wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 06:33 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

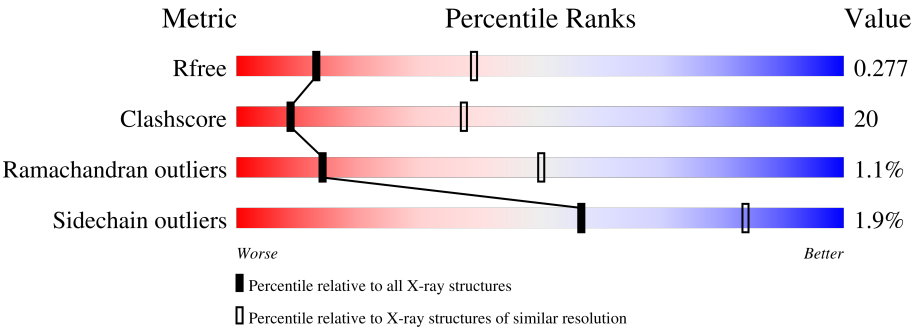
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	375	60% 38%
1	B	375	59% 39%
1	C	375	61% 37%
1	D	375	58% 40%
1	E	375	58% 38%
1	F	375	60% 37%
1	G	375	61% 38%

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Mol	Chain	Length	Quality of chain
1	H	375	59% 39%

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
2	GOL	A	395	-	X	-	-
2	GOL	B	394	-	X	-	-
2	GOL	C	392	-	X	-	-
2	GOL	D	393	-	X	-	-
2	GOL	F	391	-	X	-	-
5	CIT	D	381	-	X	-	-
5	CIT	D	384	-	X	-	-
5	CIT	G	382	-	X	-	-
5	CIT	G	383	-	X	-	-

2 Entry composition (i)

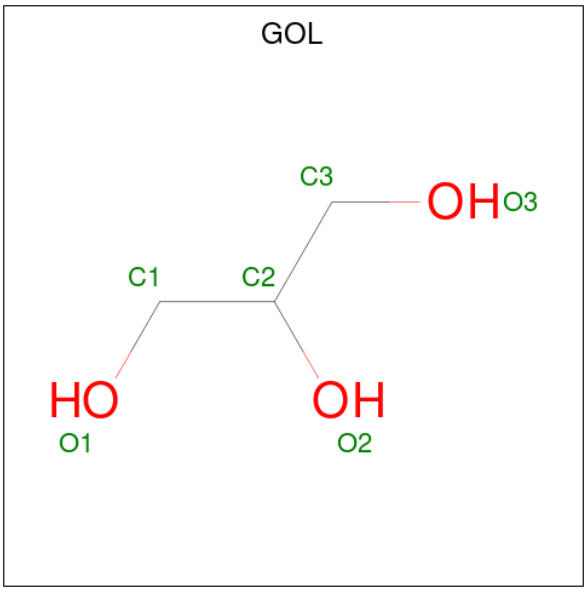
There are 6 unique types of molecules in this entry. The entry contains 23615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

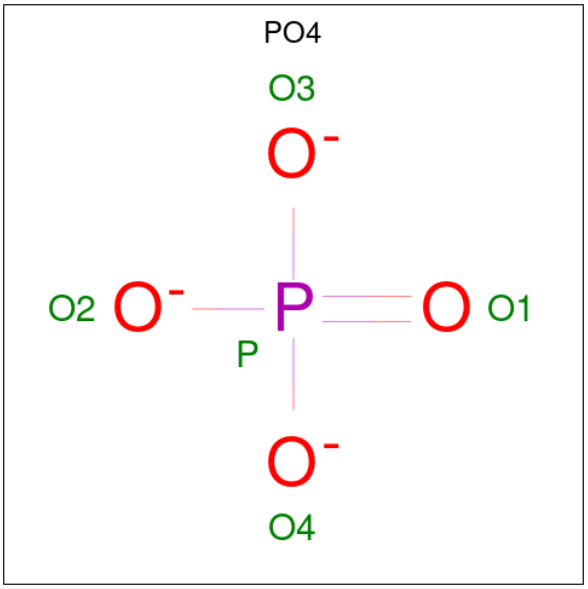
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	B	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	C	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	D	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	E	371	Total	C	N	O	S	0	0	0
			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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

