Full wwPDB X-ray Structure Validation Report ⓘ

Jul 22, 2024 – 06:17 PM JST

PDB ID	:	8XW6
Title	:	Crystal structure of Streptococcus pneumoniae pyruvate kinase in complex with oxalate and fructose 1,6-bisphosphate and ATP
Authors	:	Nakashima, R.; Taguchi, A.
Deposited on	:	2024-01-16
Resolution	:	1.99 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:

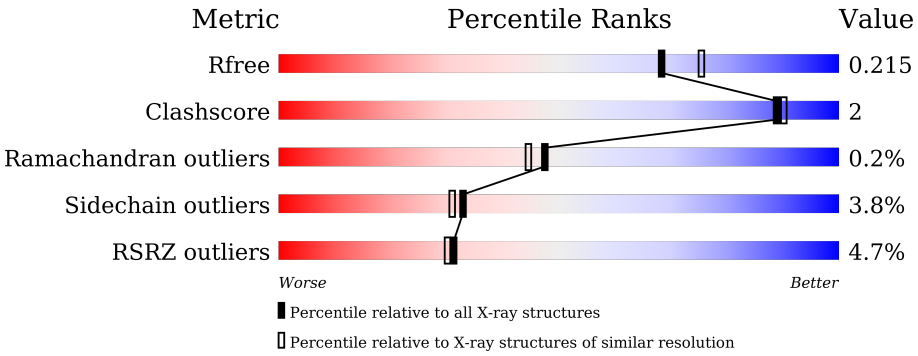
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

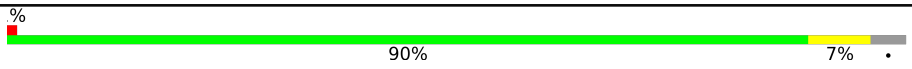
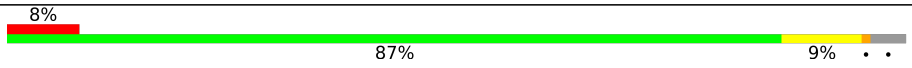
The reported resolution of this entry is 1.99 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	521	
1	B	521	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8277 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	B	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8DQ84
A	-18	GLY	-	expression tag	UNP Q8DQ84
A	-17	SER	-	expression tag	UNP Q8DQ84
A	-16	SER	-	expression tag	UNP Q8DQ84
A	-15	HIS	-	expression tag	UNP Q8DQ84
A	-14	HIS	-	expression tag	UNP Q8DQ84
A	-13	HIS	-	expression tag	UNP Q8DQ84
A	-12	HIS	-	expression tag	UNP Q8DQ84
A	-11	HIS	-	expression tag	UNP Q8DQ84
A	-10	HIS	-	expression tag	UNP Q8DQ84
A	-9	SER	-	expression tag	UNP Q8DQ84
A	-8	SER	-	expression tag	UNP Q8DQ84
A	-7	GLY	-	expression tag	UNP Q8DQ84
A	-6	LEU	-	expression tag	UNP Q8DQ84
A	-5	VAL	-	expression tag	UNP Q8DQ84
A	-4	PRO	-	expression tag	UNP Q8DQ84
A	-3	ARG	-	expression tag	UNP Q8DQ84
A	-2	GLY	-	expression tag	UNP Q8DQ84
A	-1	SER	-	expression tag	UNP Q8DQ84
A	0	HIS	-	expression tag	UNP Q8DQ84
B	-19	MET	-	initiating methionine	UNP Q8DQ84
B	-18	GLY	-	expression tag	UNP Q8DQ84
B	-17	SER	-	expression tag	UNP Q8DQ84
B	-16	SER	-	expression tag	UNP Q8DQ84
B	-15	HIS	-	expression tag	UNP Q8DQ84

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8DQ84
B	-13	HIS	-	expression tag	UNP Q8DQ84
B	-12	HIS	-	expression tag	UNP Q8DQ84
B	-11	HIS	-	expression tag	UNP Q8DQ84
B	-10	HIS	-	expression tag	UNP Q8DQ84
B	-9	SER	-	expression tag	UNP Q8DQ84
B	-8	SER	-	expression tag	UNP Q8DQ84
B	-7	GLY	-	expression tag	UNP Q8DQ84
B	-6	LEU	-	expression tag	UNP Q8DQ84
B	-5	VAL	-	expression tag	UNP Q8DQ84
B	-4	PRO	-	expression tag	UNP Q8DQ84
B	-3	ARG	-	expression tag	UNP Q8DQ84
B	-2	GLY	-	expression tag	UNP Q8DQ84
B	-1	SER	-	expression tag	UNP Q8DQ84
B	0	HIS	-	expression tag	UNP Q8DQ84

