



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1X9J  
Title : Structure of butyrate kinase 2 reveals both open- and citrate-induced closed conformations: implications for substrate-induced fit conformational changes  
Authors : Diao, J.S.; Sanders, D.A.; Hasson, M.S.  
Deposited on : 2004-08-21  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

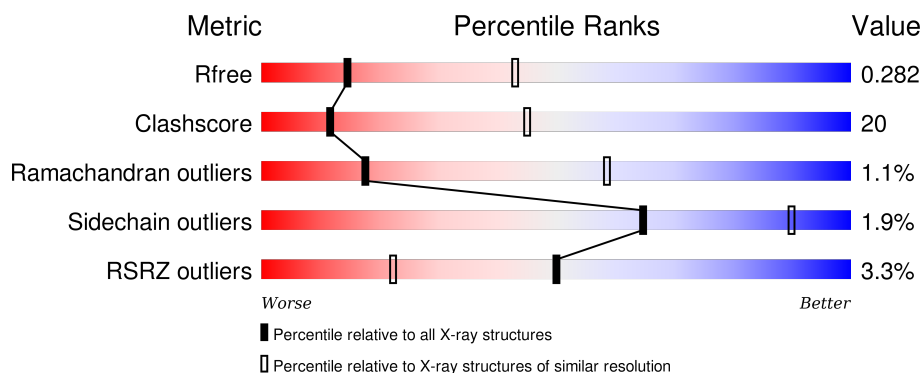
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	375	<div> <div>4%</div> <div>60%</div> <div>38%</div> <div>..</div> </div>
1	B	375	<div> <div>3%</div> <div>59%</div> <div>39%</div> <div>..</div> </div>
1	C	375	<div> <div>3%</div> <div>61%</div> <div>37%</div> <div>..</div> </div>
1	D	375	<div> <div>4%</div> <div>58%</div> <div>40%</div> <div>..</div> </div>
1	E	375	<div> <div>%</div> <div>58%</div> <div>38%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	375	
1	G	375	
1	H	375	

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
5	GOL	A	395	-	X	-	X
5	GOL	B	394	-	X	-	-
5	GOL	C	392	-	X	-	X
5	GOL	D	393	-	X	-	-
5	GOL	F	391	-	X	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23615 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 Probable butyrate kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	B	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	C	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	D	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	E	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	F	372	Total	C	N	O	S	0	0	0
			2931	1860	520	538	13			
1	G	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	H	372	Total	C	N	O	S	0	0	0
			2931	1860	520	538	13			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

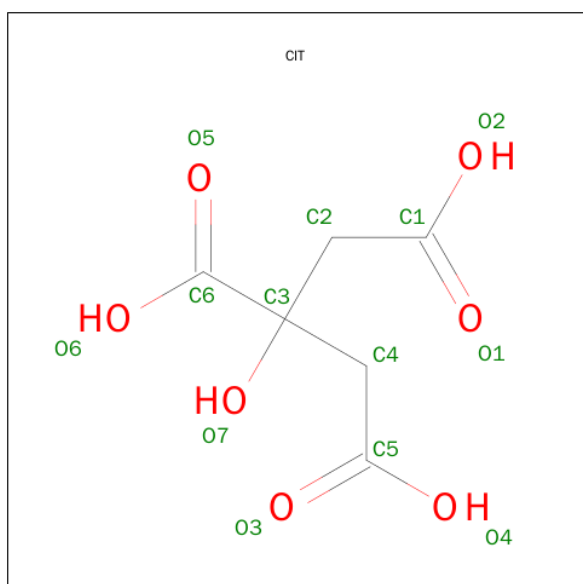
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



