



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:24 AM UTC

PDB ID : 1A5U / pdb_00001a5u
Title : PYRUVATE KINASE COMPLEX WITH BIS MG-ATP-NA-OXALATE
Authors : Larsen, T.M.; Benning, M.M.; Rayment, I.; Reed, G.H.
Deposited on : 1998-02-18
Resolution : 2.35 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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

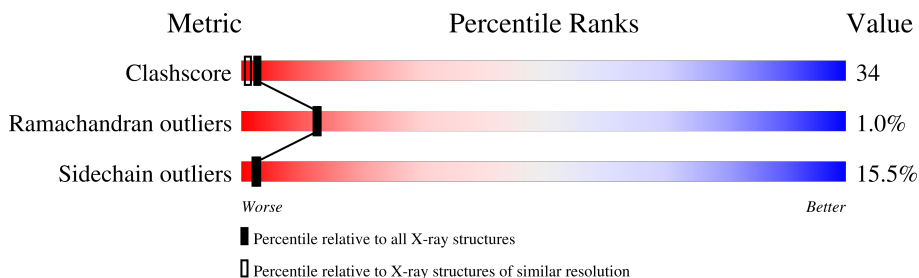
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	35% 44% 17% ..
1	B	530	49% 40% 9% .
1	C	530	34% 48% 15% ..
1	D	530	49% 38% 10% .
1	E	530	45% 41% 10% ..
1	F	530	43% 44% 10% ..
1	G	530	41% 45% 12% ..
1	H	530	54% 37% 7% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	533	-	X	X	-
3	OXL	B	1133	-	X	-	-
3	OXL	C	1733	-	X	-	-
3	OXL	D	2333	-	X	-	-
3	OXL	E	3533	-	X	-	-
3	OXL	F	4133	-	X	X	-
3	OXL	G	4733	-	X	X	-
3	OXL	H	5333	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33890 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	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	B	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	C	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	D	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	E	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	F	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	G	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	H	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

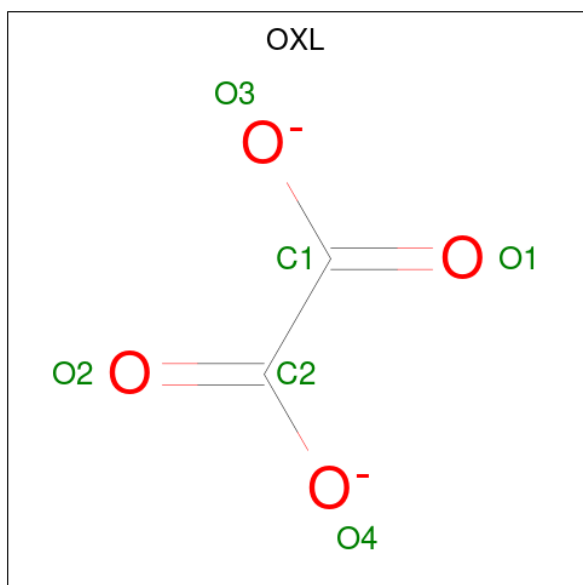
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

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

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).

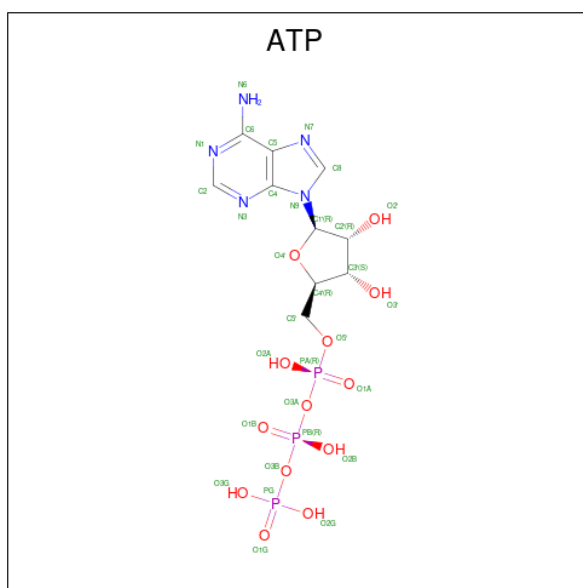


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

- 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 31	C 10	N 5	O 13	P 3	0	0
5	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	E	1	Total 31	C 10	N 5	O 13	P 3	0	0

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

- Molecule 6 is water.

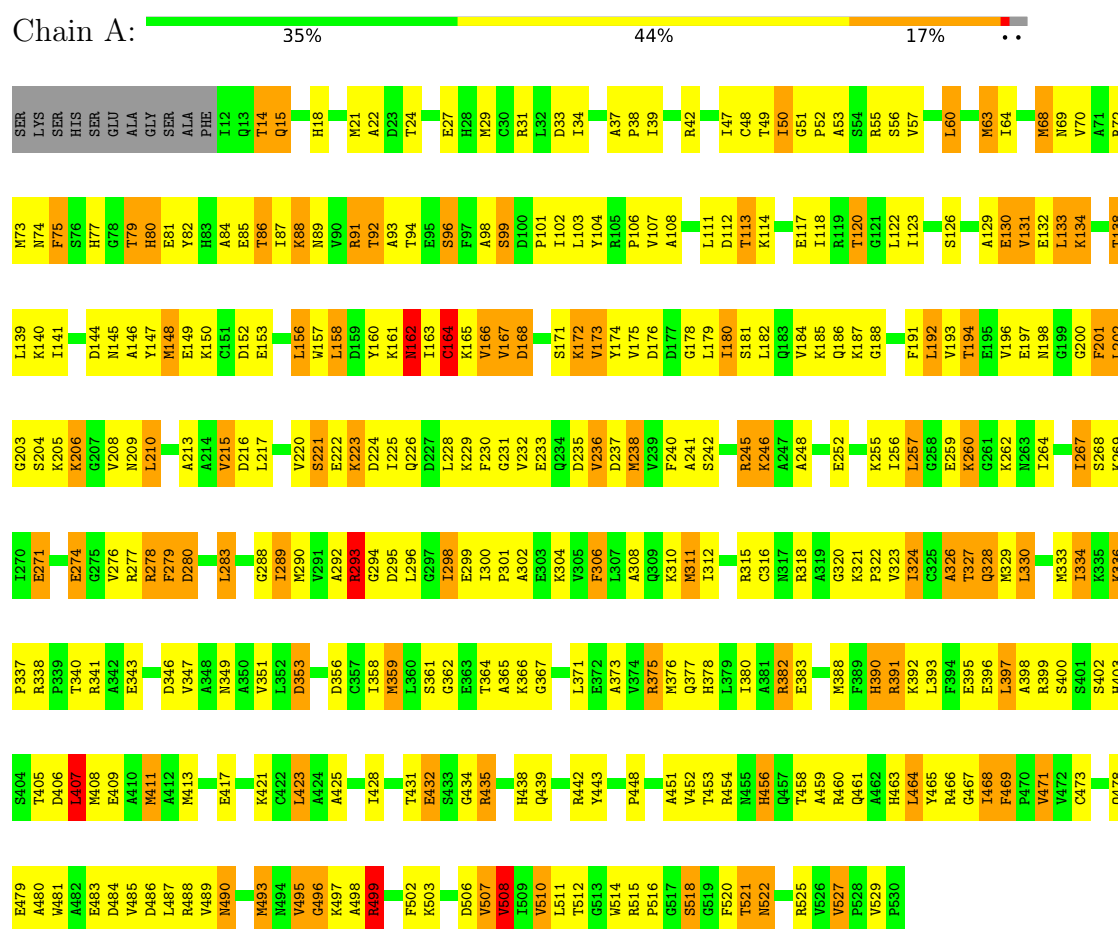
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	176	Total	O	0	0
			176	176		
6	B	260	Total	O	0	0
			260	260		
6	C	166	Total	O	0	0
			166	166		
6	D	250	Total	O	0	0
			250	250		
6	E	267	Total	O	0	0
			267	267		
6	F	185	Total	O	0	0
			185	185		
6	G	210	Total	O	0	0
			210	210		
6	H	296	Total	O	0	0
			296	296		