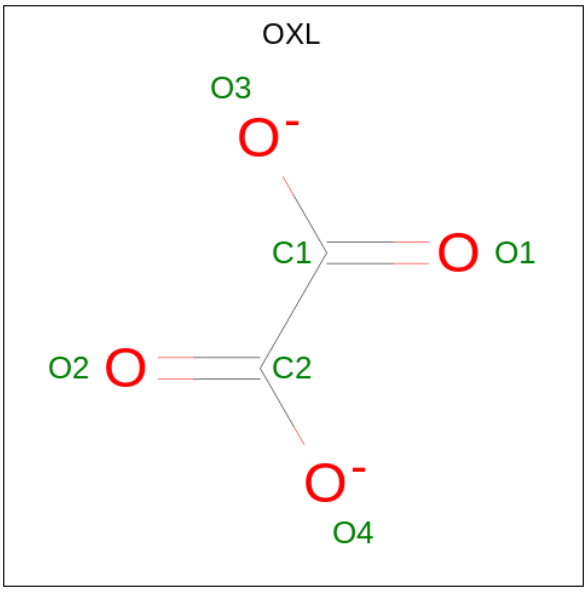
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0

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

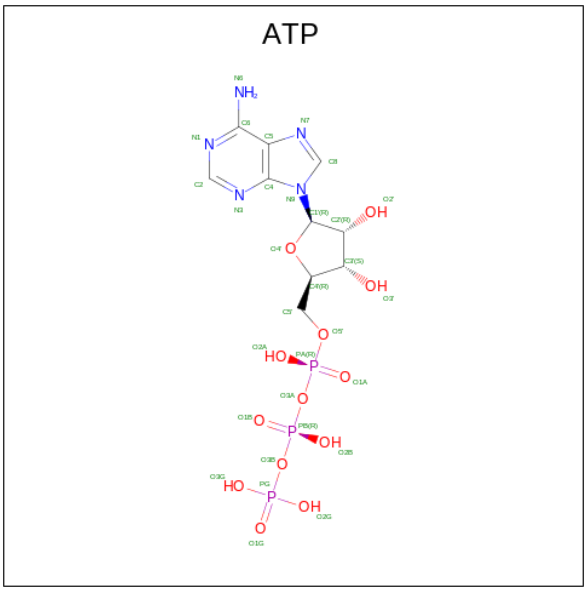
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



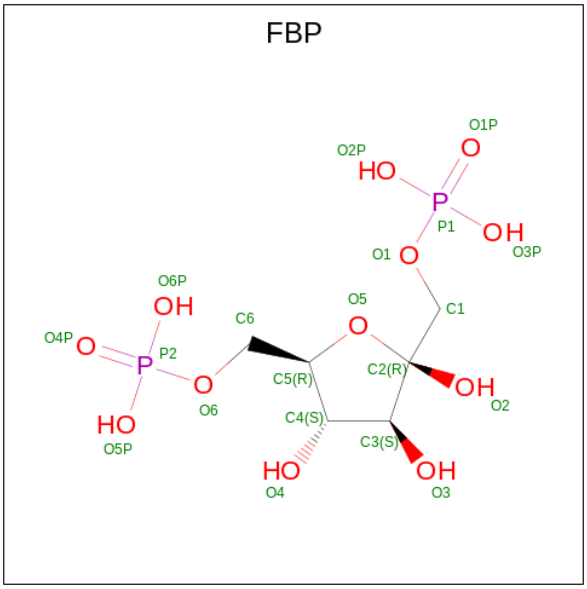
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 2 4	0	0
4	B	1	Total C O 6 2 4	0	0

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



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

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

- Molecule 7 is water.

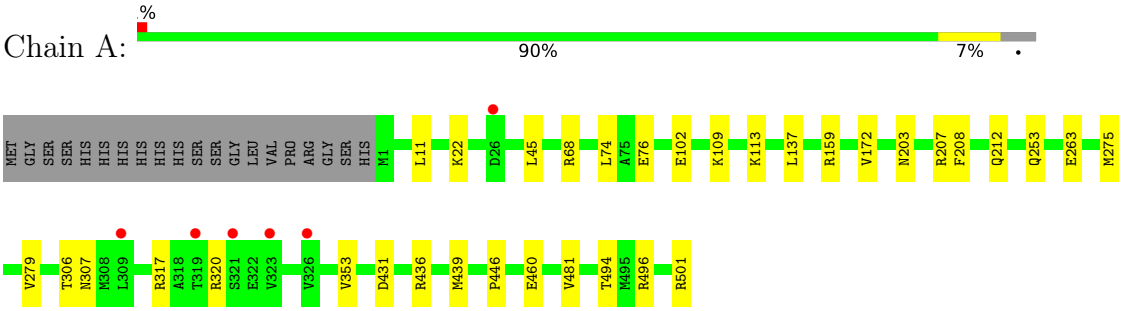
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	296	Total	O	0	0
			296	296		
7	B	213	Total	O	0	0
			213	213		

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.