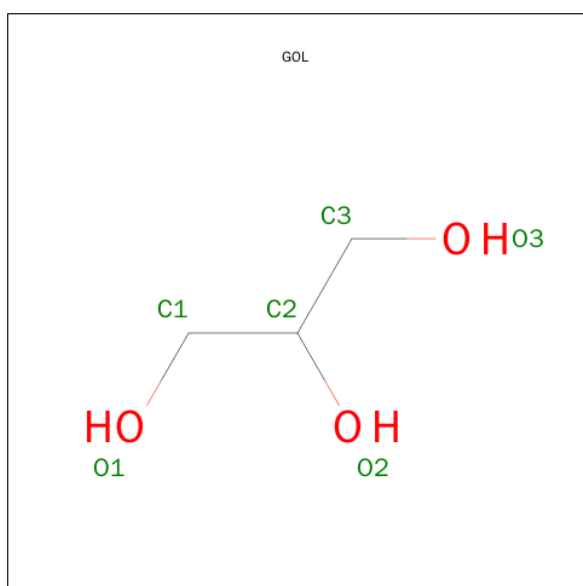
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 13 6 7	0	0
4	G	1	Total C O 13 6 7	0	0
4	G	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0

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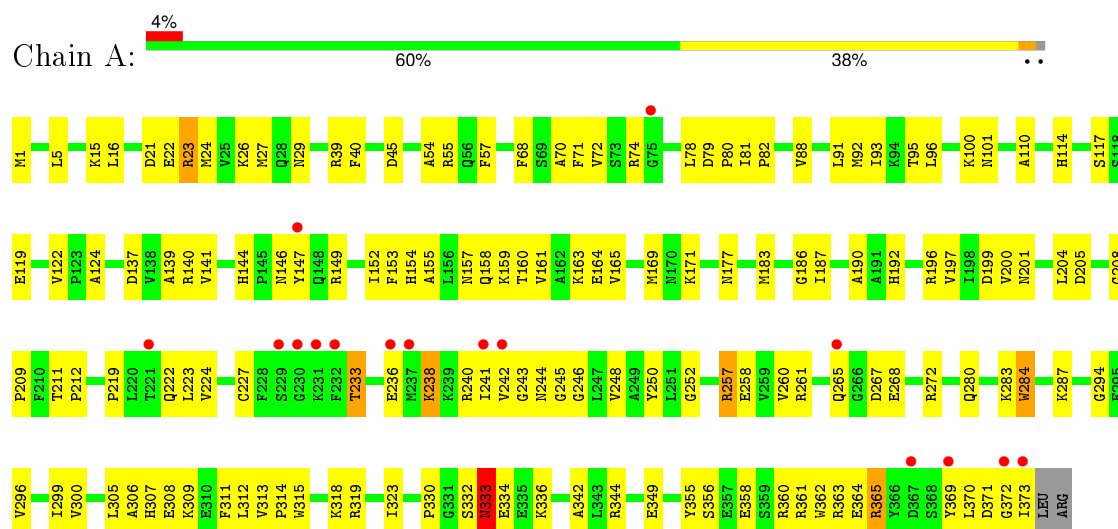
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	7	Total 7	O 7	0	0
6	C	5	Total 5	O 5	0	0
6	D	10	Total 10	O 10	0	0
6	E	4	Total 4	O 4	0	0
6	F	3	Total 3	O 3	0	0
6	G	8	Total 8	O 8	0	0
6	H	2	Total 2	O 2	0	0