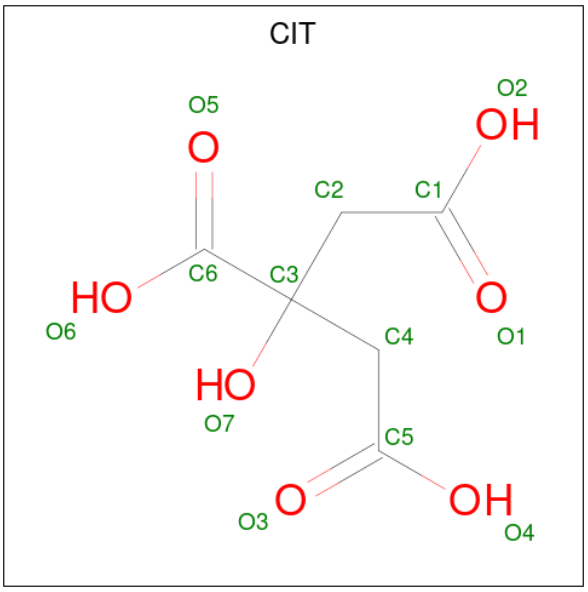


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 6 is water.

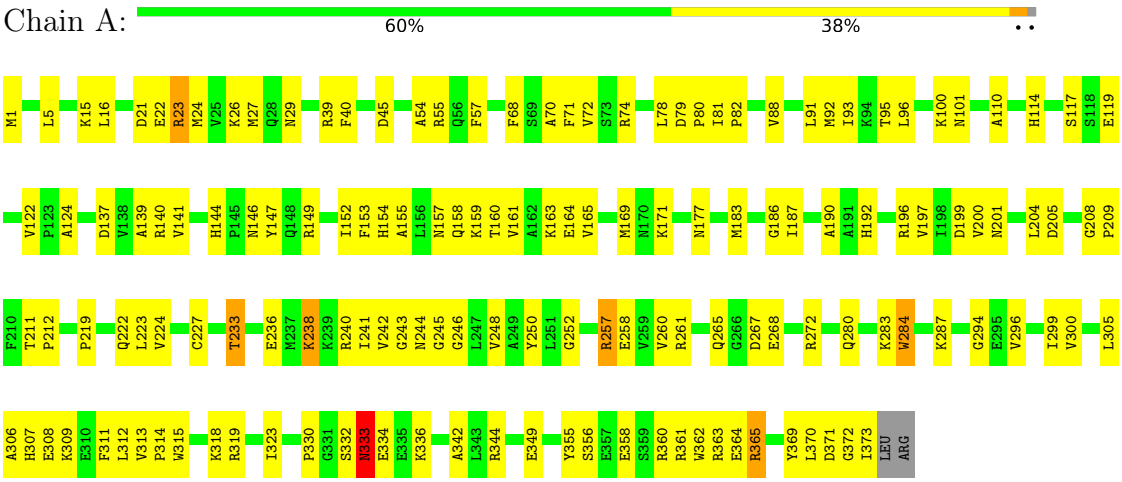
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	7	Total O 7 7	0	0
6	C	5	Total O 5 5	0	0
6	D	10	Total O 10 10	0	0
6	E	4	Total O 4 4	0	0
6	F	3	Total O 3 3	0	0
6	G	8	Total O 8 8	0	0
6	H	2	Total O 2 2	0	0

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.

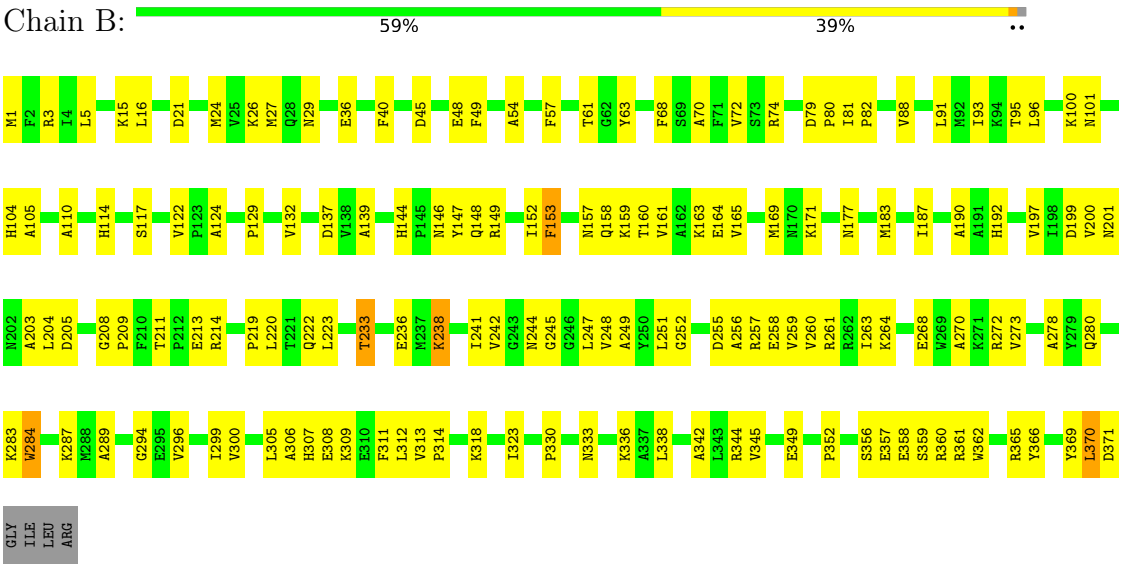
• Molecule 1: Probable butyrate kinase 2