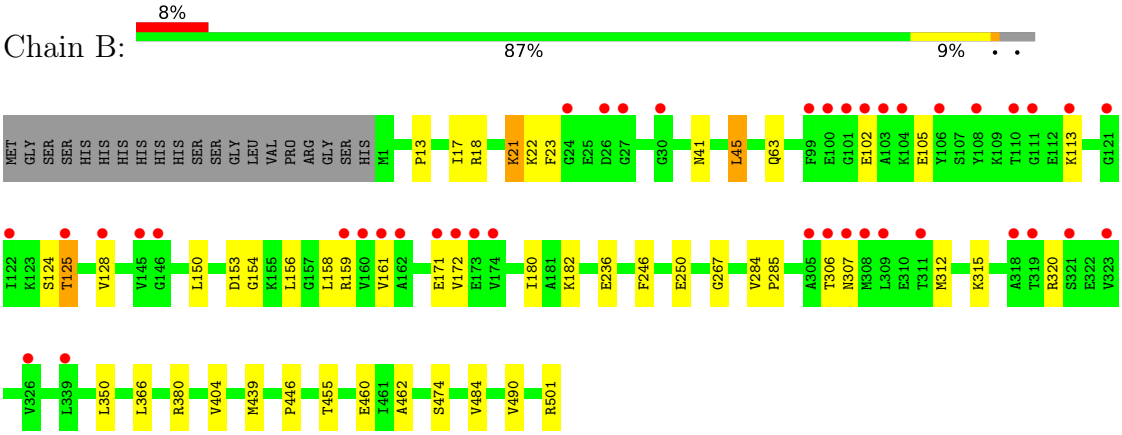
• Molecule 1: Pyruvate kinase

Chain A:



• Molecule 1: Pyruvate kinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	81.58Å 81.58Å 402.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 1.99 46.96 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.96-1.99) 99.2 (46.96-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.178 , 0.211 0.186 , 0.215	Depositor DCC
R_{free} test set	4661 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8277	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: ATP, FBP, K, OXL, 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	0.77	0/3885	0.89	1/5238 (0.0%)
1	B	0.78	0/3885	0.89	2/5238 (0.0%)
All	All	0.77	0/7770	0.89	3/10476 (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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	380	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	380	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	501	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	GLU	Peptide

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	3840	0	3887	14	0
1	B	3840	0	3887	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
5	A	31	0	12	0	0
6	A	20	0	10	0	0
6	B	20	0	10	0	0
7	A	296	0	0	1	0
7	B	213	0	0	1	0
All	All	8277	0	7806	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:H	1:B:307:ASN:HD22	1.30	0.79
1:A:307:ASN:HD22	1:B:320:ARG:H	1.37	0.70
1:A:76:GLU:OE1	1:A:436:ARG:NH2	2.22	0.67
1:B:18:ARG:O	1:B:21:LYS:HG3	1.96	0.66
1:A:317:ARG:HD2	1:B:154:GLY:O	1.97	0.65
1:A:203:ASN:HD21	1:A:207:ARG:HE	1.49	0.58
1:A:275:MET:O	1:A:279:VAL:HG22	2.09	0.53
1:A:317:ARG:NH2	7:A:708:HOH:O	2.45	0.49
1:B:439:MET:HG2	7:B:881:HOH:O	2.12	0.49
1:B:161:VAL:HG22	1:B:171:GLU:O	2.13	0.48
1:B:13:PRO:HB2	1:B:23:PHE:CD1	2.50	0.47
1:A:439:MET:HG3	1:A:446:PRO:HG2	1.98	0.46
1:B:17:ILE:HD11	1:B:41:ASN:HD21	1.81	0.46
1:B:150:LEU:HB3	1:B:154:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:O	1:A:212:GLN:HG2	2.17	0.44
1:B:439:MET:HG3	1:B:446:PRO:HG2	2.01	0.43
1:A:159:ARG:O	1:A:172:VAL:HA	2.19	0.43
1:A:11:LEU:HB3	1:A:68:ARG:HD3	2.00	0.42
1:B:156:LEU:CD2	1:B:180:ILE:CG1	2.97	0.42
1:B:246:PHE:CD1	1:B:267:GLY:HA3	2.54	0.42
1:B:45:LEU:HD22	1:B:350:LEU:HA	2.02	0.42
1:A:481:VAL:HA	1:A:494:THR:O	2.20	0.42
1:A:45:LEU:HG	1:A:353:VAL:HG21	2.02	0.41
1:B:159:ARG:O	1:B:172:VAL:HA	2.20	0.41
1:B:125:THR:CG2	1:B:128:VAL:HB	2.51	0.41
1:B:284:VAL:N	1:B:285:PRO:CD	2.84	0.41
1:B:404:VAL:HG11	1:B:462:ALA:HB1	2.02	0.40
1:B:312:MET:HA	1:B:315:LYS:O	2.21	0.40
1:A:203:ASN:ND2	1:A:207:ARG:HE	2.18	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	499/521 (96%)	487 (98%)	11 (2%)	1 (0%)	47	44
1	B	499/521 (96%)	488 (98%)	10 (2%)	1 (0%)	47	44
All	All	998/1042 (96%)	975 (98%)	21 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	THR
1	B	306	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	411/428 (96%)	401 (98%)	10 (2%)	49	51
1	B	411/428 (96%)	390 (95%)	21 (5%)	24	19
All	All	822/856 (96%)	791 (96%)	31 (4%)	33	31

