



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 23, 2021 – 04:50 PM EST

PDB ID : 2AP9  
Title : Crystal structure of acetylglutamate kinase from Mycobacterium tuberculosis CDC1551  
Authors : Rajashankar, K.R.; Kniewel, R.; Lee, K.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2005-08-15  
Resolution : 2.80 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.

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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	:	2.16
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)	:	2.16

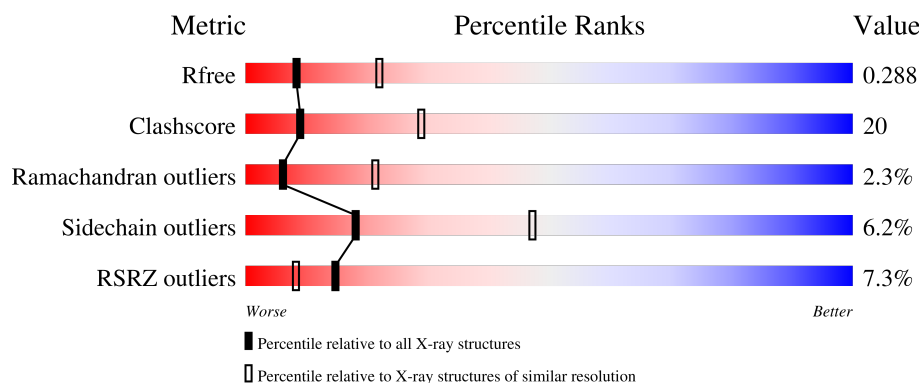
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\leq 5\%$ . 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	299	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>39%</div> <div>..</div> </div> </div>
1	B	299	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>39%</div> <div>..</div> </div> </div>
1	C	299	<div> <div>8%</div> <div> <div></div> <div>57%</div> <div>37%</div> <div>..</div> </div> </div>
1	D	299	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>37%</div> <div>5% ..</div> </div> </div>
1	E	299	<div> <div>17%</div> <div> <div></div> <div>54%</div> <div>39%</div> <div>6% ..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	299	<div><div></div><div>6%</div><div>56%</div><div>37%</div><div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13141 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 acetylglutamate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	Se	0	0	0
			2221	1400	399	412	3	7			
1	B	292	Total	C	N	O	S	Se	0	0	0
			2156	1362	380	404	3	7			
1	C	292	Total	C	N	O	S	Se	0	0	0
			2156	1362	380	404	3	7			
1	D	292	Total	C	N	O	S	Se	0	0	0
			2156	1362	380	404	3	7			
1	E	295	Total	C	N	O	S	Se	0	0	0
			2180	1376	387	407	3	7			
1	F	292	Total	C	N	O	S	Se	0	0	0
			2156	1362	380	404	3	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MSE	MET	modified residue	UNP P0A4Y6
A	55	MSE	MET	modified residue	UNP P0A4Y6
A	78	MSE	MET	modified residue	UNP P0A4Y6
A	105	MSE	MET	modified residue	UNP P0A4Y6
A	167	MSE	MET	modified residue	UNP P0A4Y6
A	213	MSE	MET	modified residue	UNP P0A4Y6
A	248	LEU	SER	conflict	UNP P0A4Y6
A	250	MSE	MET	modified residue	UNP P0A4Y6
A	297	GLU	-	expression tag	UNP P0A4Y6
A	298	GLY	-	expression tag	UNP P0A4Y6
A	299	HIS	-	expression tag	UNP P0A4Y6
A	300	HIS	-	expression tag	UNP P0A4Y6
A	301	HIS	-	expression tag	UNP P0A4Y6
A	302	HIS	-	expression tag	UNP P0A4Y6
A	303	HIS	-	expression tag	UNP P0A4Y6
A	304	HIS	-	expression tag	UNP P0A4Y6
B	42	MSE	MET	modified residue	UNP P0A4Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	55	MSE	MET	modified residue	UNP P0A4Y6
B	78	MSE	MET	modified residue	UNP P0A4Y6
B	105	MSE	MET	modified residue	UNP P0A4Y6
B	167	MSE	MET	modified residue	UNP P0A4Y6
B	213	MSE	MET	modified residue	UNP P0A4Y6
B	248	LEU	SER	conflict	UNP P0A4Y6
B	250	MSE	MET	modified residue	UNP P0A4Y6
