Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 10:41 AM EDT

PDB ID	:	6ECH
Title	:	Pyruvate Kinase Isoform L-type with phosphorylated Ser12 (pS12) in complex with FBP
Authors	:	Padyana, A.; Tong, S.
Deposited on	:	2018-08-07
Resolution	:	2.19 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

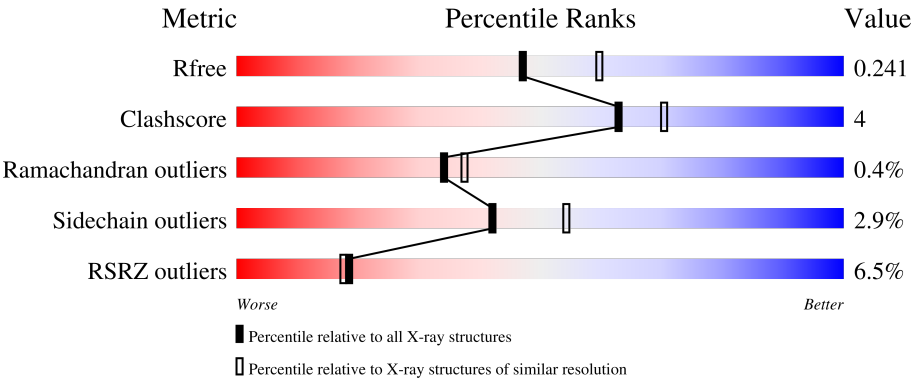
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	550	5% 85% 11% ·
1	B	550	4% 86% 8% · 5%
1	C	550	8% 86% 9% · ·
1	D	550	8% 86% 9% · ·

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	MG	A	603	-	-	-	X
6	EDO	C	611	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17686 atoms, of which 0 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	528	Total	C	N	O	S	0	2	0
			4038	2537	722	761	18			
1	B	525	Total	C	N	O	S	0	1	0
			4001	2516	715	752	18			
1	C	528	Total	C	N	O	S	0	2	0
			4054	2546	734	756	18			
1	D	527	Total	C	N	O	S	0	0	0
			4012	2522	717	755	18			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P12928
A	544	HIS	-	expression tag	UNP P12928
A	545	HIS	-	expression tag	UNP P12928
A	546	HIS	-	expression tag	UNP P12928
A	547	HIS	-	expression tag	UNP P12928
A	548	HIS	-	expression tag	UNP P12928
A	549	HIS	-	expression tag	UNP P12928
B	0	HIS	-	expression tag	UNP P12928
B	544	HIS	-	expression tag	UNP P12928
B	545	HIS	-	expression tag	UNP P12928
B	546	HIS	-	expression tag	UNP P12928
B	547	HIS	-	expression tag	UNP P12928
B	548	HIS	-	expression tag	UNP P12928
B	549	HIS	-	expression tag	UNP P12928
C	0	HIS	-	expression tag	UNP P12928
C	544	HIS	-	expression tag	UNP P12928
C	545	HIS	-	expression tag	UNP P12928
C	546	HIS	-	expression tag	UNP P12928
C	547	HIS	-	expression tag	UNP P12928
C	548	HIS	-	expression tag	UNP P12928
C	549	HIS	-	expression tag	UNP P12928

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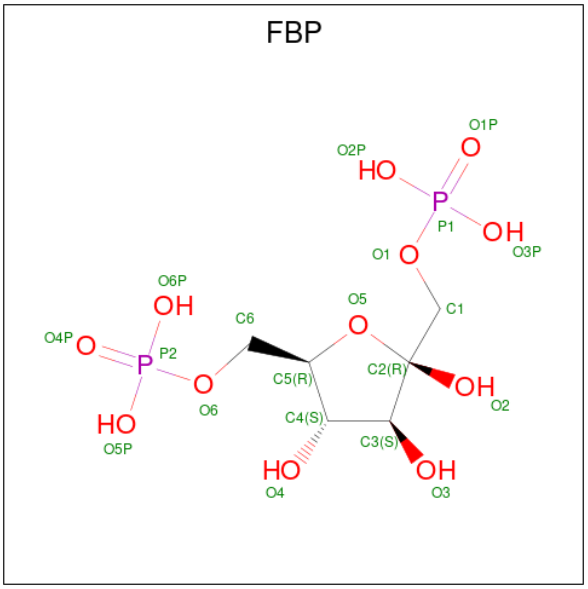
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP P12928
D	544	HIS	-	expression tag	UNP P12928
D	545	HIS	-	expression tag	UNP P12928
D	546	HIS	-	expression tag	UNP P12928
D	547	HIS	-	expression tag	UNP P12928
D	548	HIS	-	expression tag	UNP P12928
D	549	HIS	-	expression tag	UNP P12928

- 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 20 6 12 2	0	0
2	B	1	Total C O P 20 6 12 2	0	0
2	C	1	Total C O P 20 6 12 2	0	0
2	D	1	Total C O P 20 6 12 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Mg 4 4	0	0

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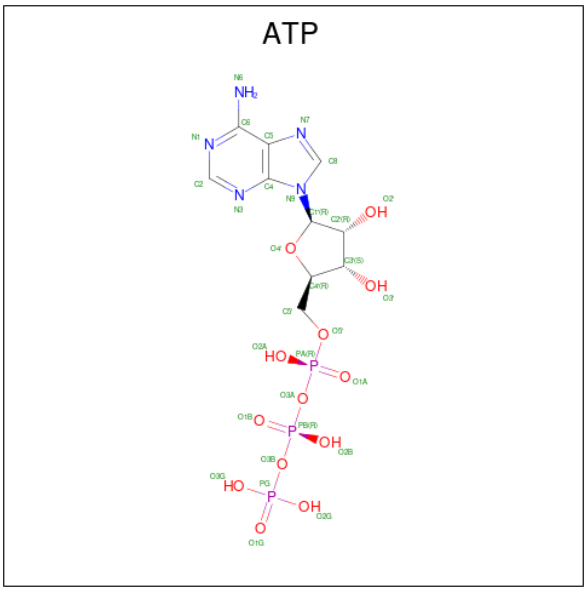
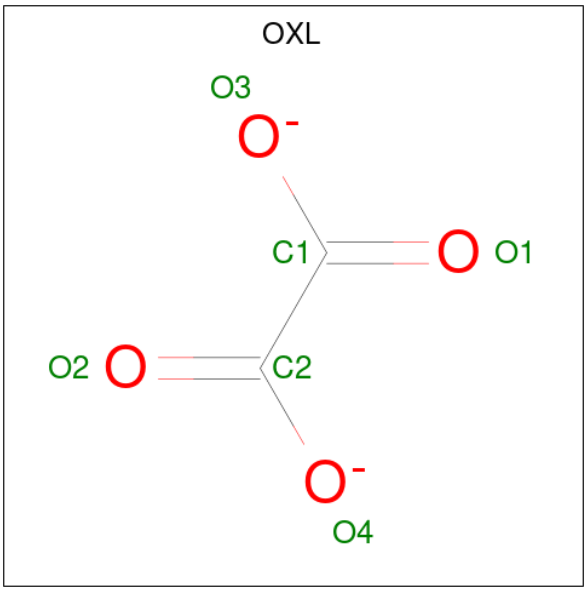
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Mg 4 4	0	0
3	C	2	Total Mg 2 2	0	0
3	D	3	Total Mg 3 3	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



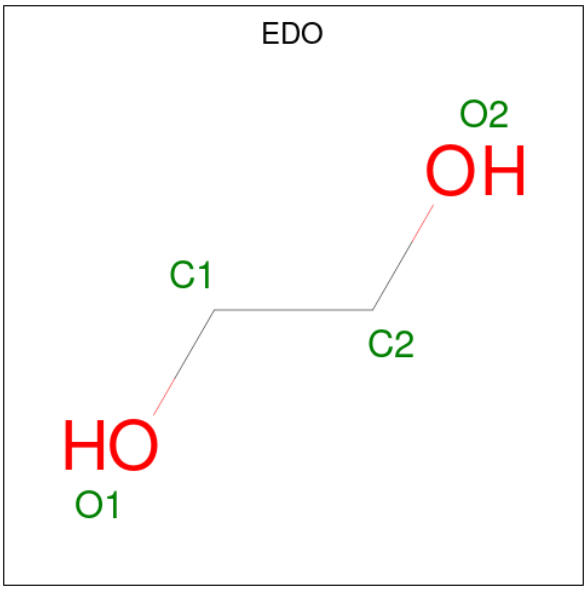
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 31 10 5 13 3	0	0
4	B	1	Total C N O P 31 10 5 13 3	0	0
4	D	1	Total C N O P 31 10 5 13 3	0	0

- Molecule 5 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 2 4	0	0
5	B	1	Total C O 6 2 4	0	0
5	C	1	Total C O 6 2 4	0	0
5	D	1	Total C O 6 2 4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

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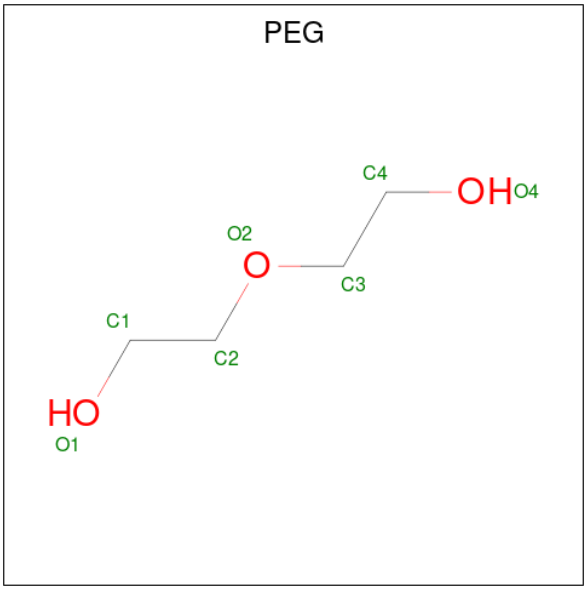
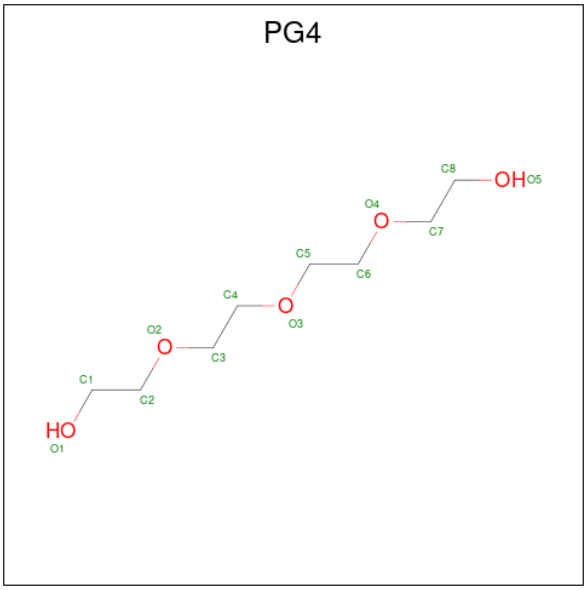
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



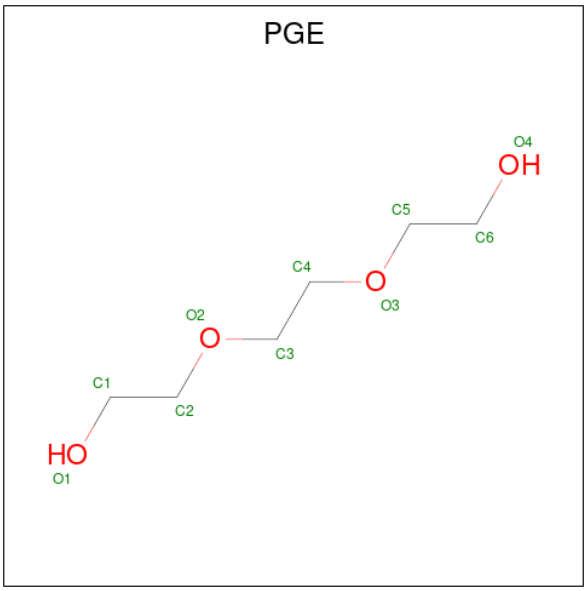
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 13 8 5	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 10 6 4	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total Cl 1 1	0	0