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	74	LEU
1	A	109	LYS
1	A	113	LYS
1	A	137	LEU
1	A	253	GLN
1	A	263	GLU
1	A	431	ASP
1	A	460	GLU
1	A	496	ARG
1	B	21	LYS
1	B	22	LYS
1	B	45	LEU
1	B	63	GLN
1	B	102	GLU
1	B	105	GLU
1	B	113	LYS
1	B	124	SER
1	B	125	THR
1	B	153	ASP
1	B	158	LEU
1	B	182	LYS
1	B	236	GLU
1	B	250	GLU
1	B	366	LEU
1	B	455	THR
1	B	460	GLU

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Mol	Chain	Res	Type
1	B	474	SER
1	B	484	VAL
1	B	490	VAL
1	B	501	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	307	ASN
1	A	368	ASN
1	A	381	ASN
1	B	41	ASN
1	B	63	GLN
1	B	190	ASN
1	B	307	ASN
1	B	381	ASN

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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	OXL	B	603	3	5,5,5	1.29	1 (20%)	6,6,6	1.41	0
4	OXL	A	604	3	5,5,5	1.39	1 (20%)	6,6,6	1.61	2 (33%)
6	FBP	A	606	-	18,20,20	0.70	0	23,32,32	1.00	2 (8%)
5	ATP	A	605	3,2	26,33,33	0.74	0	31,52,52	1.13	2 (6%)
6	FBP	B	604	-	18,20,20	1.04	2 (11%)	23,32,32	1.17	2 (8%)

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
4	OXL	B	603	3	-	0/4/4/4	-
4	OXL	A	604	3	-	1/4/4/4	-
6	FBP	A	606	-	-	5/13/32/32	0/1/1/1
5	ATP	A	605	3,2	-	3/18/38/38	0/3/3/3
6	FBP	B	604	-	-	6/13/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	OXL	O4-C2	-3.00	1.21	1.30
4	B	603	OXL	O3-C1	-2.27	1.24	1.30
6	B	604	FBP	P1-O3P	-2.18	1.46	1.54
6	B	604	FBP	O4-C4	-2.04	1.38	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	605	ATP	O3G-PG-O3B	3.46	116.25	104.64
6	B	604	FBP	O3P-P1-O1	2.70	113.93	106.73
6	B	604	FBP	O2-C2-O5	-2.29	105.08	109.50
4	A	604	OXL	O3-C1-C2	2.24	119.80	113.16
4	A	604	OXL	O1-C1-C2	-2.12	113.98	120.78
6	A	606	FBP	O5P-P2-O4P	2.05	118.70	110.68
6	A	606	FBP	O5-C5-C6	-2.04	104.97	109.45
5	A	605	ATP	O3B-PG-O1G	-2.01	100.02	111.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

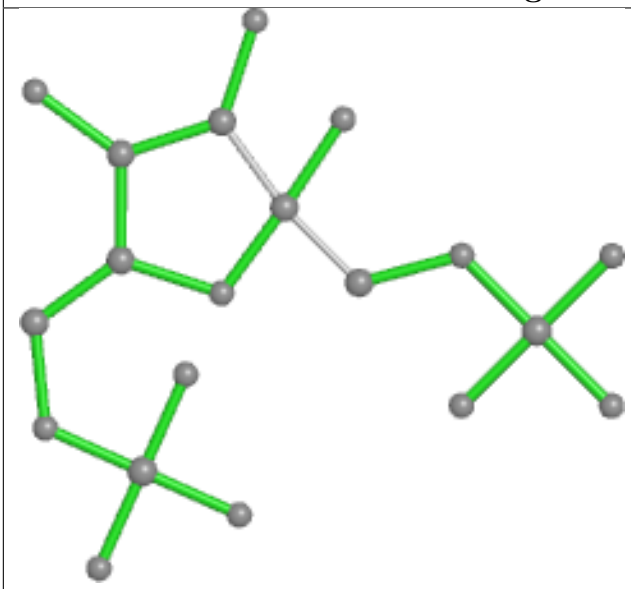
Mol	Chain	Res	Type	Atoms
6	A	606	FBP	C1-O1-P1-O2P
6	A	606	FBP	C1-O1-P1-O3P
6	A	606	FBP	O1-C1-C2-O2
6	A	606	FBP	O1-C1-C2-C3
6	A	606	FBP	O1-C1-C2-O5
6	B	604	FBP	C1-O1-P1-O3P
6	B	604	FBP	O1-C1-C2-C3
6	B	604	FBP	O1-C1-C2-O5
6	B	604	FBP	C1-O1-P1-O1P
5	A	605	ATP	PG-O3B-PB-O1B
5	A	605	ATP	PB-O3A-PA-O2A
6	B	604	FBP	O1-C1-C2-O2
4	A	604	OXL	O3-C1-C2-O4
6	B	604	FBP	C1-O1-P1-O2P
5	A	605	ATP	PG-O3B-PB-O2B

There are no ring outliers.