Chain A:



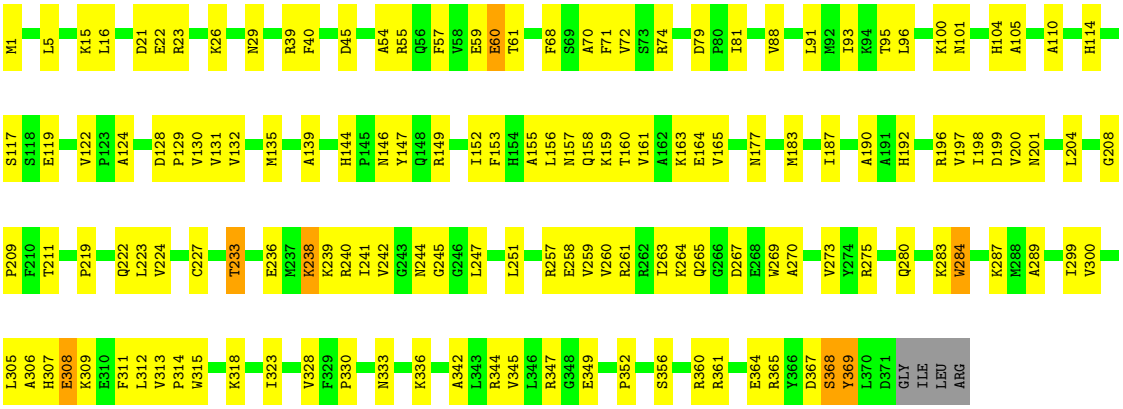
• Molecule 1: Probable butyrate kinase 2

Chain B:



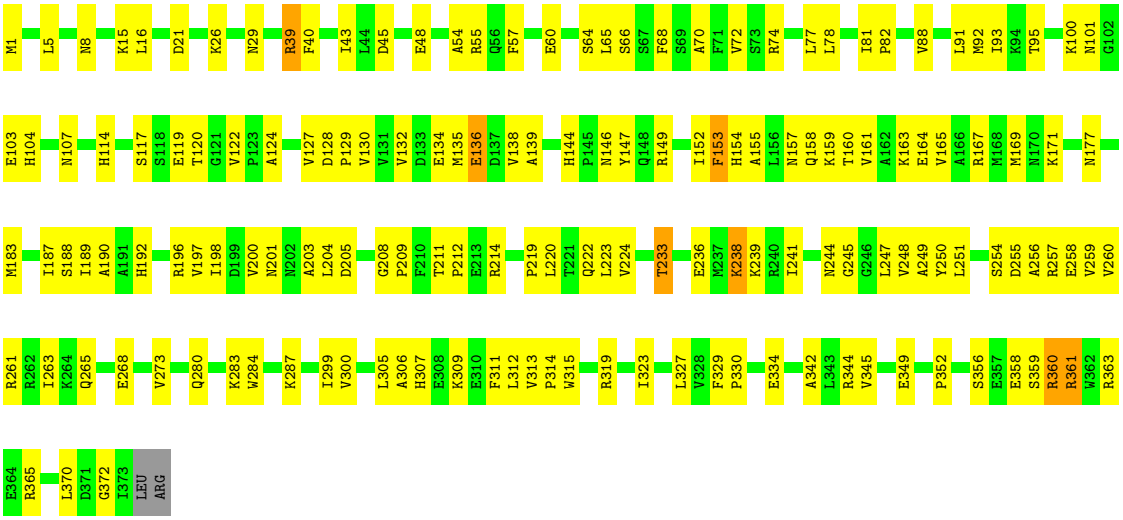
• Molecule 1: Probable butyrate kinase 2