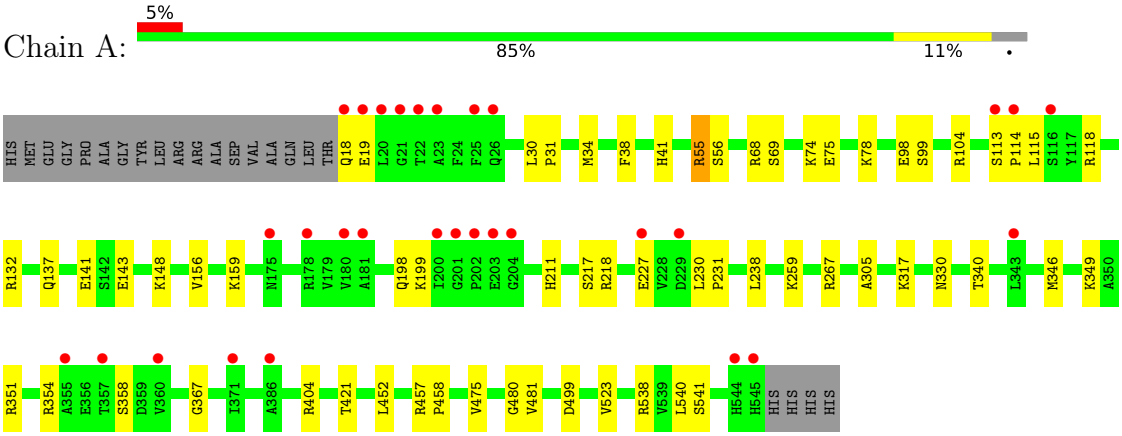
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	320	Total O 320 320	0	0
11	B	281	Total O 281 281	0	0
11	C	306	Total O 306 306	0	0
11	D	294	Total O 294 294	0	0

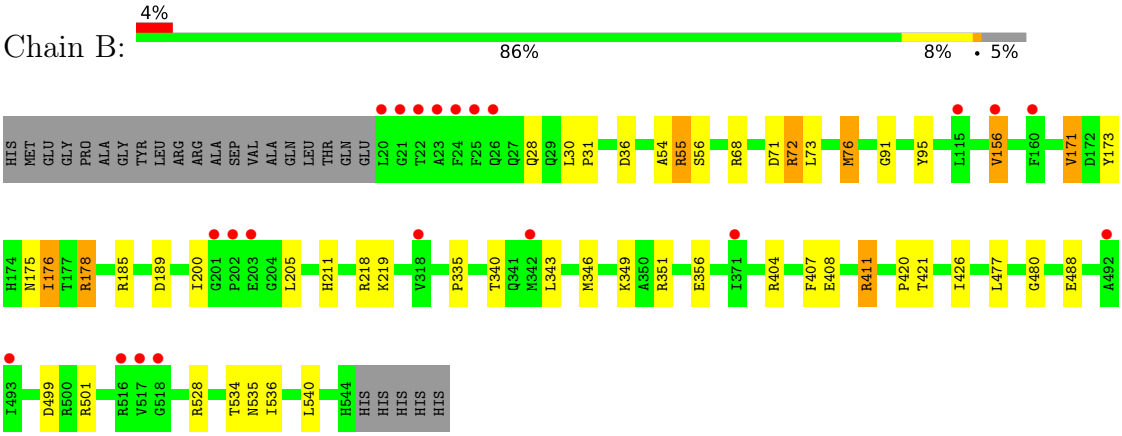
3 Residue-property plots (i)

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.

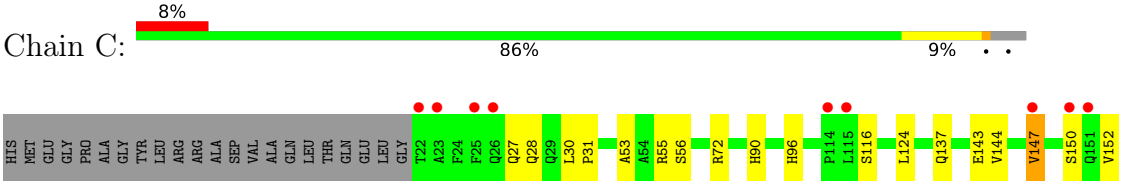
• Molecule 1: Pyruvate kinase PKLR

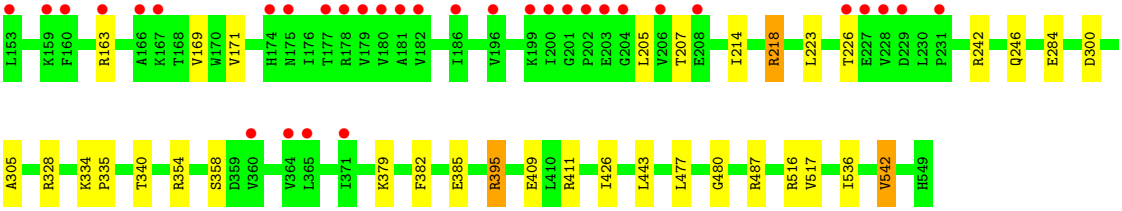


• Molecule 1: Pyruvate kinase PKLR

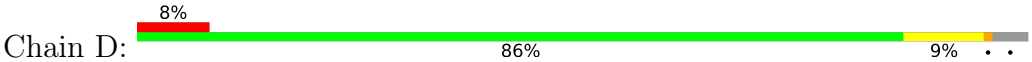


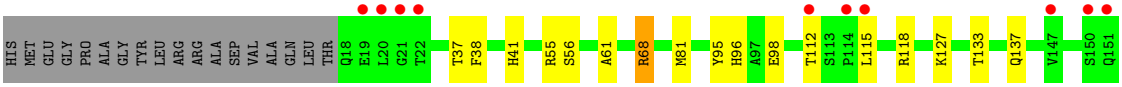
• Molecule 1: Pyruvate kinase PKLR

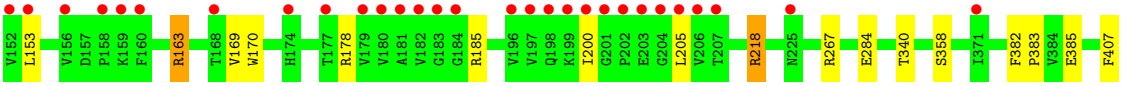


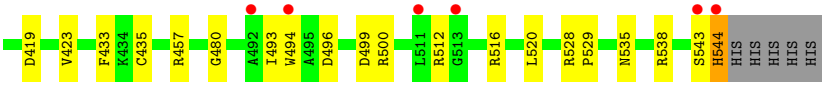


• Molecule 1: Pyruvate kinase PKLR









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.55Å 108.90Å 296.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.19 49.47 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.52-2.19) 100.0 (49.47-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.181 , 0.238 0.189 , 0.241	Depositor DCC
R_{free} test set	7124 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17686	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PG4, EDO, PEG, CL, PGE, OXL, FBP, ATP, 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	0.57	0/4104	0.69	0/5560
1	B	0.56	0/4066	0.70	1/5509 (0.0%)
1	C	0.55	0/4125	0.70	0/5587
1	D	0.55	0/4077	0.69	1/5523 (0.0%)
All	All	0.56	0/16372	0.69	2/22179 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	4
1	C	0	4
1	D	0	5
All	All	0	19

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	68	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	72	ARG	CG-CD-NE	-5.51	100.22	111.80

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Sidechain
1	A	132	ARG	Sidechain
1	A	218	ARG	Sidechain
1	A	267	ARG	Sidechain
1	A	457	ARG	Sidechain
1	A	55	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	55	ARG	Sidechain
1	B	72	ARG	Sidechain
1	C	163	ARG	Sidechain
1	C	328	ARG	Sidechain
1	C	516	ARG	Sidechain
1	C	72	ARG	Sidechain
1	D	185	ARG	Sidechain
1	D	218	ARG	Sidechain
1	D	267	ARG	Sidechain
1	D	457	ARG	Sidechain
1	D	55	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4038	0	4098	40	0
1	B	4001	0	4072	37	0
1	C	4054	0	4105	36	0
1	D	4012	0	4080	27	0
2	A	20	0	10	0	0
2	B	20	0	10	2	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	D	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	0	1	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
6	A	28	0	42	9	0
6	B	36	0	54	5	0
6	C	36	0	54	7	0
6	D	32	0	48	3	0
7	A	7	0	10	3	0
7	D	7	0	10	0	0
8	A	13	0	18	2	0
9	B	10	0	14	5	0
10	D	1	0	0	0	0
11	A	320	0	0	10	0
11	B	281	0	0	8	0
11	C	306	0	0	8	0
11	D	294	0	0	7	0
All	All	17686	0	16681	142	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 4.