3 Residue-property plots

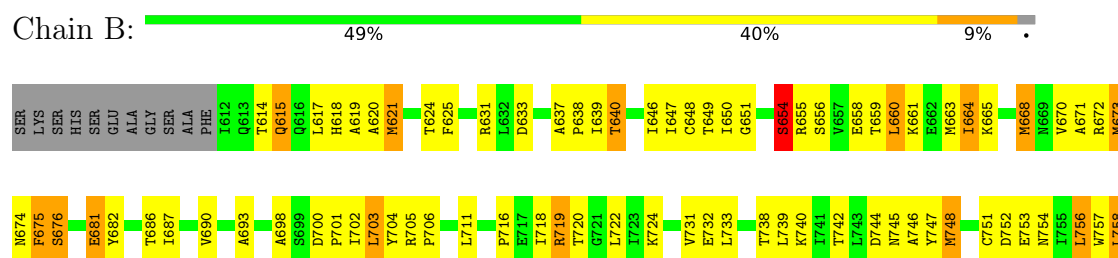
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

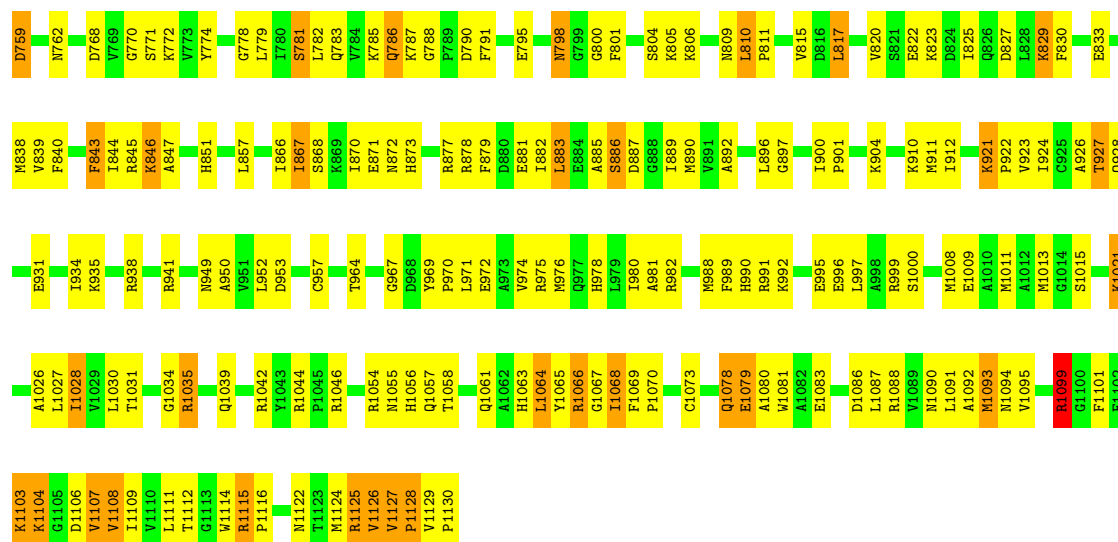
Note EDS was not executed.

• Molecule 1: PYRUVATE KINASE



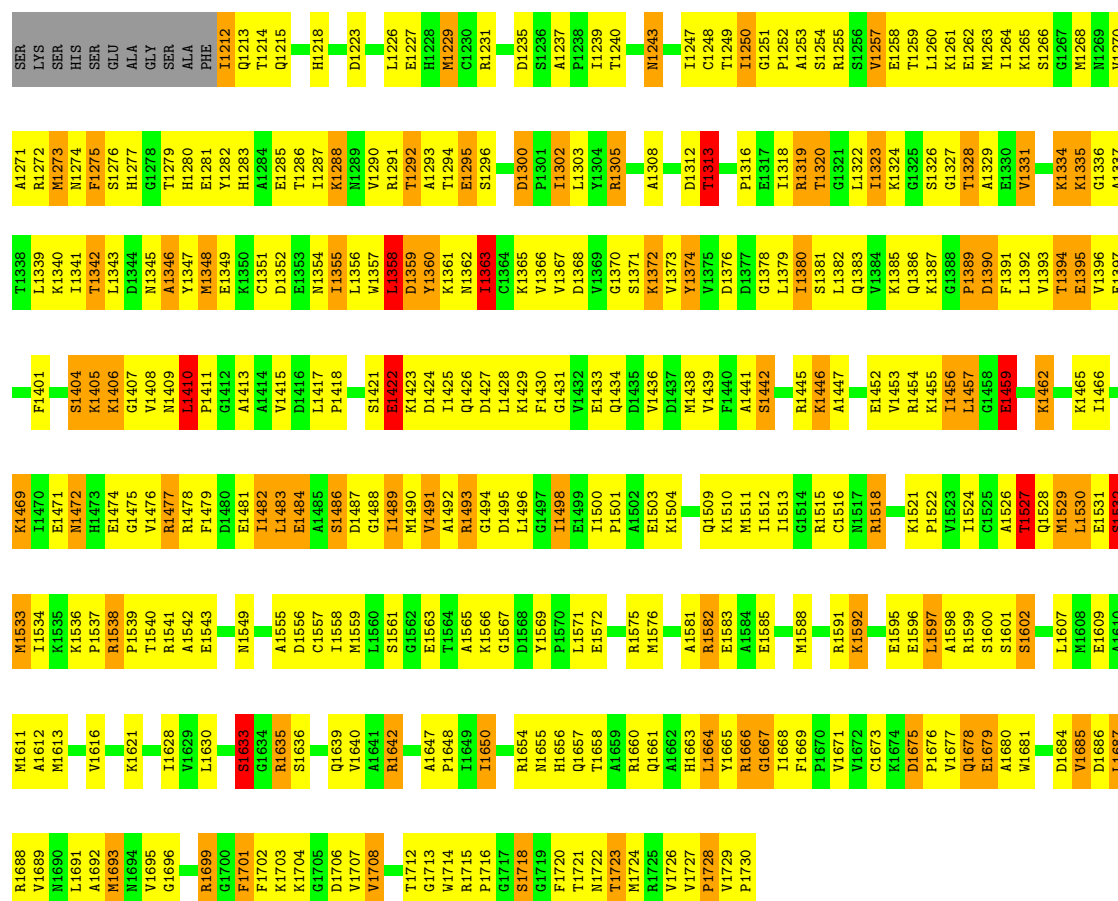
• Molecule 1: PYRUVATE KINASE





• Molecule 1: PYRUVATE KINASE

Chain C: 34% 48% 15% . .