B	297	GLU	-	expression tag	UNP P0A4Y6
B	298	GLY	-	expression tag	UNP P0A4Y6
B	299	HIS	-	expression tag	UNP P0A4Y6
B	300	HIS	-	expression tag	UNP P0A4Y6
B	301	HIS	-	expression tag	UNP P0A4Y6
B	302	HIS	-	expression tag	UNP P0A4Y6
B	303	HIS	-	expression tag	UNP P0A4Y6
B	304	HIS	-	expression tag	UNP P0A4Y6
C	42	MSE	MET	modified residue	UNP P0A4Y6
C	55	MSE	MET	modified residue	UNP P0A4Y6
C	78	MSE	MET	modified residue	UNP P0A4Y6
C	105	MSE	MET	modified residue	UNP P0A4Y6
C	167	MSE	MET	modified residue	UNP P0A4Y6
C	213	MSE	MET	modified residue	UNP P0A4Y6
C	248	LEU	SER	conflict	UNP P0A4Y6
C	250	MSE	MET	modified residue	UNP P0A4Y6
C	297	GLU	-	expression tag	UNP P0A4Y6
C	298	GLY	-	expression tag	UNP P0A4Y6
C	299	HIS	-	expression tag	UNP P0A4Y6
C	300	HIS	-	expression tag	UNP P0A4Y6
C	301	HIS	-	expression tag	UNP P0A4Y6
C	302	HIS	-	expression tag	UNP P0A4Y6
C	303	HIS	-	expression tag	UNP P0A4Y6
C	304	HIS	-	expression tag	UNP P0A4Y6
D	42	MSE	MET	modified residue	UNP P0A4Y6
D	55	MSE	MET	modified residue	UNP P0A4Y6
D	78	MSE	MET	modified residue	UNP P0A4Y6
D	105	MSE	MET	modified residue	UNP P0A4Y6
D	167	MSE	MET	modified residue	UNP P0A4Y6
D	213	MSE	MET	modified residue	UNP P0A4Y6
D	248	LEU	SER	conflict	UNP P0A4Y6
D	250	MSE	MET	modified residue	UNP P0A4Y6
D	297	GLU	-	expression tag	UNP P0A4Y6
D	298	GLY	-	expression tag	UNP P0A4Y6
D	299	HIS	-	expression tag	UNP P0A4Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	300	HIS	-	expression tag	UNP P0A4Y6
D	301	HIS	-	expression tag	UNP P0A4Y6
D	302	HIS	-	expression tag	UNP P0A4Y6
D	303	HIS	-	expression tag	UNP P0A4Y6
D	304	HIS	-	expression tag	UNP P0A4Y6
E	42	MSE	MET	modified residue	UNP P0A4Y6
E	55	MSE	MET	modified residue	UNP P0A4Y6
E	78	MSE	MET	modified residue	UNP P0A4Y6
E	105	MSE	MET	modified residue	UNP P0A4Y6
E	167	MSE	MET	modified residue	UNP P0A4Y6
E	213	MSE	MET	modified residue	UNP P0A4Y6
E	248	LEU	SER	conflict	UNP P0A4Y6
E	250	MSE	MET	modified residue	UNP P0A4Y6
E	297	GLU	-	expression tag	UNP P0A4Y6
E	298	GLY	-	expression tag	UNP P0A4Y6
E	299	HIS	-	expression tag	UNP P0A4Y6
E	300	HIS	-	expression tag	UNP P0A4Y6
E	301	HIS	-	expression tag	UNP P0A4Y6
E	302	HIS	-	expression tag	UNP P0A4Y6
E	303	HIS	-	expression tag	UNP P0A4Y6
E	304	HIS	-	expression tag	UNP P0A4Y6
F	42	MSE	MET	modified residue	UNP P0A4Y6
F	55	MSE	MET	modified residue	UNP P0A4Y6
F	78	MSE	MET	modified residue	UNP P0A4Y6
F	105	MSE	MET	modified residue	UNP P0A4Y6
F	167	MSE	MET	modified residue	UNP P0A4Y6
F	213	MSE	MET	modified residue	UNP P0A4Y6
F	248	LEU	SER	conflict	UNP P0A4Y6
F	250	MSE	MET	modified residue	UNP P0A4Y6
F	297	GLU	-	expression tag	UNP P0A4Y6
F	298	GLY	-	expression tag	UNP P0A4Y6
F	299	HIS	-	expression tag	UNP P0A4Y6
F	300	HIS	-	expression tag	UNP P0A4Y6
F	301	HIS	-	expression tag	UNP P0A4Y6
F	302	HIS	-	expression tag	UNP P0A4Y6
F	303	HIS	-	expression tag	UNP P0A4Y6
F	304	HIS	-	expression tag	UNP P0A4Y6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