All (142) 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:382:PHE:HB3	1:C:385:GLU:HG2	1.63	0.80
1:D:435:CYS:HB2	1:D:520:LEU:HD12	1.68	0.76
1:C:354:ARG:HH12	6:C:608:EDO:H11	1.52	0.73
1:C:242:ARG:CZ	11:C:702:HOH:O	2.37	0.71
1:C:242:ARG:NE	11:C:702:HOH:O	2.26	0.68
1:D:493:ILE:HB	1:D:496:ASP:OD2	1.94	0.67
1:D:382:PHE:HB3	1:D:385:GLU:HG2	1.75	0.67
1:A:351:ARG:NH2	1:B:211:HIS:ND1	2.43	0.67
1:D:137:GLN:OE1	1:D:163:ARG:HG3	1.97	0.65
1:B:91:GLY:H	9:B:608:PGE:H32	1.61	0.65
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.80	0.63
1:A:55:ARG:H	6:A:608:EDO:H12	1.64	0.62
1:A:211:HIS:ND1	1:B:351:ARG:NH1	2.47	0.62
1:C:218:ARG:HD2	11:C:965:HOH:O	1.99	0.62
1:C:354:ARG:HH12	6:C:608:EDO:C1	2.13	0.62
1:C:143:GLU:CD	1:C:214:ILE:HD11	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:O	1:A:34:MET:HG2	2.01	0.61
1:A:458:PRO:HG2	7:A:615:PEG:H11	1.82	0.60
1:B:156:VAL:HG23	1:B:176:ILE:HD11	1.83	0.60
1:A:538:ARG:HG2	1:C:536:ILE:HG12	1.84	0.59
1:C:300:ASP:OD1	6:C:611:EDO:C2	2.50	0.59
1:D:68:ARG:NH2	1:D:95:TYR:O	2.36	0.59
1:A:480:GLY:HA3	7:A:615:PEG:H12	1.83	0.59
1:A:18:GLN:N	11:A:705:HOH:O	2.35	0.58
1:A:354:ARG:HH22	6:A:612:EDO:H12	1.69	0.58
1:D:516:ARG:NH2	11:D:705:HOH:O	2.34	0.57
1:A:75[A]:GLU:OE1	1:A:78:LYS:NZ	2.36	0.57
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.69	0.56
1:A:118:ARG:NH2	11:A:707:HOH:O	2.38	0.56
1:B:501:ARG:NH2	2:B:601:FBP:O3P	2.39	0.56
1:B:501:ARG:HH22	2:B:601:FBP:P1	2.29	0.56
6:A:612:EDO:C1	11:B:842:HOH:O	2.54	0.55
1:A:421[B]:THR:HG23	11:A:760:HOH:O	2.07	0.55
1:D:96:HIS:HD2	11:D:887:HOH:O	1.90	0.55
1:A:68:ARG:NH2	11:A:708:HOH:O	2.39	0.55
1:A:421[B]:THR:HG21	11:A:881:HOH:O	2.06	0.55
6:A:612:EDO:H12	11:B:842:HOH:O	2.06	0.55
1:A:480:GLY:HA3	7:A:615:PEG:C1	2.38	0.54
1:A:523:VAL:HG21	1:A:540:LEU:HD12	1.89	0.54
1:A:113:SER:O	1:A:115:LEU:N	2.40	0.54
1:C:147:VAL:HG22	1:C:150:SER:HB3	1.90	0.53
1:C:517:VAL:HA	1:C:542:VAL:HG22	1.89	0.53
1:A:305:ALA:HB1	5:A:607:OXL:C2	2.39	0.53
1:A:330:ASN:HD21	1:A:367:GLY:HA3	1.74	0.53
1:A:113:SER:C	1:A:115:LEU:H	2.11	0.53
1:B:55:ARG:H	6:B:610:EDO:C1	2.23	0.52
1:B:175:ASN:ND2	1:B:178:ARG:HH11	2.07	0.52
1:D:115:LEU:O	1:D:512:ARG:NE	2.41	0.51
1:A:56:SER:HB2	1:A:480:GLY:HA2	1.92	0.51
1:C:382:PHE:HB3	1:C:385:GLU:CG	2.38	0.51
1:B:68:ARG:NH1	1:B:95:TYR:O	2.36	0.51
1:D:38:PHE:O	1:D:41:HIS:HB3	2.12	0.50
1:B:91:GLY:N	9:B:608:PGE:H32	2.27	0.50
1:C:242:ARG:CZ	1:C:246:GLN:HE22	2.24	0.50
1:A:55:ARG:N	6:A:608:EDO:H12	2.26	0.50
1:B:91:GLY:H	9:B:608:PGE:C3	2.25	0.50
1:B:421[A]:THR:HG23	1:B:534:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ARG:HG2	1:C:426:ILE:HD11	1.94	0.50
1:D:118:ARG:NH1	11:D:706:HOH:O	2.34	0.49
1:B:54:ALA:HA	6:B:610:EDO:H21	1.94	0.49
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.27	0.49
1:C:300:ASP:OD1	6:C:611:EDO:H22	2.12	0.49
1:A:346:MET:HA	1:A:349:LYS:O	2.12	0.48
1:C:90:HIS:O	1:C:96:HIS:HE1	1.95	0.48
1:B:420:PRO:HB2	11:B:718:HOH:O	2.12	0.48
1:C:300:ASP:OD1	6:C:611:EDO:H21	2.14	0.48
1:D:200:ILE:HG12	1:D:205:LEU:HD23	1.94	0.48
1:B:540:LEU:HD22	6:B:611:EDO:C1	2.44	0.47
1:C:300:ASP:HA	6:C:611:EDO:H22	1.94	0.47
1:B:536:ILE:HG12	1:D:538:ARG:HG2	1.96	0.47
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.96	0.47
1:C:284:GLU:HG2	1:C:305:ALA:HB3	1.96	0.47
1:C:335:PRO:HB3	1:C:477:LEU:O	2.14	0.47
1:C:27:GLN:HG2	11:C:958:HOH:O	2.14	0.47
1:C:55:ARG:HB2	1:C:395:ARG:HG3	1.97	0.47
1:C:28:GLN:HG2	11:C:804:HOH:O	2.14	0.46
1:C:205:LEU:O	1:C:207:THR:HG23	2.16	0.46
1:B:421[B]:THR:HG23	11:B:762:HOH:O	2.15	0.46
1:C:218:ARG:NH1	11:C:709:HOH:O	2.42	0.46
1:C:53:ALA:O	1:C:395:ARG:NH1	2.44	0.46
1:B:408:GLU:HG2	11:D:884:HOH:O	2.16	0.45
1:D:494:TRP:NE1	1:D:529:PRO:HG3	2.31	0.45
1:D:494:TRP:CD1	1:D:529:PRO:HG3	2.51	0.45
6:B:610:EDO:O2	11:B:701:HOH:O	2.21	0.45
1:A:421[B]:THR:OG1	1:A:452:LEU:HD12	2.16	0.45
1:D:61:ALA:HB3	1:D:81:MET:SD	2.57	0.45
1:A:38:PHE:O	1:A:41:HIS:HB3	2.17	0.44
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.99	0.44
1:B:189:ASP:CG	1:B:219:LYS:HD2	2.38	0.44
1:C:30:LEU:N	1:C:31:PRO:CD	2.80	0.44
1:A:230:LEU:O	1:A:231:PRO:C	2.56	0.44
1:B:421[B]:THR:CG2	11:B:762:HOH:O	2.64	0.44
1:B:156:VAL:CG2	1:B:176:ILE:HD11	2.48	0.44
1:B:200:ILE:HG12	1:B:205:LEU:HD23	2.00	0.44
1:A:475:VAL:HB	1:A:481:VAL:HG11	2.00	0.44
1:B:218:ARG:HH11	9:B:608:PGE:H32	1.83	0.44
1:D:435:CYS:CB	1:D:520:LEU:HD12	2.44	0.44
1:A:351:ARG:HD2	11:A:997:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HA	1:B:76:MET:HG3	2.00	0.43
1:B:218:ARG:HE	9:B:608:PGE:H4	1.83	0.43
1:C:124:LEU:C	1:C:124:LEU:HD23	2.39	0.43
1:C:409:GLU:OE2	1:D:37:THR:HB	2.18	0.43
1:B:421[B]:THR:HG22	1:B:534:THR:HB	2.01	0.43
1:A:317:LYS:NZ	11:A:729:HOH:O	2.50	0.42
1:B:171:VAL:HG11	1:B:176:ILE:HG12	2.01	0.42
1:D:382:PHE:N	1:D:383:PRO:CD	2.82	0.42
1:A:217:SER:HB2	6:A:610:EDO:H12	2.01	0.42
1:C:487:ARG:NH1	11:C:705:HOH:O	2.35	0.42
1:D:528:ARG:HB2	1:D:529:PRO:CD	2.49	0.42
6:B:611:EDO:H22	11:B:896:HOH:O	2.18	0.42
1:D:133:THR:HA	1:D:170:TRP:O	2.20	0.42
1:A:118:ARG:HH12	6:A:611:EDO:H11	1.84	0.42
1:C:143:GLU:OE1	1:C:214:ILE:HD11	2.20	0.42
6:A:608:EDO:H22	6:A:611:EDO:C2	2.49	0.42
1:D:544:HIS:C	1:D:544:HIS:CD2	2.92	0.42
1:B:343:LEU:HD23	1:B:356:GLU:HB3	2.02	0.42
1:A:30:LEU:N	1:A:31:PRO:CD	2.82	0.42
1:A:68:ARG:HD2	1:A:99:SER:OG	2.19	0.42
1:A:68:ARG:HH12	1:A:98:GLU:HB3	1.84	0.42
1:B:335:PRO:HB3	1:B:477:LEU:O	2.19	0.42
1:C:334:LYS:HE2	6:C:611:EDO:H11	2.02	0.41
1:D:433:PHE:CD2	6:D:607:EDO:H22	2.55	0.41
1:A:541:SER:H	8:A:616:PG4:C3	2.33	0.41
1:B:28:GLN:HG2	11:B:878:HOH:O	2.20	0.41
1:A:137:GLN:NE2	11:A:735:HOH:O	2.54	0.41
1:B:346:MET:HA	1:B:349:LYS:O	2.20	0.41
1:C:443:LEU:N	1:C:443:LEU:HD23	2.36	0.41
6:D:613:EDO:H21	11:D:921:HOH:O	2.20	0.41
1:A:69:SER:HB2	6:A:613:EDO:H12	2.03	0.41
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.93	0.41
1:B:30:LEU:N	1:B:31:PRO:CD	2.83	0.41
1:D:56:SER:HB2	1:D:480:GLY:HA2	2.01	0.41
11:A:753:HOH:O	1:B:36:ASP:HB3	2.21	0.41
6:D:613:EDO:C1	11:D:875:HOH:O	2.69	0.41
1:B:173:TYR:O	1:B:176:ILE:HG13	2.20	0.41
1:B:407:PHE:CE2	1:B:411:ARG:HD3	2.56	0.41
1:A:74:LYS:HE3	11:A:846:HOH:O	2.20	0.41
1:C:90:HIS:O	1:C:96:HIS:CE1	2.72	0.41
1:C:242:ARG:HD2	11:C:888:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ASP:O	1:D:423:VAL:HG23	2.20	0.40
1:D:218:ARG:NH2	11:D:735:HOH:O	2.53	0.40
1:A:541:SER:H	8:A:616:PG4:H31	1.86	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	528/550 (96%)	512 (97%)	14 (3%)	2 (0%)	34	37
1	B	524/550 (95%)	513 (98%)	9 (2%)	2 (0%)	34	37
1	C	528/550 (96%)	517 (98%)	10 (2%)	1 (0%)	47	55
1	D	525/550 (96%)	508 (97%)	14 (3%)	3 (1%)	25	26
All	All	2105/2200 (96%)	2050 (97%)	47 (2%)	8 (0%)	34	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	A	340	THR
1	B	340	THR
1	B	535	ASN
1	C	340	THR
1	D	535	ASN
1	D	112	THR
1	D	340	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/446 (97%)	418 (97%)	14 (3%)	39	50
1	B	428/446 (96%)	418 (98%)	10 (2%)	50	63
1	C	433/446 (97%)	419 (97%)	14 (3%)	39	50
1	D	429/446 (96%)	417 (97%)	12 (3%)	43	56
All	All	1722/1784 (96%)	1672 (97%)	50 (3%)	42	54

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

Mol	Chain	Res	Type
1	A	19	GLU
1	A	141	GLU
1	A	143	GLU
1	A	148	LYS
1	A	156	VAL
1	A	159	LYS
1	A	198	GLN
1	A	199	LYS
1	A	227	GLU
1	A	238	LEU
1	A	259	LYS
1	A	358	SER
1	A	404	ARG
1	A	499	ASP
1	B	71	ASP
1	B	76	MET
1	B	156	VAL
1	B	171	VAL
1	B	176	ILE
1	B	178	ARG
1	B	185	ARG
1	B	411	ARG
1	B	488	GLU
1	B	499	ASP

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Mol	Chain	Res	Type
1	C	116	SER
1	C	137	GLN
1	C	144	VAL
1	C	147	VAL
1	C	152	VAL
1	C	169	VAL
1	C	171	VAL
1	C	218	ARG
1	C	223	LEU
1	C	226	THR
1	C	358	SER
1	C	379	LYS
1	C	395	ARG
1	C	542	VAL
1	D	127	LYS
1	D	153	LEU
1	D	163	ARG
1	D	169	VAL
1	D	178	ARG
1	D	284	GLU
1	D	358	SER
1	D	407	PHE
1	D	499	ASP
1	D	500	ARG
1	D	543	SER
1	D	544	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	161	GLN
1	A	246	GLN
1	A	275	GLN
1	A	330	ASN
1	B	27	GLN
1	B	161	GLN
1	B	175	ASN
1	B	222	ASN
1	B	236	GLN
1	C	96	HIS
1	C	161	GLN

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Mol	Chain	Res	Type
1	C	222	ASN
1	C	246	GLN
1	C	286	HIS
1	C	545	HIS
1	C	546	HIS
1	D	28	GLN
1	D	96	HIS
1	D	102	ASN
1	D	161	GLN
1	D	211	HIS
1	D	222	ASN
1	D	286	HIS
1	D	503	GLN
1	D	544	HIS

