



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:16 AM UTC

PDB ID : 1A49 / pdb\_00001a49  
Title : BIS MG-ATP-K-OXALATE COMPLEX OF PYRUVATE KINASE  
Authors : Larsen, T.M.; Benning, M.M.; Rayment, I.; Reed, G.H.  
Deposited on : 1998-02-12  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

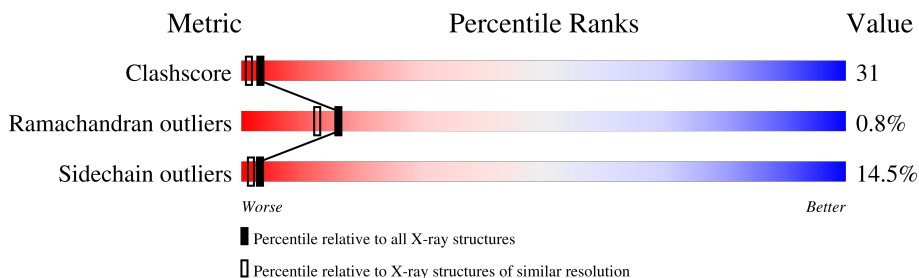
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	38% 43% 15% ..
1	B	530	49% 38% 10% ..
1	C	530	37% 42% 16% ..
1	D	530	45% 41% 12% ..
1	E	530	45% 41% 10% ..
1	F	530	44% 42% 11% ..
1	G	530	40% 45% 12% ..
1	H	530	53% 36% 8% ..

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	OXL	A	533	-	-	X	-
3	OXL	F	4133	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34001 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
			Total	C	N	O	S			
1	A	519	3978	2498	708	744	28	0	0	0
1	B	519	3978	2498	708	744	28	0	0	0
1	C	519	3978	2498	708	744	28	0	0	0
1	D	519	3978	2498	708	744	28	0	0	0
1	E	519	3978	2498	708	744	28	0	0	0
1	F	519	3978	2498	708	744	28	0	0	0
1	G	519	3978	2498	708	744	28	0	0	0
1	H	519	3978	2498	708	744	28	0	0	0

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

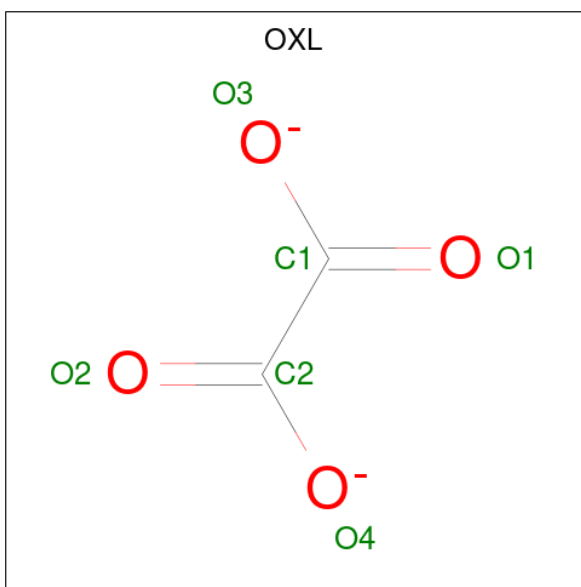
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	K 1	0	0
2	B	1	Total 1	K 1	0	0
2	C	1	Total 1	K 1	0	0
2	D	1	Total 1	K 1	0	0
2	E	1	Total 1	K 1	0	0
2	F	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C<sub>2</sub>O<sub>4</sub>).

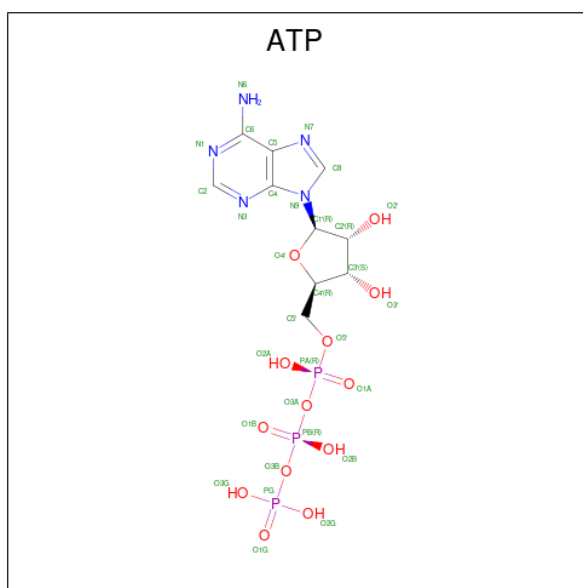


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0
3	E	1	Total C O 6 2 4	0	0
3	F	1	Total C O 6 2 4	0	0
3	G	1	Total C O 6 2 4	0	0
3	H	1	Total C O 6 2 4	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	1	Total Mg 1 1	0	0
4	C	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0
4	G	2	Total Mg 2 2	0	0
4	H	1	Total Mg 1 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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
5	C	1	Total C N O P 31 10 5 13 3	0	0
5	D	1	Total C N O P 31 10 5 13 3	0	0
5	E	1	Total C N O P 31 10 5 13 3	0	0

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total 195	O 195	0	0
6	B	270	Total 270	O 270	0	0
6	C	178	Total 178	O 178	0	0
6	D	272	Total 272	O 272	0	0
6	E	279	Total 279	O 279	0	0
6	F	197	Total 197	O 197	0	0
6	G	228	Total 228	O 228	0	0
6	H	302	Total 302	O 302	0	0

### 3 Residue-property plots i

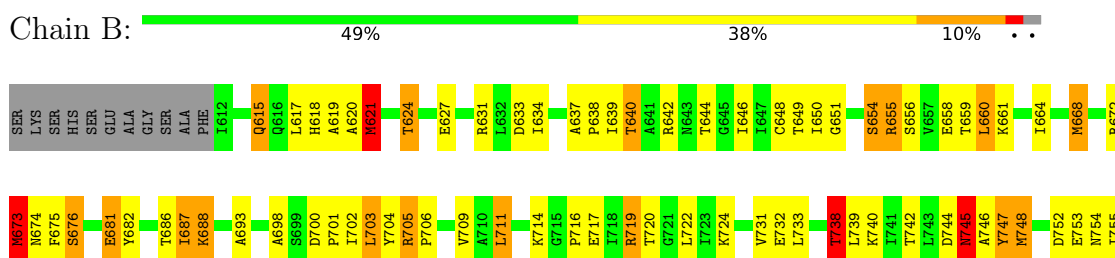
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