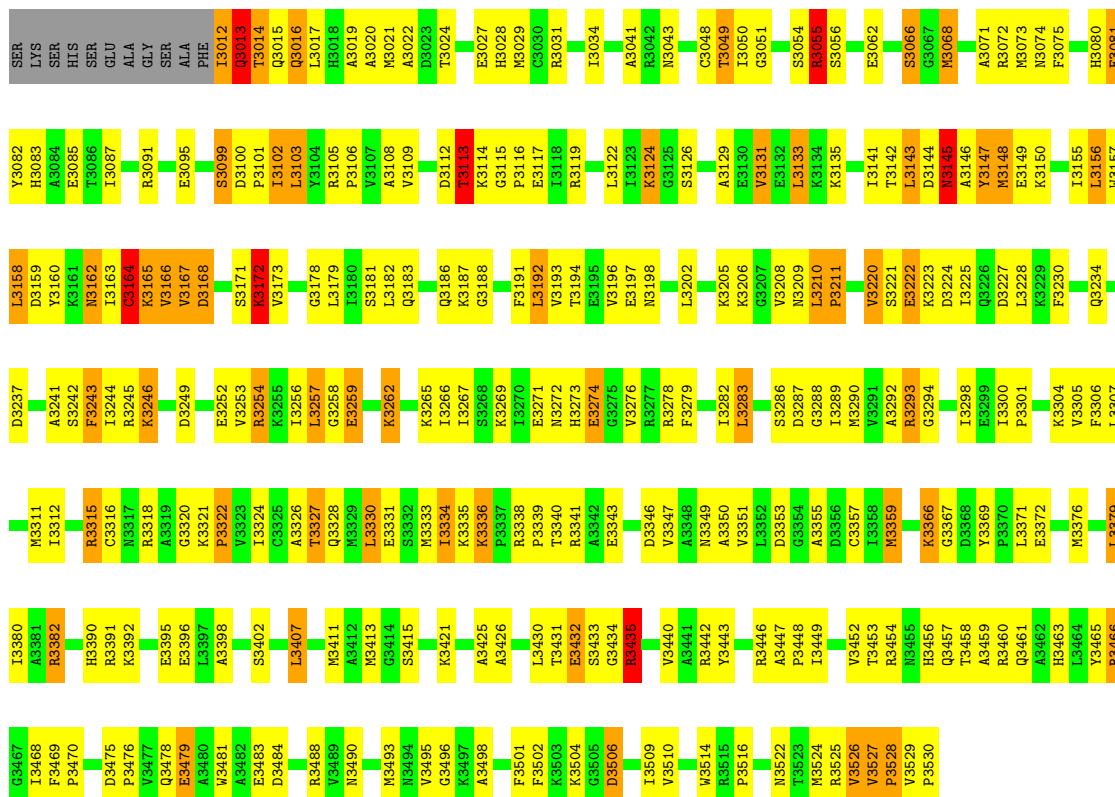


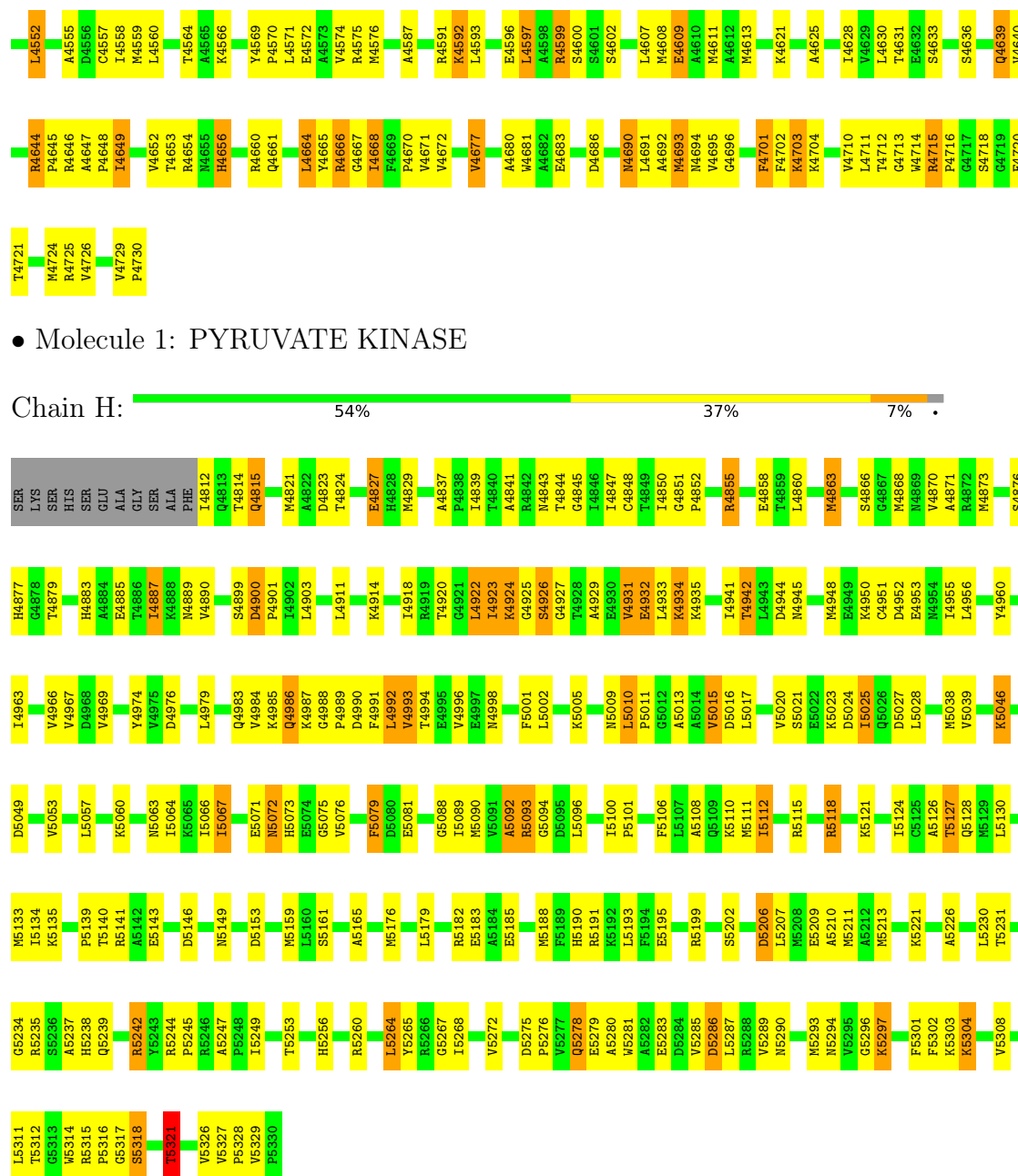
• Molecule 1: PYRUVATE KINASE

Chain D: 49% 38% 10% .



Chain E: 45% 41% 10% ..





• Molecule 1: PYRUVATE KINASE

Chain H: 54% 37% 7%

4 Data and refinement statistics

Xtriage (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, α , β , γ	95.30Å 216.50Å 258.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35	Depositor
% Data completeness (in resolution range)	85.0 (30.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33890	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.27	5/4041 (0.1%)	1.66	58/5452 (1.1%)
1	B	1.19	4/4041 (0.1%)	1.61	36/5452 (0.7%)
1	C	1.13	2/4041 (0.0%)	1.64	30/5452 (0.6%)
1	D	1.19	0/4041	1.63	42/5452 (0.8%)
1	E	1.17	0/4041	1.67	38/5452 (0.7%)
1	F	1.14	0/4041	1.62	32/5452 (0.6%)
1	G	1.17	2/4041 (0.0%)	1.65	42/5452 (0.8%)
1	H	1.19	3/4041 (0.1%)	1.58	26/5452 (0.5%)
All	All	1.18	16/32328 (0.0%)	1.63	304/43616 (0.7%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	ASN	N-CA	25.81	1.82	1.46
1	A	241	ALA	C-N	-14.20	1.15	1.33
1	A	162	ASN	C-N	-7.63	1.23	1.33
1	A	162	ASN	CA-CB	7.43	1.66	1.53
1	G	4713	GLY	CA-C	6.00	1.56	1.52

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	CYS	O-C-N	13.88	141.05	122.59
1	A	162	ASN	N-CA-CB	-11.01	91.04	110.42
1	C	1368	ASP	CB-CA-C	-10.24	92.74	110.45
1	E	3367	GLY	N-CA-C	10.03	123.36	112.33
1	A	222	GLU	N-CA-C	-9.72	100.76	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3978	0	4054	365	2
1	B	3978	0	4056	239	0
1	C	3978	0	4056	373	5
1	D	3978	0	4055	278	5
1	E	3978	0	4056	262	12
1	F	3978	0	4056	275	2
1	G	3978	0	4056	298	2
1	H	3978	0	4056	212	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
3	B	6	0	0	1	0
3	C	6	0	0	1	0
3	D	6	0	0	1	0
3	E	6	0	0	1	0
3	F	6	0	0	3	0
3	G	6	0	0	2	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	4	0
5	C	31	0	12	4	0
5	D	31	0	12	1	0
5	E	31	0	12	2	0
5	F	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	31	0	12	0	0