Chain C:



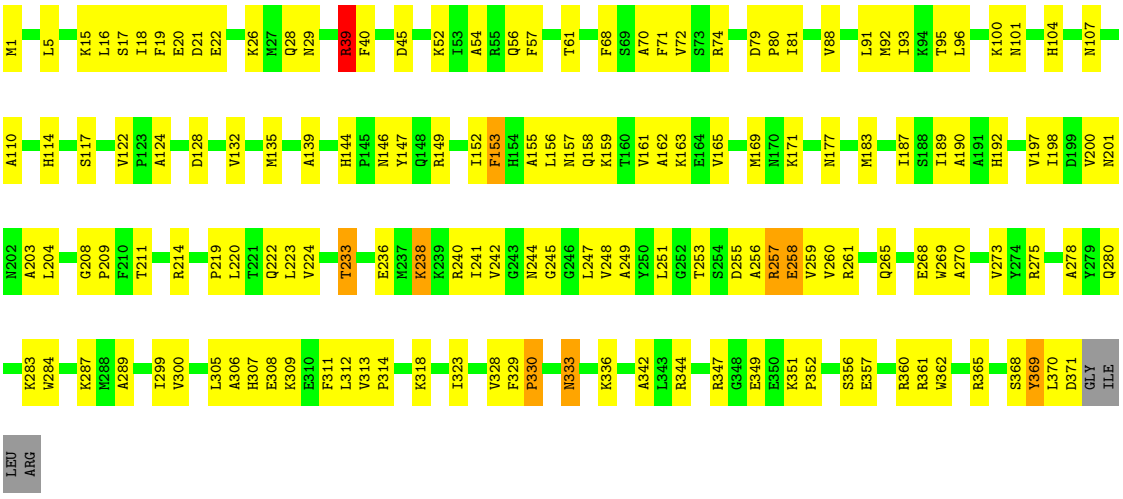
• Molecule 1: Probable butyrate kinase 2

Chain D:



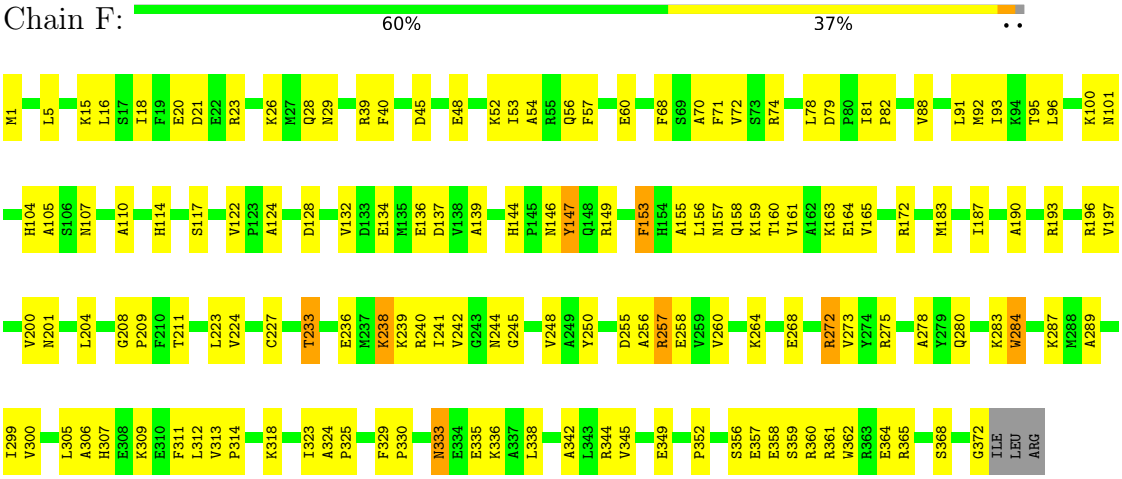
• Molecule 1: Probable butyrate kinase 2

Chain E:



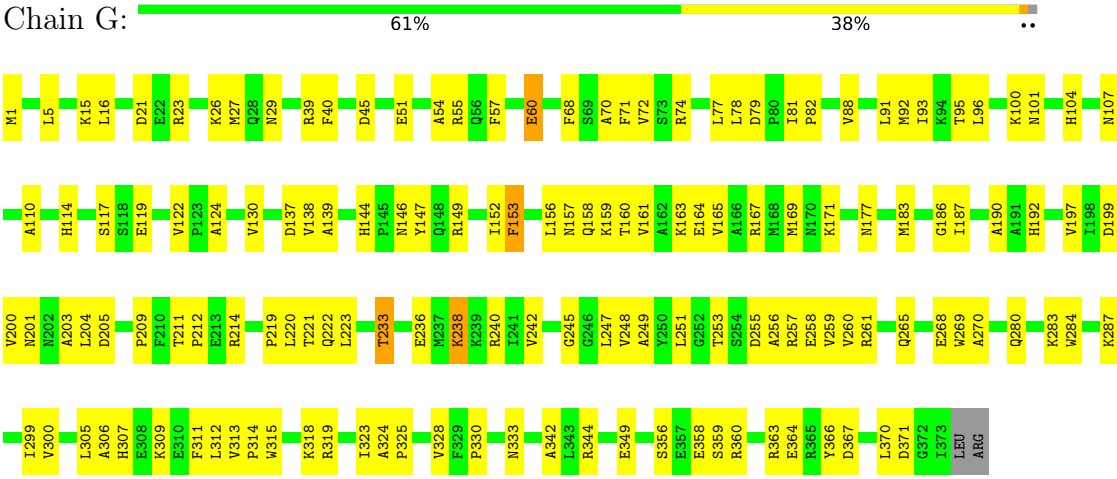
• Molecule 1: Probable butyrate kinase 2

Chain F:



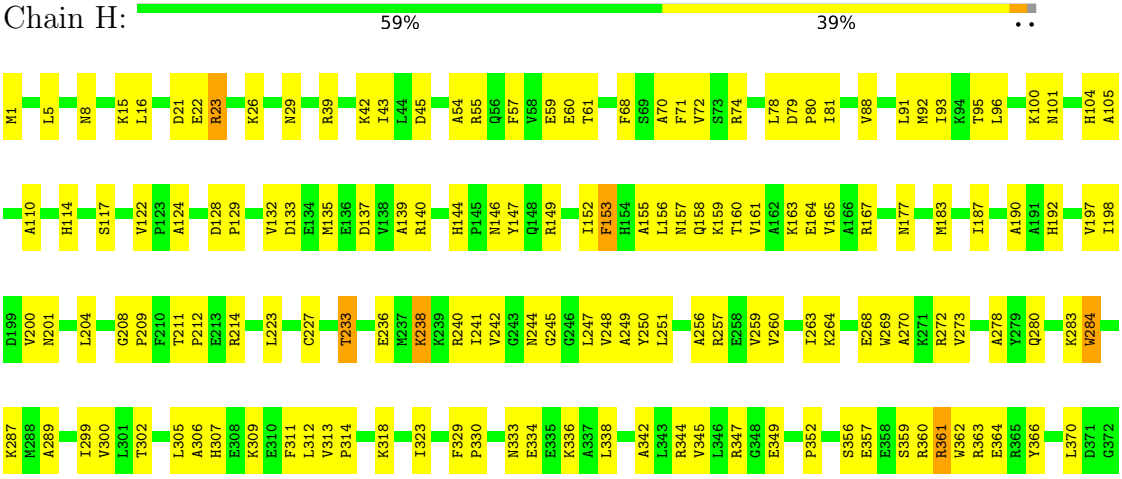
• Molecule 1: Probable butyrate kinase 2

Chain G:



• Molecule 1: Probable butyrate kinase 2

Chain H:




ILE
LEU
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.25 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.261 , 0.284 0.256 , 0.277	Depositor DCC
R_{free} test set	8832 reflections (8.99%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 29.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.278 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23615	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, CIT, PO4, GOL

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(^{o})	Ideal(^{o})
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

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	A	6	0	4	0	0
2	B	6	0	4	0	0
2	C	6	0	4	0	0
2	D	6	0	4	0	0
2	F	6	0	4	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	1	0	0	0	0
5	D	26	0	10	3	0
5	G	26	0	10	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:HB3	1:A:257:ARG:HH11	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%)	8 36
1	B	369/375 (98%)	326 (88%)	39 (11%)	4 (1%)	14 50
1	C	369/375 (98%)	325 (88%)	38 (10%)	6 (2%)	9 40
1	D	371/375 (99%)	327 (88%)	41 (11%)	3 (1%)	19 57
1	E	369/375 (98%)	325 (88%)	40 (11%)	4 (1%)	14 50
1	F	370/375 (99%)	325 (88%)	43 (12%)	2 (0%)	29 68
1	G	371/375 (99%)	322 (87%)	45 (12%)	4 (1%)	14 50
1	H	370/375 (99%)	326 (88%)	41 (11%)	3 (1%)	19 57
All	All	2960/3000 (99%)	2601 (88%)	326 (11%)	33 (1%)	14 50