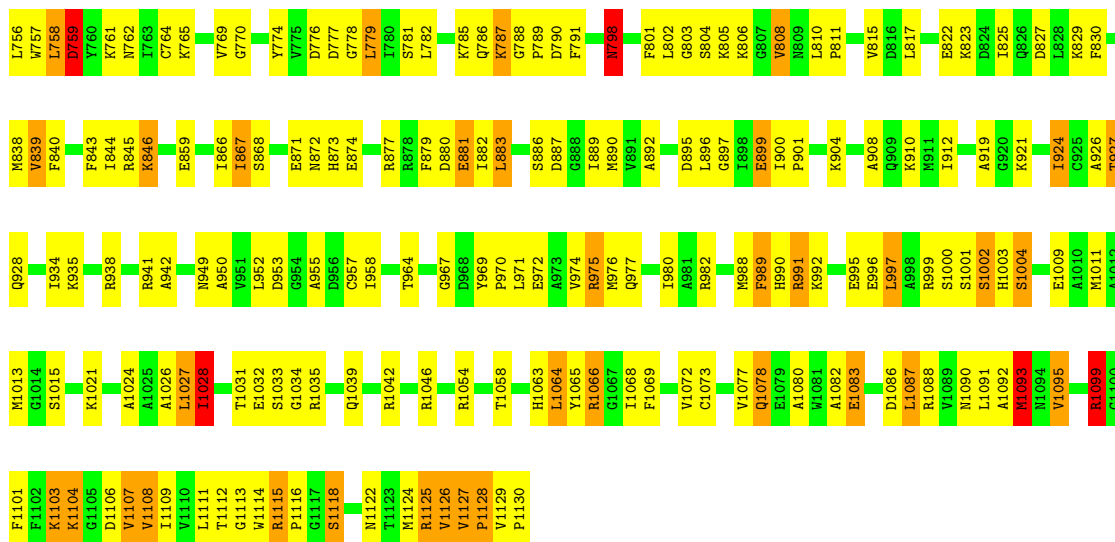
Note EDS was not executed.