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 62 ligands modelled in this entry, 14 are monoatomic - leaving 48 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	$\#\|Z\|>2$
9	PGE	B	608	-	9,9,9	0.90	0	8,8,8	1.22	1 (12%)
6	EDO	A	608	-	3,3,3	0.83	0	2,2,2	0.93	0
6	EDO	B	613	-	3,3,3	0.75	0	2,2,2	0.65	0
6	EDO	C	607	-	3,3,3	0.82	0	2,2,2	0.51	0
6	EDO	C	613	-	3,3,3	0.67	0	2,2,2	0.21	0
6	EDO	A	610	-	3,3,3	0.90	0	2,2,2	0.82	0
6	EDO	C	612	-	3,3,3	0.55	0	2,2,2	0.15	0
4	ATP	B	606	3	26,33,33	1.00	1 (3%)	31,52,52	1.62	7 (22%)
6	EDO	B	617	-	3,3,3	0.47	0	2,2,2	0.61	0
6	EDO	A	611	-	3,3,3	0.42	0	2,2,2	0.43	0
4	ATP	A	606	3	26,33,33	1.07	2 (7%)	31,52,52	1.62	4 (12%)
6	EDO	B	614	-	3,3,3	0.40	0	2,2,2	0.90	0
6	EDO	C	610	-	3,3,3	0.55	0	2,2,2	0.87	0
4	ATP	D	605	3	26,33,33	1.13	3 (11%)	31,52,52	1.58	6 (19%)
6	EDO	A	609	-	3,3,3	0.59	0	2,2,2	0.30	0
6	EDO	B	612	-	3,3,3	0.42	0	2,2,2	0.63	0
6	EDO	A	612	-	3,3,3	0.74	0	2,2,2	0.49	0
6	EDO	B	611	-	3,3,3	0.49	0	2,2,2	0.25	0
6	EDO	B	610	-	3,3,3	0.57	0	2,2,2	0.35	0
7	PEG	A	615	-	6,6,6	1.15	0	5,5,5	1.10	0
6	EDO	D	608	-	3,3,3	0.80	0	2,2,2	0.52	0
6	EDO	C	605	-	3,3,3	0.39	0	2,2,2	0.45	0
2	FBP	B	601	-	18,20,20	0.75	0	23,32,32	1.37	4 (17%)
5	OXL	A	607	3	5,5,5	1.81	1 (20%)	6,6,6	1.28	0
6	EDO	C	608	-	3,3,3	0.59	0	2,2,2	0.54	0
6	EDO	D	611	-	3,3,3	0.44	0	2,2,2	0.59	0
5	OXL	D	606	3	5,5,5	1.82	2 (40%)	6,6,6	0.86	0
6	EDO	B	616	-	3,3,3	0.72	0	2,2,2	0.21	0
6	EDO	D	609	-	3,3,3	0.57	0	2,2,2	0.39	0
6	EDO	D	610	-	3,3,3	0.23	0	2,2,2	0.87	0
6	EDO	D	613	-	3,3,3	0.43	0	2,2,2	0.37	0
2	FBP	D	601	-	18,20,20	0.92	0	23,32,32	1.60	5 (21%)
2	FBP	A	601	-	18,20,20	0.94	1 (5%)	23,32,32	1.29	3 (13%)
6	EDO	C	606	-	3,3,3	0.28	0	2,2,2	0.49	0
8	PG4	A	616	-	12,12,12	0.61	0	11,11,11	0.98	1 (9%)
5	OXL	C	604	3	5,5,5	1.54	1 (20%)	6,6,6	1.77	2 (33%)
6	EDO	D	612	-	3,3,3	0.40	0	2,2,2	0.80	0
6	EDO	A	613	-	3,3,3	0.77	0	2,2,2	0.23	0
2	FBP	C	601	-	18,20,20	0.65	0	23,32,32	1.12	1 (4%)
6	EDO	D	607	-	3,3,3	0.37	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PEG	D	615	-	6,6,6	0.67	0	5,5,5	0.64	0
5	OXL	B	607	3	5,5,5	1.71	1 (20%)	6,6,6	2.52	4 (66%)
6	EDO	C	611	-	3,3,3	0.60	0	2,2,2	0.52	0
6	EDO	A	614	-	3,3,3	0.57	0	2,2,2	0.34	0
6	EDO	B	609	-	3,3,3	0.35	0	2,2,2	0.66	0
6	EDO	C	609	-	3,3,3	0.61	0	2,2,2	0.19	0
6	EDO	B	615	-	3,3,3	0.38	0	2,2,2	0.57	0
6	EDO	D	614	-	3,3,3	0.40	0	2,2,2	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PGE	B	608	-	-	4/7/7/7	-
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	B	613	-	-	1/1/1/1	-
6	EDO	C	607	-	-	0/1/1/1	-
6	EDO	C	613	-	-	1/1/1/1	-
6	EDO	A	610	-	-	1/1/1/1	-
6	EDO	C	612	-	-	1/1/1/1	-
4	ATP	B	606	3	-	4/18/38/38	0/3/3/3
6	EDO	B	617	-	-	0/1/1/1	-
6	EDO	A	611	-	-	1/1/1/1	-
4	ATP	A	606	3	-	1/18/38/38	0/3/3/3
6	EDO	B	614	-	-	1/1/1/1	-
6	EDO	C	610	-	-	1/1/1/1	-
4	ATP	D	605	3	-	5/18/38/38	0/3/3/3
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	B	612	-	-	0/1/1/1	-
6	EDO	A	612	-	-	1/1/1/1	-
6	EDO	B	611	-	-	1/1/1/1	-
6	EDO	B	610	-	-	1/1/1/1	-
7	PEG	A	615	-	-	1/4/4/4	-
6	EDO	D	608	-	-	0/1/1/1	-
6	EDO	C	605	-	-	1/1/1/1	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
5	OXL	A	607	3	-	0/4/4/4	-
6	EDO	C	608	-	-	1/1/1/1	-
6	EDO	D	611	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OXL	D	606	3	-	1/4/4/4	-
6	EDO	B	616	-	-	1/1/1/1	-
6	EDO	D	609	-	-	1/1/1/1	-
6	EDO	D	610	-	-	0/1/1/1	-
6	EDO	D	613	-	-	1/1/1/1	-
2	FBP	D	601	-	-	3/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
6	EDO	C	606	-	-	1/1/1/1	-
8	PG4	A	616	-	-	6/10/10/10	-
5	OXL	C	604	3	-	0/4/4/4	-
6	EDO	D	612	-	-	0/1/1/1	-
6	EDO	A	613	-	-	1/1/1/1	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
6	EDO	D	607	-	-	1/1/1/1	-
7	PEG	D	615	-	-	1/4/4/4	-
5	OXL	B	607	3	-	0/4/4/4	-
6	EDO	C	611	-	-	1/1/1/1	-
6	EDO	A	614	-	-	1/1/1/1	-
6	EDO	B	609	-	-	0/1/1/1	-
6	EDO	C	609	-	-	0/1/1/1	-
6	EDO	B	615	-	-	1/1/1/1	-
6	EDO	D	614	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	ATP	O4'-C1'	3.01	1.45	1.41
5	B	607	OXL	C2-C1	-2.81	1.46	1.54
4	B	606	ATP	C5-C4	2.80	1.48	1.40
5	A	607	OXL	C2-C1	-2.69	1.46	1.54
4	D	605	ATP	C5-C4	2.62	1.47	1.40
4	D	605	ATP	O4'-C1'	2.41	1.44	1.41
5	C	604	OXL	O1-C1	2.30	1.28	1.22
4	A	606	ATP	C5-N7	-2.19	1.31	1.39
5	D	606	OXL	C2-C1	-2.14	1.48	1.54
5	D	606	OXL	O1-C1	2.13	1.28	1.22
2	A	601	FBP	O5-C2	-2.08	1.40	1.43
4	D	605	ATP	C4-N3	2.04	1.38	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	605	ATP	N3-C2-N1	-3.82	122.70	128.68
4	A	606	ATP	O3G-PG-O2G	3.80	122.14	107.64
4	A	606	ATP	N3-C2-N1	-3.56	123.12	128.68
4	B	606	ATP	N3-C2-N1	-3.50	123.20	128.68
5	B	607	OXL	O1-C1-C2	-3.47	109.64	120.78
5	B	607	OXL	O3-C1-C2	3.39	123.22	113.16
2	D	601	FBP	O6-P2-O4P	-3.24	97.39	106.47
4	A	606	ATP	O2A-PA-O1A	3.19	128.02	112.24
2	D	601	FBP	O3P-P1-O2P	3.17	119.74	107.64
2	B	601	FBP	O2P-P1-O1P	3.15	123.02	110.68
4	A	606	ATP	C1'-N9-C4	-3.15	121.11	126.64
5	C	604	OXL	O4-C2-C1	3.08	122.31	113.16
4	B	606	ATP	O2G-PG-O3B	-2.93	94.80	104.64
4	B	606	ATP	C2-N1-C6	2.87	123.67	118.75
5	B	607	OXL	O4-C2-C1	2.76	121.37	113.16
4	D	605	ATP	C2-N1-C6	2.66	123.30	118.75
4	B	606	ATP	O3G-PG-O2G	2.60	117.56	107.64
2	D	601	FBP	O3P-P1-O1	-2.48	100.12	106.73
2	D	601	FBP	O3P-P1-O1P	2.47	120.35	110.68
4	B	606	ATP	O2A-PA-O1A	2.47	124.44	112.24
4	B	606	ATP	O3G-PG-O1G	2.46	120.33	110.68
2	A	601	FBP	O5P-P2-O6	-2.43	100.26	106.73
4	D	605	ATP	O2G-PG-O1G	2.40	120.08	110.68
2	B	601	FBP	O1-P1-O1P	-2.39	99.76	106.47
4	B	606	ATP	N6-C6-N1	2.37	123.50	118.57
4	D	605	ATP	PB-O3B-PG	-2.33	124.82	132.83
4	D	605	ATP	N6-C6-N1	2.29	123.33	118.57
9	B	608	PGE	O3-C5-C6	2.29	120.12	110.07
5	C	604	OXL	O3-C1-C2	2.27	119.89	113.16
2	B	601	FBP	O6P-P2-O5P	2.23	116.15	107.64
2	C	601	FBP	O1-P1-O1P	-2.16	100.42	106.47
5	B	607	OXL	O2-C2-C1	-2.12	113.99	120.78
4	D	605	ATP	O2A-PA-O1A	2.10	122.62	112.24
2	D	601	FBP	O5P-P2-O6	2.10	112.31	106.73
2	A	601	FBP	P2-O6-C6	2.08	124.02	118.30
8	A	616	PG4	O2-C2-C1	2.03	119.00	110.07
2	B	601	FBP	O5-C5-C6	2.03	113.92	109.45
2	A	601	FBP	O1-P1-O1P	2.02	112.13	106.47

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
4	B	606	ATP	PB-O3B-PG-O3G
8	A	616	PG4	C1-C2-O2-C3
2	B	601	FBP	C4-C5-C6-O6
9	B	608	PGE	O2-C3-C4-O3
2	A	601	FBP	O5-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
7	A	615	PEG	O1-C1-C2-O2
9	B	608	PGE	C3-C4-O3-C5
9	B	608	PGE	O3-C5-C6-O4
6	A	610	EDO	O1-C1-C2-O2
6	A	612	EDO	O1-C1-C2-O2
6	C	606	EDO	O1-C1-C2-O2
6	C	608	EDO	O1-C1-C2-O2
6	C	611	EDO	O1-C1-C2-O2
6	C	612	EDO	O1-C1-C2-O2
6	D	607	EDO	O1-C1-C2-O2
6	D	611	EDO	O1-C1-C2-O2
6	D	613	EDO	O1-C1-C2-O2
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
7	D	615	PEG	O1-C1-C2-O2
6	C	605	EDO	O1-C1-C2-O2
4	B	606	ATP	PB-O3A-PA-O1A
4	D	605	ATP	PA-O3A-PB-O1B
8	A	616	PG4	O2-C3-C4-O3
6	A	611	EDO	O1-C1-C2-O2
6	A	613	EDO	O1-C1-C2-O2
6	B	613	EDO	O1-C1-C2-O2
6	B	615	EDO	O1-C1-C2-O2
6	B	616	EDO	O1-C1-C2-O2
6	C	613	EDO	O1-C1-C2-O2
9	B	608	PGE	C1-C2-O2-C3
8	A	616	PG4	C3-C4-O3-C5
4	A	606	ATP	PB-O3B-PG-O2G
4	D	605	ATP	PB-O3B-PG-O2G
8	A	616	PG4	C8-C7-O4-C6
2	D	601	FBP	O5-C5-C6-O6
4	D	605	ATP	PB-O3A-PA-O2A
6	A	614	EDO	O1-C1-C2-O2
6	B	610	EDO	O1-C1-C2-O2
6	B	614	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	C	610	EDO	O1-C1-C2-O2
8	A	616	PG4	O1-C1-C2-O2
4	B	606	ATP	PB-O3A-PA-O2A
8	A	616	PG4	O3-C5-C6-O4
4	D	605	ATP	PB-O3A-PA-O1A
5	D	606	OXL	O3-C1-C2-O4
2	D	601	FBP	C6-O6-P2-O4P
6	B	611	EDO	O1-C1-C2-O2
4	D	605	ATP	PA-O3A-PB-O2B
6	D	609	EDO	O1-C1-C2-O2
4	B	606	ATP	PB-O3B-PG-O1G

There are no ring outliers.

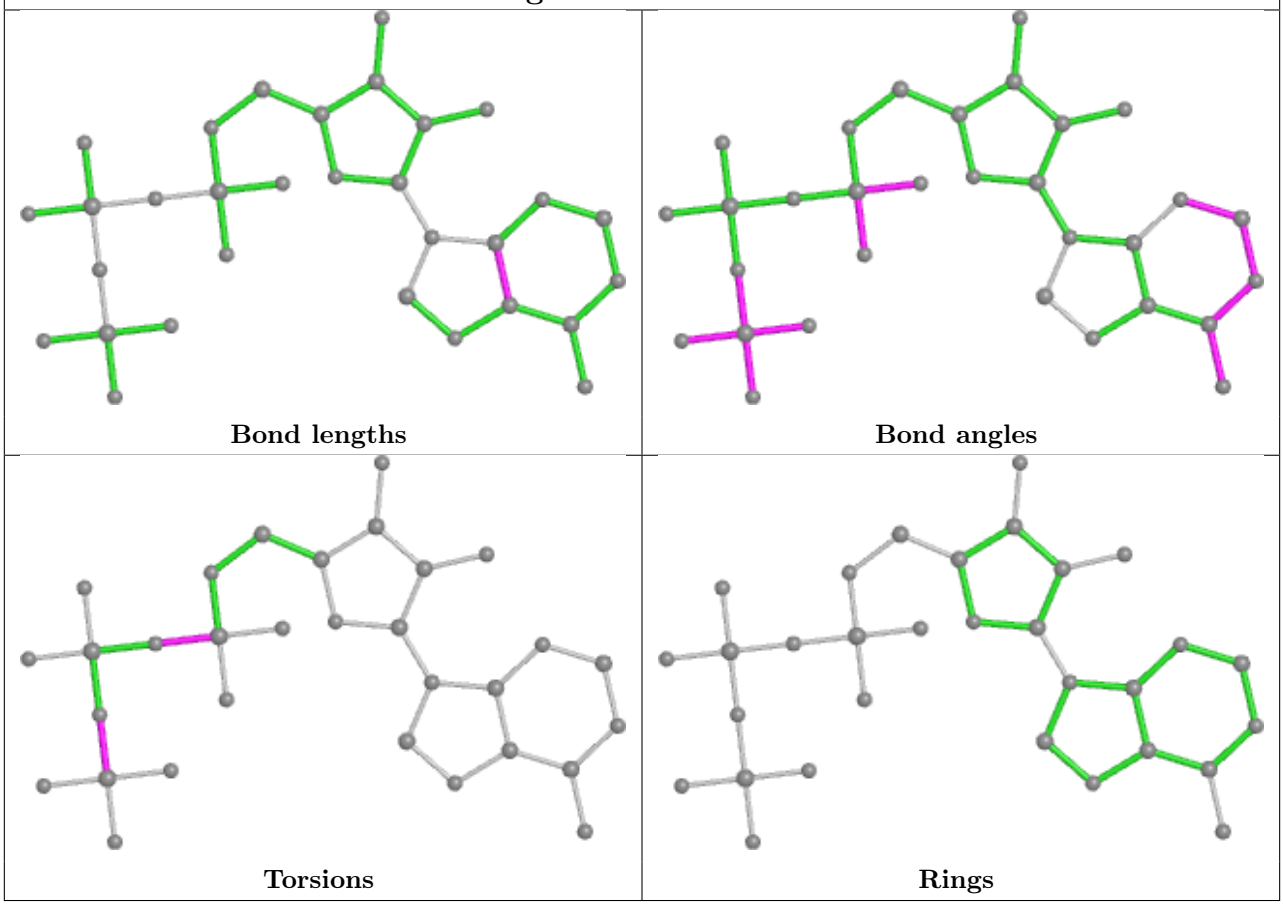
16 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	608	PGE	5	0
6	A	608	EDO	3	0
6	A	610	EDO	1	0
6	A	611	EDO	2	0
6	A	612	EDO	3	0
6	B	611	EDO	2	0
6	B	610	EDO	3	0
7	A	615	PEG	3	0
2	B	601	FBP	2	0
5	A	607	OXL	1	0
6	C	608	EDO	2	0
6	D	613	EDO	2	0
8	A	616	PG4	2	0
6	A	613	EDO	1	0
6	D	607	EDO	1	0
6	C	611	EDO	5	0