6	A	176	0	0	10	0
6	B	260	0	0	13	0
6	C	166	0	0	12	0
6	D	250	0	0	18	0
6	E	267	0	0	17	0
6	F	185	0	0	11	0
6	G	210	0	0	6	0
6	H	296	0	0	15	2
All	All	33890	0	32517	2187	24

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 34.

The worst 5 of 2187 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:162:ASN:N	1:A:162:ASN:CA	1.82	1.40
1:E:3493:MET:HE2	1:E:3530:PRO:HD2	1.23	1.14
1:C:1678:GLN:HB2	1:C:1684:ASP:HB2	1.31	1.13
1:D:1850:ILE:HD11	1:D:1868:MET:HE1	1.13	1.12
1:H:4850:ILE:HD11	1:H:4868:MET:HE1	1.16	1.12

The worst 5 of 24 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]	0.67	1.53
1:E:3149:GLU:CD	1:H:4934:LYS:NZ[3_655]	1.03	1.17
1:E:3149:GLU:CD	1:H:4934:LYS:CE[3_655]	1.23	0.97
1:D:1924:LYS:NZ	1:H:4858:GLU:OE1[1_455]	1.38	0.82
1:E:3149:GLU:OE1	1:H:4934:LYS:CD[3_655]	1.43	0.77

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%)	476 (92%)	36 (7%)	5 (1%)	12	12
1	B	517/530 (98%)	485 (94%)	30 (6%)	2 (0%)	30	34
1	C	517/530 (98%)	464 (90%)	42 (8%)	11 (2%)	5	4
1	D	517/530 (98%)	487 (94%)	27 (5%)	3 (1%)	21	24
1	E	517/530 (98%)	484 (94%)	26 (5%)	7 (1%)	9	7
1	F	517/530 (98%)	486 (94%)	27 (5%)	4 (1%)	16	17
1	G	517/530 (98%)	487 (94%)	27 (5%)	3 (1%)	21	24
1	H	517/530 (98%)	485 (94%)	27 (5%)	5 (1%)	12	12
All	All	4136/4240 (98%)	3854 (93%)	242 (6%)	40 (1%)	12	12

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1337	ALA
1	C	1533	MET
1	F	3729	ALA
1	F	3789	PRO
1	G	4389	PRO

5.3.2 Protein sidechains ⓘ

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%)	342 (80%)	84 (20%)	1	1
1	B	426/434 (98%)	369 (87%)	57 (13%)	4	3
1	C	426/434 (98%)	341 (80%)	85 (20%)	1	1
1	D	426/434 (98%)	375 (88%)	51 (12%)	5	4
1	E	426/434 (98%)	361 (85%)	65 (15%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	426/434 (98%)	358 (84%)	68 (16%)	2	2
1	G	426/434 (98%)	358 (84%)	68 (16%)	2	2
1	H	426/434 (98%)	377 (88%)	49 (12%)	5	5
All	All	3408/3472 (98%)	2881 (84%)	527 (16%)	2	2

