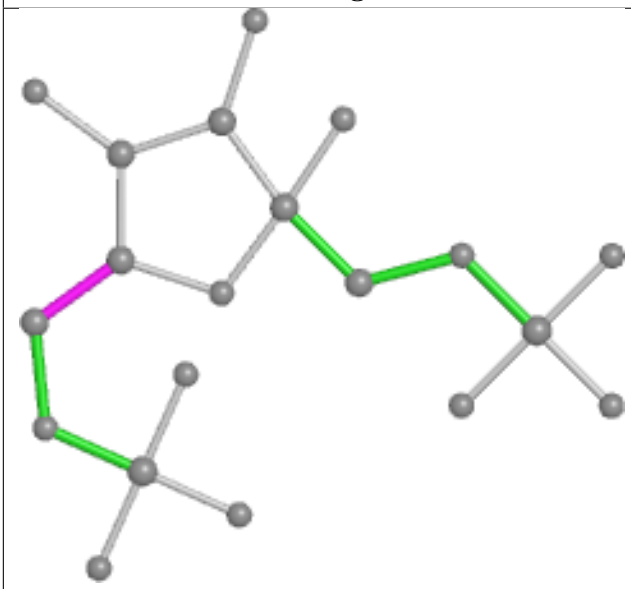
Ligand FBP G 601



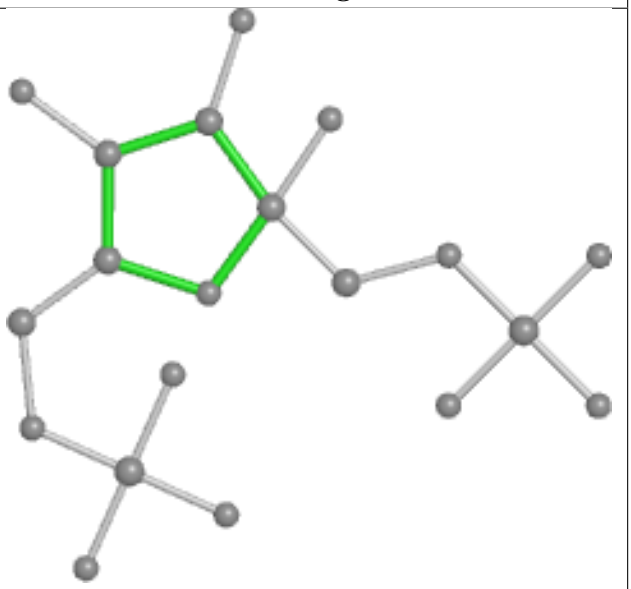
Bond lengths



Bond angles

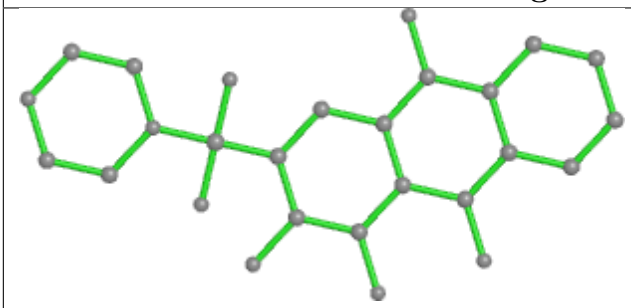


Torsions



Rings

Ligand I9N G 603



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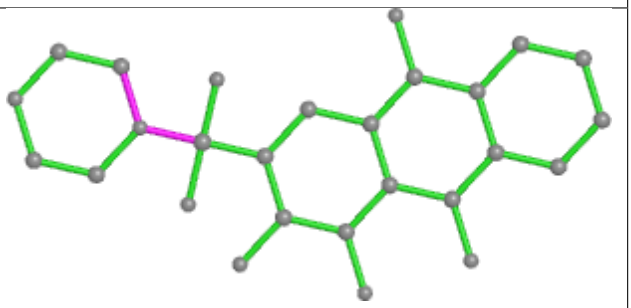
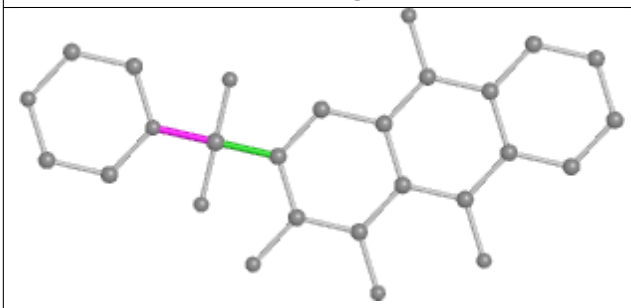
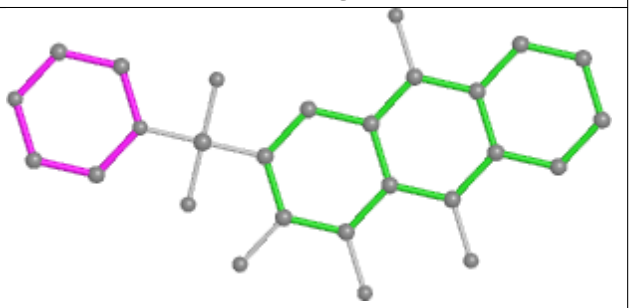


Bond angles

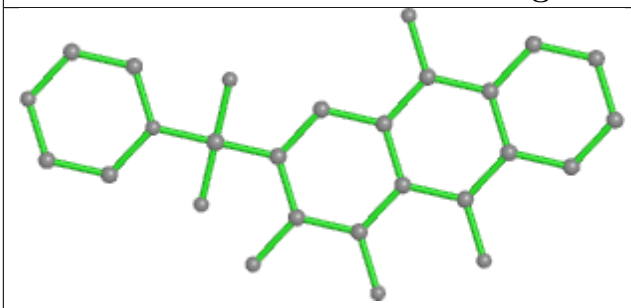


Torsions

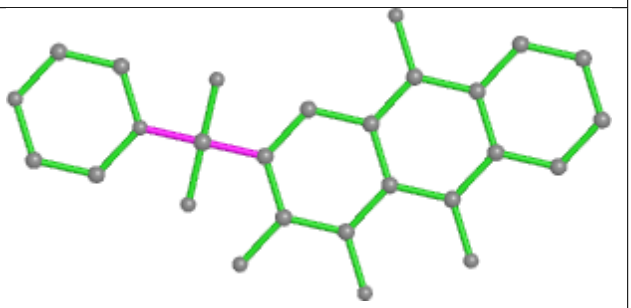


Rings

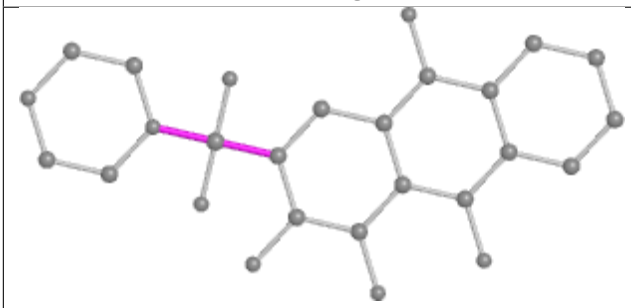
Ligand I9N C 603



Bond lengths



Bond angles



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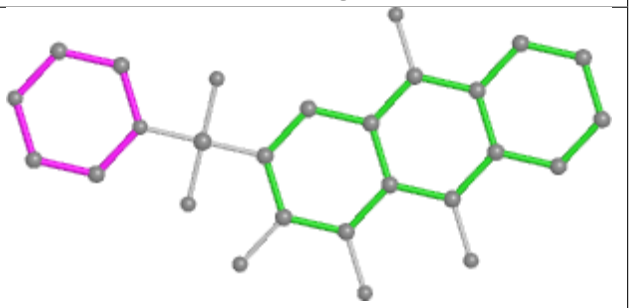
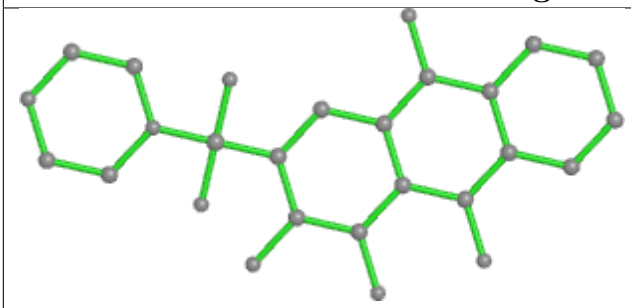
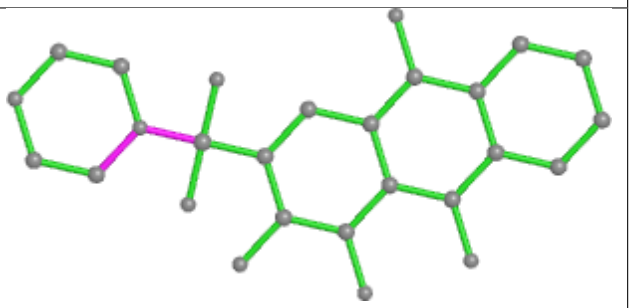


Rings

Ligand I9N E 603



Bond lengths



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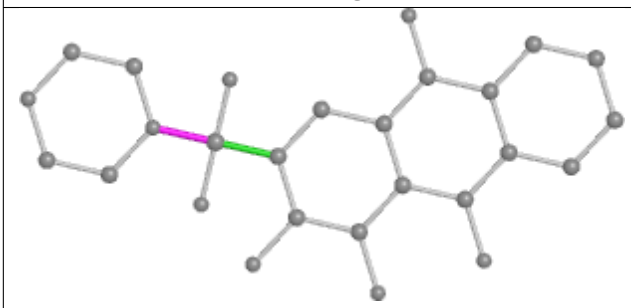

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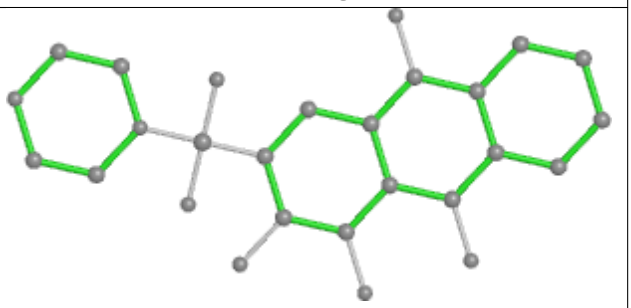