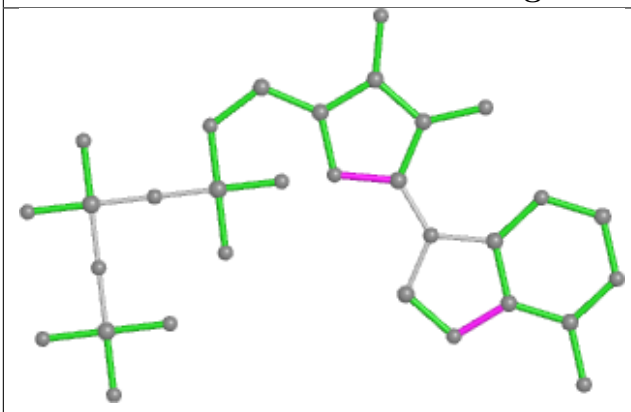
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

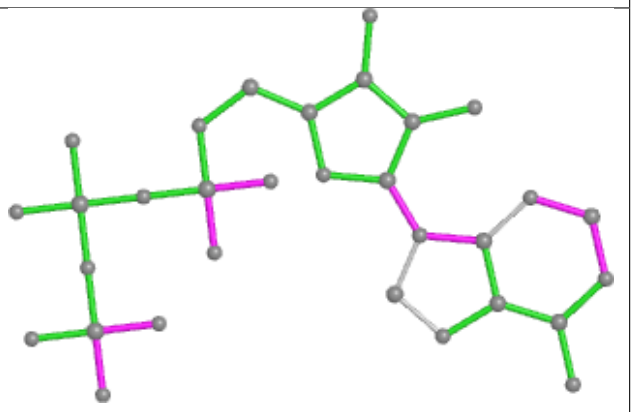
Ligand ATP B 606



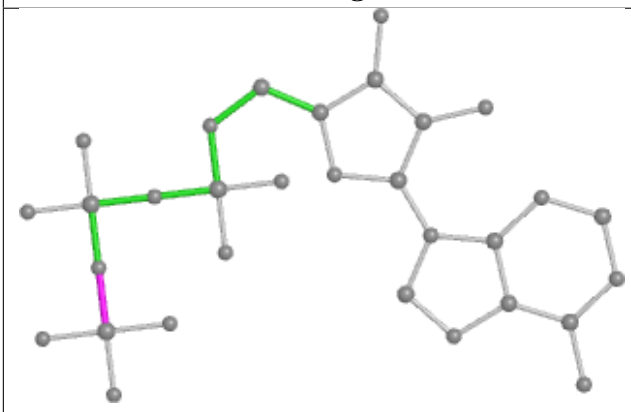
Ligand ATP A 606



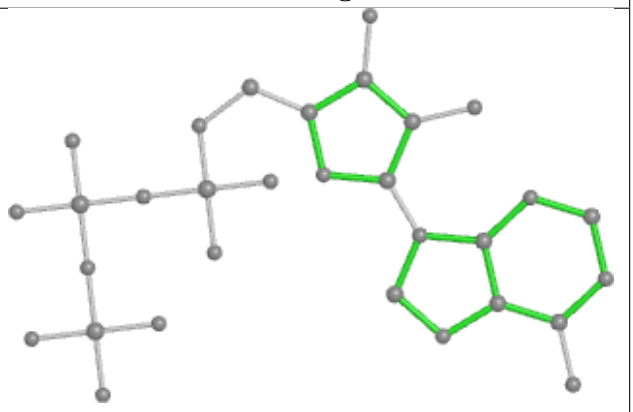
Bond lengths



Bond angles

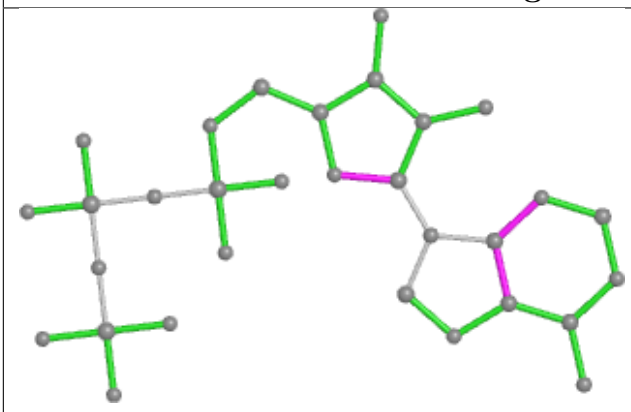


Torsions

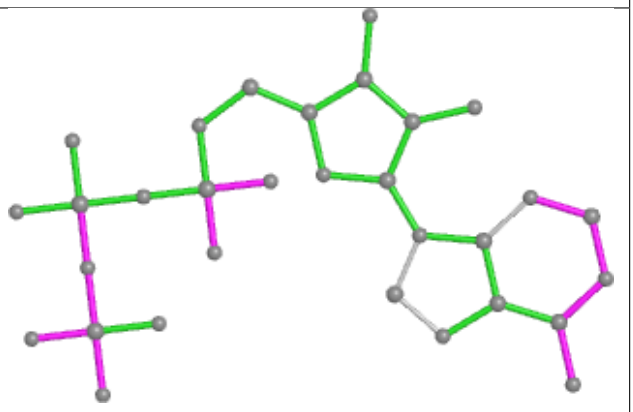


Rings

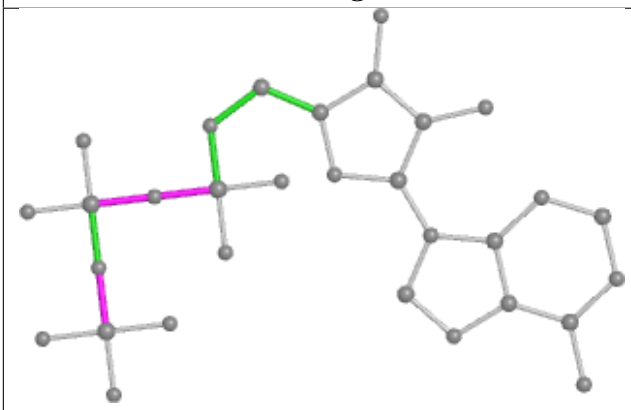
Ligand ATP D 605



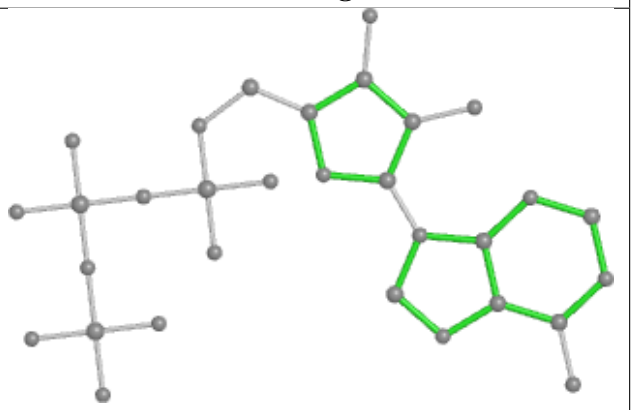
Bond lengths



Bond angles

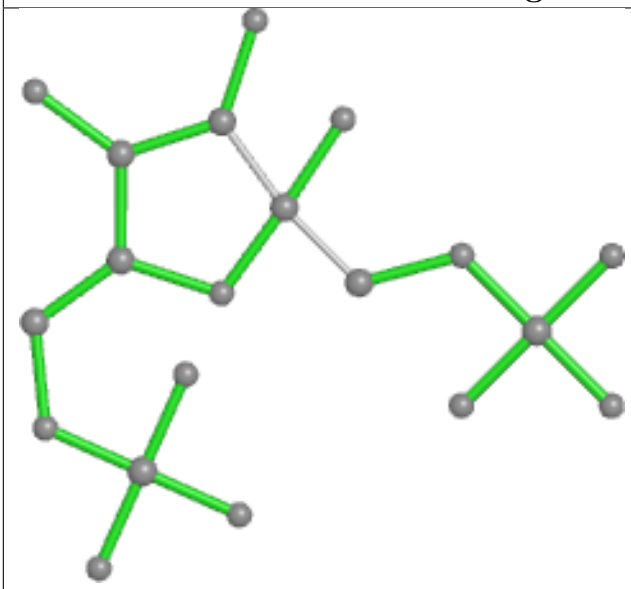


Torsions

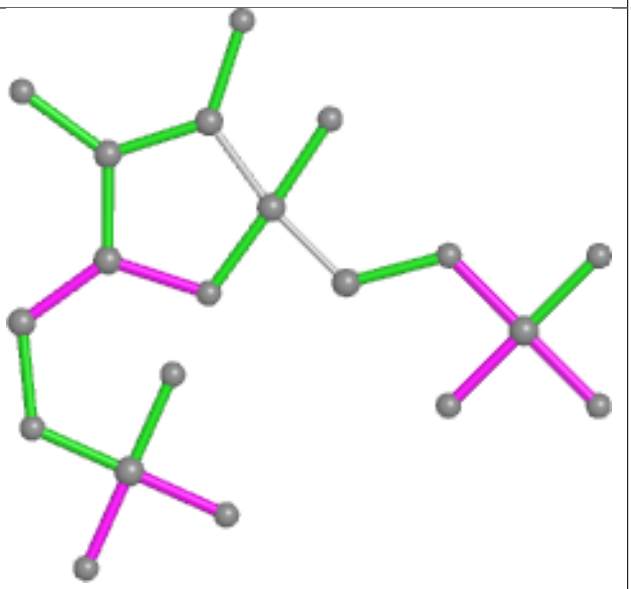


Rings

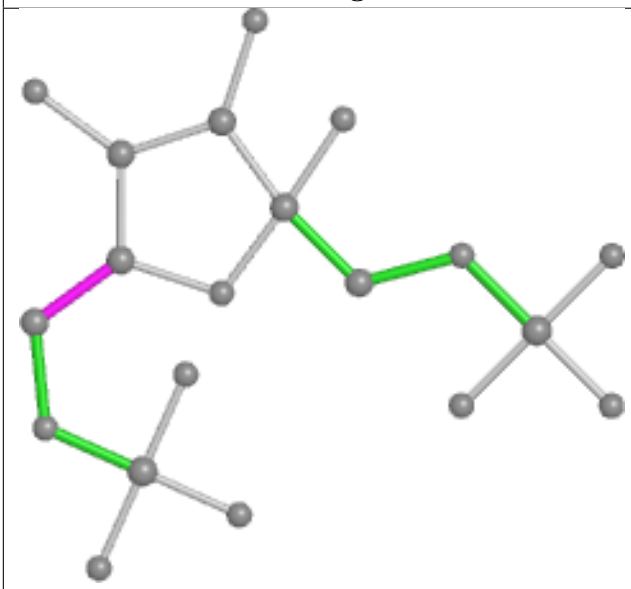
Ligand FBP B 601



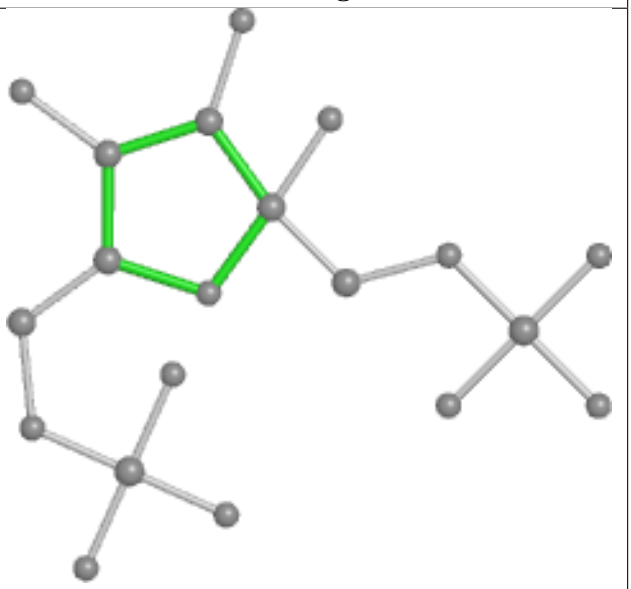
Bond lengths



Bond angles

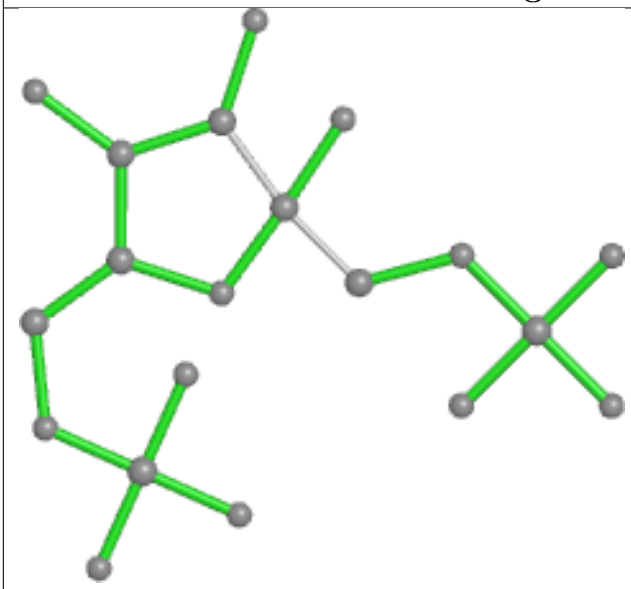


Torsions

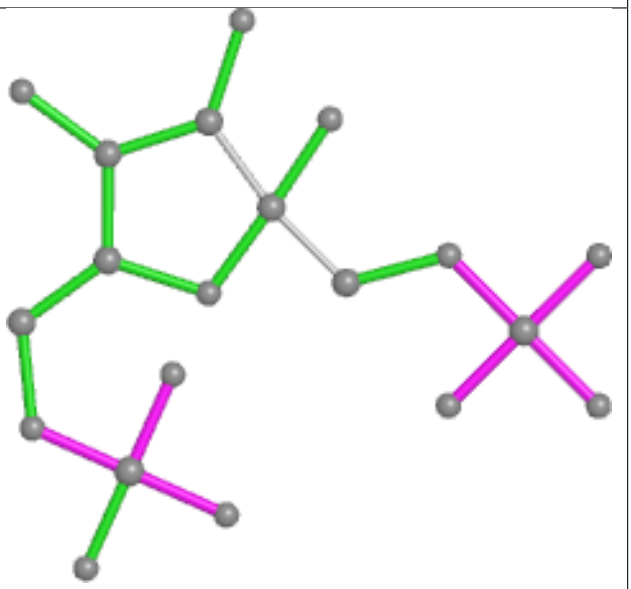


Rings

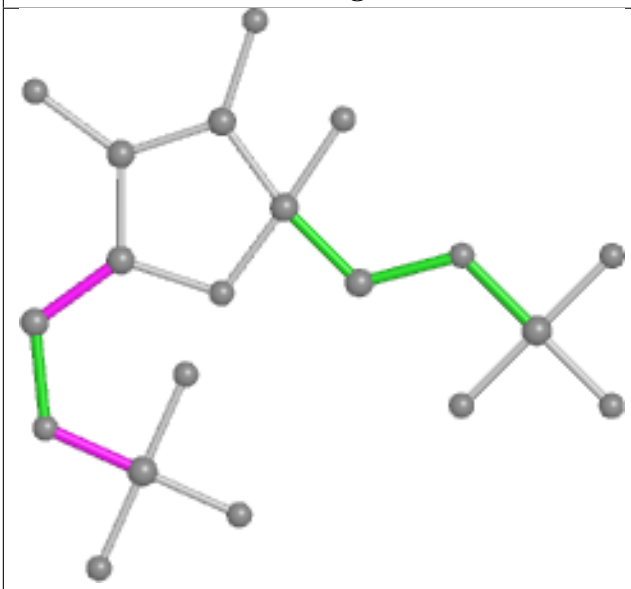
Ligand FBP D 601



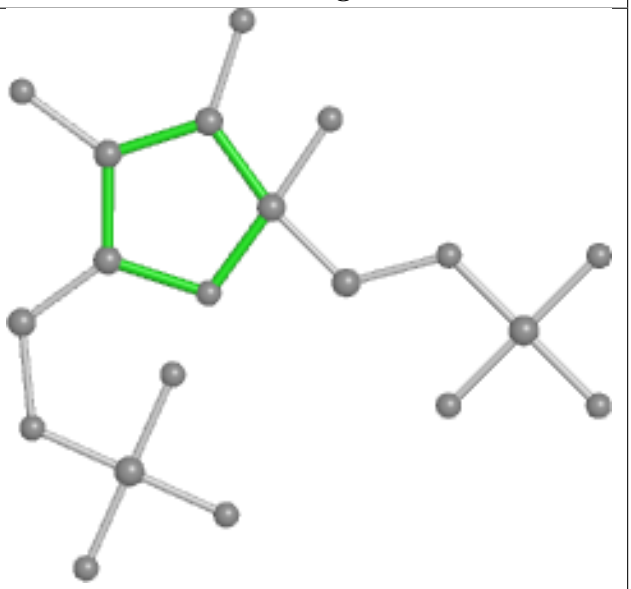
Bond lengths



Bond angles

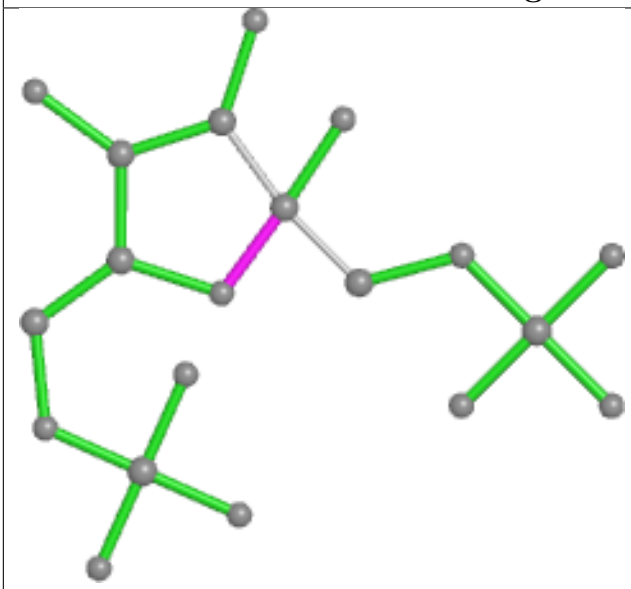


Torsions

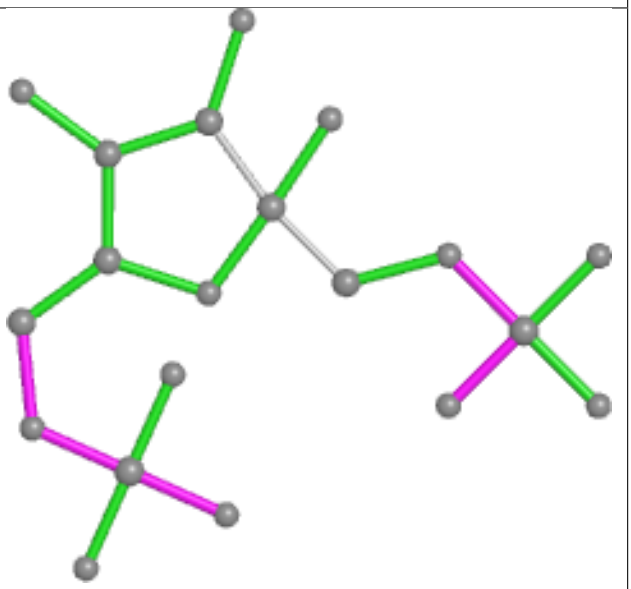


Rings

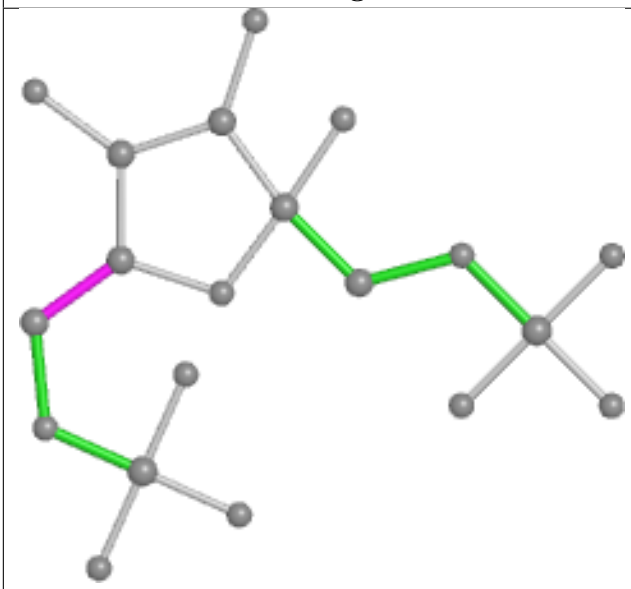
Ligand FBP A 601



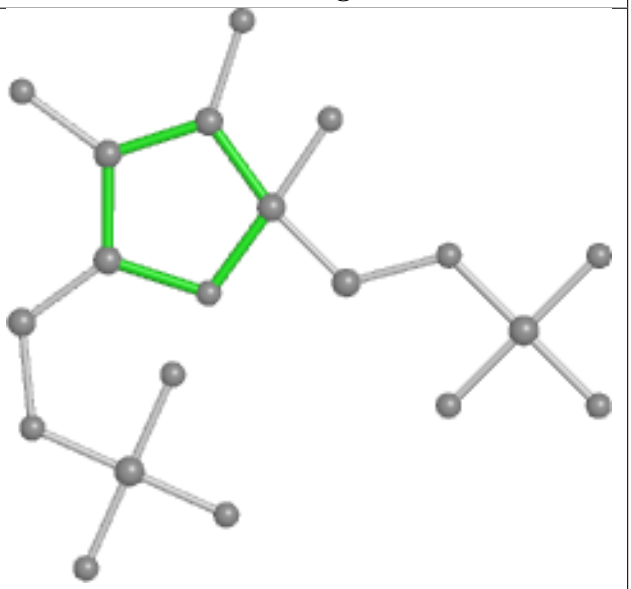
Bond lengths



Bond angles

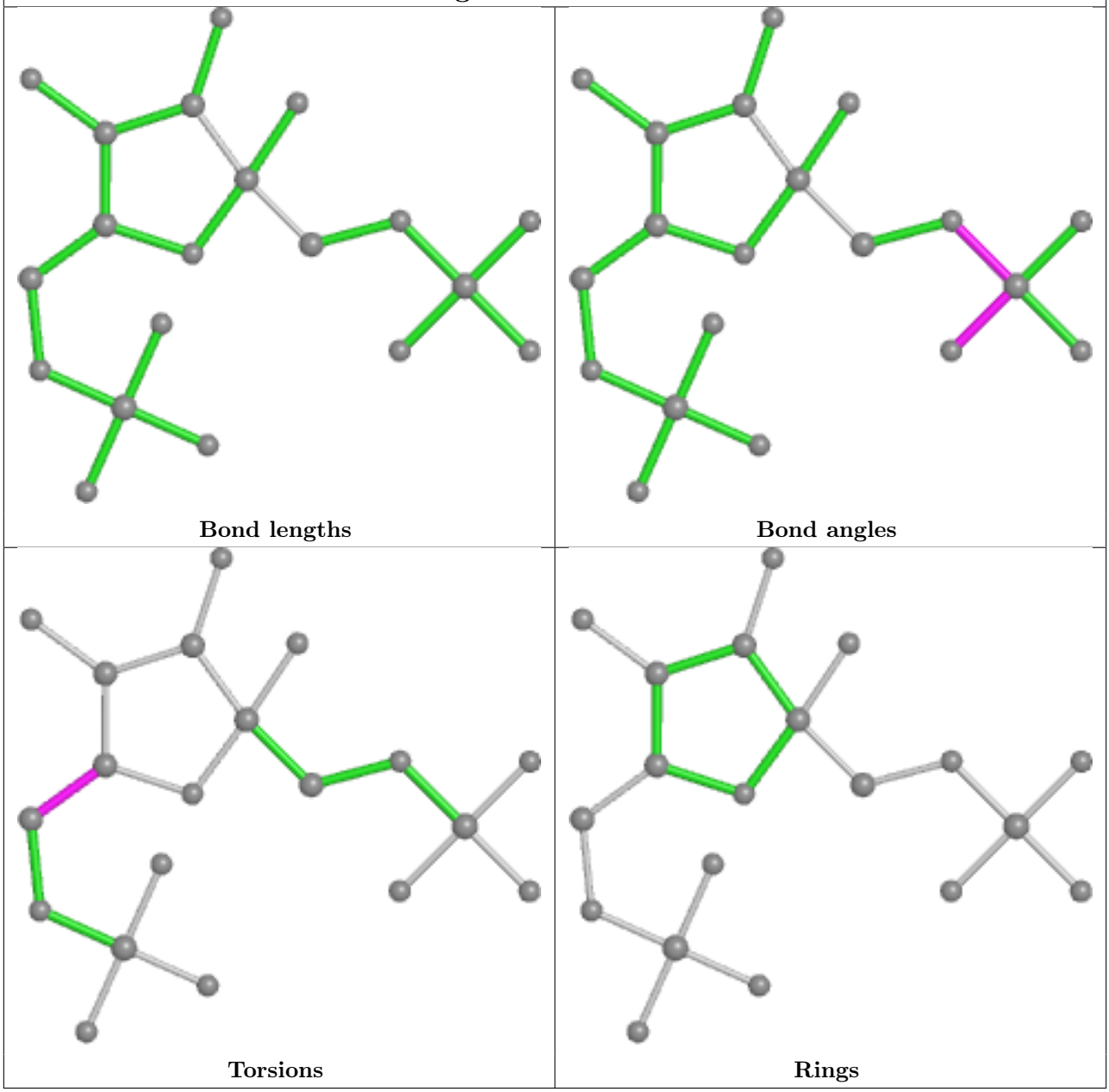


Torsions



Rings

Ligand FBP C 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	528/550 (96%)	0.07	30 (5%)	23	22	27, 40, 73, 110	0
1	B	525/550 (95%)	0.08	21 (4%)	38	36	30, 44, 70, 106	0
1	C	528/550 (96%)	0.22	42 (7%)	12	11	29, 42, 76, 123	0
1	D	527/550 (95%)	0.28	45 (8%)	10	9	29, 44, 77, 124	0
All	All	2108/2200 (95%)	0.16	138 (6%)	18	17	27, 43, 74, 124	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	115	LEU	7.4
1	B	22	THR	6.2
1	C	229	ASP	6.2
1	C	228	VAL	5.9
1	D	181	ALA	5.4
1	D	200	ILE	5.2
1	A	20	LEU	4.9
1	B	517	VAL	4.9
1	D	182	VAL	4.8
1	A	22	THR	4.6
1	A	21	GLY	4.6
1	D	22	THR	4.5
1	B	21	GLY	4.4
1	D	201	GLY	4.4
1	B	20	LEU	4.4
1	D	184	GLY	4.1
1	D	492	ALA	4.1
1	D	159	LYS	4.0
1	D	180	VAL	4.0
1	D	204	GLY	3.9
1	C	181	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	205	LEU	3.9
1	D	207	THR	3.9
1	D	206	VAL	3.8
1	B	25	PHE	3.7
1	C	180	VAL	3.6
1	C	182	VAL	3.6
1	B	493	ILE	3.5
1	C	227	GLU	3.5
1	D	225	ASN	3.5
1	D	544	HIS	3.5
1	C	26	GLN	3.5
1	C	178	ARG	3.4
1	B	23	ALA	3.4
1	C	202	PRO	3.4
1	D	202	PRO	3.4