#### • Molecule 1: PYRUVATE KINASE

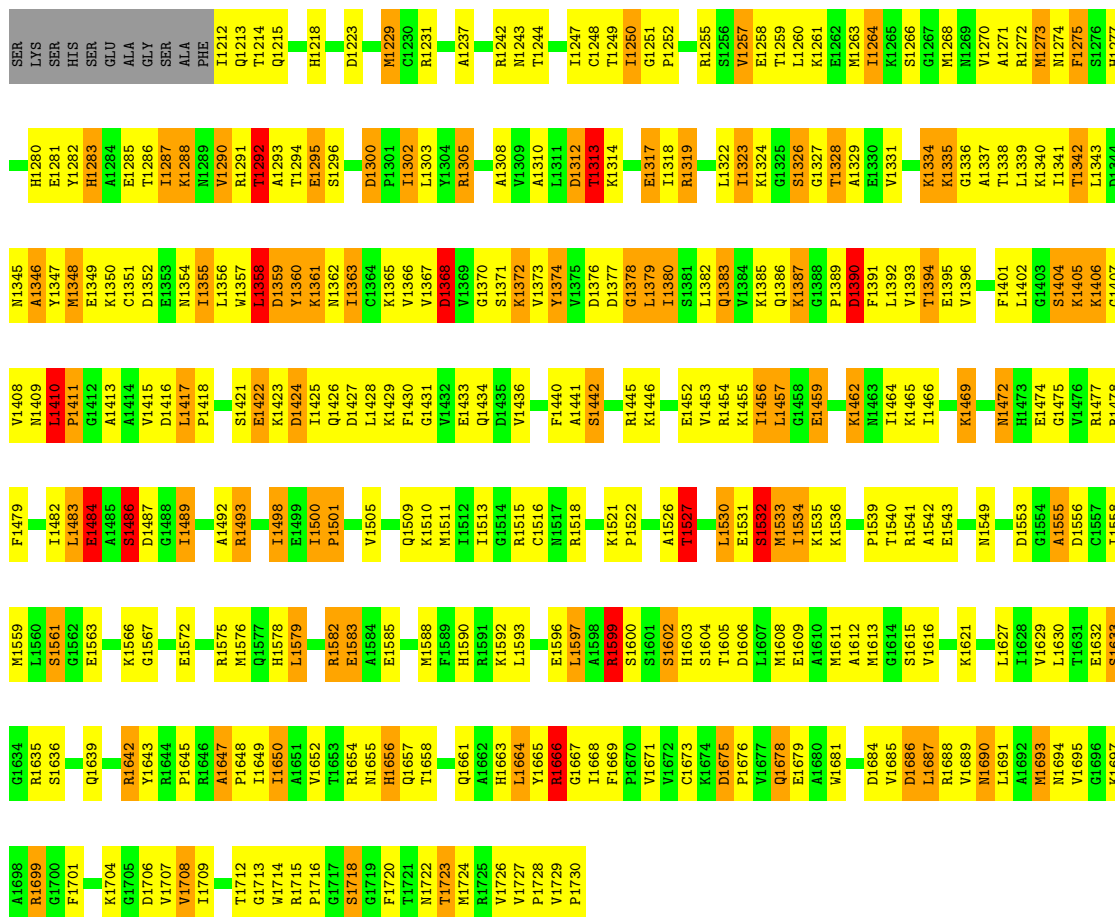


#### • Molecule 1: PYRUVATE KINASE



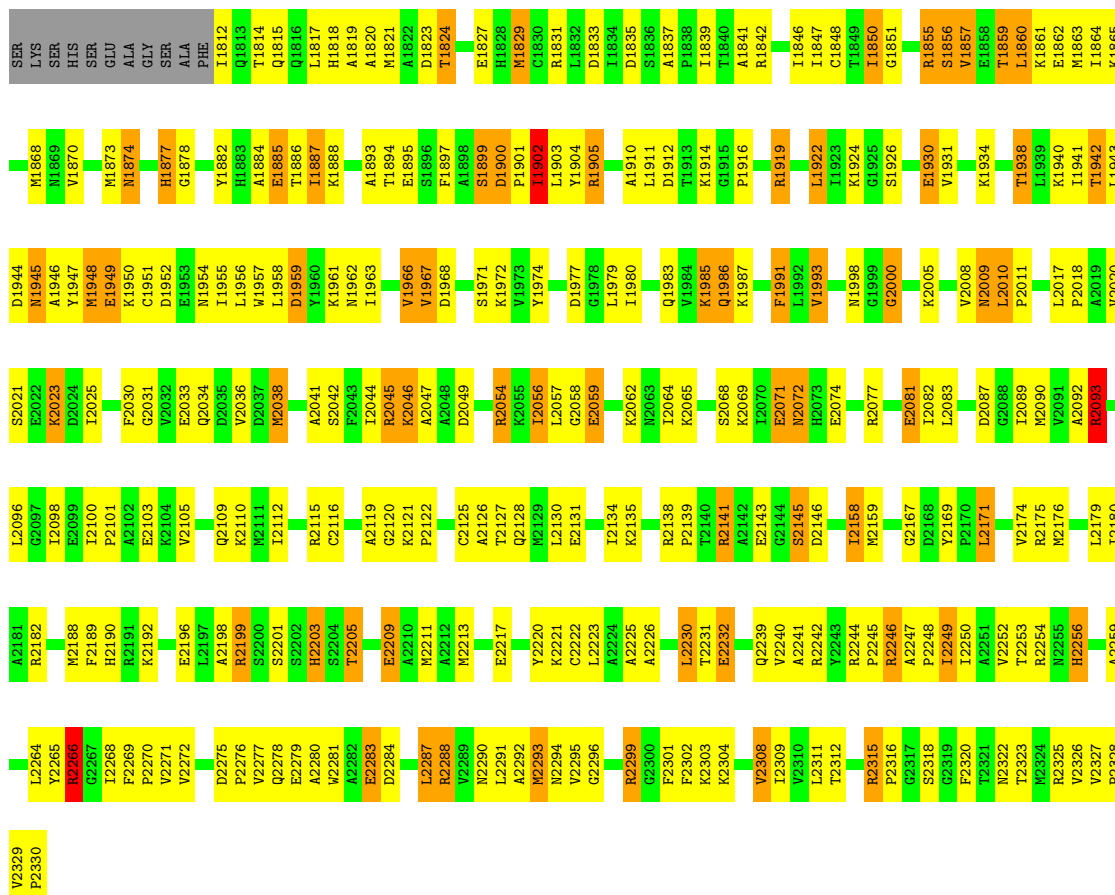


● Molecule 1: PYRUVATE KINASE

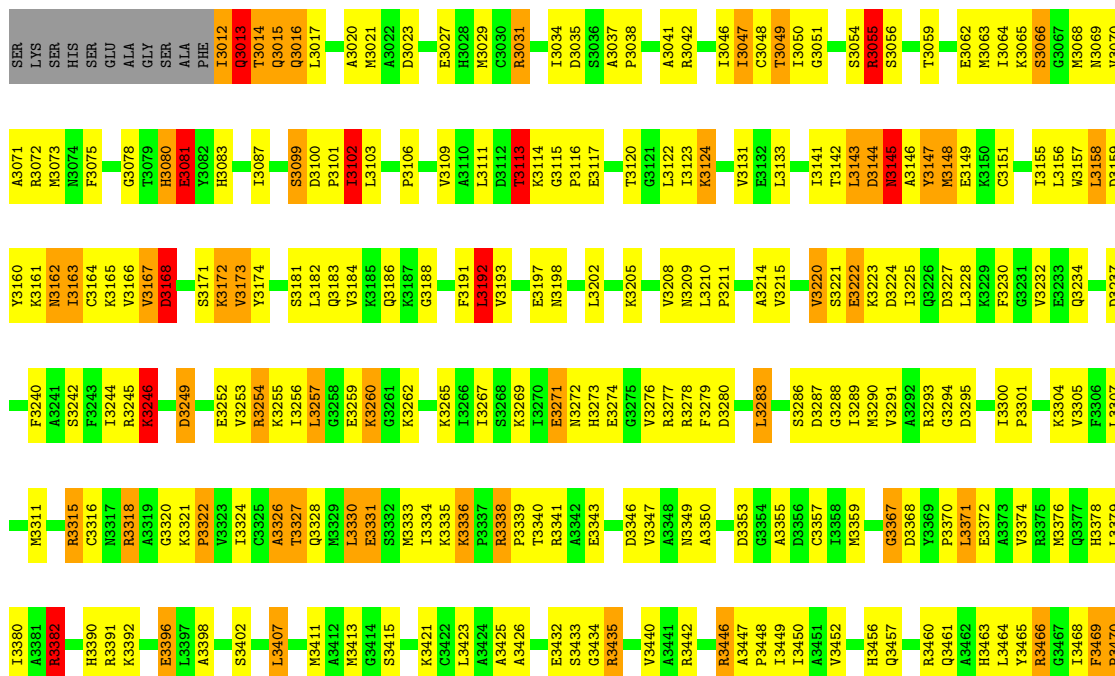


● Molecule 1: PYRUVATE KINASE

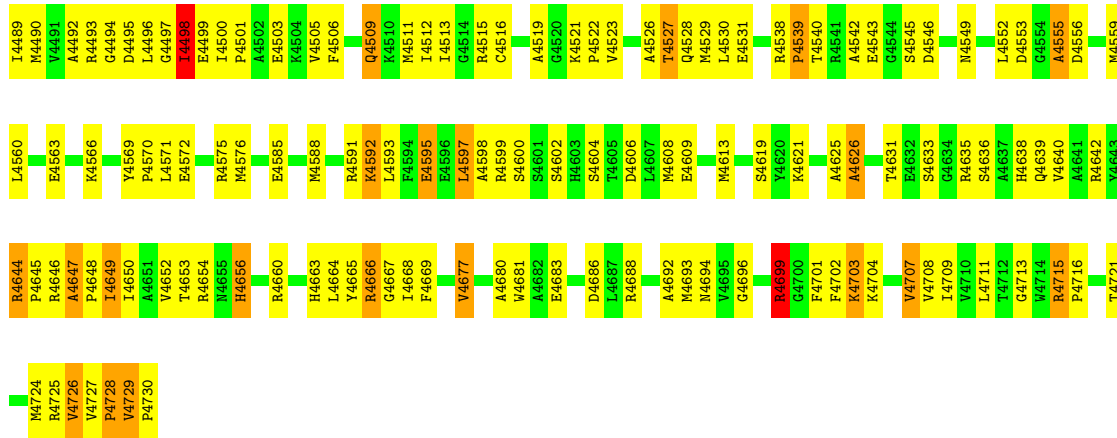




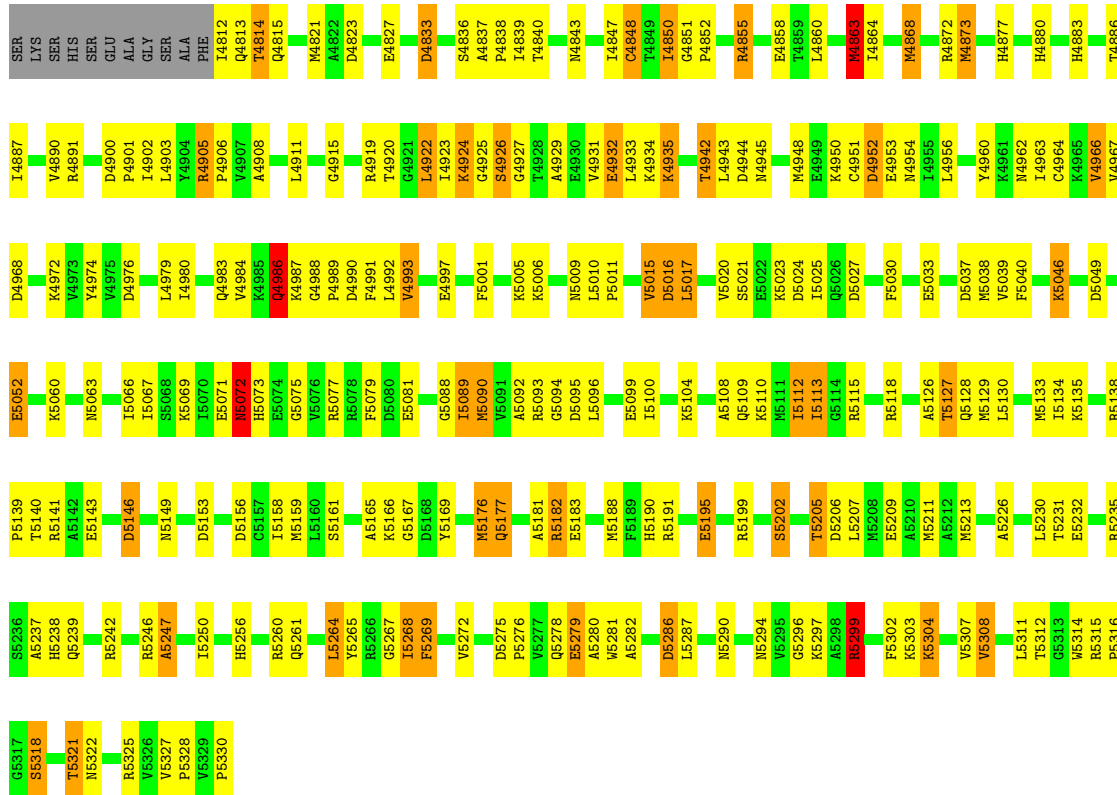
• Molecule 1: PYRUVATE KINASE







• Molecule 1: PYRUVATE KINASE



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.30Å 216.50Å 258.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	87.0 (30.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, $R_{free}$	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	34001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.76	42/4041 (1.0%)	1.52	35/5452 (0.6%)
1	B	1.80	63/4041 (1.6%)	1.51	25/5452 (0.5%)
1	C	1.71	40/4041 (1.0%)	1.54	35/5452 (0.6%)
1	D	1.80	48/4041 (1.2%)	1.47	25/5452 (0.5%)
1	E	1.78	40/4041 (1.0%)	1.53	25/5452 (0.5%)
1	F	1.70	36/4041 (0.9%)	1.47	28/5452 (0.5%)
1	G	1.77	48/4041 (1.2%)	1.53	32/5452 (0.6%)
1	H	1.78	50/4041 (1.2%)	1.46	25/5452 (0.5%)
All	All	1.76	367/32328 (1.1%)	1.50	230/43616 (0.5%)

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	B	0	1
1	C	0	1
1	H	1	0
All	All	1	2

The worst 5 of 367 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1561	SER	CA-C	-12.63	1.46	1.52
1	G	4644	ARG	C-O	-9.80	1.19	1.23
1	A	158	LEU	CA-C	-9.78	1.40	1.52
1	D	2315	ARG	N-CA	-8.70	1.37	1.45
1	B	1092	ALA	C-N	-8.44	1.21	1.33

The worst 5 of 230 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3168	ASP	CA-CB-CG	11.91	124.51	112.60
1	B	758	LEU	CA-C-N	10.36	134.16	120.28
1	B	758	LEU	C-N-CA	10.36	134.16	120.28
1	G	4368	ASP	CA-CB-CG	8.98	121.58	112.60
1	E	3490	ASN	CA-CB-CG	-8.89	103.71	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	5205	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	759	ASP	Mainchain
1	C	1599	ARG	Mainchain

## 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	3978	0	4055	339	2
1	B	3978	0	4056	224	1
1	C	3978	0	4055	326	3
1	D	3978	0	4055	262	5
1	E	3978	0	4056	240	14
1	F	3978	0	4055	252	2
1	G	3978	0	4055	287	2
1	H	3978	0	4055	199	18