5 of 527 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	4597	LEU
1	G	4718	SER
1	G	4592	LYS
1	H	5286	ASP
1	C	1491	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1998	ASN
1	G	4549	ASN
1	E	3145	ASN
1	G	4528	GLN
1	H	5149	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
5	ATP	F	4135	2,4	32,33,33	2.83	10 (31%)	48,52,52	1.12	5 (10%)
3	OXL	C	1733	4	5,5,5	1.70	2 (40%)	6,6,6	1.99	4 (66%)
3	OXL	D	2333	4	5,5,5	1.65	3 (60%)	6,6,6	2.26	4 (66%)
3	OXL	F	4133	4	5,5,5	1.36	0	6,6,6	1.70	2 (33%)
5	ATP	G	4735	2,4	32,33,33	3.00	9 (28%)	48,52,52	0.92	1 (2%)
3	OXL	G	4733	4	5,5,5	1.38	0	6,6,6	1.71	2 (33%)
3	OXL	H	5333	4	5,5,5	1.68	2 (40%)	6,6,6	2.09	4 (66%)
5	ATP	A	535	2,4	32,33,33	2.14	10 (31%)	48,52,52	1.48	3 (6%)
3	OXL	E	3533	4	5,5,5	1.37	0	6,6,6	1.70	2 (33%)
5	ATP	E	3535	2,4	32,33,33	2.29	7 (21%)	48,52,52	0.86	2 (4%)
3	OXL	A	533	4	5,5,5	1.81	2 (40%)	6,6,6	0.92	0
5	ATP	C	1735	4	32,33,33	2.33	10 (31%)	48,52,52	1.25	6 (12%)
3	OXL	B	1133	4	5,5,5	1.74	2 (40%)	6,6,6	2.09	3 (50%)
5	ATP	D	2335	2,4	32,33,33	2.34	9 (28%)	48,52,52	1.32	7 (14%)

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
5	ATP	F	4135	2,4	-	0/22/38/38	0/3/3/3
3	OXL	C	1733	4	-	4/4/4/4	-
3	OXL	D	2333	4	-	4/4/4/4	-
3	OXL	F	4133	4	-	4/4/4/4	-
5	ATP	G	4735	2,4	-	4/22/38/38	0/3/3/3
3	OXL	G	4733	4	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	H	5333	4	-	4/4/4/4	-
5	ATP	A	535	2,4	-	3/22/38/38	0/3/3/3
3	OXL	E	3533	4	-	4/4/4/4	-
5	ATP	E	3535	2,4	-	4/22/38/38	0/3/3/3
3	OXL	A	533	4	-	4/4/4/4	-
5	ATP	C	1735	4	-	3/22/38/38	0/3/3/3
3	OXL	B	1133	4	-	4/4/4/4	-
5	ATP	D	2335	2,4	-	4/22/38/38	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	E	3535	ATP	PB-O3B	-8.98	1.49	1.59
5	C	1735	ATP	PB-O3B	-8.02	1.50	1.59
5	D	2335	ATP	PB-O3B	-7.89	1.51	1.59

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	535	ATP	O2B-PB-O3B	7.44	127.39	107.27
5	D	2335	ATP	O2G-PG-O1G	4.37	127.86	110.83
5	A	535	ATP	O2G-PG-O1G	3.71	125.28	110.83
5	C	1735	ATP	O2G-PG-O1G	3.64	125.02	110.83
5	D	2335	ATP	O2B-PB-O3B	-3.58	97.60	107.27

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

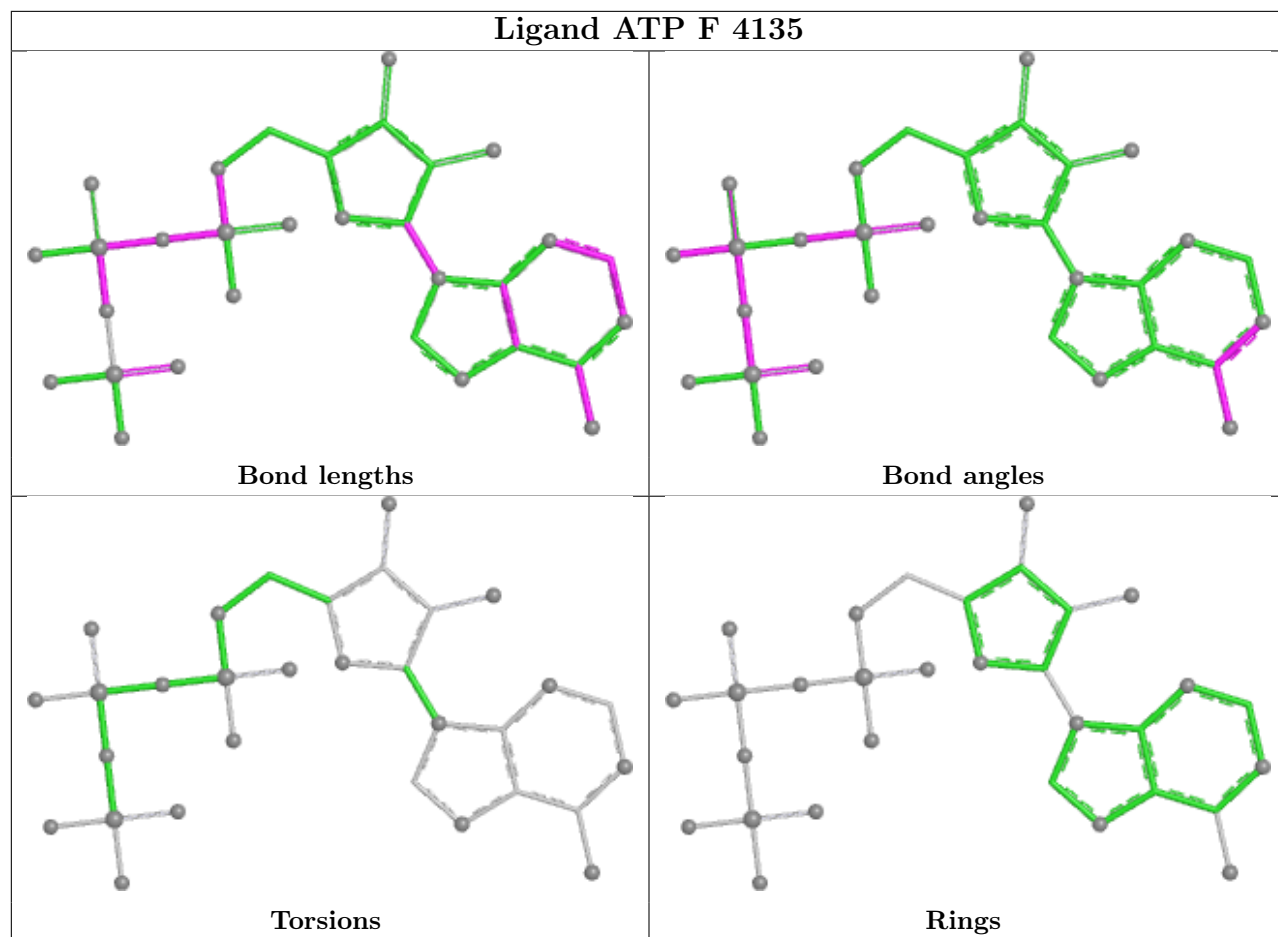
Mol	Chain	Res	Type	Atoms
5	E	3535	ATP	PB-O3B-PG-O3G
3	A	533	OXL	O3-C1-C2-O4
3	B	1133	OXL	O3-C1-C2-O4
3	C	1733	OXL	O3-C1-C2-O4
3	E	3533	OXL	O3-C1-C2-O4