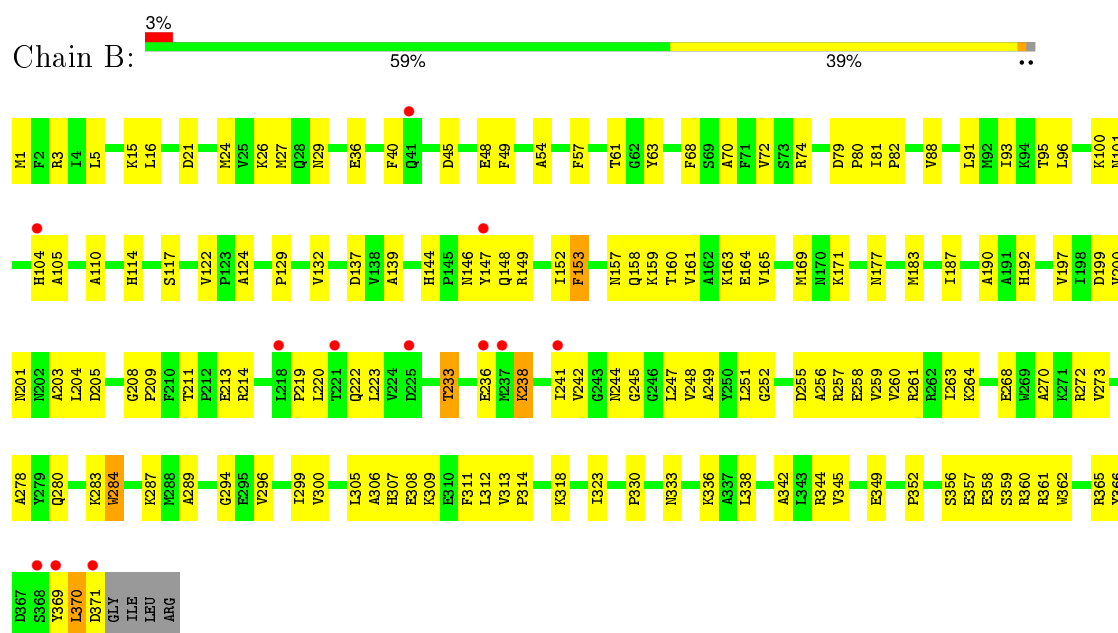
### 3 Residue-property plots

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.