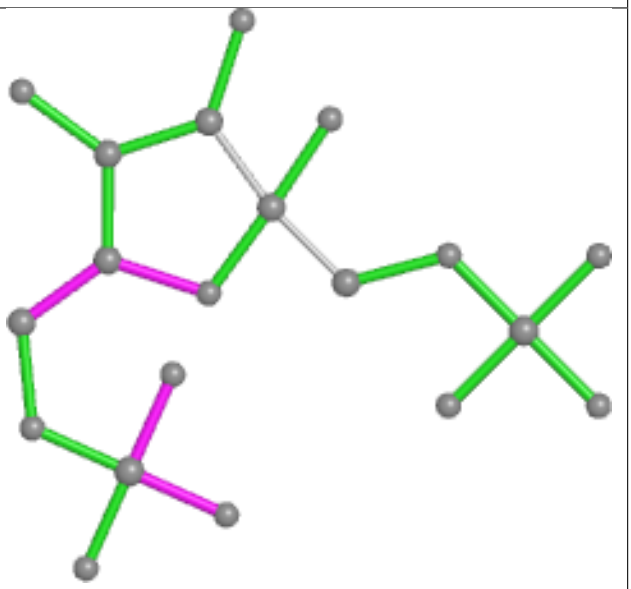
No monomer is involved in short contacts.

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.