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	6	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	6	0	0	1	0
3	E	6	0	0	0	0
3	F	6	0	0	3	0
3	G	6	0	0	1	0
3	H	6	0	0	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	A	31	0	12	3	0
5	C	31	0	12	3	0
5	D	31	0	12	1	0
5	E	31	0	12	0	0
5	F	31	0	12	0	0
5	G	31	0	12	1	0
6	A	195	0	0	11	0
6	B	270	0	0	16	0
6	C	178	0	0	11	0
6	D	272	0	0	21	0
6	E	279	0	0	15	0
6	F	197	0	0	9	0
6	G	228	0	0	7	0
6	H	302	0	0	13	3
All	All	34001	0	32514	2022	25

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 31.

The worst 5 of 2022 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:499:ARG:NH2	6:A:6596:HOH:O	1.57	1.36
1:D:1850:ILE:HD11	1:D:1868:MET:HE1	1.17	1.16
1:E:3493:MET:HE2	1:E:3530:PRO:HD2	1.23	1.14
1:C:1693:MET:HE2	1:C:1729:VAL:HG22	1.25	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3048:CYS:HB2	1:E:3068:MET:HE3	1.32	1.10

The worst 5 of 25 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3149:GLU:OE1	1:H:4934:LYS:CE[3_655]	0.65	1.55
1:E:3149:GLU:CD	1:H:4934:LYS:NZ[3_655]	1.12	1.08
1:E:3081:GLU:OE1	1:H:4924:LYS:NZ[3_655]	1.15	1.05
1:E:3149:GLU:CD	1:H:4934:LYS:CE[3_655]	1.22	0.98
1:D:1924:LYS:NZ	1:H:4858:GLU:OE1[1_455]	1.29	0.91

## 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	517/530 (98%)	480 (93%)	33 (6%)	4 (1%)	16	12
1	B	517/530 (98%)	492 (95%)	20 (4%)	5 (1%)	12	9
1	C	517/530 (98%)	471 (91%)	41 (8%)	5 (1%)	12	9
1	D	517/530 (98%)	493 (95%)	21 (4%)	3 (1%)	21	18
1	E	517/530 (98%)	488 (94%)	24 (5%)	5 (1%)	12	9
1	F	517/530 (98%)	490 (95%)	23 (4%)	4 (1%)	16	12
1	G	517/530 (98%)	488 (94%)	25 (5%)	4 (1%)	16	12
1	H	517/530 (98%)	490 (95%)	24 (5%)	3 (1%)	21	18
All	All	4136/4240 (98%)	3892 (94%)	211 (5%)	33 (1%)	16	12

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	PRO
1	C	1533	MET
1	E	3506	ASP
1	F	3729	ALA
1	F	3789	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/434 (98%)	346 (81%)	80 (19%)	1	1
1	B	426/434 (98%)	374 (88%)	52 (12%)	5	2
1	C	426/434 (98%)	345 (81%)	81 (19%)	1	1
1	D	426/434 (98%)	375 (88%)	51 (12%)	5	3
1	E	426/434 (98%)	366 (86%)	60 (14%)	3	2
1	F	426/434 (98%)	365 (86%)	61 (14%)	3	1
1	G	426/434 (98%)	364 (85%)	62 (15%)	3	1
1	H	426/434 (98%)	380 (89%)	46 (11%)	6	4
All	All	3408/3472 (98%)	2915 (86%)	493 (14%)	3	1