1	C	200	ILE	3.3
1	D	197	VAL	3.3
1	A	201	GLY	3.2
1	C	151	GLN	3.2
1	D	511	LEU	3.1
1	C	179	VAL	3.1
1	D	196	VAL	3.1
1	D	21	GLY	3.1
1	A	202	PRO	3.0
1	B	202	PRO	3.0
1	C	25	PHE	3.0
1	B	26	GLN	3.0
1	C	147	VAL	3.0
1	C	204	GLY	3.0
1	A	544	HIS	2.9
1	D	150	SER	2.9
1	C	22	THR	2.9
1	D	203	GLU	2.9
1	B	516	ARG	2.9
1	C	114	PRO	2.9
1	C	153	LEU	2.9
1	A	200	ILE	2.9
1	D	198	GLN	2.8
1	A	343	LEU	2.8
1	D	151	GLN	2.8
1	D	19	GLU	2.8
1	A	116	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	492	ALA	2.7
1	A	227	GLU	2.7
1	A	113	SER	2.7
1	A	545	HIS	2.7
1	C	199	LYS	2.7
1	D	160	PHE	2.7
1	A	180	VAL	2.6
1	D	174	HIS	2.6
1	B	115	LEU	2.6
1	C	166	ALA	2.6
1	D	371	ILE	2.5
1	D	20	LEU	2.5
1	A	114	PRO	2.5
1	C	206	VAL	2.5
1	C	364	VAL	2.5
1	D	199	LYS	2.5
1	B	201	GLY	2.5
1	C	167	LYS	2.5
1	C	175	ASN	2.4
1	A	19	GLU	2.4
1	C	203	GLU	2.4
1	B	24	PHE	2.4
1	A	23	ALA	2.4
1	C	196	VAL	2.4
1	A	371	ILE	2.4
1	C	201	GLY	2.4
1	D	183	GLY	2.4
1	C	160	PHE	2.4
1	D	179	VAL	2.4
1	A	203	GLU	2.3
1	D	147	VAL	2.3
1	C	23	ALA	2.3
1	A	360	VAL	2.3
1	D	543	SER	2.3
1	D	112	THR	2.3
1	C	186	ILE	2.3
1	B	518	GLY	2.3
1	C	365	LEU	2.3
1	A	25	PHE	2.3
1	C	226	THR	2.3
1	D	158	PRO	2.3
1	A	355	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	18	GLN	2.3
1	C	163	ARG	2.2
1	D	156	VAL	2.2
1	C	231	PRO	2.2
1	D	494	TRP	2.2
1	C	150	SER	2.2
1	C	360	VAL	2.2
1	D	168	THR	2.2
1	B	156	VAL	2.2
1	A	175	ASN	2.2
1	B	203	GLU	2.2
1	C	159	LYS	2.2
1	A	181	ALA	2.2
1	A	229	ASP	2.2
1	D	114	PRO	2.2
1	D	513	GLY	2.1
1	C	208	GLU	2.1
1	A	178	ARG	2.1
1	B	371	ILE	2.1
1	D	153	LEU	2.1
1	A	204	GLY	2.1
1	A	26	GLN	2.1
1	C	115	LEU	2.1
1	A	386	ALA	2.1
1	B	160	PHE	2.1
1	A	357	THR	2.0
1	D	177	THR	2.0
1	B	318	VAL	2.0
1	D	152	VAL	2.0
1	B	342	MET	2.0
1	C	174	HIS	2.0
1	C	177	THR	2.0
1	C	371	ILE	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	EDO	C	609	4/4	0.57	0.24	75,82,85,88	0
3	MG	D	602	1/1	0.60	0.28	41,41,41,41	0
6	EDO	C	608	4/4	0.63	0.25	56,67,68,73	0
6	EDO	C	613	4/4	0.63	0.24	63,70,73,73	0
7	PEG	A	615	7/7	0.63	0.36	48,63,77,78	0
7	PEG	D	615	7/7	0.67	0.26	60,74,83,86	0
8	PG4	A	616	13/13	0.67	0.19	58,75,86,90	0
6	EDO	A	608	4/4	0.69	0.27	50,55,59,63	0
6	EDO	B	611	4/4	0.71	0.16	79,79,80,81	0
6	EDO	B	614	4/4	0.77	0.27	61,69,70,74	0
6	EDO	B	616	4/4	0.77	0.21	72,75,76,77	0
3	MG	B	604	1/1	0.78	0.23	35,35,35,35	0
3	MG	A	605	1/1	0.78	0.31	69,69,69,69	0