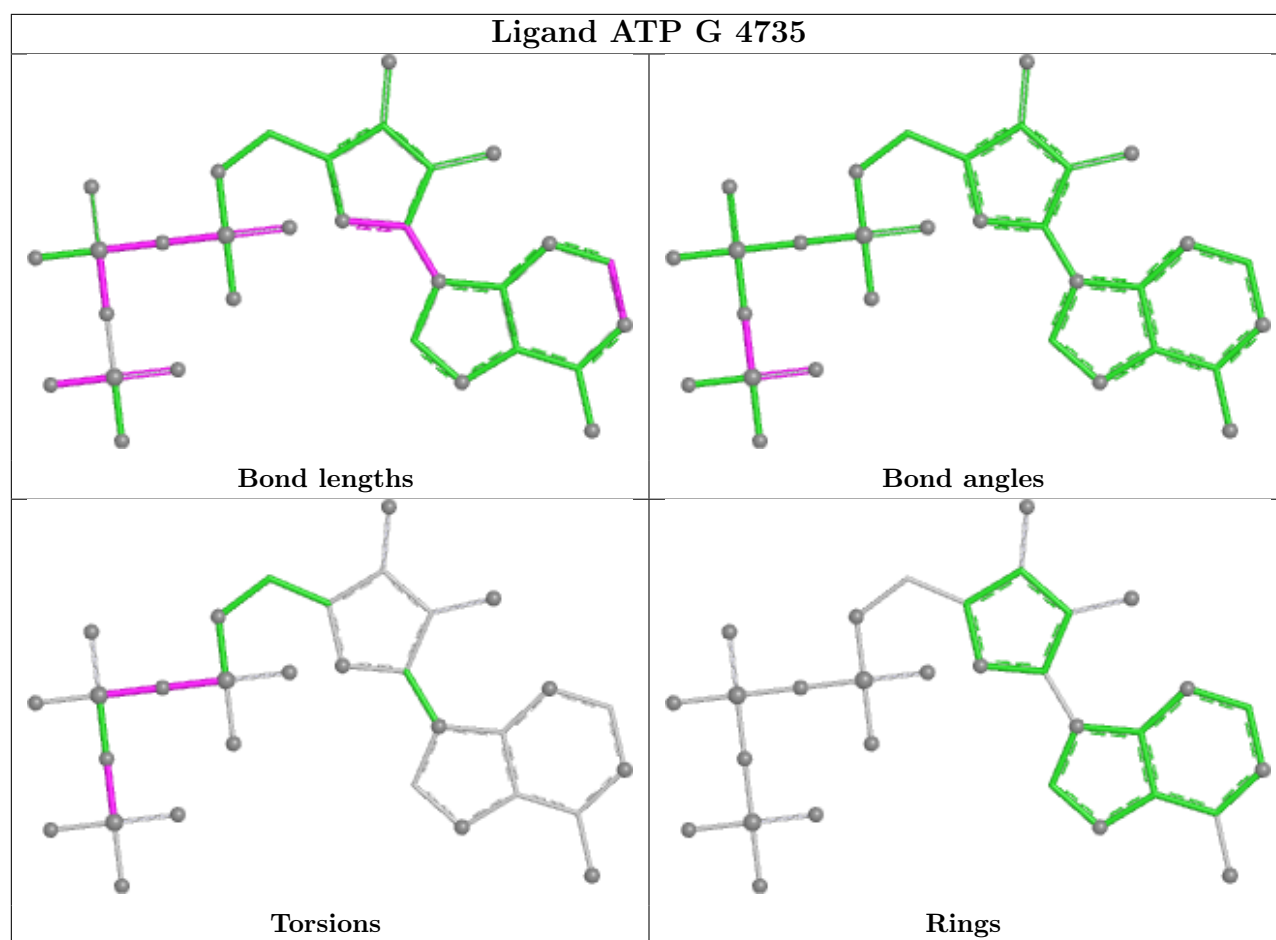
There are no ring outliers.

12 monomers are involved in 23 short contacts:

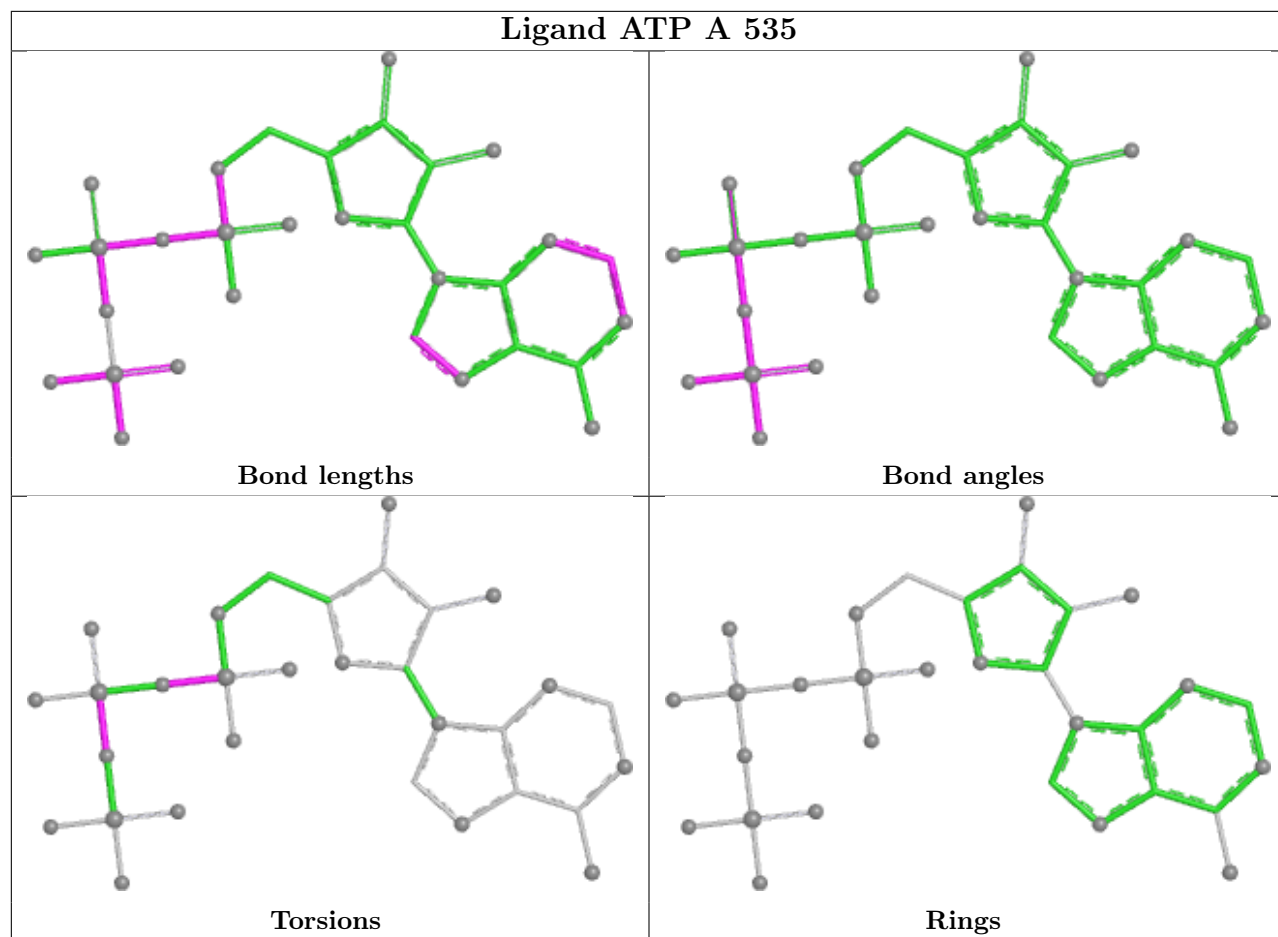
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1733	OXL	1	0
3	D	2333	OXL	1	0
3	F	4133	OXL	3	0
3	G	4733	OXL	2	0
3	H	5333	OXL	1	0
5	A	535	ATP	4	0
3	E	3533	OXL	1	0
5	E	3535	ATP	2	0
3	A	533	OXL	2	0
5	C	1735	ATP	4	0
3	B	1133	OXL	1	0
5	D	2335	ATP	1	0