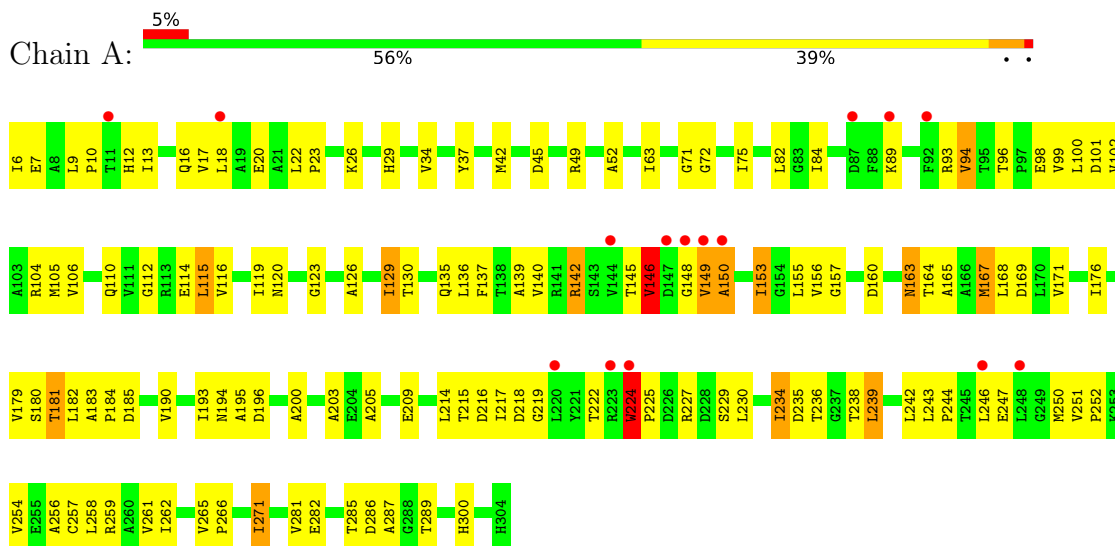
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0
4	B	24	Total O 24 24	0	0
4	C	13	Total O 13 13	0	0
4	D	17	Total O 17 17	0	0
4	E	15	Total O 15 15	0	0
4	F	10	Total O 10 10	0	0