3	MG	A	603	1/1	0.79	0.42	49,49,49,49	0
6	EDO	C	607	4/4	0.79	0.19	57,59,65,65	0
6	EDO	B	610	4/4	0.80	0.12	56,59,59,65	0
6	EDO	A	612	4/4	0.81	0.30	63,63,68,68	0
9	PGE	B	608	10/10	0.81	0.25	46,68,79,86	0
3	MG	B	605	1/1	0.83	0.12	44,44,44,44	0
6	EDO	A	613	4/4	0.84	0.22	51,51,61,63	0
6	EDO	D	611	4/4	0.84	0.13	60,64,67,73	0
3	MG	C	602	1/1	0.84	0.21	47,47,47,47	0
6	EDO	B	617	4/4	0.86	0.17	66,67,68,69	0
3	MG	A	602	1/1	0.88	0.18	34,34,34,34	0
6	EDO	D	610	4/4	0.88	0.15	57,60,61,70	0
6	EDO	A	614	4/4	0.88	0.18	53,55,57,62	0
6	EDO	D	613	4/4	0.88	0.10	53,60,65,68	0
6	EDO	C	612	4/4	0.89	0.22	65,72,72,73	0
6	EDO	B	613	4/4	0.90	0.12	42,50,54,62	0
6	EDO	B	609	4/4	0.90	0.15	59,65,68,73	0
3	MG	B	602	1/1	0.91	0.16	38,38,38,38	0
6	EDO	C	606	4/4	0.91	0.22	61,62,65,72	0
3	MG	D	603	1/1	0.92	0.15	35,35,35,35	0
6	EDO	C	610	4/4	0.92	0.25	40,41,52,53	0
6	EDO	A	610	4/4	0.92	0.17	46,48,51,51	0
6	EDO	B	615	4/4	0.92	0.19	55,64,66,67	0
6	EDO	D	608	4/4	0.92	0.11	42,42,43,46	0

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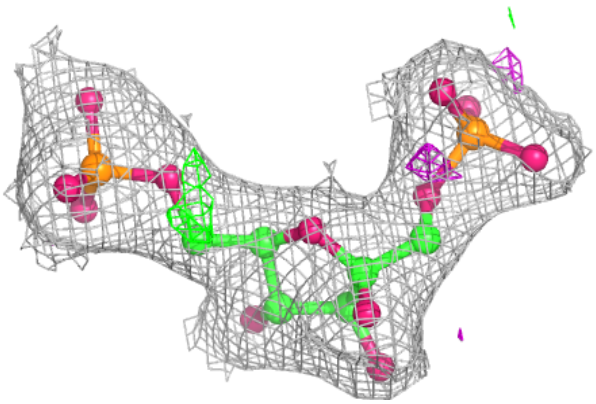
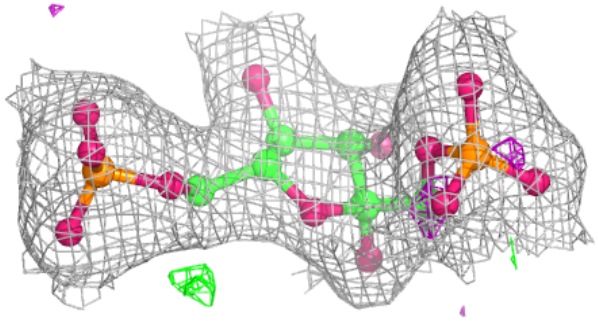
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	611	4/4	0.92	0.14	56,57,57,58	0
6	EDO	D	612	4/4	0.93	0.17	47,51,53,61	0
6	EDO	C	611	4/4	0.93	0.24	41,52,53,64	0
6	EDO	D	607	4/4	0.94	0.17	59,61,67,72	0
6	EDO	D	614	4/4	0.94	0.12	54,60,61,67	0
6	EDO	C	605	4/4	0.95	0.12	60,60,67,68	0
6	EDO	A	609	4/4	0.95	0.14	43,44,44,44	0
5	OXL	D	606	6/6	0.96	0.09	35,38,41,43	0
6	EDO	B	612	4/4	0.96	0.13	44,56,60,64	0
6	EDO	D	609	4/4	0.96	0.16	41,46,46,48	0
5	OXL	B	607	6/6	0.97	0.10	33,36,44,45	0
5	OXL	C	604	6/6	0.97	0.09	33,42,44,50	0
3	MG	B	603	1/1	0.97	0.16	25,25,25,25	0
2	FBP	B	601	20/20	0.97	0.09	39,43,47,48	0
5	OXL	A	607	6/6	0.97	0.08	32,35,37,41	0
10	CL	D	616	1/1	0.97	0.09	62,62,62,62	0
4	ATP	A	606	31/31	0.98	0.10	27,31,34,38	0
4	ATP	B	606	31/31	0.98	0.09	25,36,43,45	0
4	ATP	D	605	31/31	0.98	0.09	30,37,43,44	0
2	FBP	C	601	20/20	0.98	0.07	32,35,39,40	0
2	FBP	D	601	20/20	0.98	0.10	37,42,45,49	0
2	FBP	A	601	20/20	0.99	0.10	29,31,34,35	0
3	MG	A	604	1/1	0.99	0.19	24,24,24,24	0
3	MG	D	604	1/1	0.99	0.16	28,28,28,28	0
3	MG	C	603	1/1	0.99	0.13	26,26,26,26	0

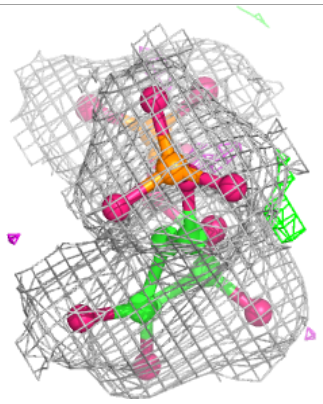
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP 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)