Rings

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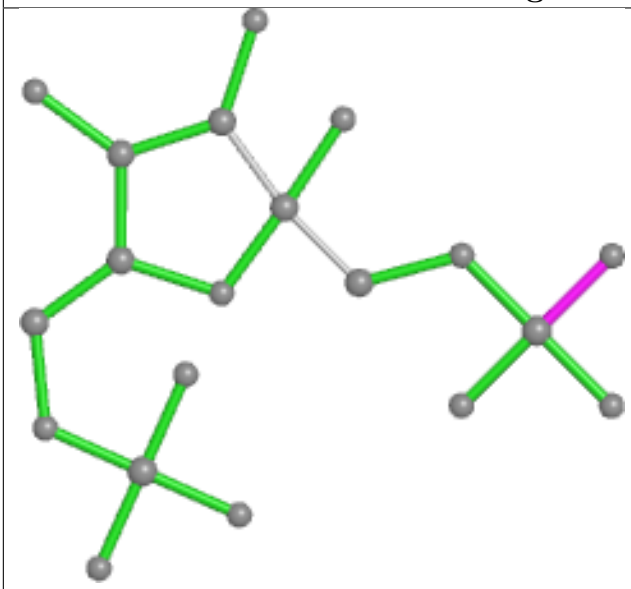

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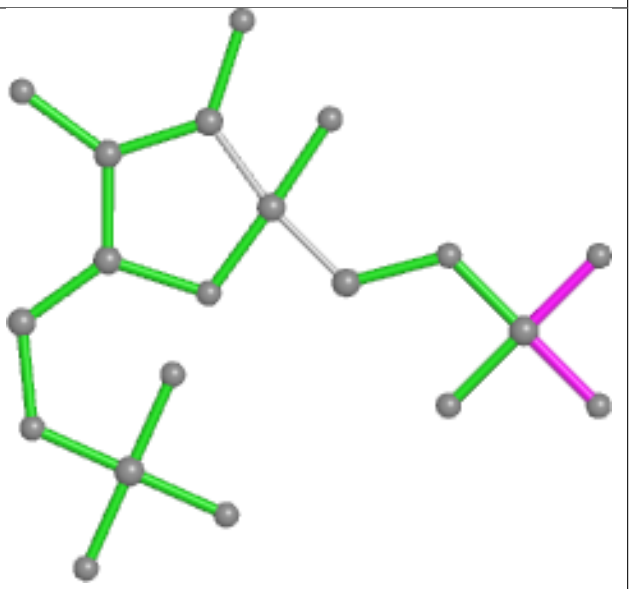

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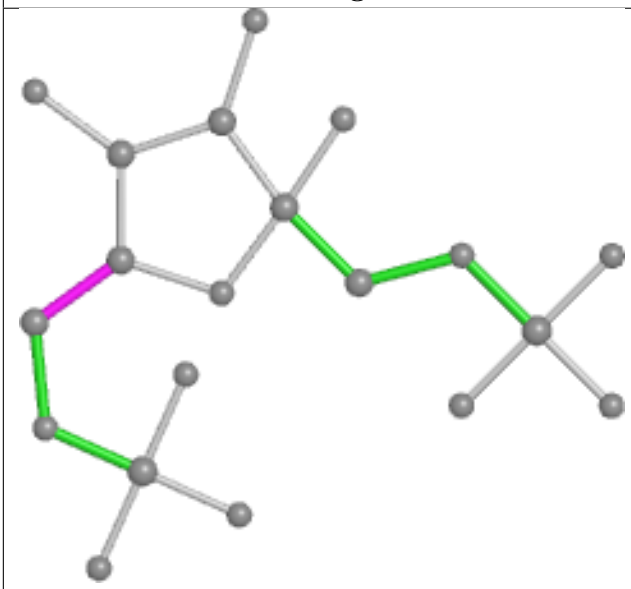
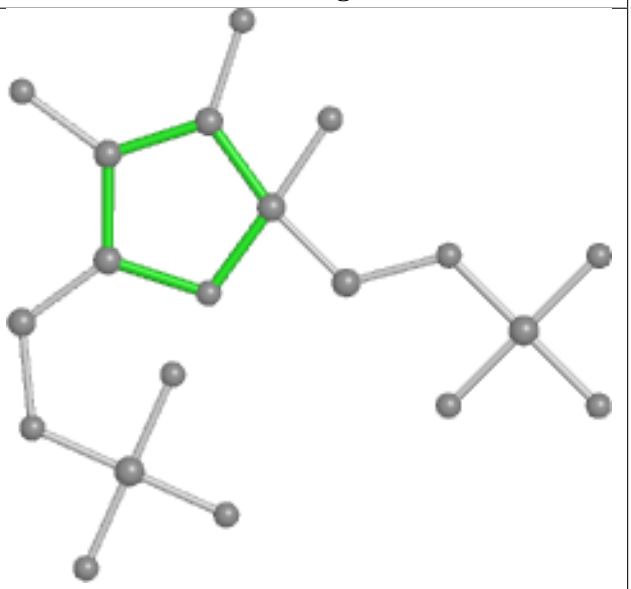
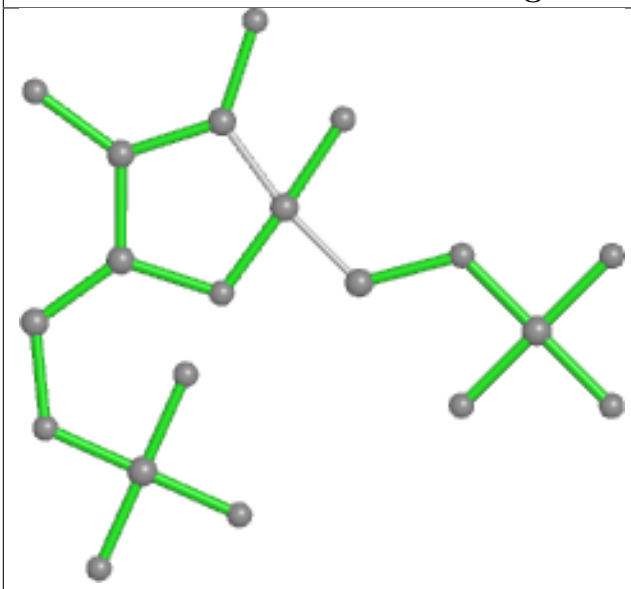


Torsions



Rings

Ligand FBP D 601



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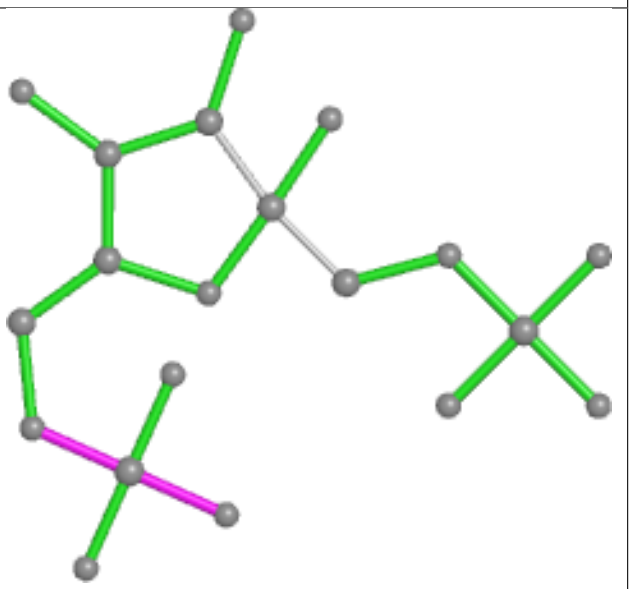

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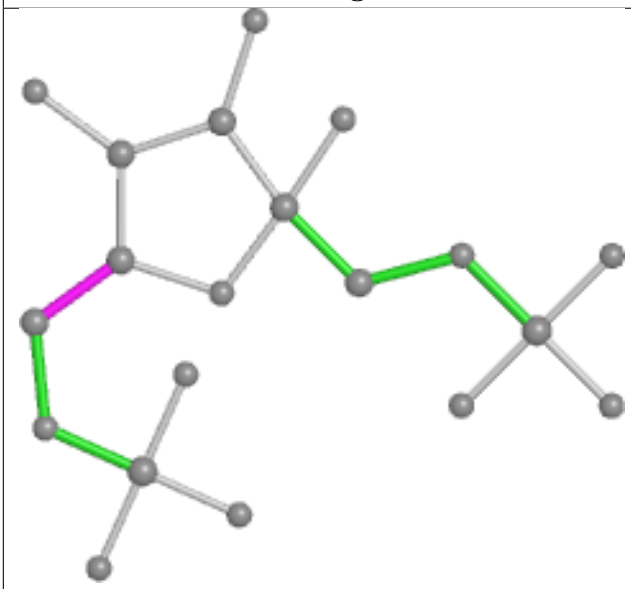

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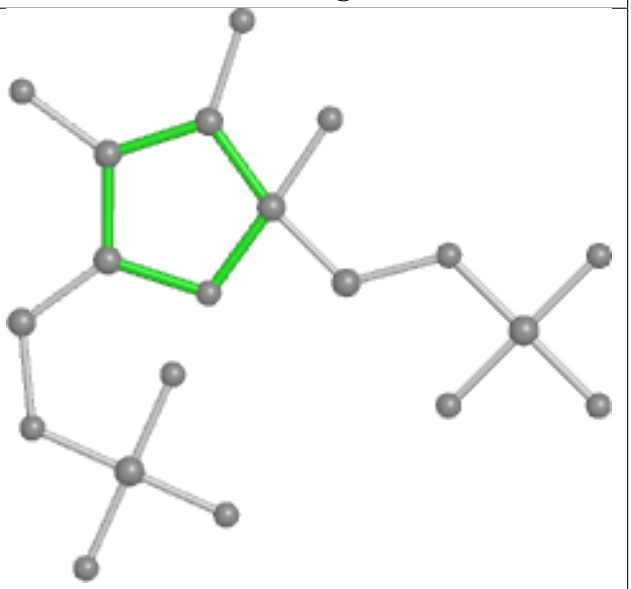
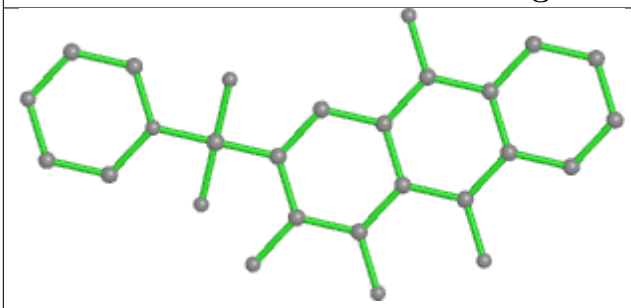
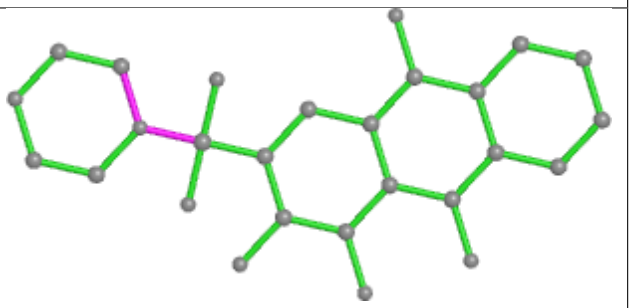