5 of 493 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1959	ASP
1	G	4707	VAL
1	E	3156	LEU
1	G	4666	ARG
1	H	5118	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	4986	GLN

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Mol	Chain	Res	Type
1	H	5072	ASN
1	D	1815	GLN
1	C	1690	ASN
1	H	5149	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 22 are monoatomic - leaving 14 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	A	533	4	5,5,5	1.47	1 (20%)	6,6,6	2.38	2 (33%)
3	OXL	H	5333	4	5,5,5	1.26	1 (20%)	6,6,6	1.75	2 (33%)
5	ATP	E	3535	2,4	32,33,33	2.29	7 (21%)	48,52,52	0.86	2 (4%)
3	OXL	C	1733	4	5,5,5	2.15	3 (60%)	6,6,6	1.78	1 (16%)
3	OXL	B	1133	4	5,5,5	1.50	2 (40%)	6,6,6	1.75	2 (33%)
3	OXL	F	4133	4	5,5,5	1.38	0	6,6,6	1.98	4 (66%)
5	ATP	F	4135	2,4	32,33,33	2.83	10 (31%)	48,52,52	1.12	5 (10%)
3	OXL	D	2333	4	5,5,5	1.45	1 (20%)	6,6,6	1.97	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ATP	G	4735	2,4	32,33,33	3.00	9 (28%)	48,52,52	0.92	1 (2%)
5	ATP	D	2335	2,4	32,33,33	2.45	9 (28%)	48,52,52	1.21	6 (12%)
3	OXL	G	4733	4	5,5,5	1.41	0	6,6,6	2.00	4 (66%)
3	OXL	E	3533	4	5,5,5	1.39	0	6,6,6	1.99	4 (66%)
5	ATP	C	1735	2,4	32,33,33	3.39	9 (28%)	48,52,52	1.02	4 (8%)
5	ATP	A	535	2,4	32,33,33	2.41	9 (28%)	48,52,52	1.38	3 (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	A	533	4	-	0/4/4/4	-
3	OXL	H	5333	4	-	0/4/4/4	-
5	ATP	E	3535	2,4	-	4/22/38/38	0/3/3/3
3	OXL	C	1733	4	-	0/4/4/4	-
3	OXL	B	1133	4	-	0/4/4/4	-
3	OXL	F	4133	4	-	0/4/4/4	-
5	ATP	F	4135	2,4	-	0/22/38/38	0/3/3/3
3	OXL	D	2333	4	-	0/4/4/4	-
5	ATP	G	4735	2,4	-	4/22/38/38	0/3/3/3
5	ATP	D	2335	2,4	-	4/22/38/38	0/3/3/3
3	OXL	G	4733	4	-	0/4/4/4	-
3	OXL	E	3533	4	-	0/4/4/4	-
5	ATP	C	1735	2,4	-	5/22/38/38	0/3/3/3
5	ATP	A	535	2,4	-	1/22/38/38	0/3/3/3

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1735	ATP	PB-O3B	-16.43	1.41	1.59
5	G	4735	ATP	PB-O3B	-12.93	1.45	1.59
5	F	4135	ATP	PB-O3B	-11.19	1.47	1.59
5	D	2335	ATP	PB-O3B	-10.59	1.48	1.59
5	A	535	ATP	PB-O3B	-9.25	1.49	1.59

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	535	ATP	O2B-PB-O3B	7.42	127.32	107.27
5	D	2335	ATP	O2B-PB-O3B	-4.26	95.76	107.27
3	A	533	OXL	O3-C1-C2	4.07	120.72	112.83
3	A	533	OXL	O1-C1-C2	-3.65	113.02	120.63
5	D	2335	ATP	O3G-PG-O3B	3.26	115.58	104.64

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

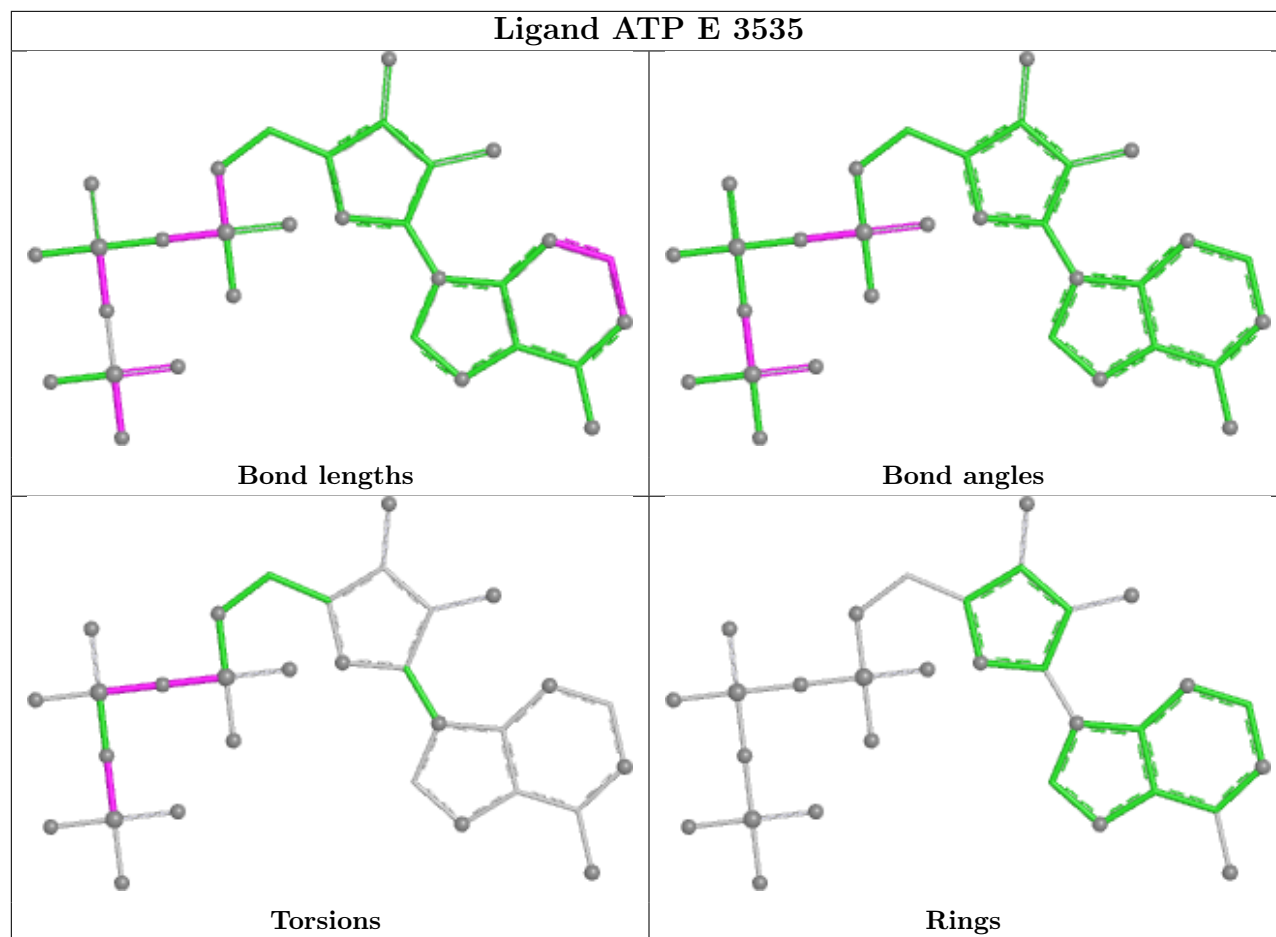
Mol	Chain	Res	Type	Atoms
5	E	3535	ATP	PB-O3B-PG-O3G
5	C	1735	ATP	PB-O3B-PG-O1G
5	E	3535	ATP	PB-O3A-PA-O1A
5	D	2335	ATP	PB-O3B-PG-O1G
5	C	1735	ATP	PA-O3A-PB-O1B