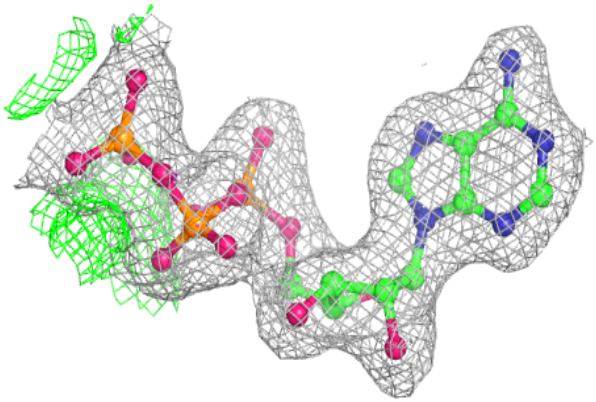


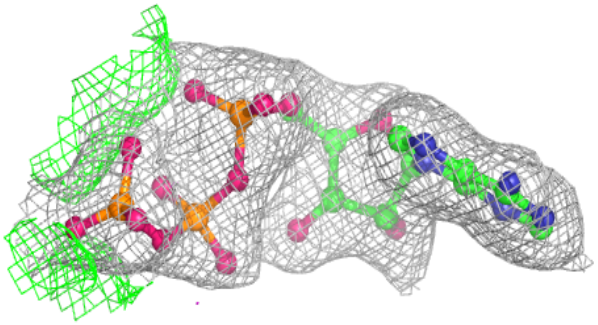


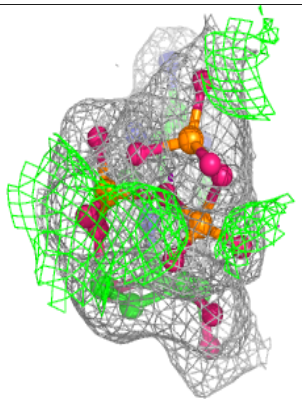


Electron density around ATP A 606:

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

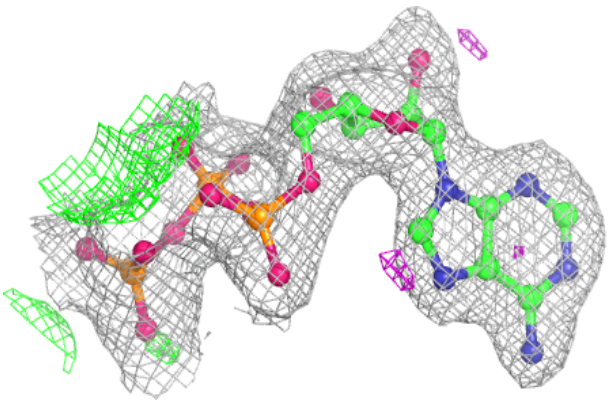


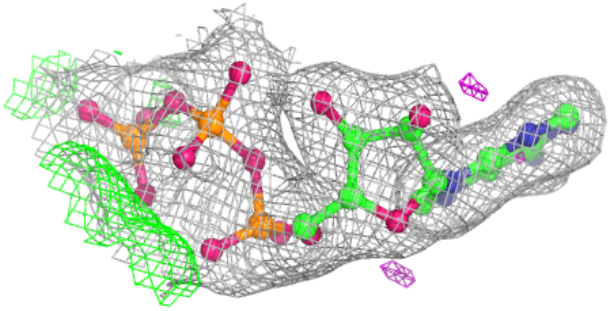


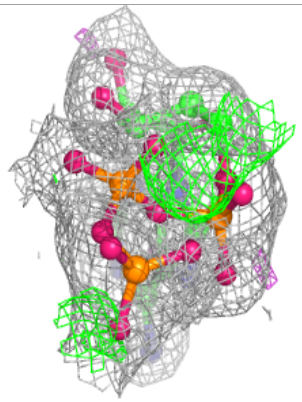


Electron density around ATP B 606:

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

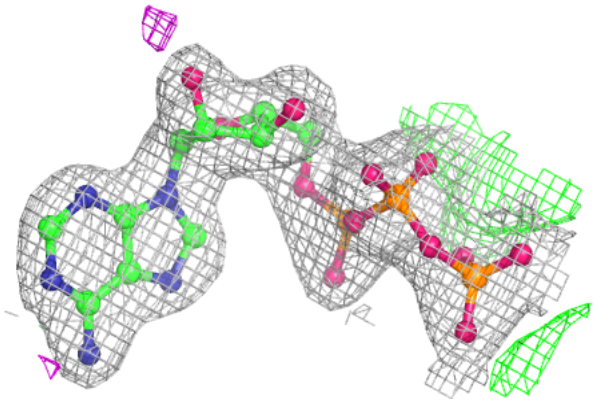


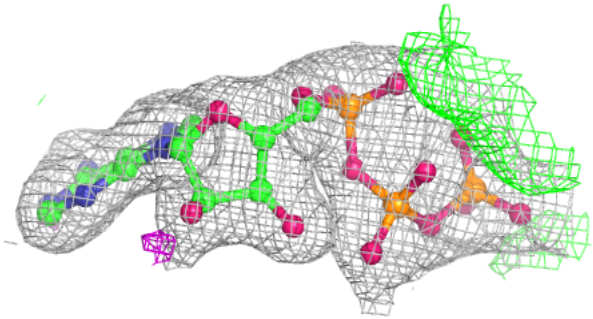


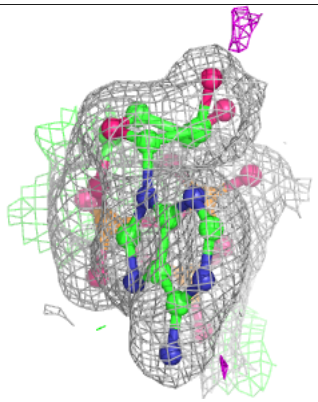


Electron density around ATP D 605:

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

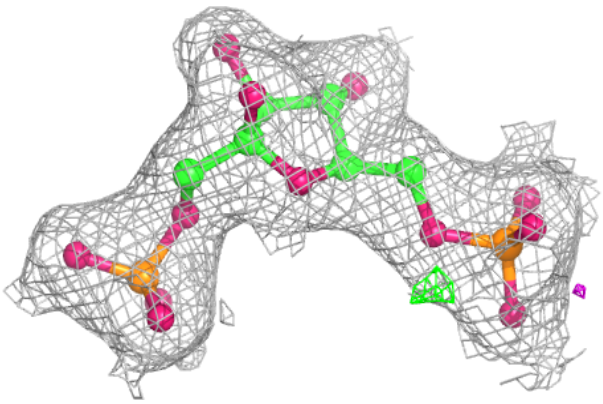


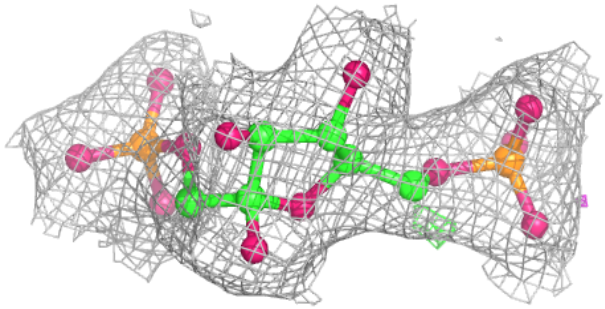


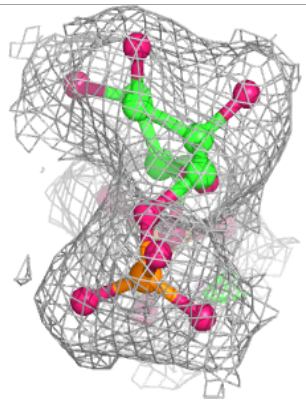


Electron density around FBP C 601:

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

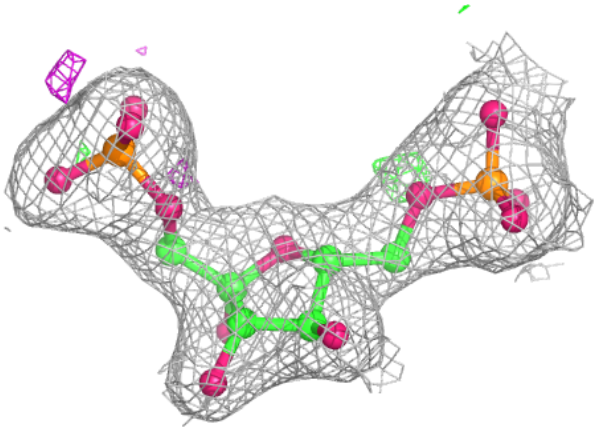


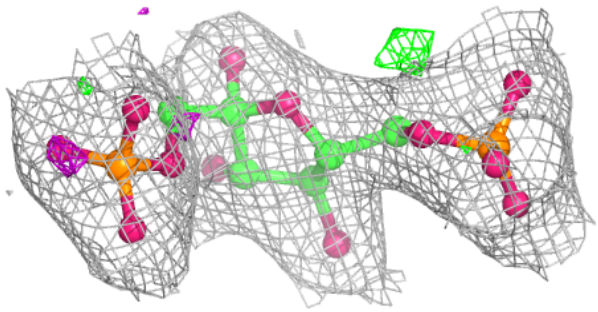


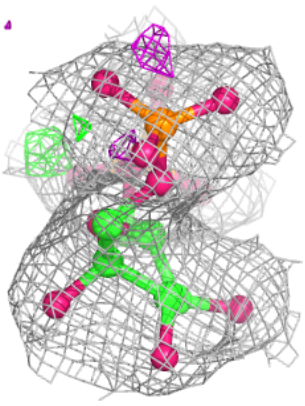


Electron density around FBP D 601:

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

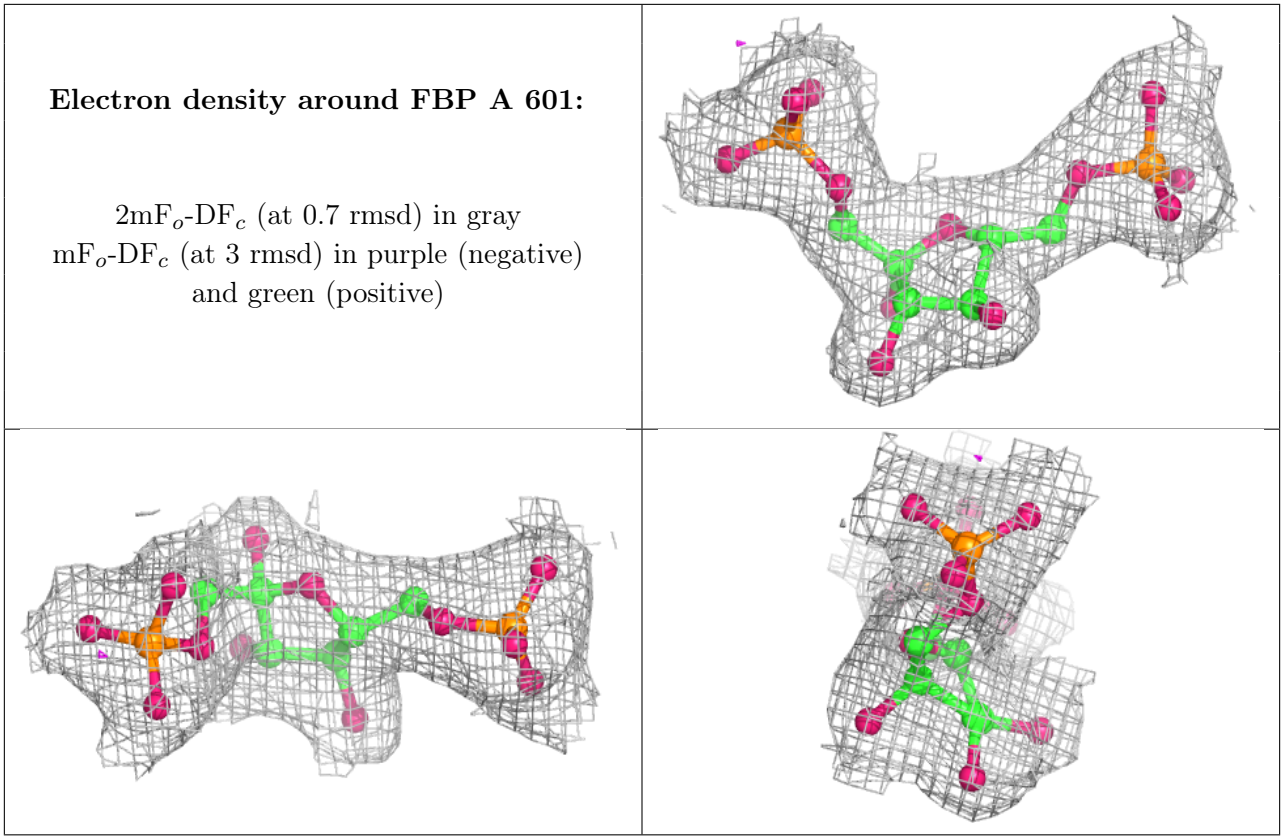






Electron density around FBP A 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.