- Molecule 1: Probable butyrate kinase 2

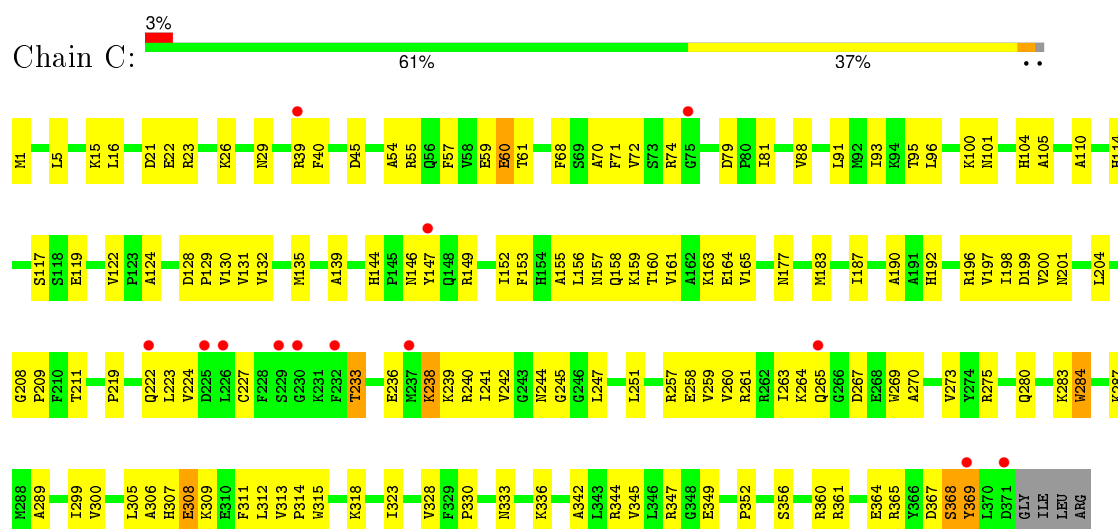


- Molecule 1: Probable butyrate kinase 2

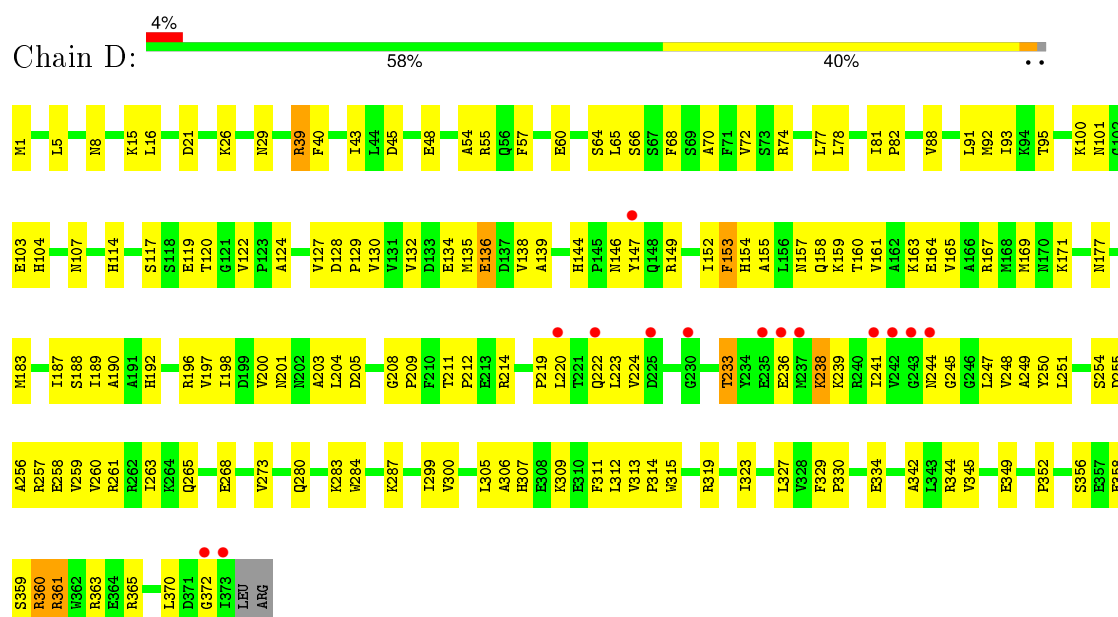


- Molecule 1: Probable butyrate kinase 2

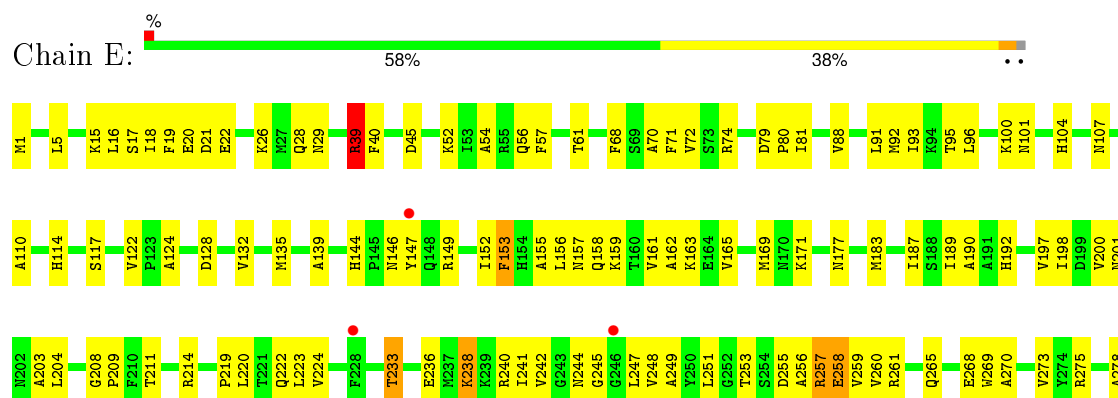


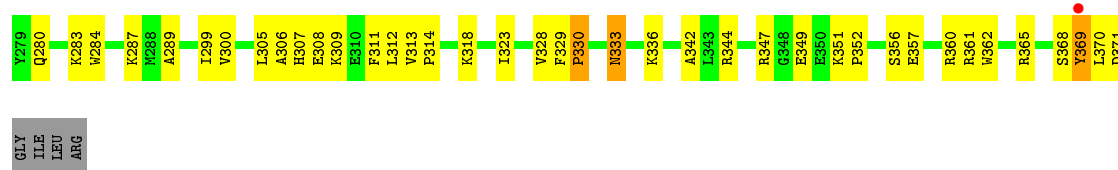


- Molecule 1: Probable butyrate kinase 2

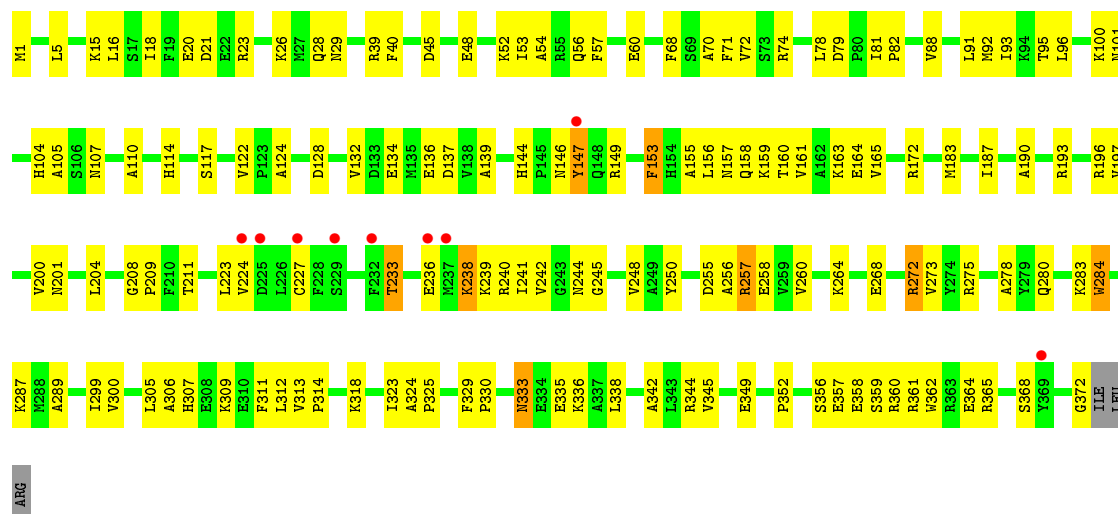


- Molecule 1: Probable butyrate kinase 2

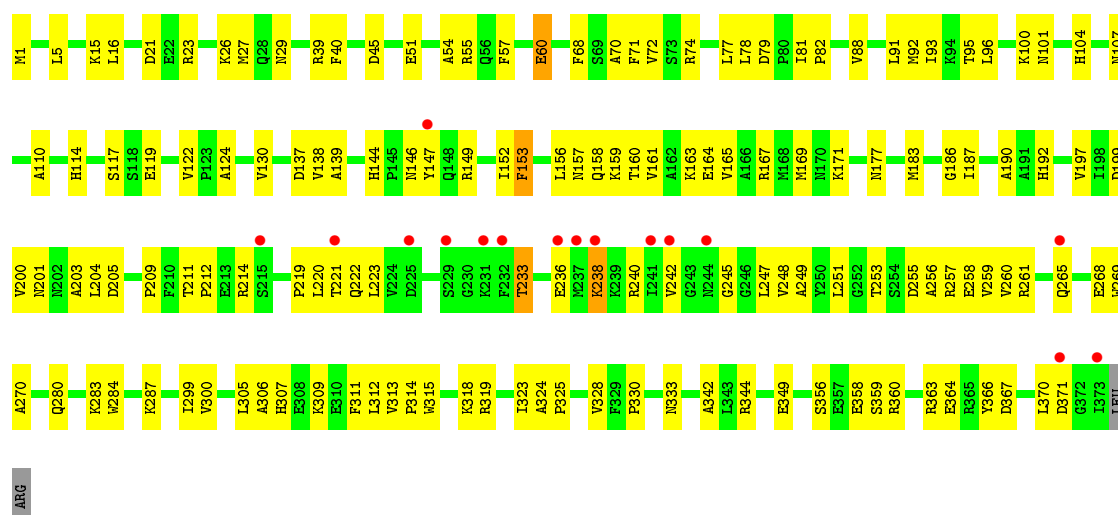




- Molecule 1: Probable butyrate kinase 2



- Molecule 1: Probable butyrate kinase 2



- Molecule 1: Probable butyrate kinase 2



R363	R364	R365	Y366	Y369	L370	E371	G372	ILE	LEU	ARG	M1	L5	N8	K15	L16	D21	E22	R23	K26	N29	R39	K42	I43	L44	D45	A54	R55	Q56	F57	V58	E59	E60	T61	F68	S69	A70	F71	V72	S73	R74	Q75	L78	D79	P80	I81	V88	L91	M92	I93	K94	T95	L96	K100	N101	H104							
											A105	A110	H114	S117	V122	P123	A124	D128	P129	V132	D133	E134	M135	E136	D137	V138	A139	R140	H144	P145	N146	Y147	Q148	R149	I152	F153	H154	A155	L156	M157	Q158	K159	T160	V161	A162	K163	E164	V165	A166	R167	M177	M183	I187	A190	A191	H192	V197					
											I198	D199	V200	N201	L204	G208	P209	F210	T211	P212	E213	R214	L220	T221	Q222	L223	V224	D225	L226	C227	K231	F232	T233	E236	M237	K238	K239	R240	I241	V242	G243	N244	G245	G246	L247	V248	A249	Y250	L251	A256	R257	E258	V259	V260	I263	K264	E268	W269	A270	R271	R272	V273