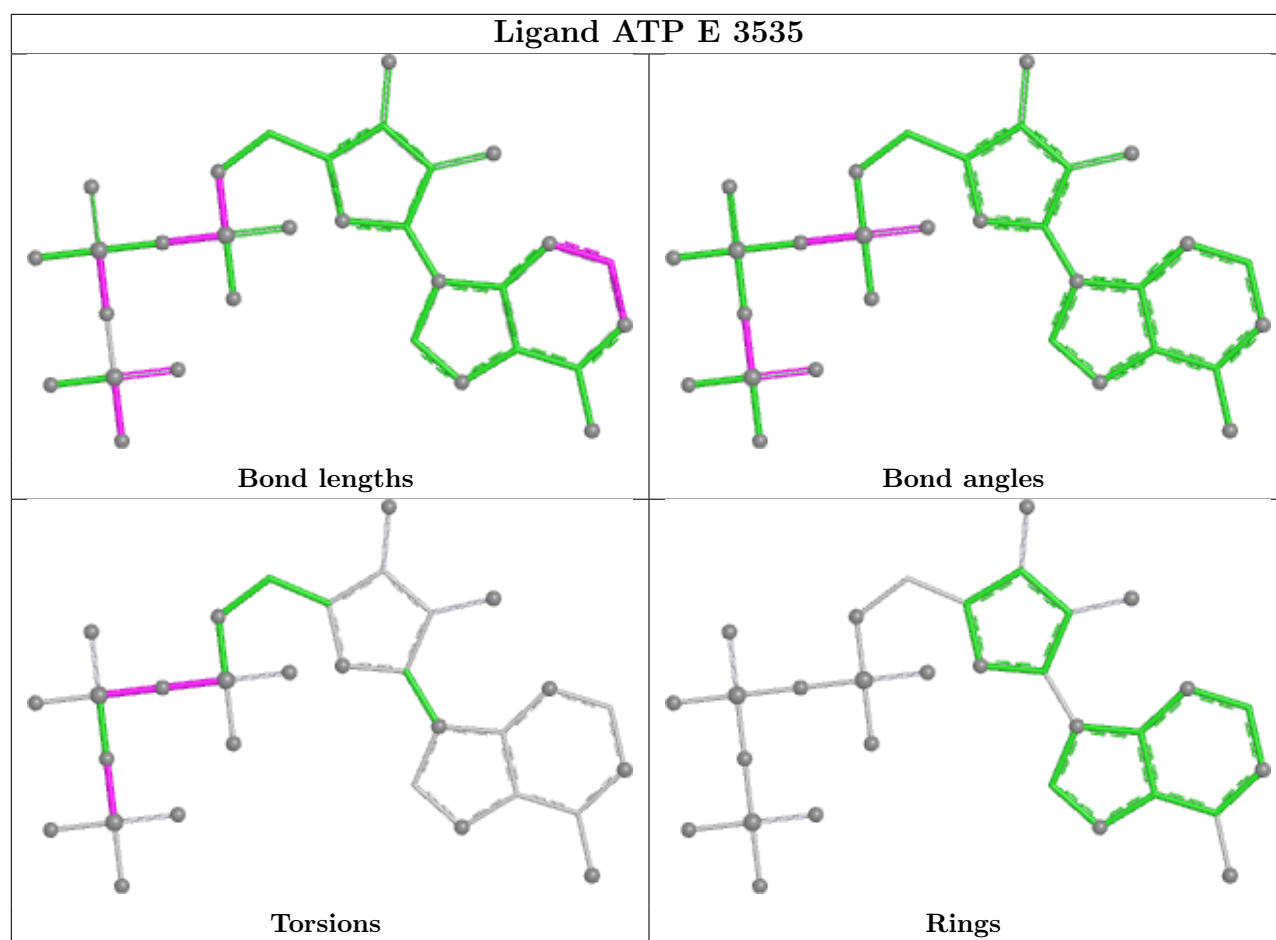
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

