wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:21 PM GMT

PDB ID	:	1A49
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

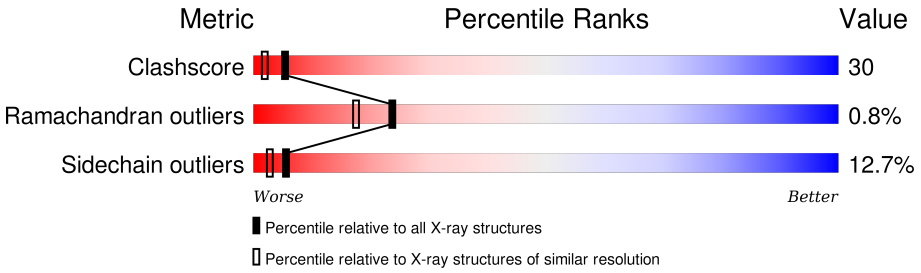
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	40% 40% 16%
1	B	530	49% 38% 10%
1	C	530	38% 44% 14%
1	D	530	45% 42% 9%
1	E	530	47% 37% 12%
1	F	530	44% 41% 11%
1	G	530	43% 43% 12%

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Mol	Chain	Length	Quality of chain
1	H	530	54% 36% 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	-

2 Entry composition

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		
2	H	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		

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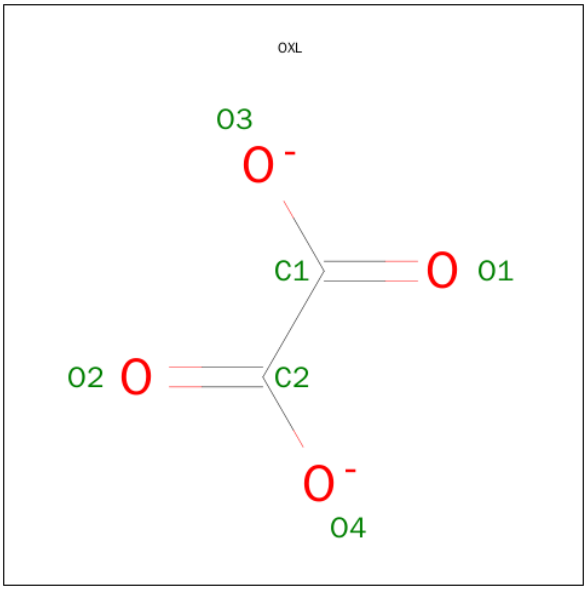
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).

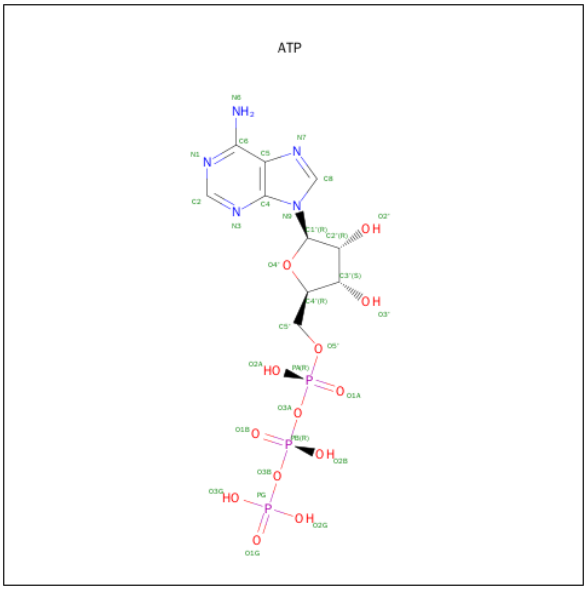


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0
3	E	1	Total C O 6 2 4	0	0
3	F	1	Total C O 6 2 4	0	0
3	G	1	Total C O 6 2 4	0	0
3	H	1	Total C O 6 2 4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
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	195	Total	O	0	0
			195	195		
6	B	270	Total	O	0	0
			270	270		
6	C	178	Total	O	0	0
			178	178		
6	D	272	Total	O	0	0
			272	272		
6	E	279	Total	O	0	0
			279	279		
6	F	197	Total	O	0	0
			197	197		
6	G	228	Total	O	0	0
			228	228		
6	H	302	Total	O	0	0
			302	302		