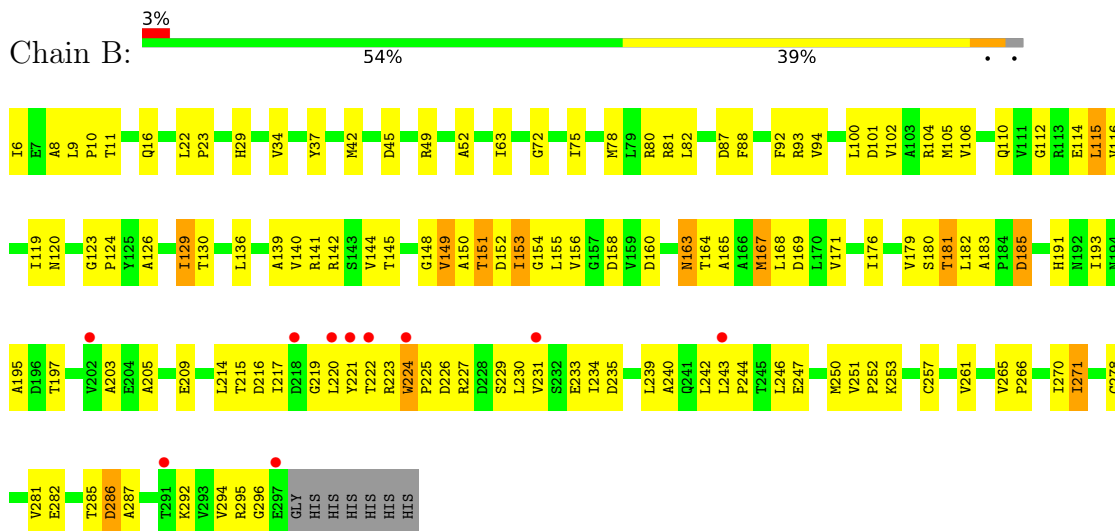
### 3 Residue-property plots

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 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: acetylglutamate kinase