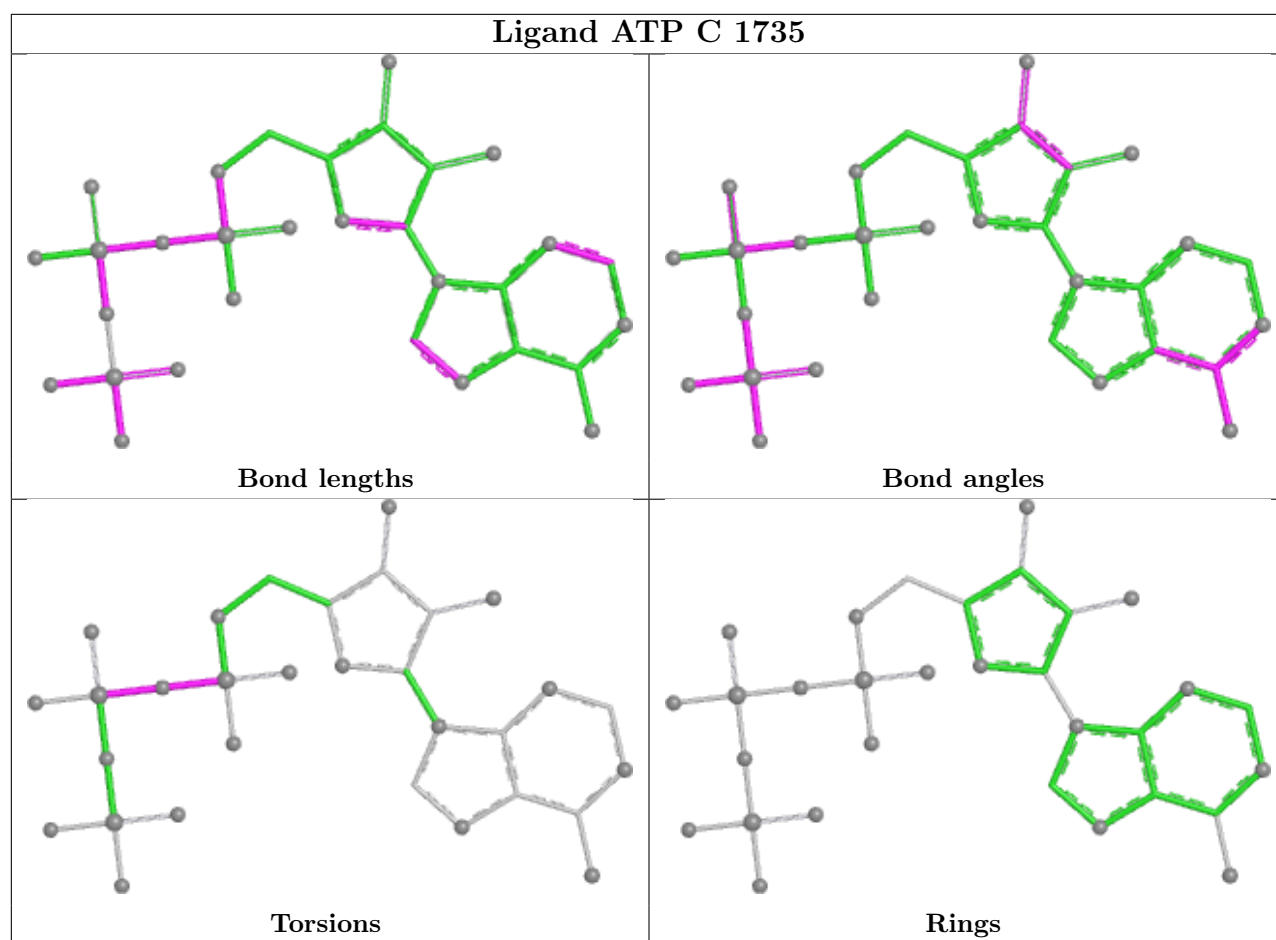


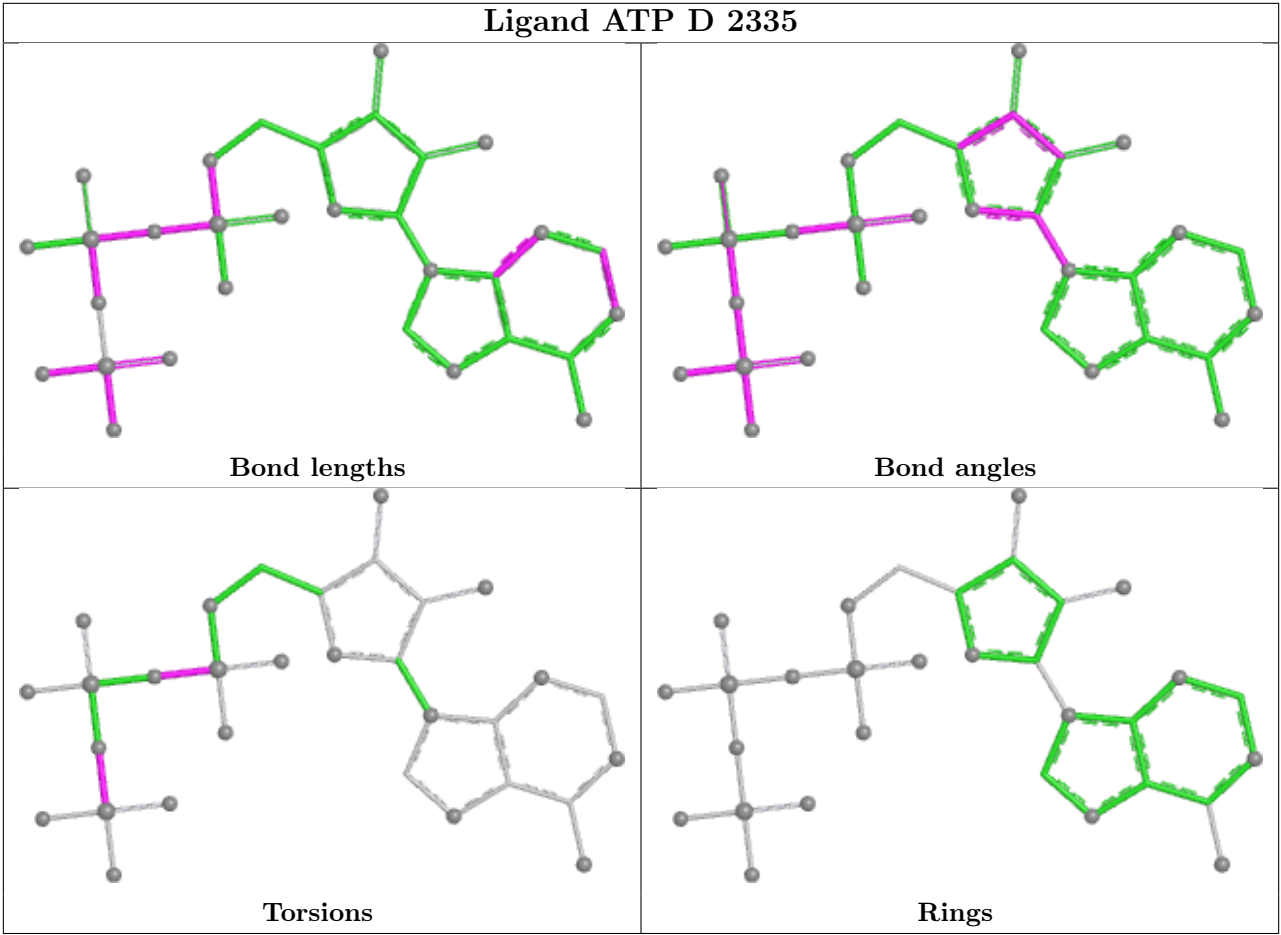


Ligand ATP A 535









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	241:ALA	C	242:SER	N	1.14

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.