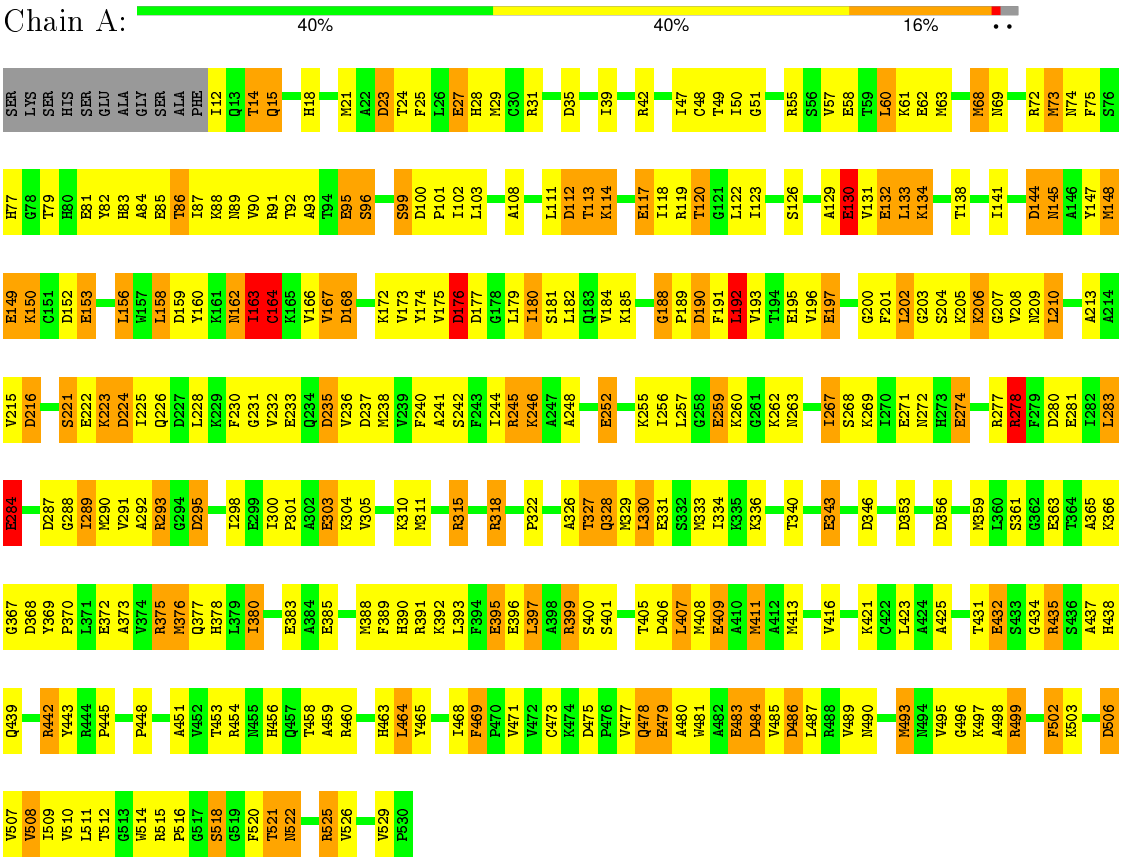
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