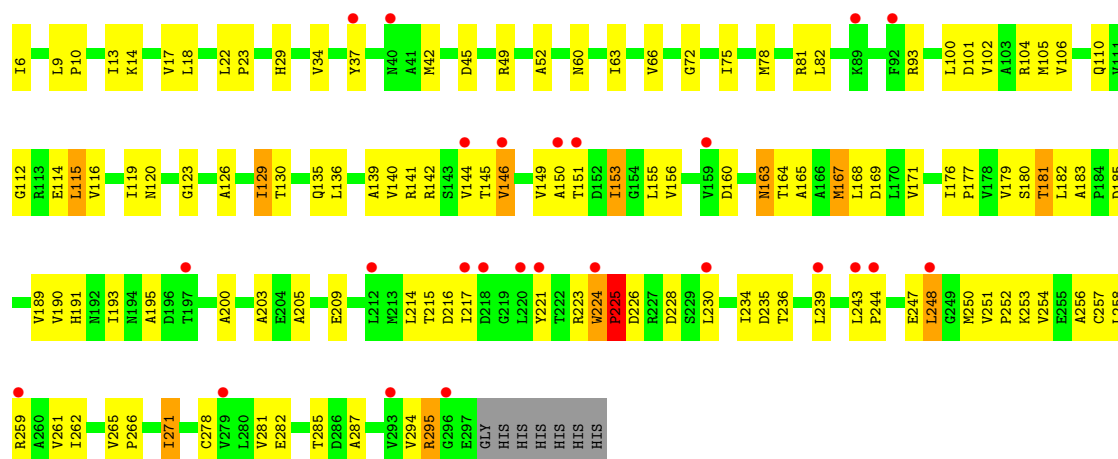
- Molecule 1: acetylglutamate kinase



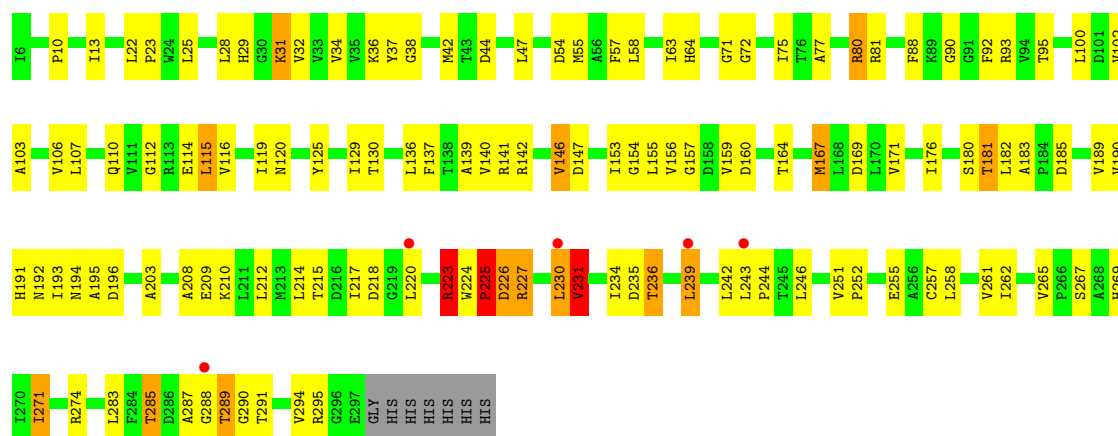
- Molecule 1: acetylglutamate kinase



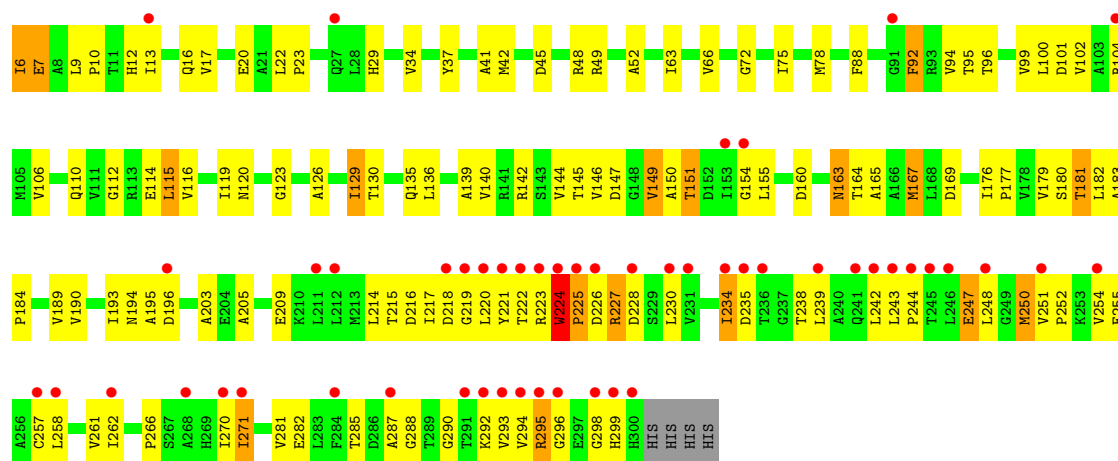




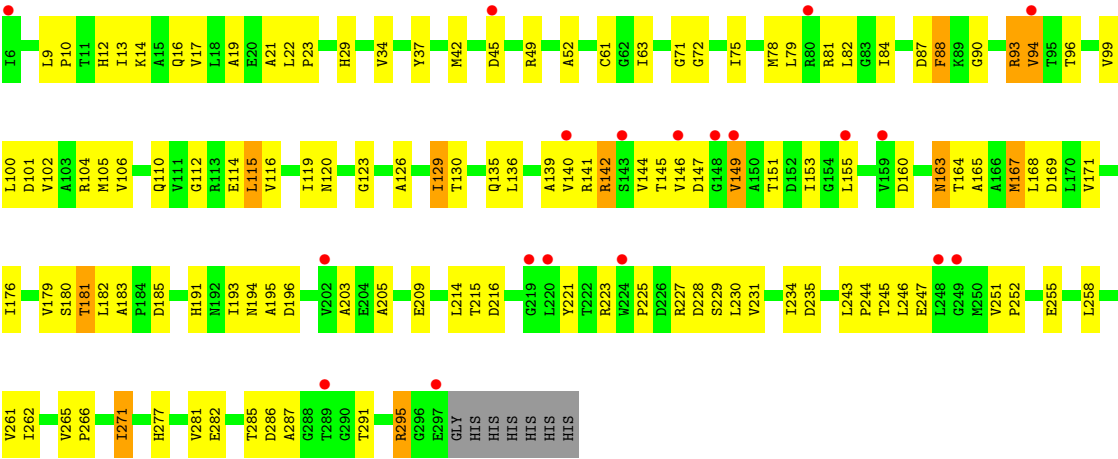
• Molecule 1: acetylglutamate kinase



• Molecule 1: acetylglutamate kinase



• Molecule 1: acetylglutamate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.02Å 123.00Å 194.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.80 48.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.9 (48.80-2.80) 93.7 (48.80-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.258 , 0.284 0.267 , 0.288	Depositor DCC
$R_{free}$ test set	4582 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.7	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: NI, 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	0.29	0/2253	0.60	1/3058 (0.0%)
1	B	0.28	0/2182	0.60	2/2963 (0.1%)
1	C	0.28	0/2182	0.75	4/2963 (0.1%)
1	D	0.28	0/2182	0.71	7/2963 (0.2%)
1	E	0.28	0/2208	0.64	4/2998 (0.1%)
1	F	0.28	0/2182	0.63	1/2963 (0.0%)
All	All	0.28	0/13189	0.65	19/17908 (0.1%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	TRP	C-N-CD	-19.46	77.79	120.60
1	C	224	TRP	C-N-CA	13.74	179.73	122.00
1	A	146	VAL	N-CA-C	-8.79	87.25	111.00
1	E	228	ASP	N-CA-C	8.08	132.81	111.00
1	E	226	ASP	N-CA-C	7.66	131.69	111.00