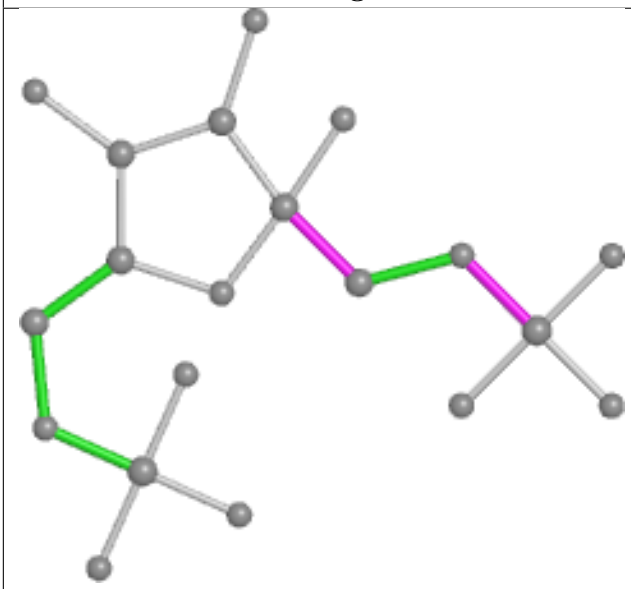
Ligand FBP A 606



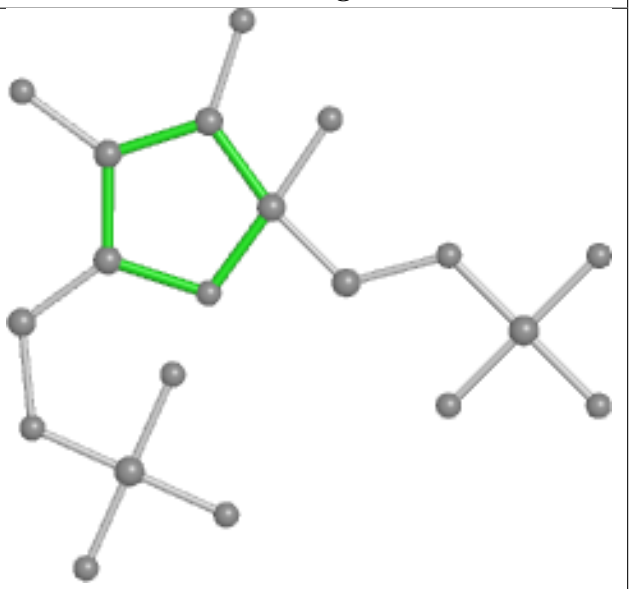
Bond lengths



Bond angles

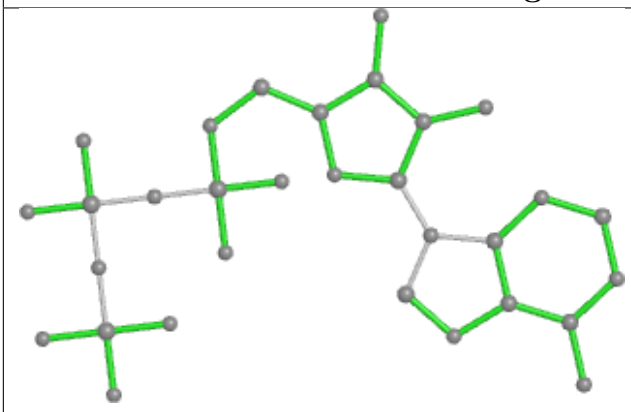


Torsions

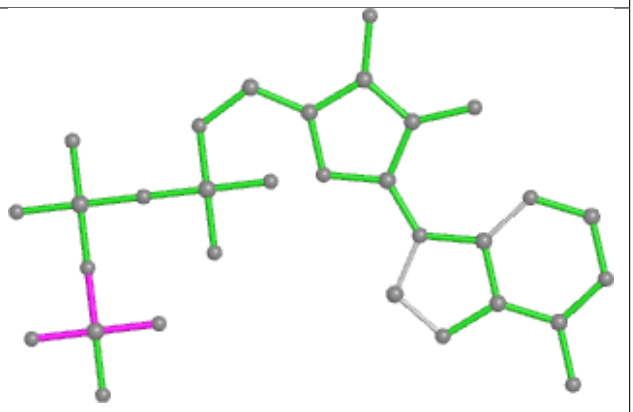


Rings

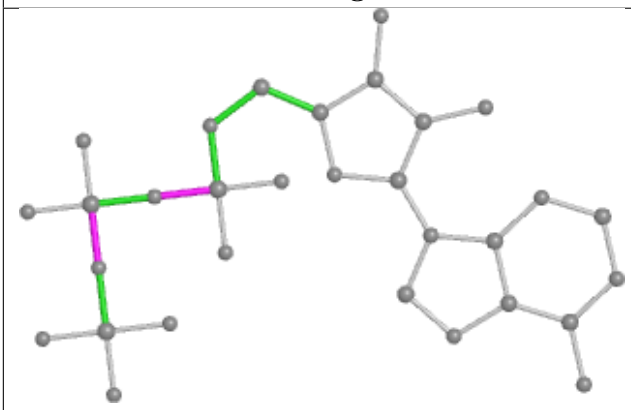
Ligand ATP A 605



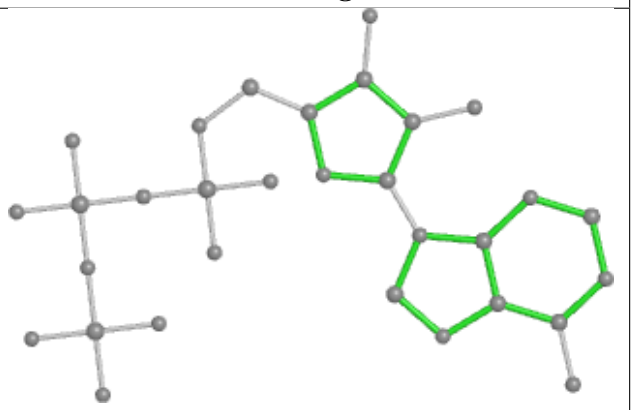
Bond lengths



Bond angles

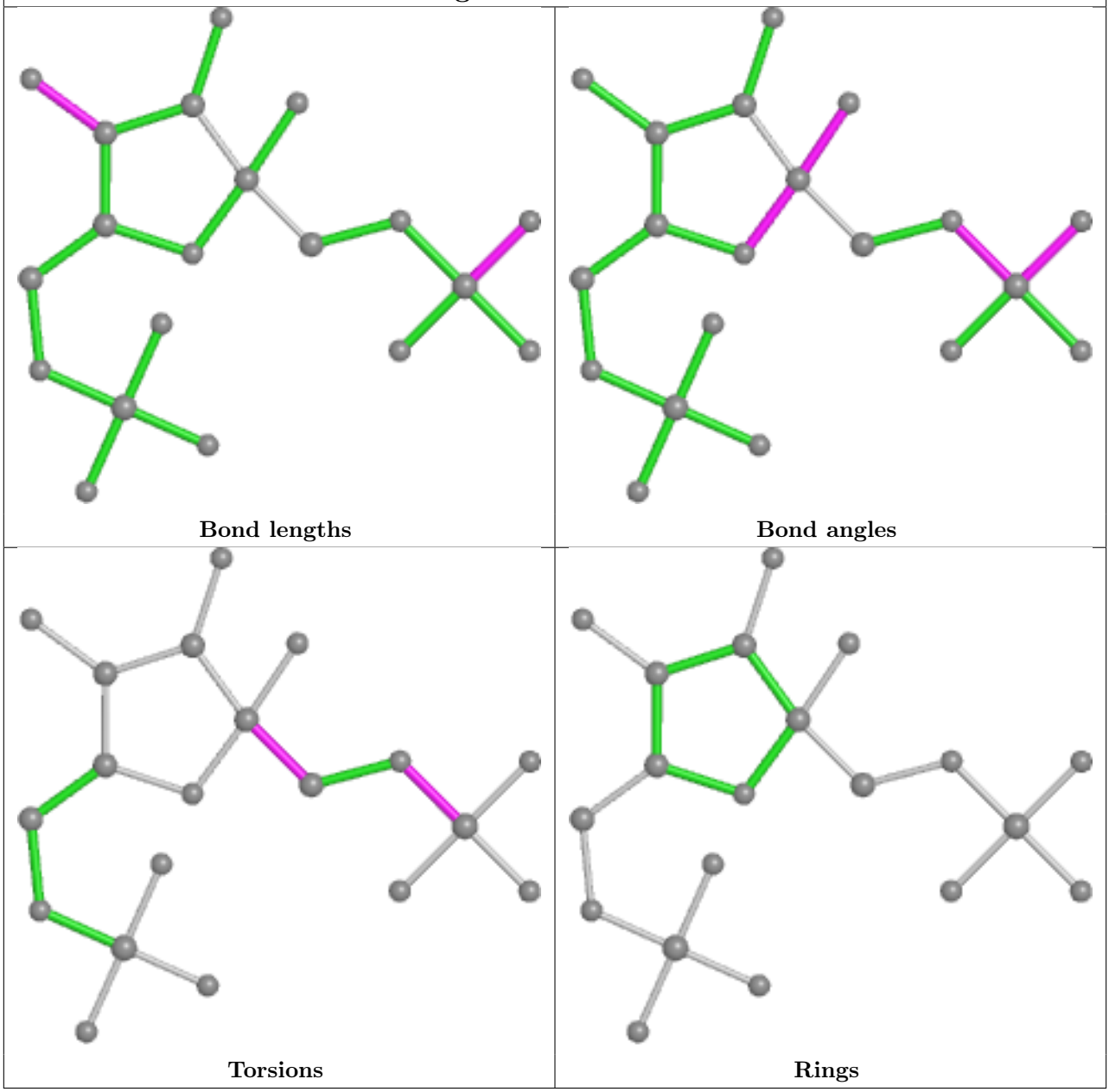


Torsions



Rings

Ligand FBP B 604



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	501/521 (96%)	-0.13	6 (1%)	79	78	35, 45, 66, 101	0
1	B	501/521 (96%)	0.35	41 (8%)	11	11	34, 49, 85, 121	0
All	All	1002/1042 (96%)	0.11	47 (4%)	31	30	34, 47, 80, 121	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	ALA	9.4
1	B	102	GLU	5.4
1	B	162	ALA	5.4
1	B	27	GLY	4.4
1	B	173	GLU	4.2
1	B	101	GLY	4.2
1	B	106	TYR	4.2
1	B	161	VAL	3.8
1	B	24	GLY	3.5
1	B	100	GLU	3.4
1	B	125	THR	3.4
1	B	309	LEU	3.3
1	B	26	ASP	3.2
1	B	339	LEU	3.1
1	B	308	MET	3.0
1	A	323	VAL	3.0
1	B	111	GLY	2.9
1	B	174	VAL	2.9
1	B	172	VAL	2.8
1	B	128	VAL	2.8
1	A	319	THR	2.7
1	B	306	THR	2.7
1	A	321	SER	2.7