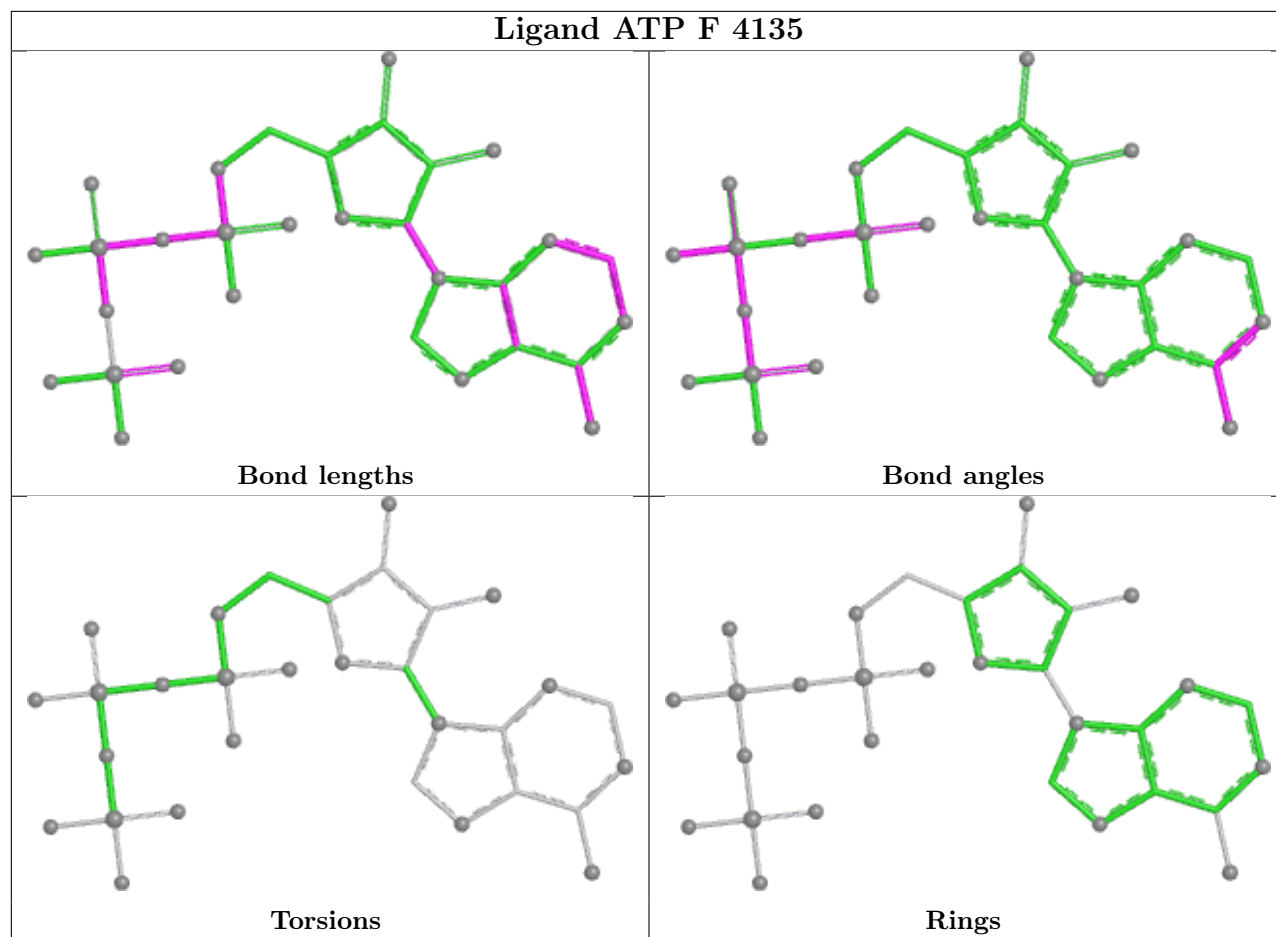
There are no ring outliers.

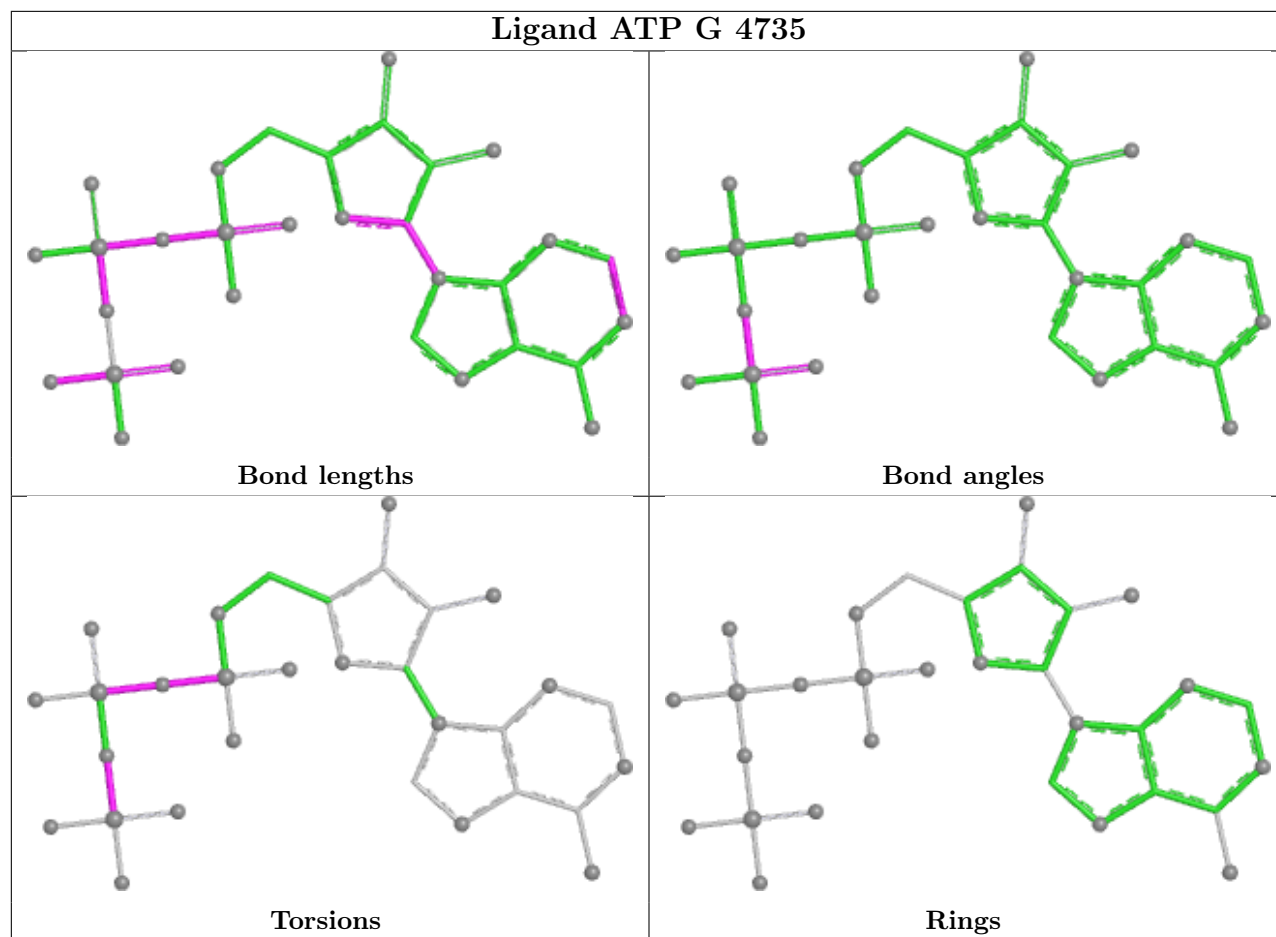
10 monomers are involved in 17 short contacts:

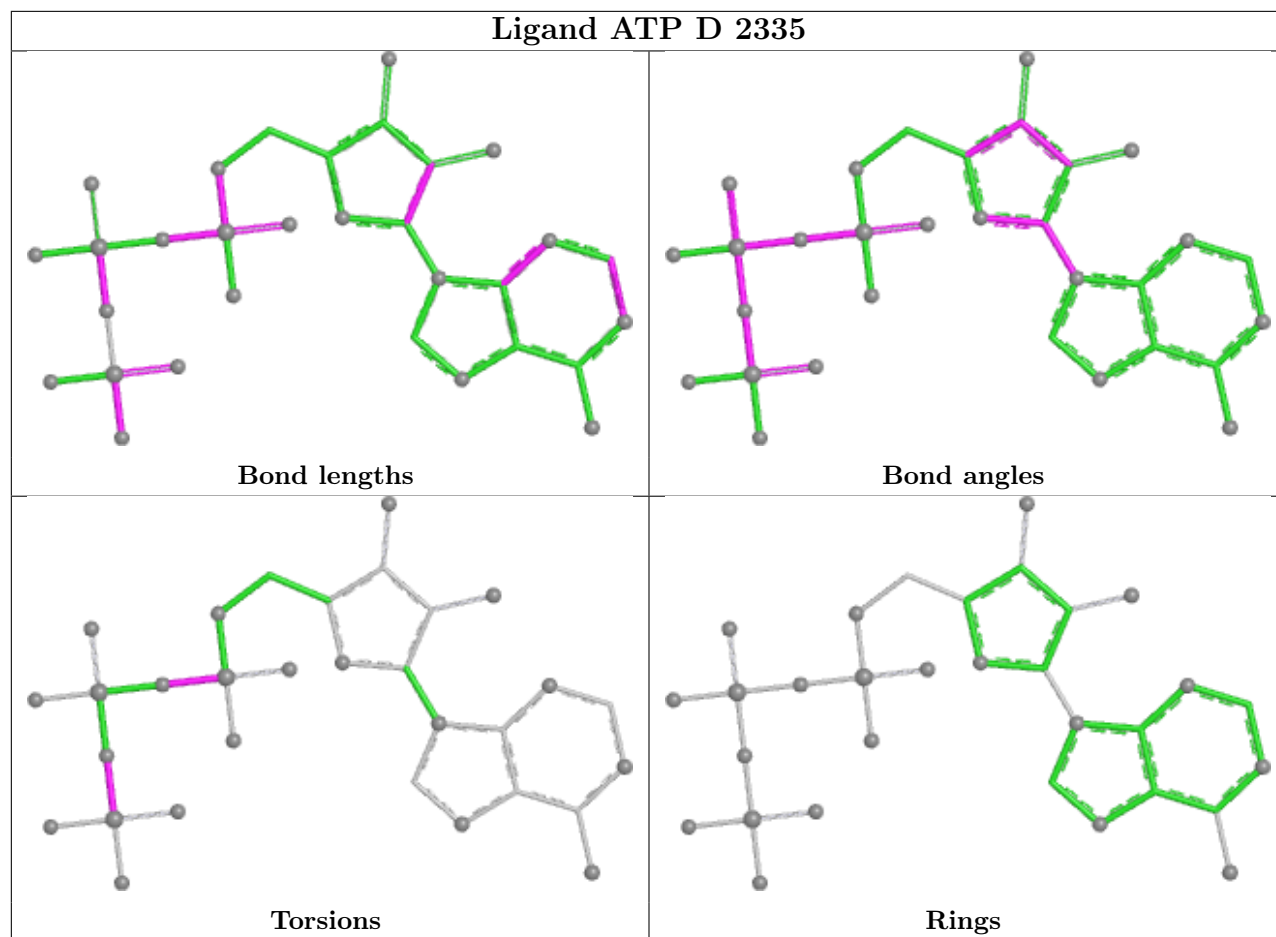
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	533	OXL	2	0
3	H	5333	OXL	1	0
3	C	1733	OXL	1	0
3	F	4133	OXL	3	0
3	D	2333	OXL	1	0
5	G	4735	ATP	1	0
5	D	2335	ATP	1	0
3	G	4733	OXL	1	0
5	C	1735	ATP	3	0
5	A	535	ATP	3	0