Rings

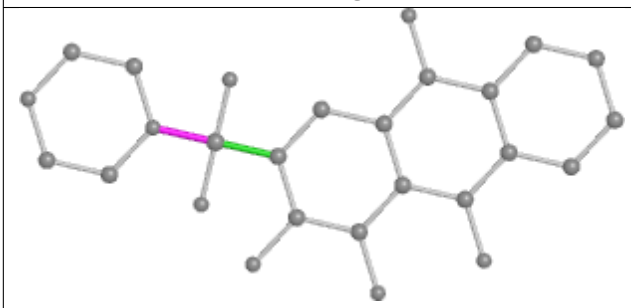
Ligand I9N B 603



Bond lengths



Bond angles



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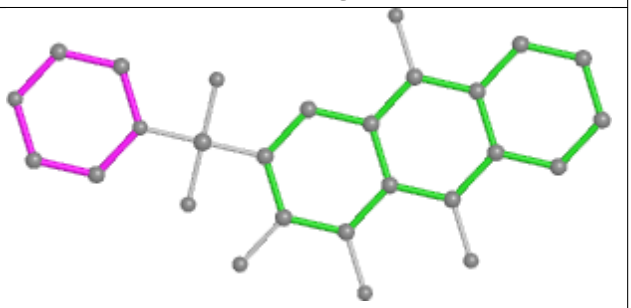
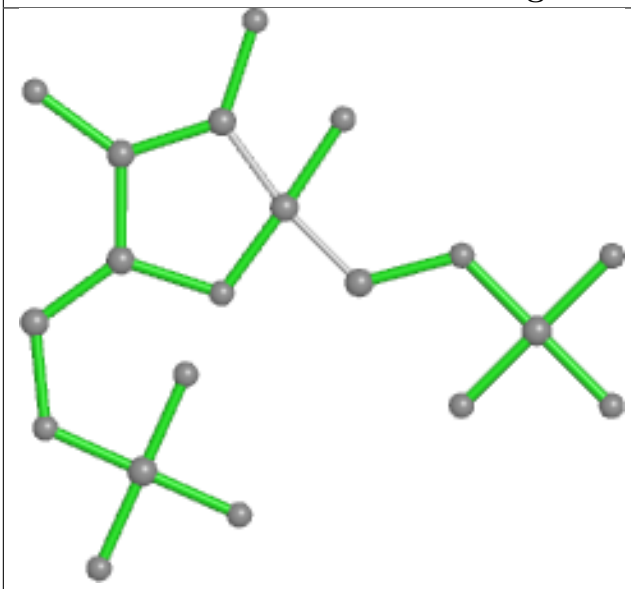
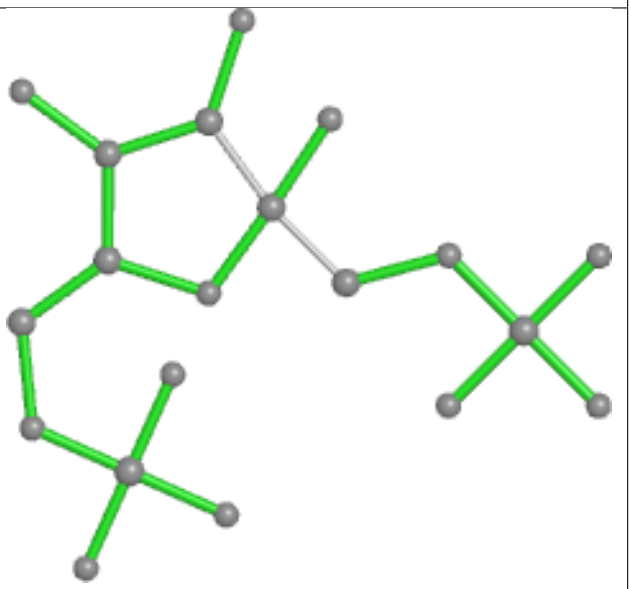