1	B	104	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	309	LEU	2.6
1	B	30	GLY	2.6
1	B	171	GLU	2.6
1	B	318	ALA	2.5
1	B	323	VAL	2.5
1	B	160	VAL	2.4
1	B	319	THR	2.4
1	A	26	ASP	2.3
1	B	145	VAL	2.2
1	B	307	ASN	2.2
1	B	121	GLY	2.2
1	B	146	GLY	2.2
1	B	326	VAL	2.2
1	B	311	THR	2.2
1	B	159	ARG	2.2
1	B	305	ALA	2.2
1	B	99	PHE	2.2
1	B	122	ILE	2.1
1	B	108	TYR	2.1
1	B	321	SER	2.1
1	A	326	VAL	2.1
1	B	110	THR	2.0
1	B	113	LYS	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.

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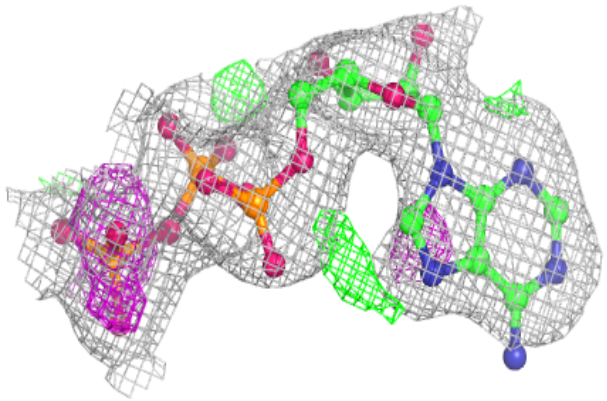
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

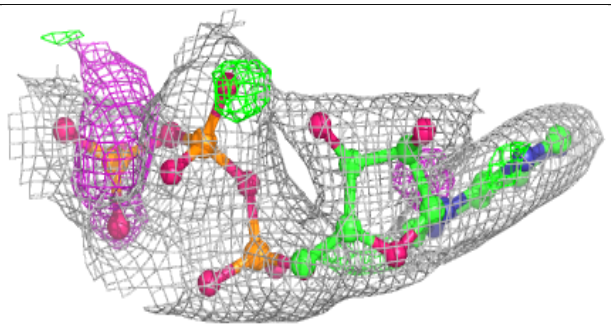
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OXL	A	604	6/6	0.87	0.16	47,53,62,63	0
4	OXL	B	603	6/6	0.91	0.12	52,53,61,66	0
3	MG	A	602	1/1	0.93	0.05	56,56,56,56	0
5	ATP	A	605	31/31	0.94	0.11	42,58,68,79	0
3	MG	B	602	1/1	0.95	0.10	47,47,47,47	0
2	K	B	601	1/1	0.98	0.08	55,55,55,55	0
2	K	A	601	1/1	0.98	0.09	46,46,46,46	0
6	FBP	A	606	20/20	0.98	0.08	42,45,52,61	0
3	MG	A	603	1/1	0.99	0.07	44,44,44,44	0
6	FBP	B	604	20/20	0.99	0.09	41,49,54,59	0