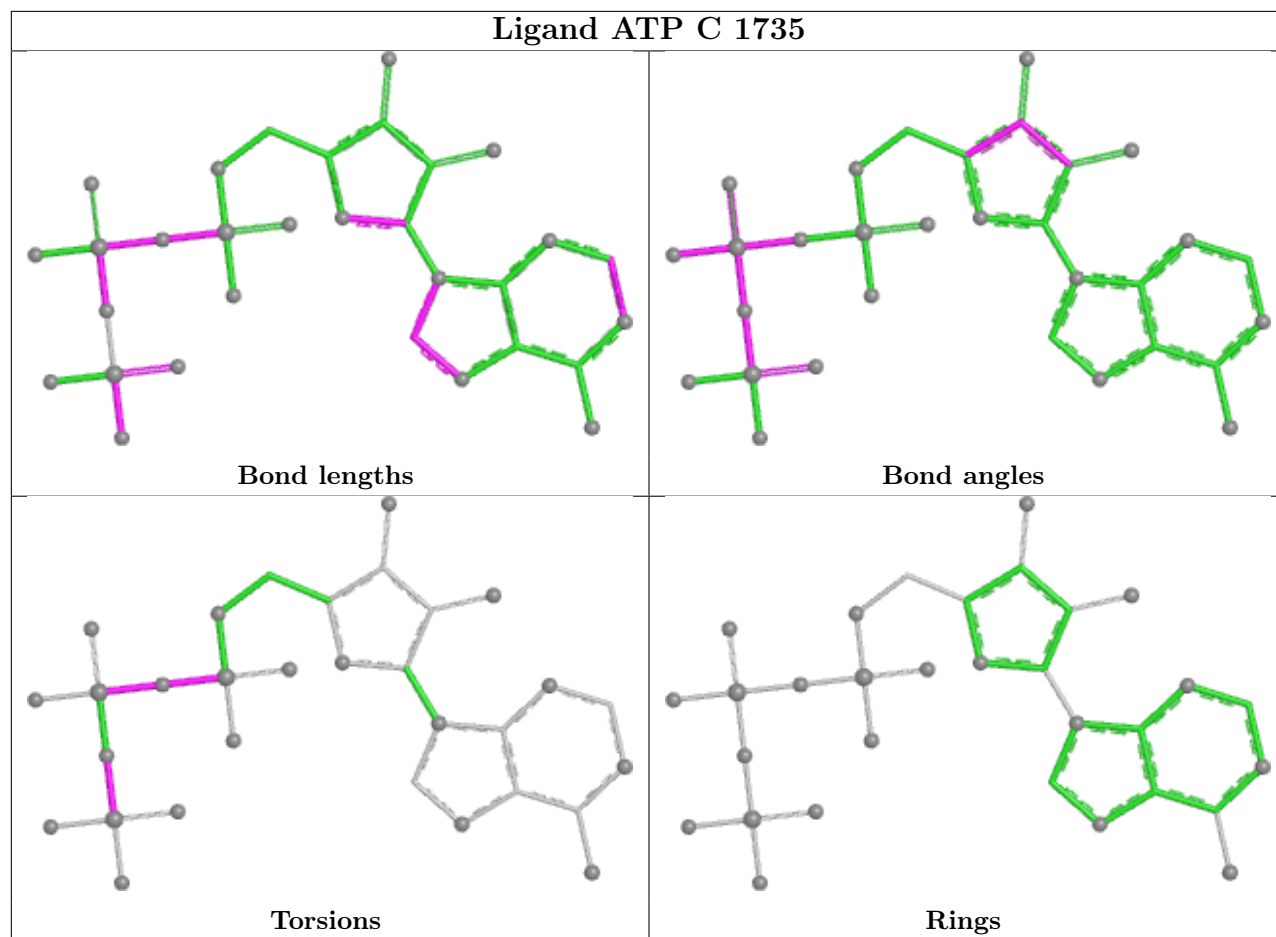
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

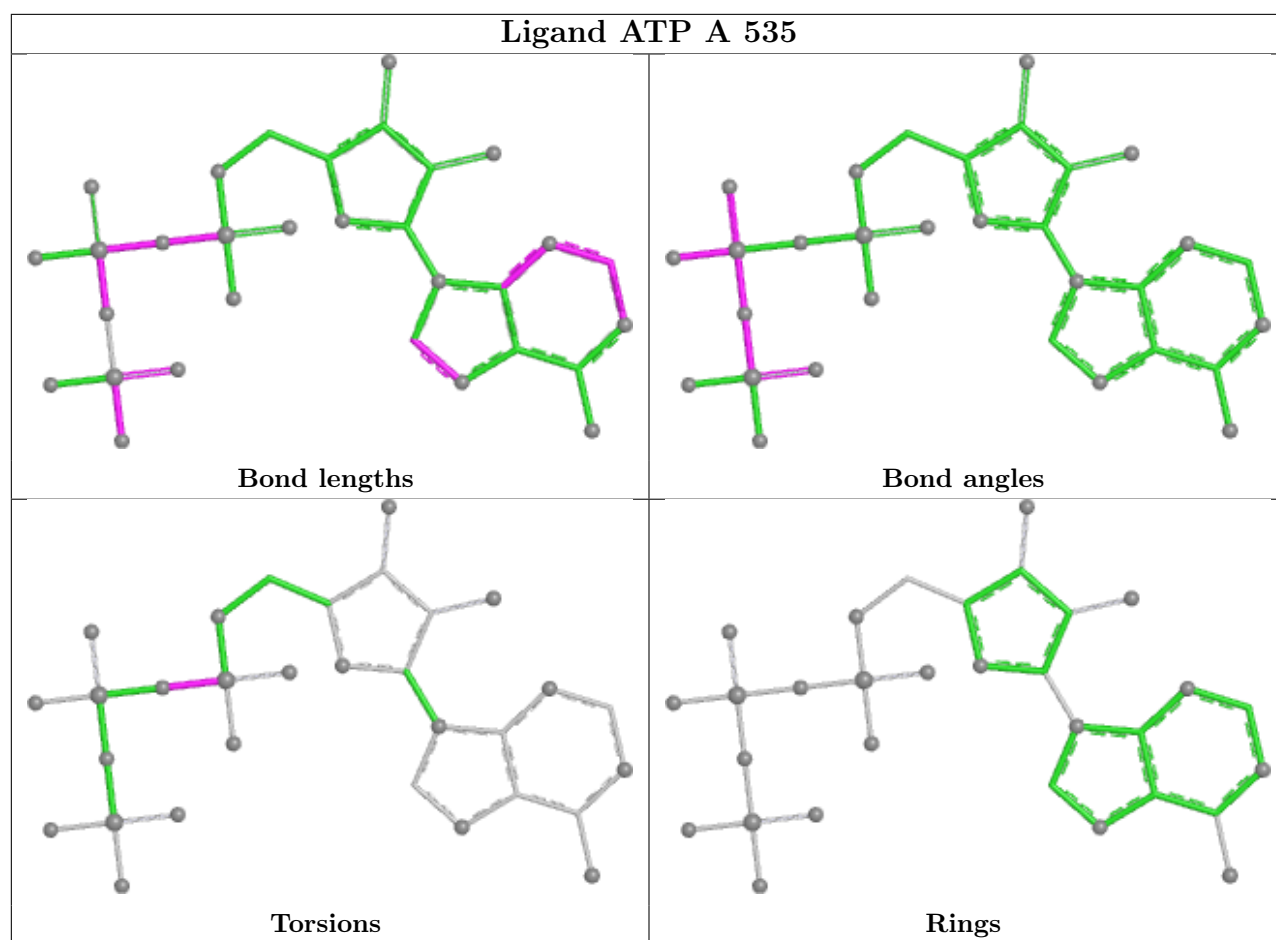












## 5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.