											A278	Y279	Q280	K283	W284	K287	W288	A289	I299	V300	L301	T302	L305	A306	H307	E308	K309	E310	F311	L312	V313	P314	K318	I323	F329	P330	N333	E334	E335	K336	A337	L338	A342	L343	R344	V345	L346	R347	G348	E349	P352	S356	E357	E358	S359	R360	R361	W362				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.68Å 193.68Å 122.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.48 – 3.00 96.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (91.48-3.00) 79.0 (96.84-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.261 , 0.284 0.260 , 0.282	Depositor DCC
$R_{free}$ test set	8832 reflections (10.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 29.4	EDS
Estimated twinning fraction	0.278 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	5 of 98195 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.69 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2748e-04.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: GOL, PO4, CIT, NA

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	0.31	0/2997	0.54	0/4036
1	B	0.30	0/2985	0.55	0/4020
1	C	0.29	0/2985	0.53	0/4020
1	D	0.32	0/2997	0.66	3/4036 (0.1%)
1	E	0.31	0/2985	0.60	3/4020 (0.1%)
1	F	0.33	0/2989	0.67	3/4025 (0.1%)
1	G	0.30	0/2997	0.53	0/4036
1	H	0.31	0/2989	0.62	2/4025 (0.0%)
All	All	0.31	0/23924	0.59	11/32218 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	360	ARG	NE-CZ-NH1	-16.16	112.22	120.30
1	F	272	ARG	NE-CZ-NH1	-15.89	112.35	120.30
1	D	360	ARG	NE-CZ-NH2	15.62	128.11	120.30
1	F	272	ARG	NE-CZ-NH2	15.51	128.05	120.30
1	E	39	ARG	NE-CZ-NH1	-11.90	114.35	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2939	0	2969	119	0
1	B	2927	0	2955	132	0
1	C	2927	0	2955	128	0
1	D	2939	0	2969	136	0
1	E	2927	0	2955	139	0
1	F	2931	0	2958	123	0
1	G	2939	0	2969	126	0
1	H	2931	0	2958	134	0
2	D	1	0	0	0	0
3	B	5	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
4	D	26	0	10	3	0
4	G	26	0	10	0	0
5	A	6	0	4	0	0
5	B	6	0	4	0	0
5	C	6	0	4	0	0
5	D	6	0	4	0	0
5	F	6	0	4	0	0
6	A	8	0	0	1	0
6	B	7	0	0	1	0
6	C	5	0	0	0	0
6	D	10	0	0	0	0
6	E	4	0	0	0	0
6	F	3	0	0	0	0
6	G	8	0	0	0	0
6	H	2	0	0	0	0
All	All	23615	0	23728	962	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 962 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:88:VAL:HG12	1:A:93:ILE:HD11	1.43	1.00
1:A:257:ARG:HH11	1:A:257:ARG:HB3	1.35	0.91
1:D:88:VAL:HG12	1:D:93:ILE:HD11	1.53	0.90
1:H:344:ARG:HG3	1:H:349:GLU:HB2	1.53	0.90
1:B:88:VAL:HG12	1:B:93:ILE:HD11	1.55	0.89