Rings

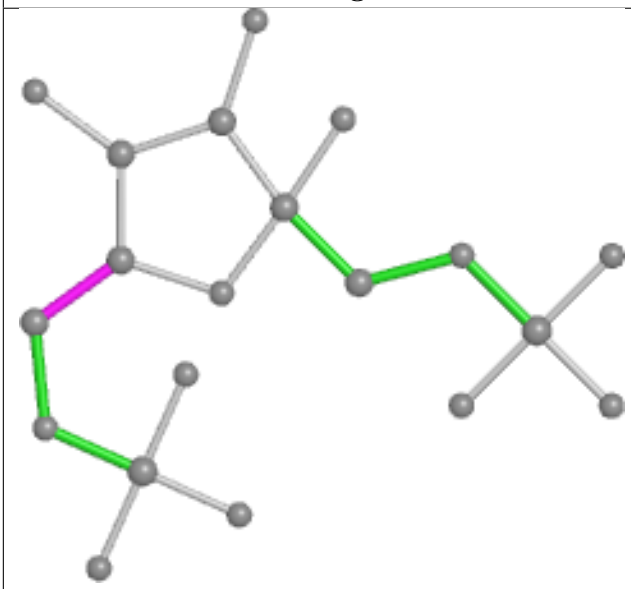
Ligand FBP F 601



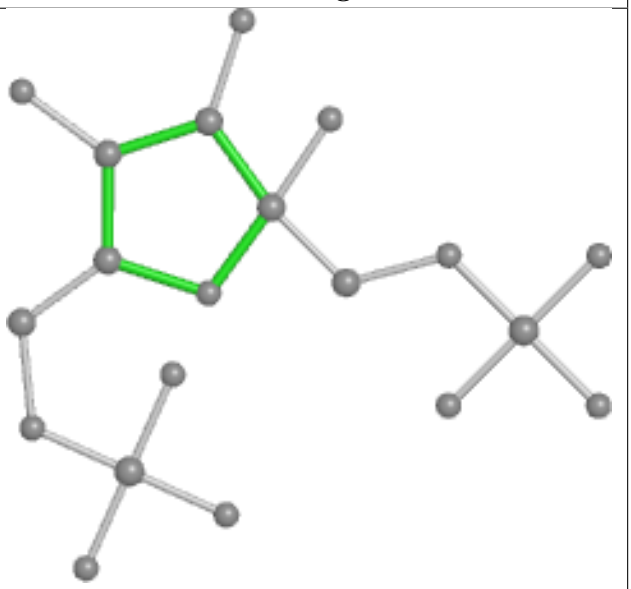
Bond lengths



Bond angles

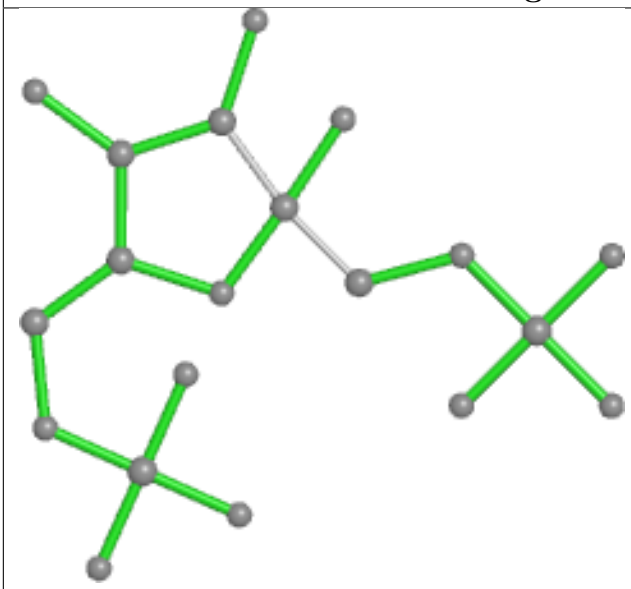


Torsions

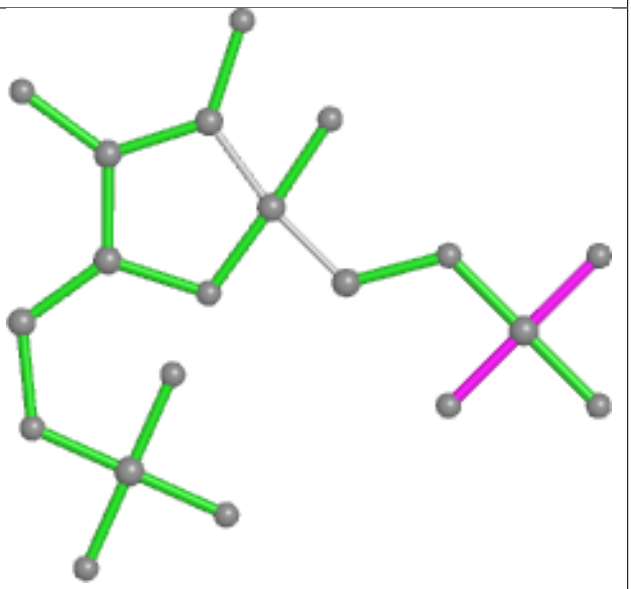


Rings

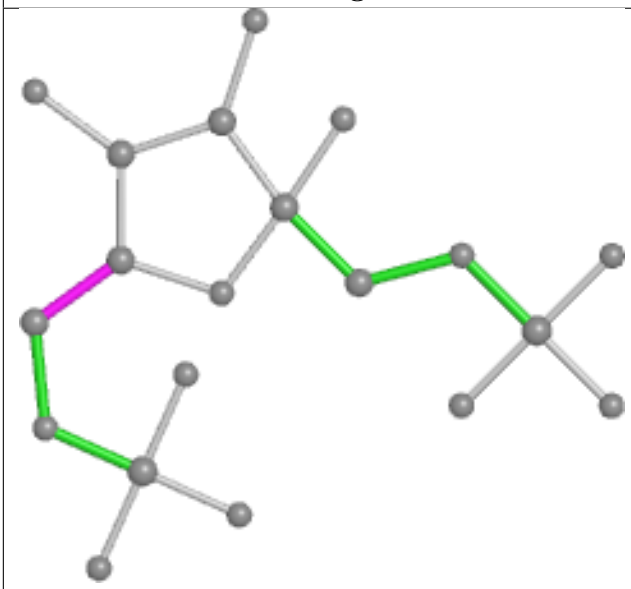
Ligand FBP A 601



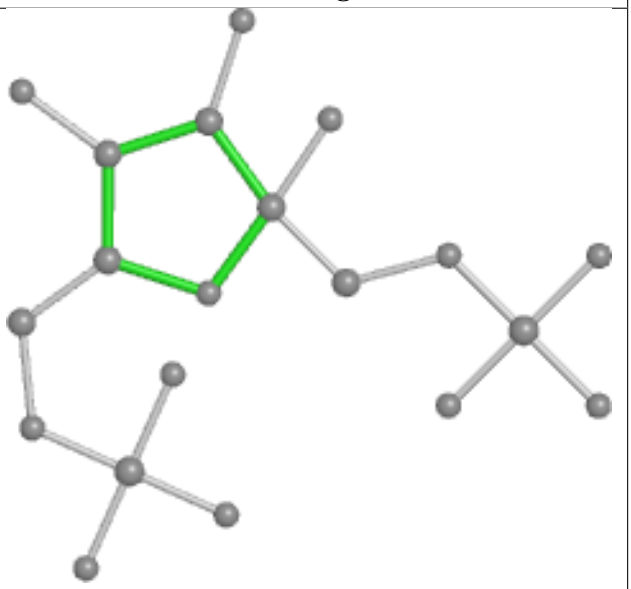
Bond lengths



Bond angles

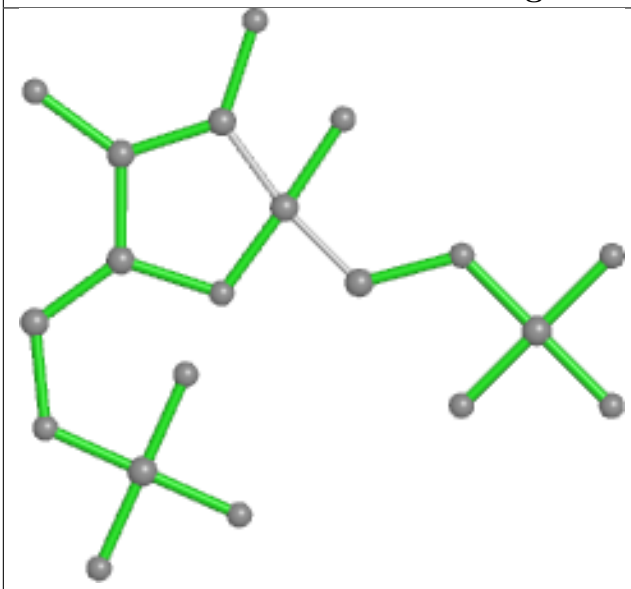


Torsions

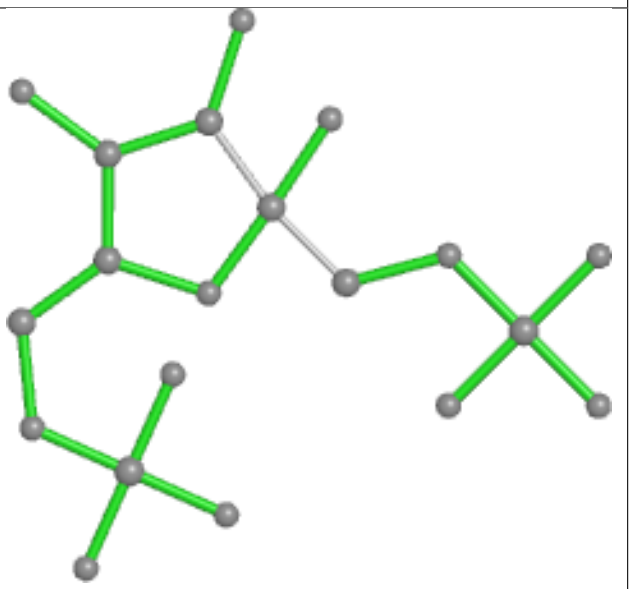


Rings

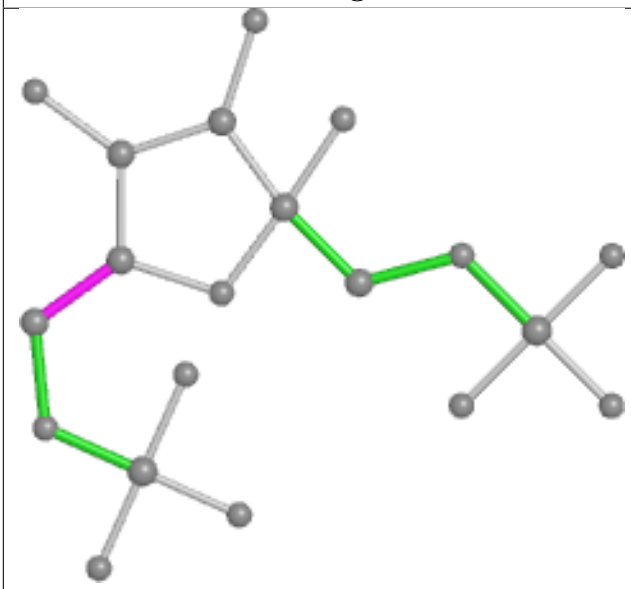
Ligand FBP C 601



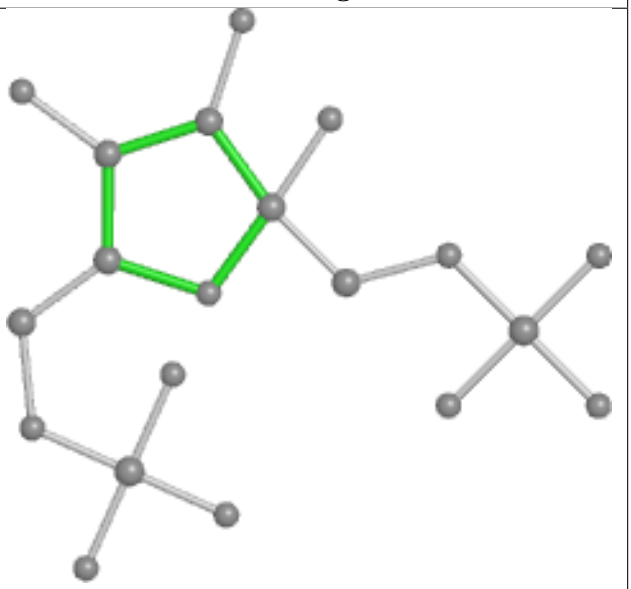
Bond lengths



Bond angles

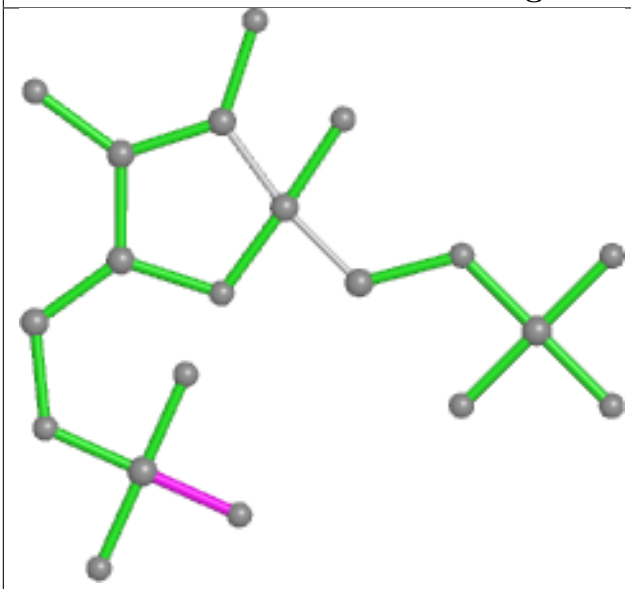


Torsions

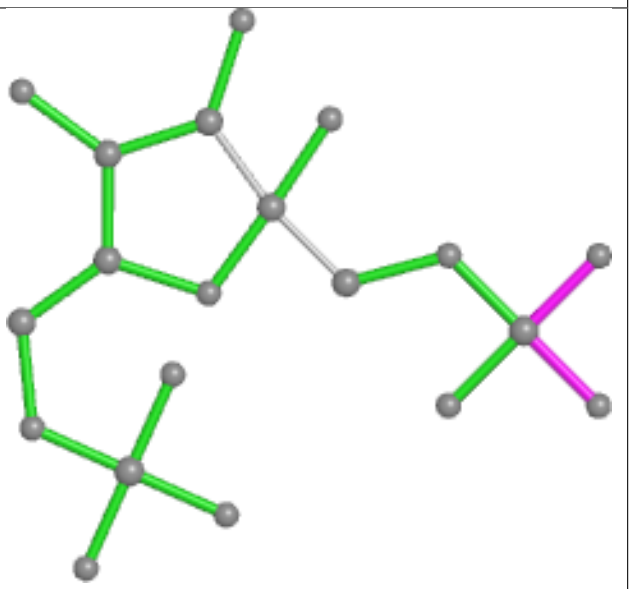


Rings

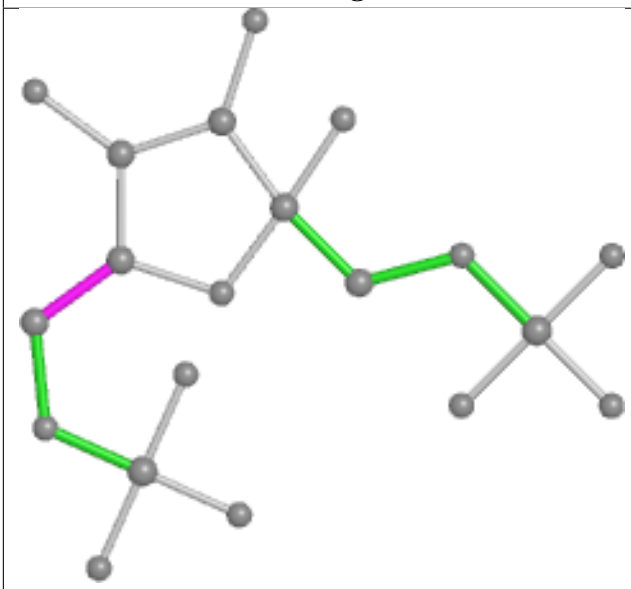
Ligand FBP B 601



Bond lengths



Bond angles



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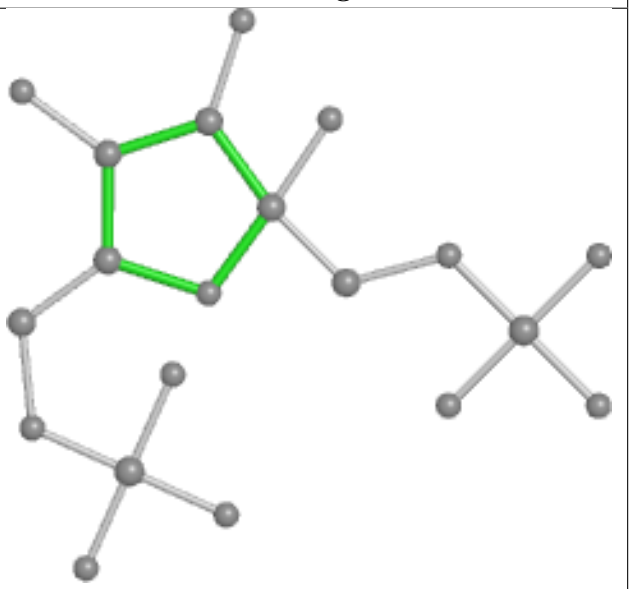
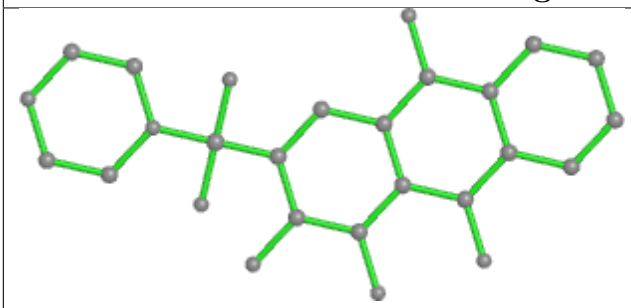
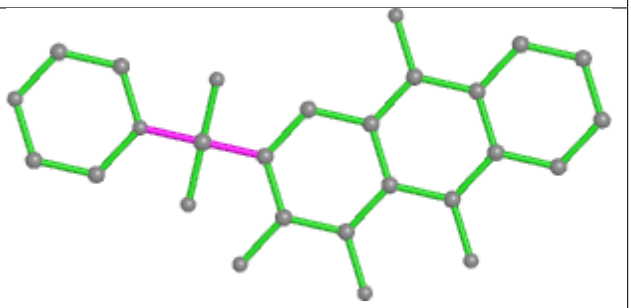


Rings

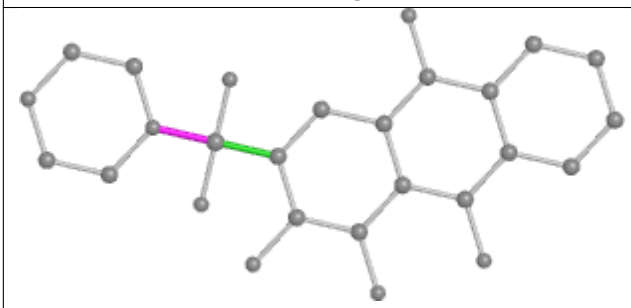
Ligand I9N F 603



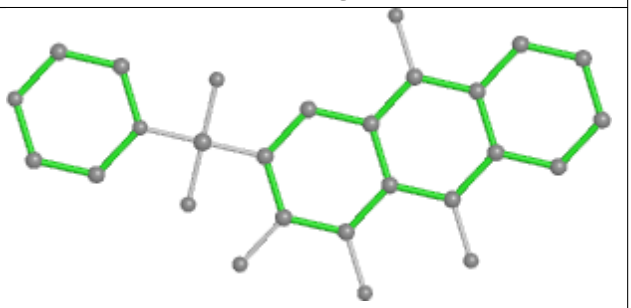
Bond lengths



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	418/447 (93%)	0.28	18 (4%)	35	39	23, 36, 58, 72	0
1	B	436/447 (97%)	-0.03	11 (2%)	57	61	16, 30, 52, 67	0
1	C	424/447 (94%)	-0.10	12 (2%)	53	57	14, 25, 45, 86	0
1	D	425/447 (95%)	-0.10	7 (1%)	72	76	15, 22, 43, 82	0
1	E	419/447 (93%)	0.07	12 (2%)	51	56	19, 34, 57, 70	0
1	F	432/447 (96%)	-0.05	13 (3%)	50	54	16, 27, 49, 65	0
1	G	422/447 (94%)	-0.17	6 (1%)	75	79	15, 23, 39, 61	1 (0%)
1	H	425/447 (95%)	-0.16	6 (1%)	75	79	14, 21, 41, 62	0