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%)	52	81
1	B	312/315 (99%)	307 (98%)	5 (2%)	62	86
1	C	312/315 (99%)	308 (99%)	4 (1%)	69	89
1	D	313/315 (99%)	307 (98%)	6 (2%)	57	84
1	E	312/315 (99%)	306 (98%)	6 (2%)	57	84
1	F	312/315 (99%)	303 (97%)	9 (3%)	42	76
1	G	313/315 (99%)	308 (98%)	5 (2%)	62	86
1	H	312/315 (99%)	306 (98%)	6 (2%)	57	84
All	All	2499/2520 (99%)	2451 (98%)	48 (2%)	57	84

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

Mol	Chain	Res	Type
1	F	23	ARG
1	F	284	TRP
1	F	137	ASP
1	F	172	ARG
1	G	60	GLU

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

Mol	Chain	Res	Type
1	E	333	ASN
1	G	56	GLN
1	F	114	HIS
1	F	222	GLN
1	G	222	GLN

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 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	$\#\|Z\| > 2$
2	GOL	F	391	-	5,5,5	4.39	5 (100%)	5,5,5	5.37	4 (80%)
5	CIT	G	382	-	12,12,12	1.77	4 (33%)	17,17,17	3.34	9 (52%)
3	PO4	E	405	-	4,4,4	1.39	1 (25%)	6,6,6	0.86	0
3	PO4	H	404	-	4,4,4	1.44	1 (25%)	6,6,6	0.85	0
2	GOL	B	394	-	5,5,5	4.45	5 (100%)	5,5,5	5.46	4 (80%)
5	CIT	D	381	-	12,12,12	1.79	4 (33%)	17,17,17	3.03	9 (52%)
2	GOL	C	392	-	5,5,5	4.42	5 (100%)	5,5,5	5.46	4 (80%)
3	PO4	B	402	-	4,4,4	1.38	1 (25%)	6,6,6	0.86	0
3	PO4	E	401	-	4,4,4	1.35	1 (25%)	6,6,6	0.89	0
3	PO4	F	403	-	4,4,4	1.39	1 (25%)	6,6,6	0.85	0
2	GOL	D	393	-	5,5,5	4.52	5 (100%)	5,5,5	5.63	4 (80%)
5	CIT	G	383	-	12,12,12	1.85	5 (41%)	17,17,17	3.26	8 (47%)
2	GOL	A	395	-	5,5,5	4.42	5 (100%)	5,5,5	5.46	4 (80%)
5	CIT	D	384	-	12,12,12	1.81	4 (33%)	17,17,17	3.21	8 (47%)

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
2	GOL	F	391	-	-	2/4/4/4	-
5	CIT	G	382	-	-	10/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	394	-	-	2/4/4/4	-
5	CIT	D	381	-	-	6/16/16/16	-
2	GOL	C	392	-	-	3/4/4/4	-
2	GOL	D	393	-	-	3/4/4/4	-
5	CIT	G	383	-	-	7/16/16/16	-
2	GOL	A	395	-	-	4/4/4/4	-
5	CIT	D	384	-	-	7/16/16/16	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	393	GOL	C3-C2	-7.13	1.22	1.51
2	A	395	GOL	C3-C2	-6.94	1.23	1.51
2	C	392	GOL	C3-C2	-6.90	1.23	1.51
2	B	394	GOL	C3-C2	-6.90	1.23	1.51
2	F	391	GOL	C3-C2	-6.87	1.23	1.51

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	393	GOL	O3-C3-C2	10.70	161.50	110.20
2	C	392	GOL	O3-C3-C2	10.59	160.98	110.20
2	B	394	GOL	O3-C3-C2	10.54	160.73	110.20
2	A	395	GOL	O3-C3-C2	10.49	160.50	110.20
2	F	391	GOL	O3-C3-C2	10.40	160.08	110.20

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	395	GOL	O1-C1-C2-C3
2	A	395	GOL	C1-C2-C3-O3
2	B	394	GOL	C1-C2-C3-O3
2	C	392	GOL	C1-C2-C3-O3
2	D	393	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	381	CIT	3	0

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.