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	371/375 (99%)	325 (88%)	39 (10%)	7 (2%)	10	43
1	B	369/375 (98%)	326 (88%)	39 (11%)	4 (1%)	17	58
1	C	369/375 (98%)	325 (88%)	38 (10%)	6 (2%)	12	48
1	D	371/375 (99%)	327 (88%)	41 (11%)	3 (1%)	24	66
1	E	369/375 (98%)	325 (88%)	40 (11%)	4 (1%)	17	58
1	F	370/375 (99%)	325 (88%)	43 (12%)	2 (0%)	34	76
1	G	371/375 (99%)	322 (87%)	45 (12%)	4 (1%)	17	58
1	H	370/375 (99%)	326 (88%)	41 (11%)	3 (1%)	24	66
All	All	2960/3000 (99%)	2601 (88%)	326 (11%)	33 (1%)	17	58

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	370	LEU
1	H	60	GLU
1	A	39	ARG
1	A	243	GLY
1	C	245	GLY

### 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	313/315 (99%)	306 (98%)	7 (2%)	60	88
1	B	312/315 (99%)	307 (98%)	5 (2%)	70	92
1	C	312/315 (99%)	308 (99%)	4 (1%)	76	93
1	D	313/315 (99%)	307 (98%)	6 (2%)	65	90
1	E	312/315 (99%)	306 (98%)	6 (2%)	65	90
1	F	312/315 (99%)	303 (97%)	9 (3%)	50	84
1	G	313/315 (99%)	308 (98%)	5 (2%)	70	92
1	H	312/315 (99%)	306 (98%)	6 (2%)	65	90
All	All	2499/2520 (99%)	2451 (98%)	48 (2%)	65	90

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	361	ARG
1	E	333	ASN
1	H	238	LYS
1	E	153	PHE
1	E	257	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	222	GLN
1	E	222	GLN
1	H	114	HIS
1	E	56	GLN
1	E	265	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is 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	GOL	A	395	-	5,5,5	4.67	5 (100%)	5,5,5	5.38	4 (80%)
5	GOL	B	394	-	5,5,5	4.70	5 (100%)	5,5,5	5.38	4 (80%)
3	PO4	B	402	-	4,4,4	0.73	0	6,6,6	0.30	0
5	GOL	C	392	-	5,5,5	4.67	5 (100%)	5,5,5	5.38	4 (80%)
4	CIT	D	381	-	3,12,12	2.68	1 (33%)	3,17,17	3.36	2 (66%)
4	CIT	D	384	-	3,12,12	2.78	1 (33%)	3,17,17	2.62	2 (66%)
5	GOL	D	393	-	5,5,5	4.77	5 (100%)	5,5,5	5.54	4 (80%)
3	PO4	E	401	-	4,4,4	0.70	0	6,6,6	0.30	0
3	PO4	E	405	-	4,4,4	0.72	0	6,6,6	0.30	0
5	GOL	F	391	-	5,5,5	4.65	5 (100%)	5,5,5	5.29	4 (80%)
3	PO4	F	403	-	4,4,4	0.73	0	6,6,6	0.30	0
4	CIT	G	382	-	3,12,12	2.59	1 (33%)	3,17,17	3.18	2 (66%)
4	CIT	G	383	-	3,12,12	2.72	1 (33%)	3,17,17	2.80	2 (66%)
3	PO4	H	404	-	4,4,4	0.75	0	6,6,6	0.30	0