All	All	3401/3576 (95%)	-0.03	85 (2%)	57	61	14, 27, 51, 86	1 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	25	PHE	9.1
1	D	21	GLY	8.3
1	D	22	THR	8.1
1	E	25	PHE	6.2
1	G	271	GLY	6.2
1	D	24	PHE	5.3
1	C	271	GLY	5.1
1	G	25	PHE	5.0
1	C	25	PHE	4.9
1	H	21	GLY	4.9
1	A	114	PRO	4.6
1	E	489	PRO	4.5
1	D	231	PRO	4.4
1	A	543	SER	4.4
1	F	511	LEU	4.2
1	H	25	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	22	THR	4.0
1	E	271	GLY	3.9
1	B	10	ARG	3.8
1	E	492	ALA	3.7
1	C	231	PRO	3.6
1	C	21	GLY	3.5
1	E	412	ARG	3.5
1	G	231	PRO	3.4
1	A	115	LEU	3.4
1	H	516	ARG	3.4
1	C	22	THR	3.4
1	B	489	PRO	3.4
1	C	26	GLN	3.3
1	B	416	LEU	3.3
1	B	490	PRO	3.3
1	F	489	PRO	3.3
1	G	21	GLY	3.2
1	G	22	THR	3.2
1	A	30	LEU	3.2
1	E	540	LEU	3.2
1	A	113	SER	3.0
1	F	516	ARG	2.9
1	F	512	ARG	2.9
1	B	543	SER	2.8
1	E	114	PRO	2.8
1	B	130	GLY	2.8
1	A	275	HIS	2.8
1	H	231	PRO	2.8
1	F	311	ILE	2.7
1	B	232	GLY	2.7
1	B	540[A]	LEU	2.6
1	A	331[A]	LEU	2.6
1	A	242	ARG	2.5
1	B	487	ARG	2.5
1	F	517	VAL	2.5
1	D	26	GLN	2.5
1	F	487	ARG	2.5
1	F	540[A]	LEU	2.5
1	A	272	PRO	2.4
1	F	490	PRO	2.4
1	A	499[A]	ASP	2.4
1	A	34	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	411	ARG	2.3
1	A	273	GLU	2.3
1	C	404	ARG	2.3
1	E	493	ILE	2.3
1	C	412	ARG	2.3
1	C	114	PRO	2.2
1	F	11	ALA	2.2
1	C	112	GLY	2.2
1	C	34	MET	2.2
1	A	493	ILE	2.2
1	F	493	ILE	2.2
1	A	492	ALA	2.2
1	E	516	ARG	2.1
1	E	34	MET	2.1
1	F	415	PRO	2.1
1	C	24	PHE	2.1
1	B	512	ARG	2.1
1	E	311	ILE	2.1
1	A	111	ALA	2.1
1	G	232	GLY	2.1
1	A	500	ARG	2.0
1	D	412	ARG	2.0
1	A	271	GLY	2.0
1	A	518	GLY	2.0
1	F	514	PHE	2.0
1	B	131	SER	2.0
1	E	331	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.