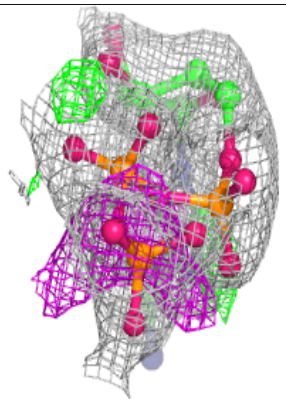
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 605:

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

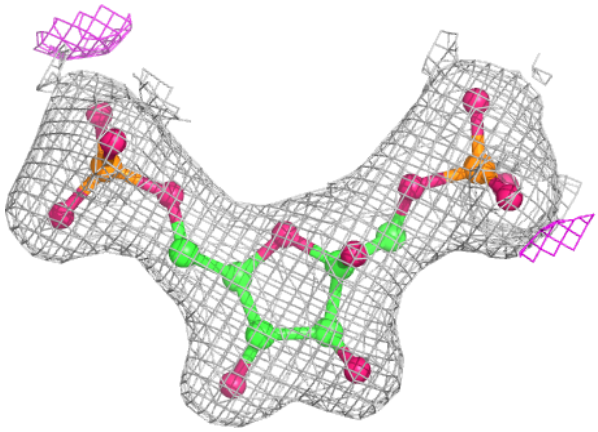


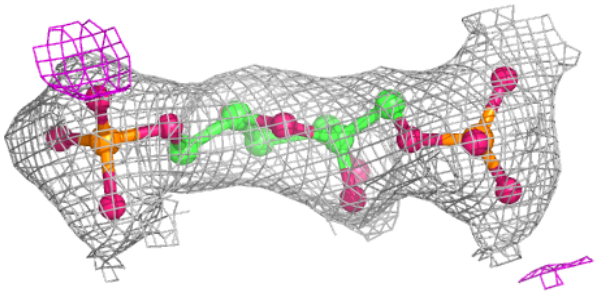


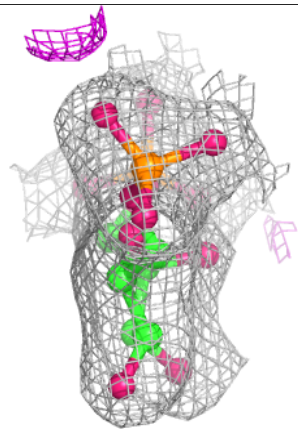


Electron density around FBP A 606:

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

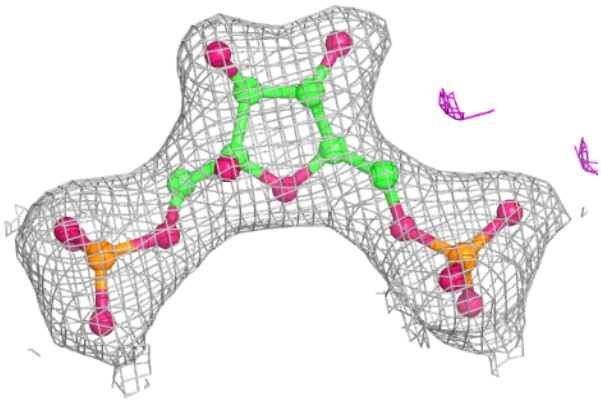


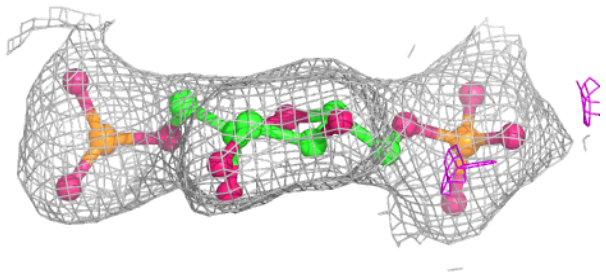


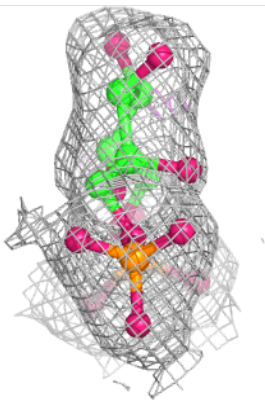


Electron density around FBP B 604:

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







6.5 Other polymers (i)

There are no such residues in this entry.