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	GOL	A	395	-	-	0/4/4/4	0/0/0/0
5	GOL	B	394	-	-	0/4/4/4	0/0/0/0
3	PO4	B	402	-	-	0/0/0/0	0/0/0/0
5	GOL	C	392	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	D	381	-	-	0/6/16/16	0/0/0/0
4	CIT	D	384	-	-	0/6/16/16	0/0/0/0
5	GOL	D	393	-	-	0/4/4/4	0/0/0/0
3	PO4	E	401	-	-	0/0/0/0	0/0/0/0
3	PO4	E	405	-	-	0/0/0/0	0/0/0/0
5	GOL	F	391	-	-	0/4/4/4	0/0/0/0
3	PO4	F	403	-	-	0/0/0/0	0/0/0/0
4	CIT	G	382	-	-	0/6/16/16	0/0/0/0
4	CIT	G	383	-	-	0/6/16/16	0/0/0/0
3	PO4	H	404	-	-	0/0/0/0	0/0/0/0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	393	GOL	C3-C2	-7.84	1.22	1.52
5	A	395	GOL	C3-C2	-7.63	1.23	1.52
5	C	392	GOL	C3-C2	-7.58	1.23	1.52
5	B	394	GOL	C3-C2	-7.58	1.23	1.52
5	F	391	GOL	C3-C2	-7.56	1.23	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	393	GOL	C3-C2-C1	-2.81	100.10	111.12
5	A	395	GOL	C3-C2-C1	-2.54	101.15	111.12
5	F	391	GOL	C3-C2-C1	-2.48	101.39	111.12
5	B	394	GOL	C3-C2-C1	-2.48	101.41	111.12
5	C	392	GOL	C3-C2-C1	-2.44	101.56	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	381	CIT	3	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 ⓘ

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	373/375 (99%)	0.12	16 (4%)	39 16	14, 49, 111, 139	0
1	B	371/375 (98%)	0.24	12 (3%)	51 23	10, 52, 117, 136	0
1	C	371/375 (98%)	0.17	13 (3%)	48 21	15, 47, 105, 138	0
1	D	373/375 (99%)	0.11	14 (3%)	44 18	18, 39, 109, 140	0
1	E	371/375 (98%)	0.03	4 (1%)	82 58	20, 43, 101, 135	0
1	F	372/375 (99%)	0.10	9 (2%)	62 32	23, 49, 105, 143	0
1	G	373/375 (99%)	0.15	16 (4%)	39 16	23, 46, 113, 142	0
1	H	372/375 (99%)	0.18	14 (3%)	44 18	21, 54, 117, 146	0
All	All	2976/3000 (99%)	0.14	98 (3%)	50 22	10, 48, 111, 146	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	242	VAL	8.4
1	A	373	ILE	7.5
1	B	237	MET	5.9
1	G	229	SER	5.8
1	D	373	ILE	5.5

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	C	392	6/6	0.64	0.42	4.02	40,43,44,44	0
5	GOL	A	395	6/6	0.32	0.46	3.57	68,71,71,71	0
5	GOL	F	391	6/6	0.67	0.34	2.24	56,58,59,59	0
4	CIT	D	384	13/13	0.62	0.32	1.89	89,91,92,92	0
4	CIT	G	383	13/13	0.62	0.37	1.34	88,92,95,96	0
4	CIT	D	381	13/13	0.51	0.31	1.26	78,80,81,81	0
4	CIT	G	382	13/13	0.70	0.31	1.13	67,68,69,70	0
3	PO4	E	405	5/5	0.81	0.25	0.80	97,98,98,99	0
5	GOL	D	393	6/6	0.75	0.27	0.41	43,44,46,49	0
3	PO4	E	401	5/5	0.91	0.23	0.38	76,76,77,78	0
5	GOL	B	394	6/6	0.75	0.27	0.23	54,54,55,55	0
3	PO4	F	403	5/5	0.82	0.22	0.10	98,99,99,100	0
3	PO4	B	402	5/5	0.91	0.21	-0.13	83,83,83,84	0
3	PO4	H	404	5/5	0.87	0.20	-0.44	76,77,78,78	0
2	NA	D	380	1/1	0.92	0.09	-3.87	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.