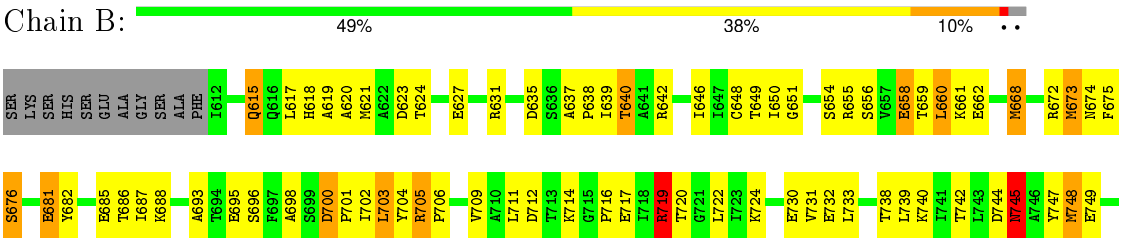
- Molecule 1: PYRUVATE KINASE

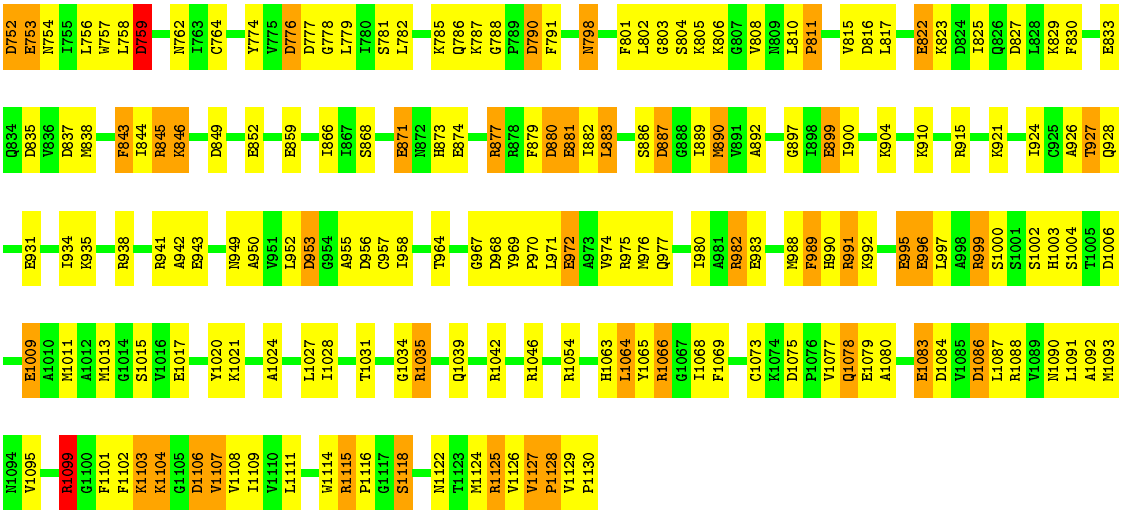
Chain A:



- Molecule 1: PYRUVATE KINASE

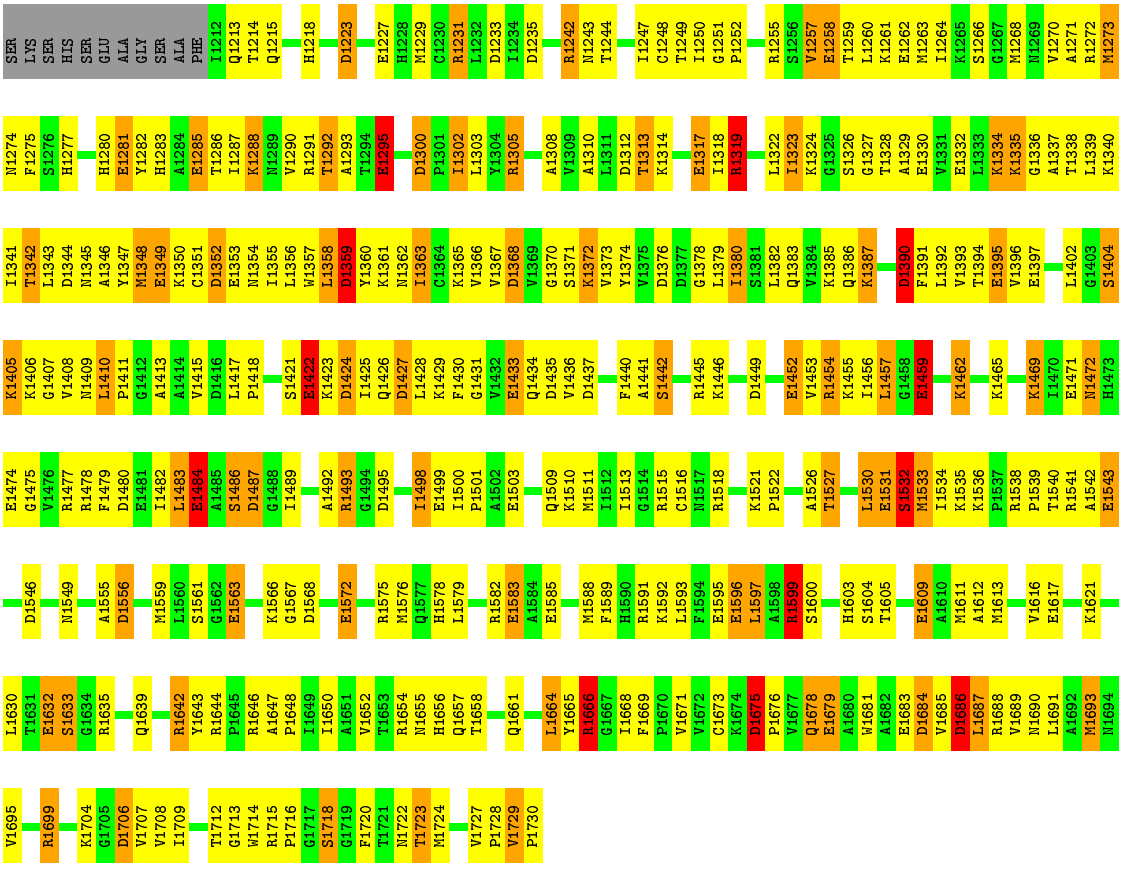
Chain B:





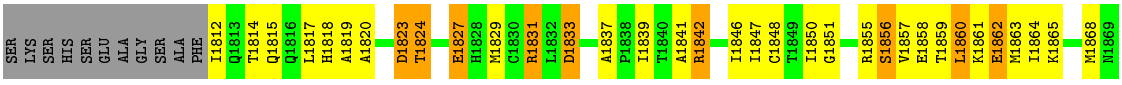
• Molecule 1: PYRUVATE KINASE

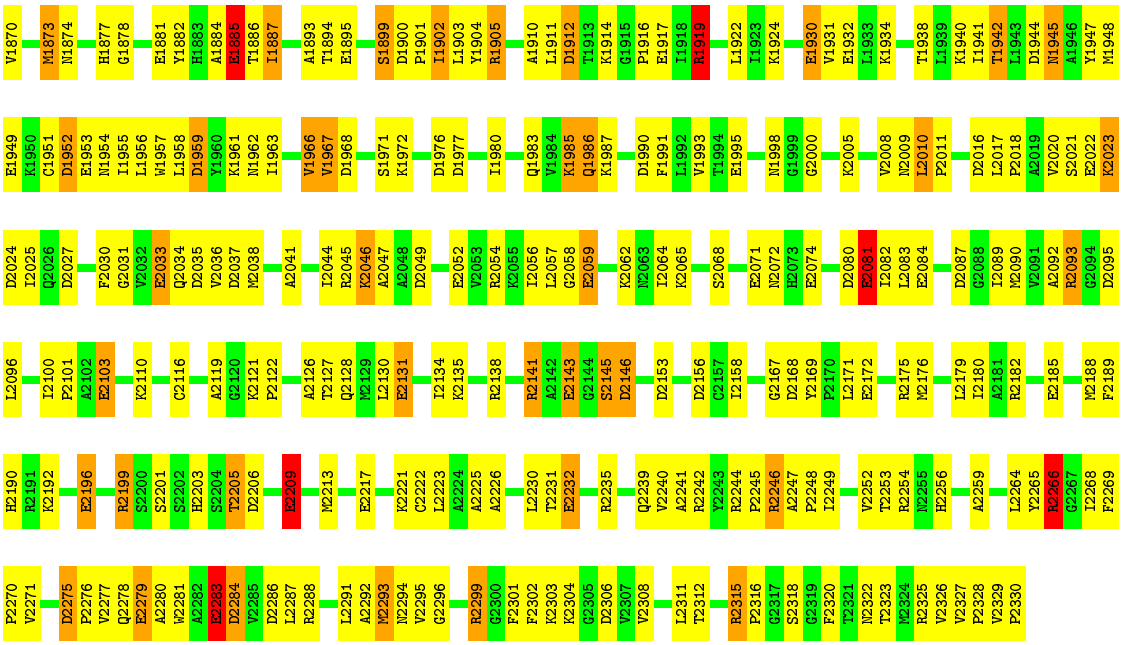
Chain C:



• Molecule 1: PYRUVATE KINASE

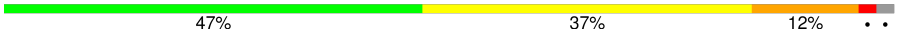
Chain D:

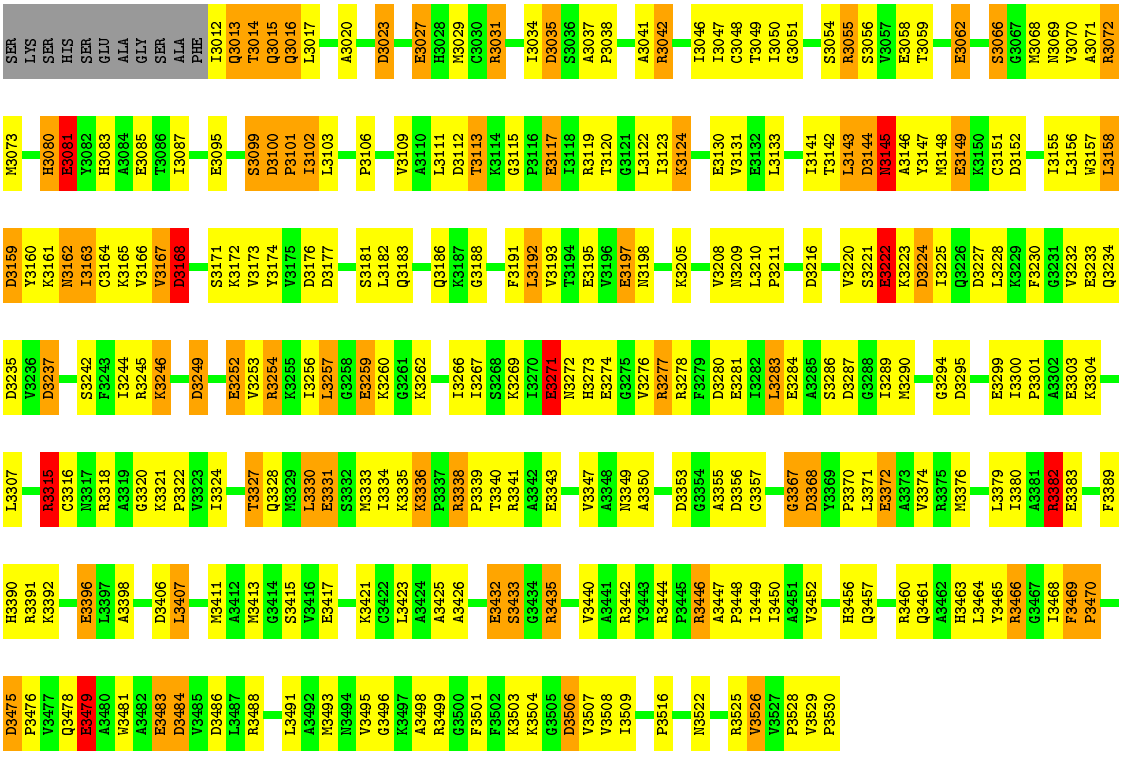




• Molecule 1: PYRUVATE KINASE

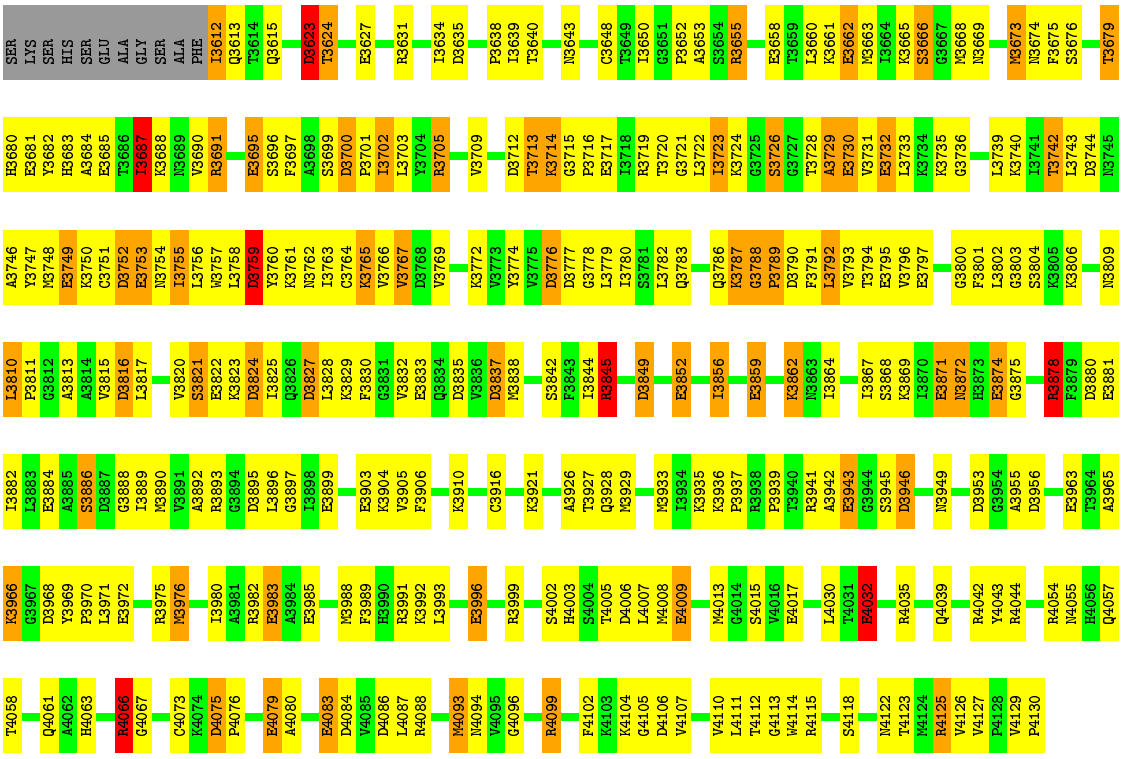
Chain E:





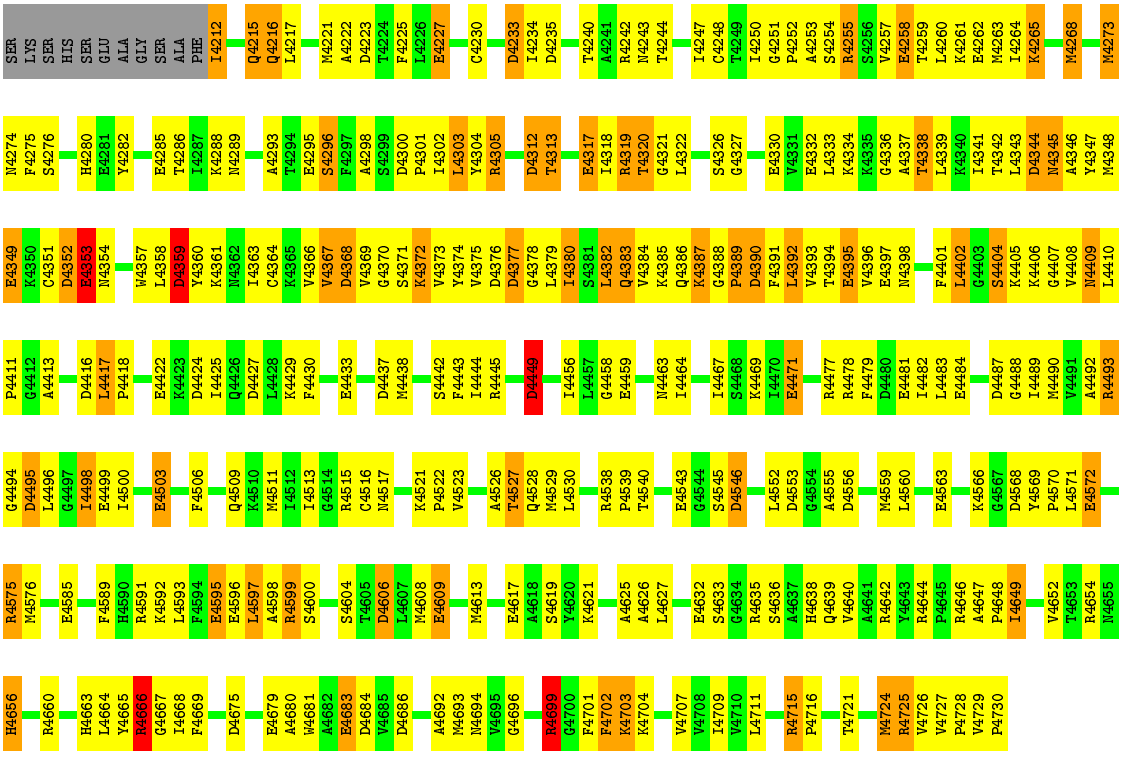
• Molecule 1: PYRUVATE KINASE

Chain F:



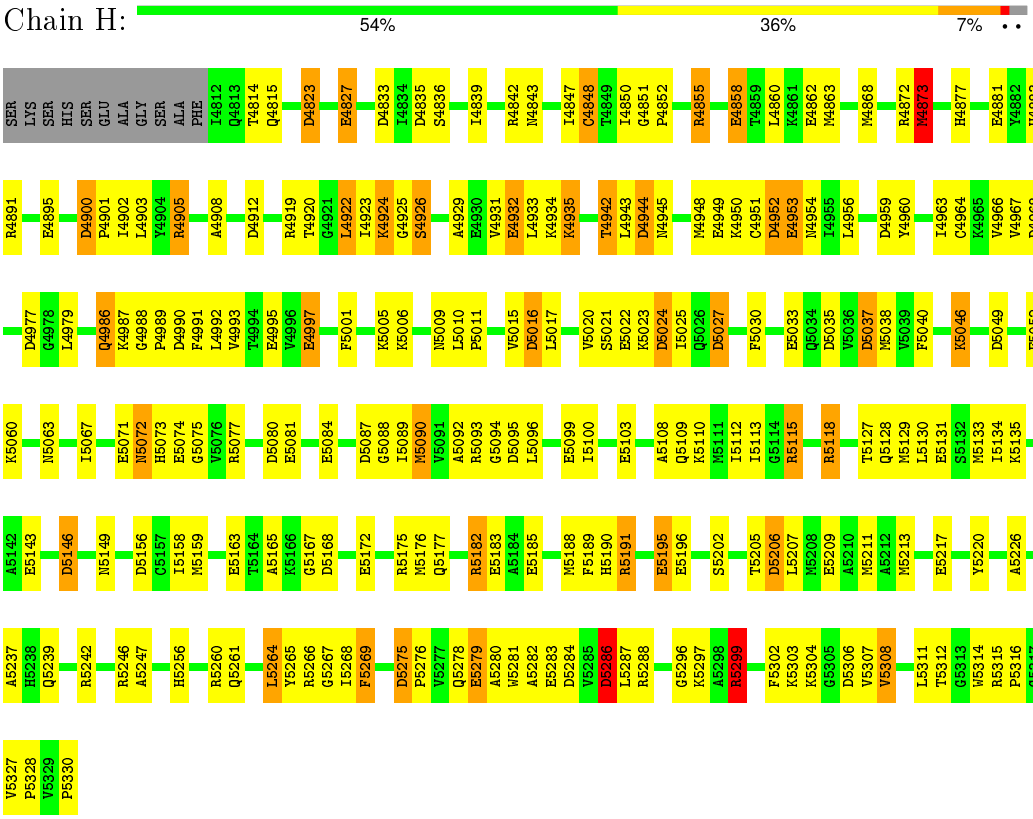
• Molecule 1: PYRUVATE KINASE

Chain G:



• Molecule 1: PYRUVATE KINASE

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 – 2.10	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 V. 5-D	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34001	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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: OXL, MG, K, 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	1.36	35/4041 (0.9%)	1.29	48/5452 (0.9%)
1	B	1.38	29/4041 (0.7%)	1.31	58/5452 (1.1%)
1	C	1.30	36/4041 (0.9%)	1.34	63/5452 (1.2%)
1	D	1.38	35/4041 (0.9%)	1.30	57/5452 (1.0%)
1	E	1.37	32/4041 (0.8%)	1.32	52/5452 (1.0%)
1	F	1.31	31/4041 (0.8%)	1.32	64/5452 (1.2%)
1	G	1.34	30/4041 (0.7%)	1.30	50/5452 (0.9%)
1	H	1.36	27/4041 (0.7%)	1.31	63/5452 (1.2%)
All	All	1.35	255/32328 (0.8%)	1.31	455/43616 (1.0%)

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

The worst 5 of 255 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4595	GLU	CD-OE1	11.92	1.38	1.25
1	B	681	GLU	CD-OE2	11.16	1.38	1.25
1	B	627	GLU	CD-OE2	10.56	1.37	1.25
1	A	27	GLU	CD-OE2	10.12	1.36	1.25
1	F	3797	GLU	CD-OE1	10.11	1.36	1.25

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1919	ARG	NE-CZ-NH1	13.83	127.21	120.30
1	C	1666	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	F	4066	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	B	1127	VAL	C-N-CD	-11.65	94.97	120.60
1	D	1919	ARG	NE-CZ-NH2	-11.52	114.54	120.30

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	326	2
1	B	3978	0	4056	216	1
1	C	3978	0	4055	321	3
1	D	3978	0	4055	251	5
1	E	3978	0	4056	221	14
1	F	3978	0	4055	240	2
1	G	3978	0	4055	276	2
1	H	3978	0	4055	187	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	0	0
3	E	6	0	0	0	0
3	F	6	0	0	1	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	17	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	12	3
All	All	34001	0	32514	1940	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 30.