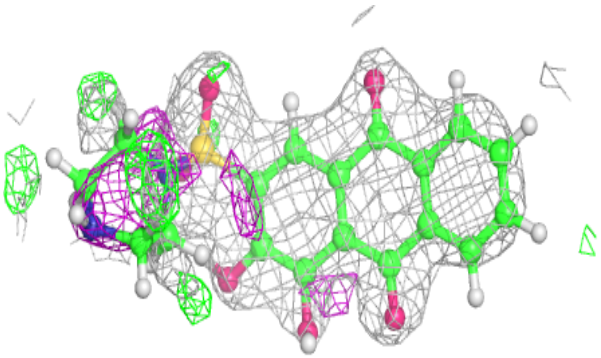
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	I9N	E	603	27/27	0.84	0.25	52,55,55,55	16
6	I9N	G	603	27/27	0.84	0.18	40,43,47,47	16
6	I9N	C	603	27/27	0.87	0.18	40,42,47,47	16
6	I9N	F	603	27/27	0.89	0.18	40,41,46,47	16
6	I9N	B	603	27/27	0.89	0.19	50,51,53,54	16
3	OXL	B	602	6/6	0.91	0.09	31,32,33,34	0
3	OXL	F	602	6/6	0.93	0.08	27,28,31,32	0
3	OXL	D	602	6/6	0.94	0.09	25,26,27,28	0
3	OXL	E	602	6/6	0.95	0.09	38,38,39,39	0
2	FBP	A	601	20/20	0.96	0.09	29,31,33,33	0
3	OXL	C	602	6/6	0.96	0.08	27,28,29,30	0
5	K	E	605	1/1	0.96	0.07	50,50,50,50	0
3	OXL	A	602	6/6	0.96	0.12	38,39,40,41	0
4	MG	A	603	1/1	0.97	0.04	37,37,37,37	0
5	K	A	604	1/1	0.97	0.08	59,59,59,59	0
2	FBP	E	601	20/20	0.97	0.09	28,29,31,32	0
3	OXL	G	602	6/6	0.97	0.06	26,27,29,29	0
2	FBP	F	601	20/20	0.98	0.08	26,28,31,32	0
4	MG	B	604	1/1	0.98	0.06	29,29,29,29	0
2	FBP	B	601	20/20	0.98	0.08	25,27,32,32	0
5	K	B	605	1/1	0.98	0.04	43,43,43,43	0
3	OXL	H	602	6/6	0.98	0.07	21,22,24,26	0
4	MG	G	604	1/1	0.99	0.05	23,23,23,23	0
2	FBP	G	601	20/20	0.99	0.08	15,16,18,19	0
2	FBP	H	601	20/20	0.99	0.09	14,16,19,20	0
5	K	C	605	1/1	0.99	0.05	34,34,34,34	0
5	K	D	604	1/1	0.99	0.08	29,29,29,29	0
2	FBP	C	601	20/20	0.99	0.09	16,17,20,20	0
5	K	G	605	1/1	0.99	0.05	33,33,33,33	0
5	K	H	604	1/1	0.99	0.08	31,31,31,31	0
2	FBP	D	601	20/20	0.99	0.09	17,18,21,21	0
4	MG	C	604	1/1	0.99	0.04	29,29,29,29	0
4	MG	D	603	1/1	0.99	0.05	24,24,24,24	0
4	MG	E	604	1/1	0.99	0.05	33,33,33,33	0
4	MG	F	604	1/1	0.99	0.05	26,26,26,26	0
5	K	F	605	1/1	1.00	0.04	42,42,42,42	0
4	MG	H	603	1/1	1.00	0.05	22,22,22,22	0

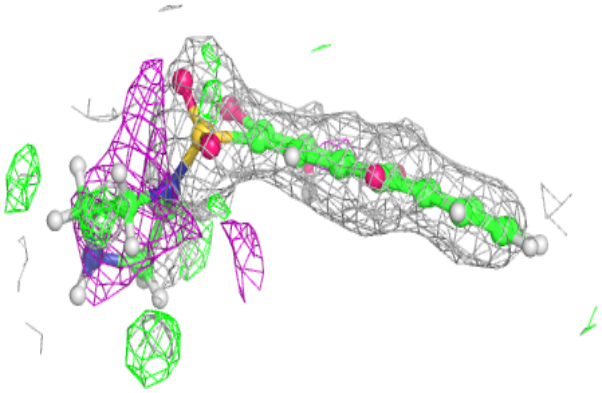
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

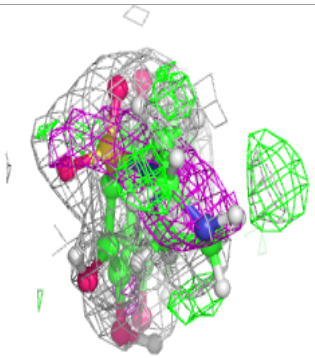
orientation to approximate a three-dimensional view.

Electron density around I9N E 603:

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

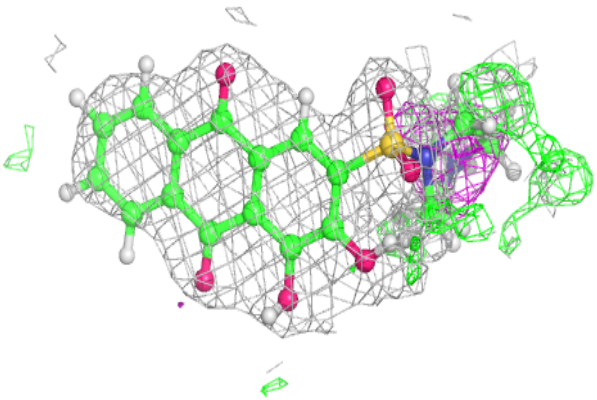


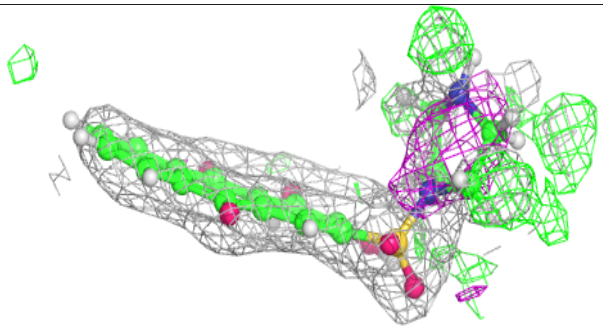


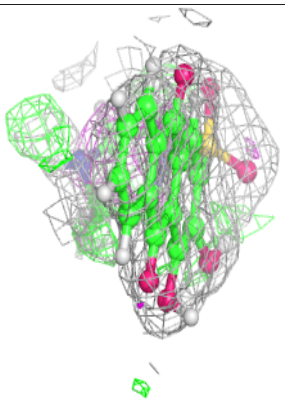


Electron density around I9N G 603:

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

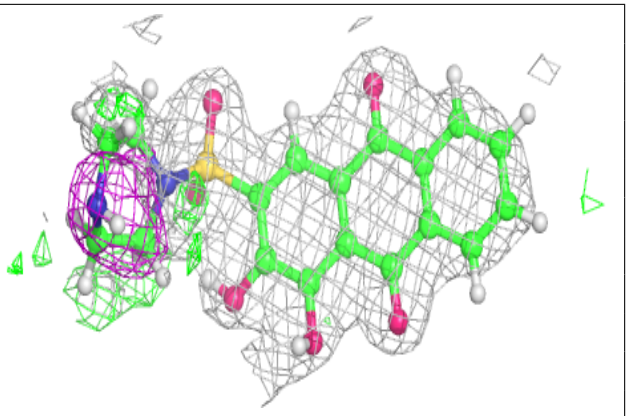


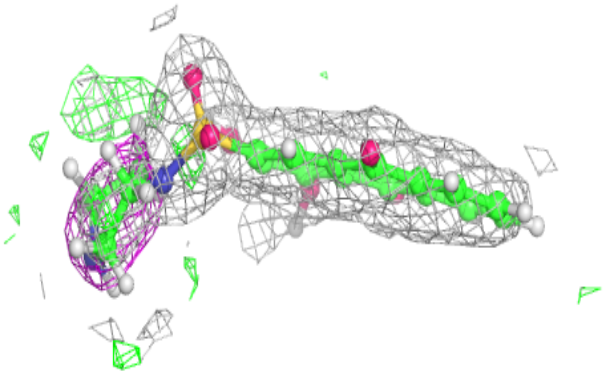


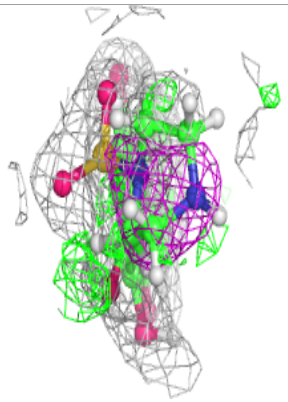


Electron density around I9N C 603:

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

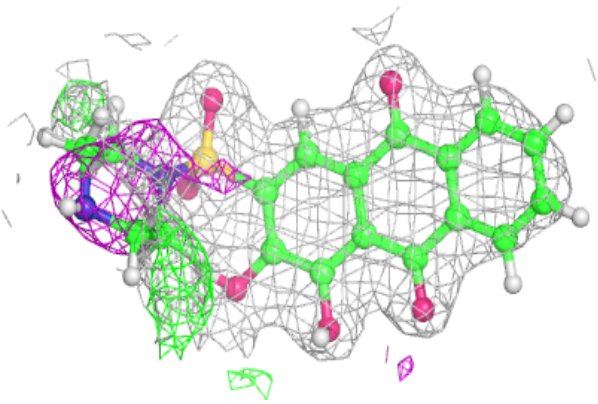


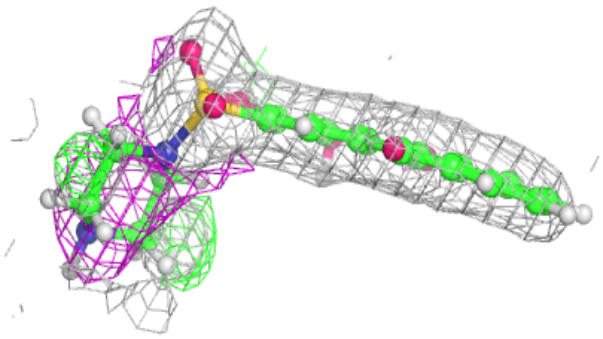


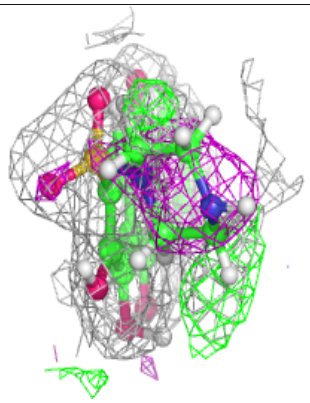


Electron density around I9N F 603:

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

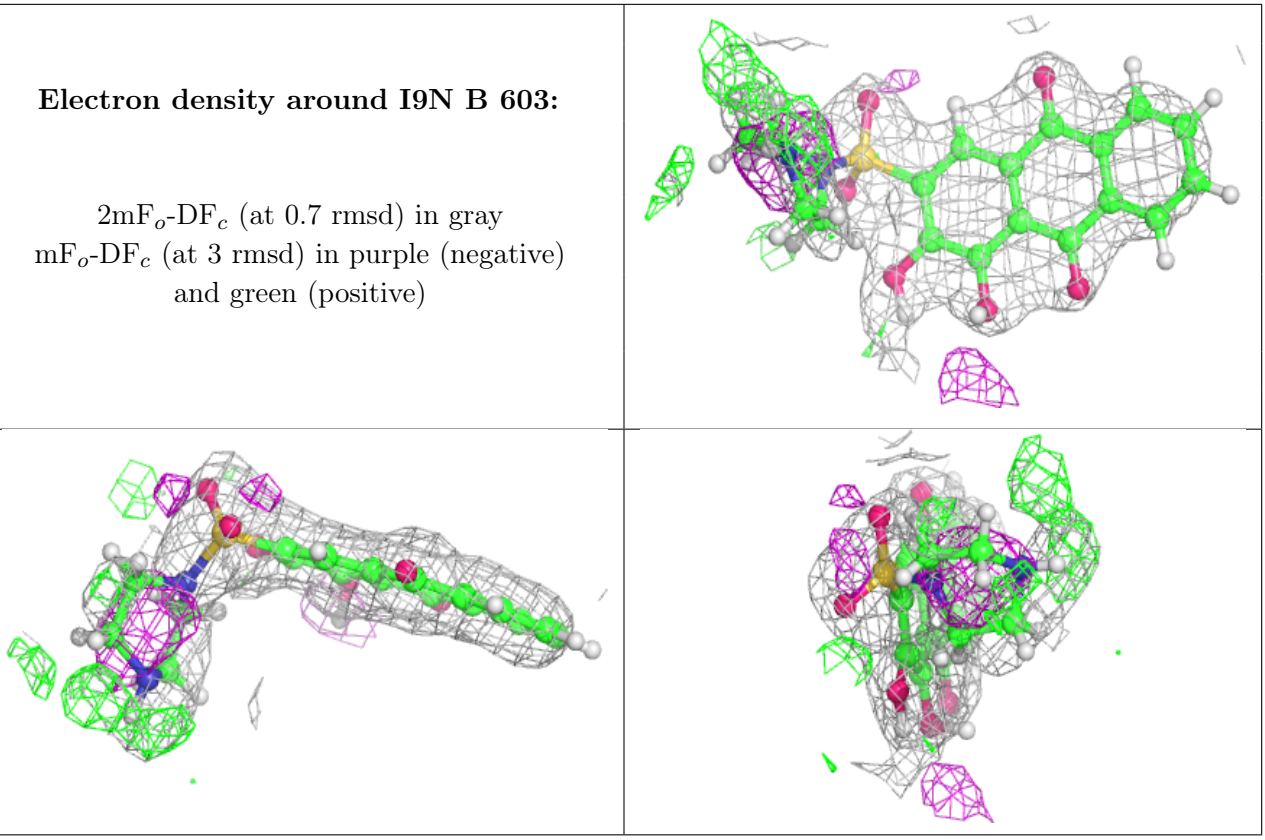






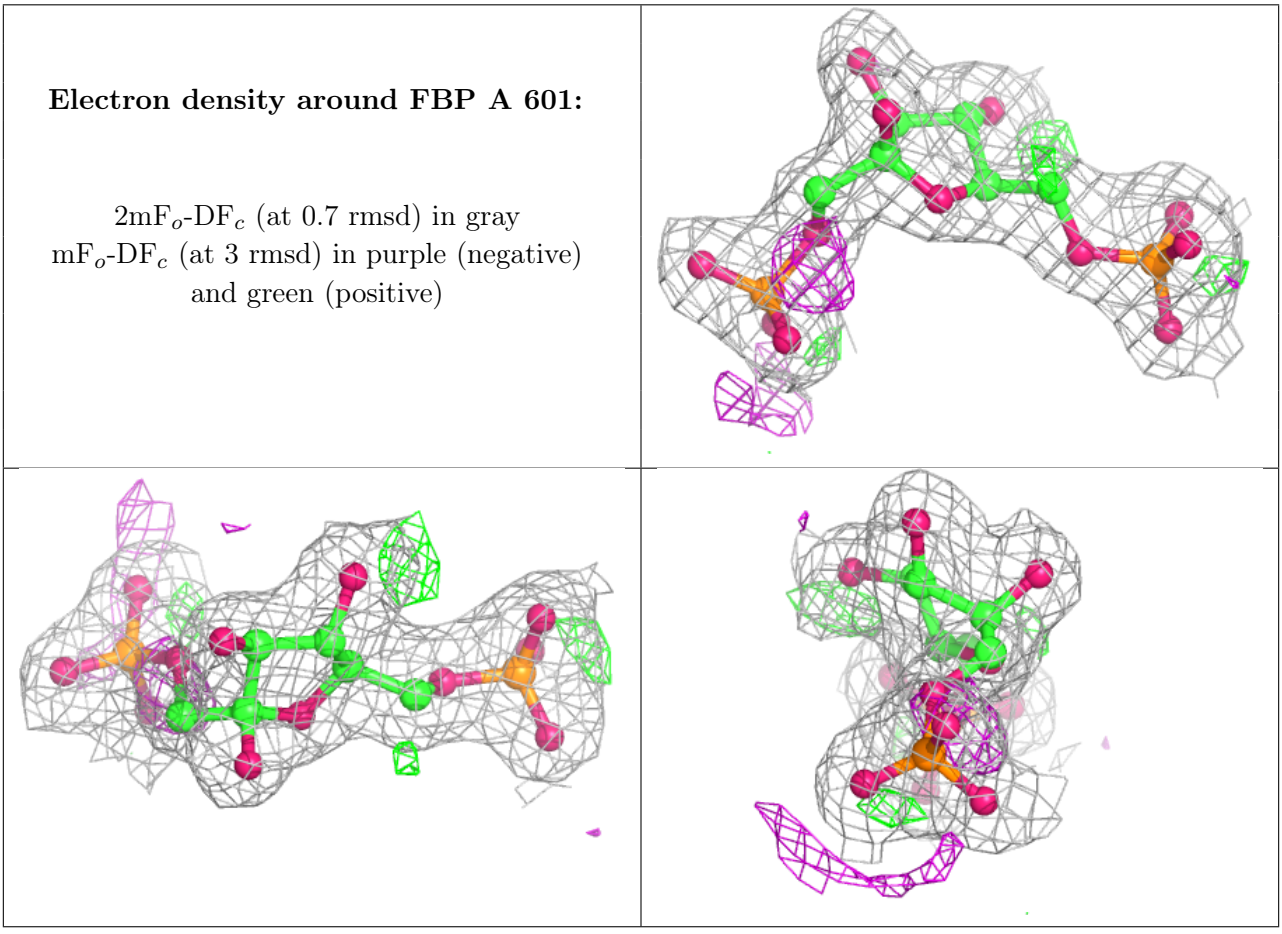
Electron density around I9N B 603:

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



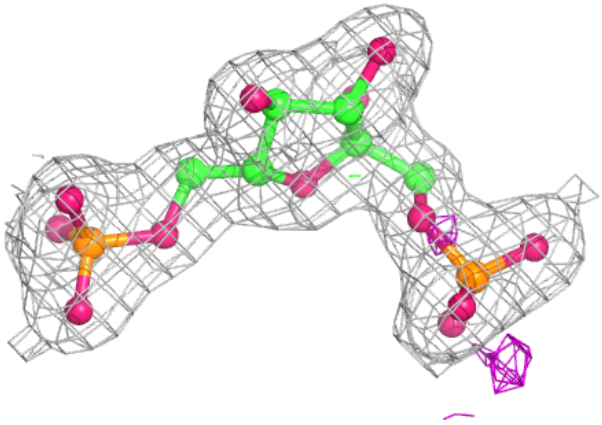
Electron density around FBP A 601:

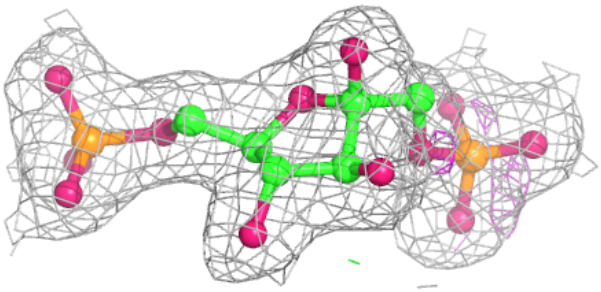
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

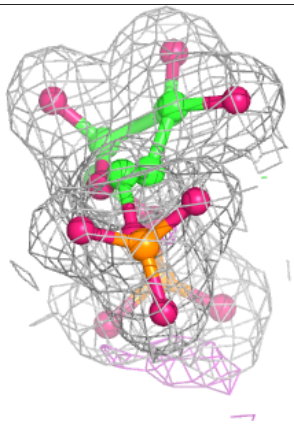


Electron density around FBP E 601:

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

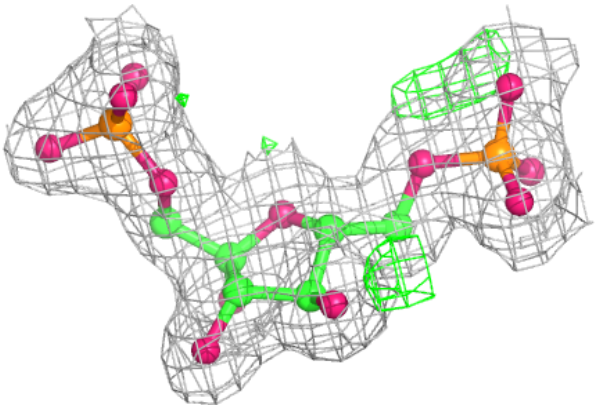


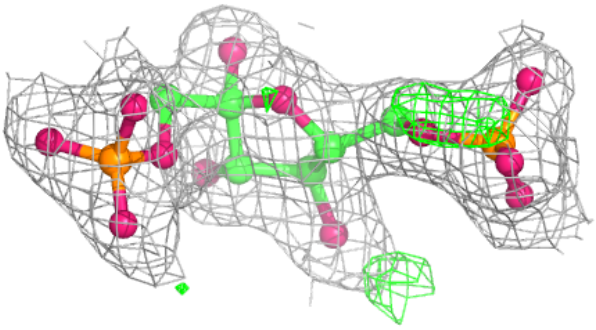


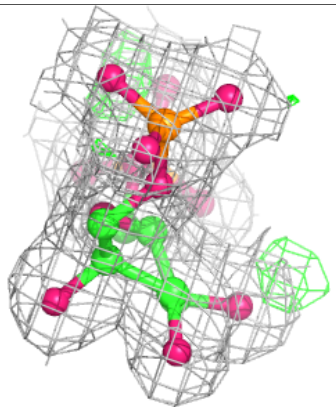


Electron density around FBP F 601:

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

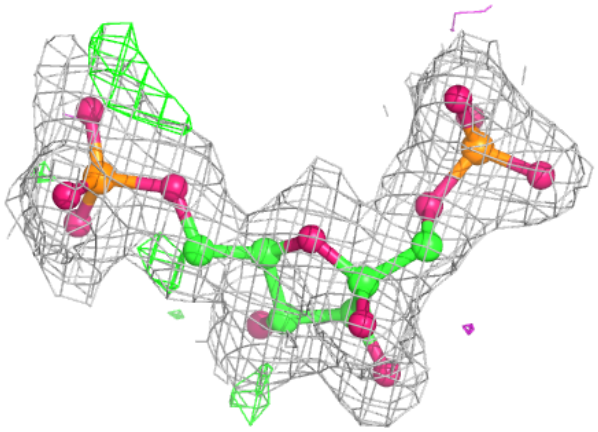


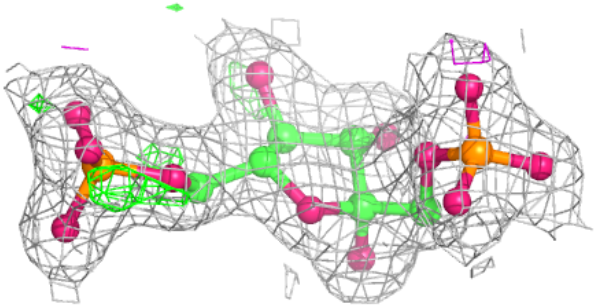


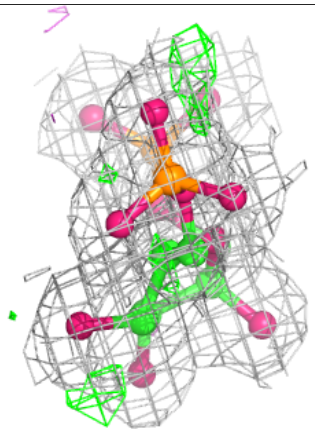


Electron density around FBP B 601:

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

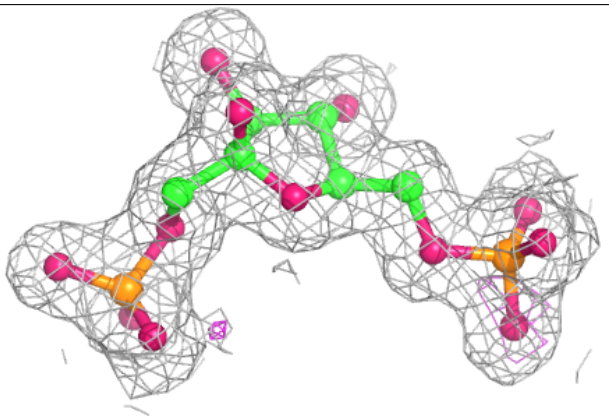


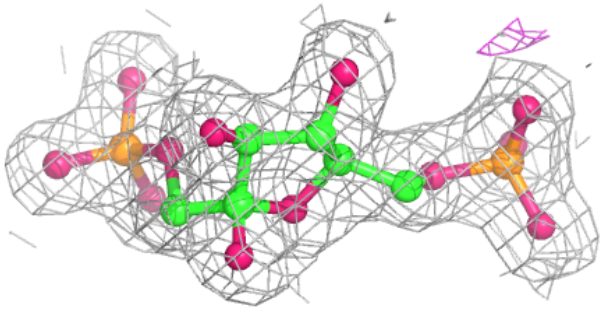




Electron density around FBP G 601:

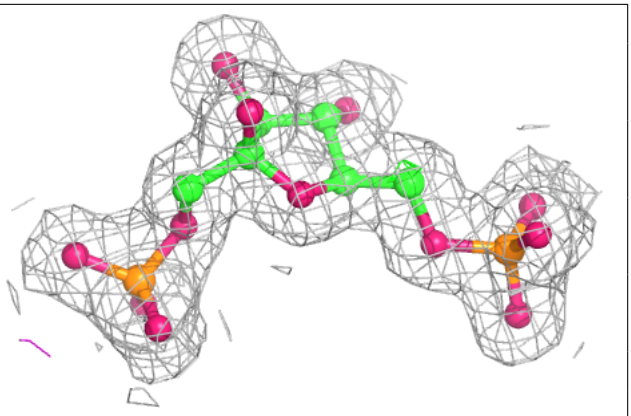
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

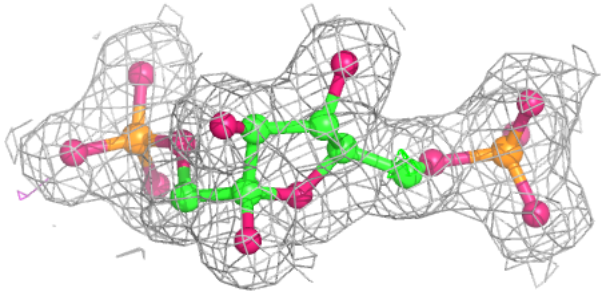


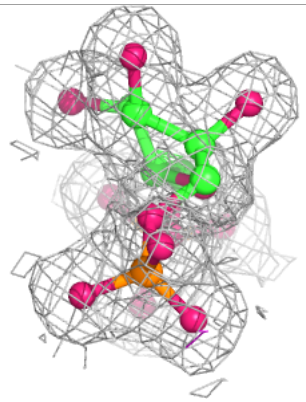


Electron density around FBP H 601:

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

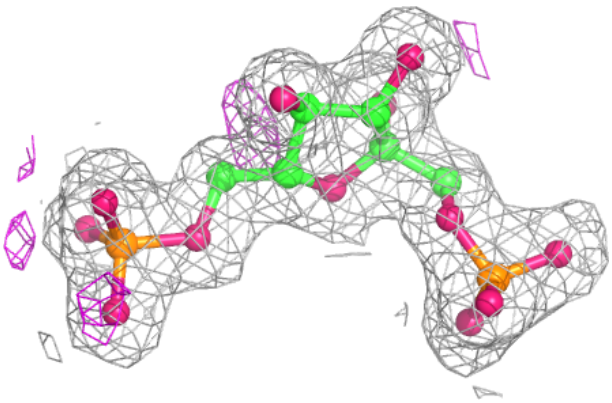


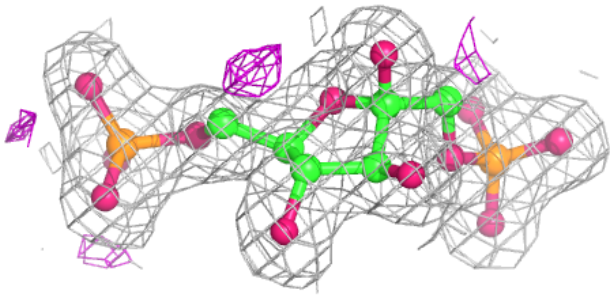




Electron density around FBP C 601:

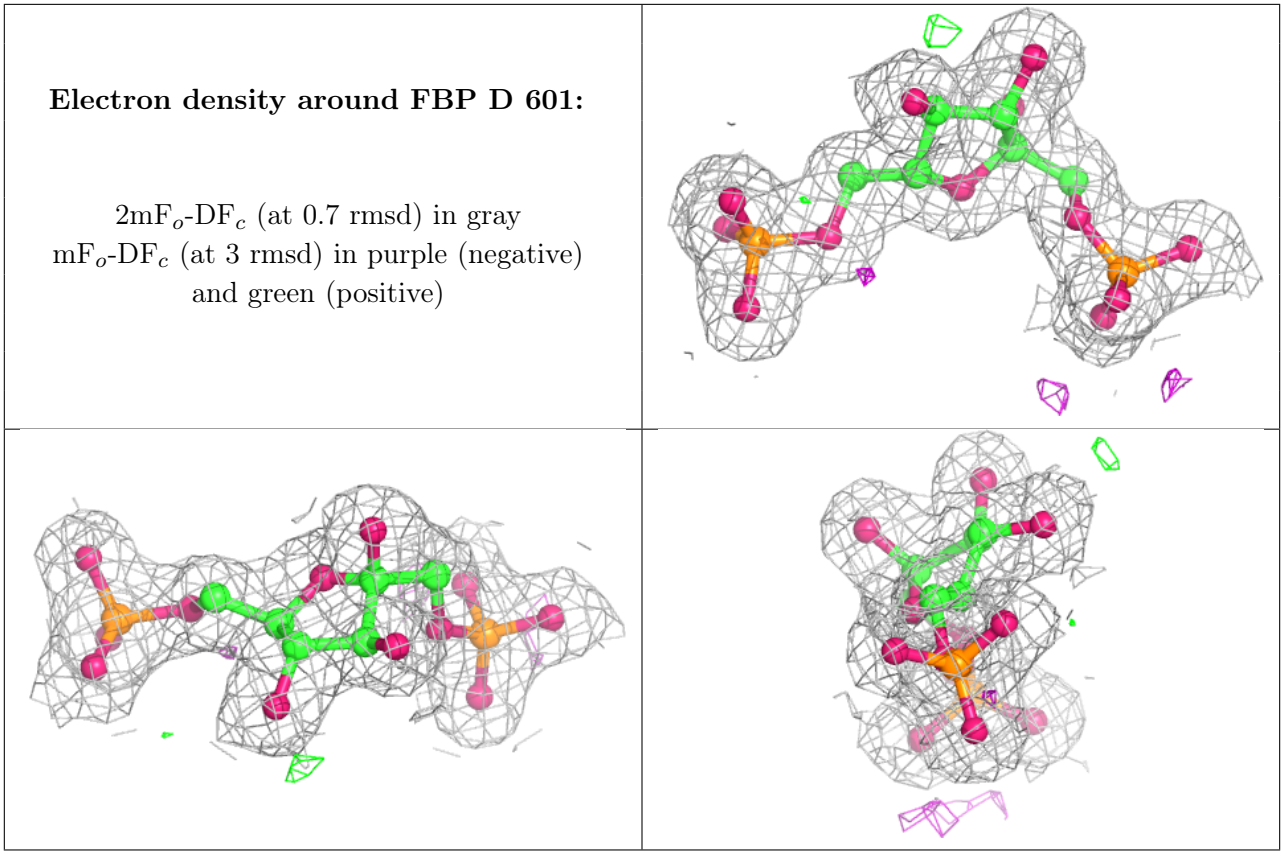
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around FBP D 601:

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



6.5 Other polymers

There are no such residues in this entry.