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	2221	0	2250	98	0
1	B	2156	0	2205	87	0
1	C	2156	0	2205	84	0
1	D	2156	0	2205	93	0
1	E	2180	0	2222	96	0
1	F	2156	0	2205	95	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
4	A	34	0	0	3	0
4	B	24	0	0	7	0
4	C	13	0	0	1	0
4	D	17	0	0	0	0
4	E	15	0	0	2	0
4	F	10	0	0	1	0
All	All	13141	0	13292	532	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 20.

The worst 5 of 532 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:218:ASP:HB3	4:A:1034:HOH:O	1.57	1.02
1:E:48:ARG:HD3	4:E:305:HOH:O	1.63	0.99
1:B:72:GLY:H	1:B:75:ILE:HD13	1.30	0.97
1:A:236:THR:HG21	1:A:262:ILE:HD11	1.45	0.96
1:E:72:GLY:H	1:E:75:ILE:HD13	1.30	0.96

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	297/299 (99%)	264 (89%)	27 (9%)	6 (2%)	7	24
1	B	290/299 (97%)	250 (86%)	31 (11%)	9 (3%)	4	14
1	C	290/299 (97%)	258 (89%)	27 (9%)	5 (2%)	9	29
1	D	290/299 (97%)	250 (86%)	32 (11%)	8 (3%)	5	17
1	E	293/299 (98%)	251 (86%)	34 (12%)	8 (3%)	5	17
1	F	290/299 (97%)	255 (88%)	30 (10%)	5 (2%)	9	29
All	All	1750/1794 (98%)	1528 (87%)	181 (10%)	41 (2%)	6	21

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	VAL
1	A	149	VAL
1	A	181	THR
1	B	181	THR
1	B	224	TRP

### 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	232/225 (103%)	217 (94%)	15 (6%)	17	44
1	B	226/225 (100%)	214 (95%)	12 (5%)	22	54
1	C	226/225 (100%)	213 (94%)	13 (6%)	20	50
1	D	226/225 (100%)	210 (93%)	16 (7%)	14	39
1	E	228/225 (101%)	213 (93%)	15 (7%)	16	44
1	F	226/225 (100%)	212 (94%)	14 (6%)	18	47
All	All	1364/1350 (101%)	1279 (94%)	85 (6%)	18	47

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	271	ILE

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Mol	Chain	Res	Type
1	D	167	MSE
1	F	163	ASN
1	C	295	ARG
1	D	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	163	ASN
1	D	40	ASN
1	F	16	GLN
1	B	163	ASN
1	F	163	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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	292/299 (97%)	0.33	15 (5%) 28 19	53, 74, 117, 135	0
1	B	285/299 (95%)	0.37	10 (3%) 44 34	51, 73, 111, 133	0
1	C	285/299 (95%)	0.55	25 (8%) 10 5	49, 76, 119, 135	0
1	D	285/299 (95%)	0.21	5 (1%) 68 61	49, 70, 121, 140	0
1	E	288/299 (96%)	0.92	51 (17%) 1 1	52, 81, 134, 146	0
1	F	285/299 (95%)	0.52	19 (6%) 17 10	53, 78, 129, 142	0
All	All	1720/1794 (95%)	0.48	125 (7%) 15 8	49, 75, 125, 146	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	299	HIS	6.8
1	A	149	VAL	6.0
1	E	220	LEU	5.9
1	E	239	LEU	5.9
1	E	254	VAL	5.8

### 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	D	1001	1/1	0.44	0.37	99,99,99,99	0
2	MG	A	1002	1/1	0.81	0.25	59,59,59,59	0
3	NI	A	1003	1/1	0.85	0.44	90,90,90,90	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.