The worst 5 of 1940 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:C:1248:CYS:HB2	1:C:1268:MET:HE3	1.25	1.19
1:E:3142:THR:HG22	1:E:3144:ASP:H	1.05	1.10
1:H:5130:LEU:HD13	1:H:5133:MET:HE3	1.20	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4665:TYR:HB2	1:G:4668:ILE:HD12	1.36	1.07

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%)	24	17
1	B	517/530 (98%)	492 (95%)	20 (4%)	5 (1%)	19	13
1	C	517/530 (98%)	471 (91%)	41 (8%)	5 (1%)	19	13
1	D	517/530 (98%)	493 (95%)	21 (4%)	3 (1%)	30	24
1	E	517/530 (98%)	488 (94%)	24 (5%)	5 (1%)	19	13
1	F	517/530 (98%)	490 (95%)	23 (4%)	4 (1%)	24	17
1	G	517/530 (98%)	488 (94%)	25 (5%)	4 (1%)	24	17
1	H	517/530 (98%)	490 (95%)	24 (5%)	3 (1%)	30	24
All	All	4136/4240 (98%)	3892 (94%)	211 (5%)	33 (1%)	24	17

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%)	349 (82%)	77 (18%)	2 1
1	B	426/434 (98%)	379 (89%)	47 (11%)	8 4
1	C	426/434 (98%)	358 (84%)	68 (16%)	3 1
1	D	426/434 (98%)	384 (90%)	42 (10%)	10 6
1	E	426/434 (98%)	372 (87%)	54 (13%)	5 3
1	F	426/434 (98%)	373 (88%)	53 (12%)	6 3
1	G	426/434 (98%)	368 (86%)	58 (14%)	5 2
1	H	426/434 (98%)	391 (92%)	35 (8%)	14 10
All	All	3408/3472 (98%)	2974 (87%)	434 (13%)	5 3

5 of 434 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1873	MET
1	E	3066	SER
1	H	4848	CYS
1	D	1930	GLU
1	D	2141	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1998	ASN

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Mol	Chain	Res	Type
1	E	3080	HIS
1	H	4986	GLN
1	D	2073	HIS
1	D	2238	HIS

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 carbohydrates 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	$\#\|Z\| > 2$
3	OXL	A	533	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	A	535	2,4	24,33,33	1.49	5 (20%)	31,52,52	1.49	4 (12%)
3	OXL	B	1133	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	C	1733	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	C	1735	2,4	24,33,33	1.63	4 (16%)	31,52,52	1.17	4 (12%)
3	OXL	D	2333	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	D	2335	2,4	24,33,33	1.55	5 (20%)	31,52,52	1.29	6 (19%)
3	OXL	E	3533	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	E	3535	2,4	24,33,33	1.65	4 (16%)	31,52,52	1.18	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OXL	F	4133	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	F	4135	2,4	24,33,33	1.62	4 (16%)	31,52,52	1.05	1 (3%)
3	OXL	G	4733	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	G	4735	2,4	24,33,33	1.65	4 (16%)	31,52,52	1.25	3 (9%)
3	OXL	H	5333	4	0,5,5	0.00	-	0,6,6	0.00	-

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	-	0/0/4/4	0/0/0/0
5	ATP	A	535	2,4	-	0/18/38/38	0/3/3/3
3	OXL	B	1133	4	-	0/0/4/4	0/0/0/0
3	OXL	C	1733	4	-	0/0/4/4	0/0/0/0
5	ATP	C	1735	2,4	-	0/18/38/38	0/3/3/3
3	OXL	D	2333	4	-	0/0/4/4	0/0/0/0
5	ATP	D	2335	2,4	-	0/18/38/38	0/3/3/3
3	OXL	E	3533	4	-	0/0/4/4	0/0/0/0
5	ATP	E	3535	2,4	-	0/18/38/38	0/3/3/3
3	OXL	F	4133	4	-	0/0/4/4	0/0/0/0
5	ATP	F	4135	2,4	-	0/18/38/38	0/3/3/3
3	OXL	G	4733	4	-	0/0/4/4	0/0/0/0
5	ATP	G	4735	2,4	-	0/18/38/38	0/3/3/3
3	OXL	H	5333	4	-	0/0/4/4	0/0/0/0

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3535	ATP	PG-O3G	-5.19	1.36	1.54
5	D	2335	ATP	PG-O3G	-4.40	1.38	1.54
5	G	4735	ATP	PG-O3G	-4.32	1.39	1.54
5	C	1735	ATP	PG-O3G	-3.99	1.40	1.54
5	C	1735	ATP	O4'-C1'	-3.94	1.36	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	3535	ATP	C2'-C1'-N9	-2.93	109.81	114.29
5	A	535	ATP	O3A-PA-O5'	-2.92	95.19	102.94
5	G	4735	ATP	C1'-N9-C4	-2.78	122.75	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	2335	ATP	O3A-PA-O5'	-2.63	95.96	102.94
5	C	1735	ATP	C2'-C1'-N9	-2.57	110.37	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.