



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 11:15 PM EDT

PDB ID : 3DJC
Title : CRYSTAL STRUCTURE OF PANTOTHENATE KINASE FROM LE-
GIONELLA PNEUMOPHILA
Authors : Patskovsky, Y.; Bonanno, J.B.; Romero, R.; Dickey, M.; Logan, C.; Wasser-
man, S.; Maletic, M.; Koss, J.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New
York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-06-23
Resolution : 2.40 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

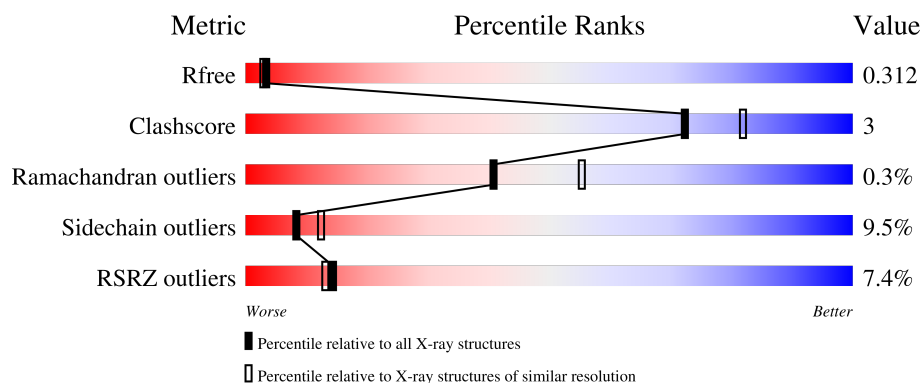
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	266	<div> <div>4%</div> <div>75%</div> <div>18%</div> <div>• •</div> </div>
1	B	266	<div> <div>2%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	C	266	<div> <div>4%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	D	266	<div> <div>3%</div> <div>82%</div> <div>11%</div> <div>• 5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	266	
1	F	266	
1	G	266	
1	H	266	
1	I	266	
1	J	266	
1	K	266	
1	L	266	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23826 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 Type III pantothenate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	5	0
			1967	1256	336	367	8			
1	B	256	Total	C	N	O	S	0	7	0
			1993	1271	346	368	8			
1	C	256	Total	C	N	O	S	0	5	0
			1973	1259	339	367	8			
1	D	254	Total	C	N	O	S	0	6	0
			1962	1251	338	365	8			
1	E	252	Total	C	N	O	S	0	4	0
			1938	1236	333	361	8			
1	F	251	Total	C	N	O	S	0	4	0
			1931	1233	331	359	8			
1	G	256	Total	C	N	O	S	0	2	0
			1960	1250	337	365	8			
1	H	255	Total	C	N	O	S	0	4	0
			1967	1255	339	365	8			
1	I	255	Total	C	N	O	S	0	6	0
			1971	1258	338	367	8			
1	J	250	Total	C	N	O	S	0	5	0
			1941	1238	335	360	8			
1	K	250	Total	C	N	O	S	0	6	0
			1941	1237	336	360	8			
1	L	250	Total	C	N	O	S	0	4	0
			1931	1234	331	358	8			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q5ZX22
A	0	SER	-	expression tag	UNP Q5ZX22
A	1	LEU	-	expression tag	UNP Q5ZX22
A	257	GLU	-	expression tag	UNP Q5ZX22
A	258	GLY	-	expression tag	UNP Q5ZX22

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	HIS	-	expression tag	UNP Q5ZX22
A	260	HIS	-	expression tag	UNP Q5ZX22
A	261	HIS	-	expression tag	UNP Q5ZX22
A	262	HIS	-	expression tag	UNP Q5ZX22
A	263	HIS	-	expression tag	UNP Q5ZX22
A	264	HIS	-	expression tag	UNP Q5ZX22
B	-1	MET	-	expression tag	UNP Q5ZX22
B	0	SER	-	expression tag	UNP Q5ZX22
B	1	LEU	-	expression tag	UNP Q5ZX22
B	257	GLU	-	expression tag	UNP Q5ZX22
B	258	GLY	-	expression tag	UNP Q5ZX22
B	259	HIS	-	expression tag	UNP Q5ZX22
B	260	HIS	-	expression tag	UNP Q5ZX22
B	261	HIS	-	expression tag	UNP Q5ZX22
B	262	HIS	-	expression tag	UNP Q5ZX22
B	263	HIS	-	expression tag	UNP Q5ZX22
B	264	HIS	-	expression tag	UNP Q5ZX22
C	-1	MET	-	expression tag	UNP Q5ZX22
C	0	SER	-	expression tag	UNP Q5ZX22
C	1	LEU	-	expression tag	UNP Q5ZX22
C	257	GLU	-	expression tag	UNP Q5ZX22
C	258	GLY	-	expression tag	UNP Q5ZX22
C	259	HIS	-	expression tag	UNP Q5ZX22
C	260	HIS	-	expression tag	UNP Q5ZX22
C	261	HIS	-	expression tag	UNP Q5ZX22
C	262	HIS	-	expression tag	UNP Q5ZX22
C	263	HIS	-	expression tag	UNP Q5ZX22
C	264	HIS	-	expression tag	UNP Q5ZX22
D	-1	MET	-	expression tag	UNP Q5ZX22
D	0	SER	-	expression tag	UNP Q5ZX22
D	1	LEU	-	expression tag	UNP Q5ZX22
D	257	GLU	-	expression tag	UNP Q5ZX22
D	258	GLY	-	expression tag	UNP Q5ZX22
D	259	HIS	-	expression tag	UNP Q5ZX22
D	260	HIS	-	expression tag	UNP Q5ZX22
D	261	HIS	-	expression tag	UNP Q5ZX22
D	262	HIS	-	expression tag	UNP Q5ZX22
D	263	HIS	-	expression tag	UNP Q5ZX22
D	264	HIS	-	expression tag	UNP Q5ZX22
E	-1	MET	-	expression tag	UNP Q5ZX22
E	0	SER	-	expression tag	UNP Q5ZX22
E	1	LEU	-	expression tag	UNP Q5ZX22

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	257	GLU	-	expression tag	UNP Q5ZX22
E	258	GLY	-	expression tag	UNP Q5ZX22
E	259	HIS	-	expression tag	UNP Q5ZX22
E	260	HIS	-	expression tag	UNP Q5ZX22
E	261	HIS	-	expression tag	UNP Q5ZX22
E	262	HIS	-	expression tag	UNP Q5ZX22
E	263	HIS	-	expression tag	UNP Q5ZX22
E	264	HIS	-	expression tag	UNP Q5ZX22
F	-1	MET	-	expression tag	UNP Q5ZX22
F	0	SER	-	expression tag	UNP Q5ZX22
F	1	LEU	-	expression tag	UNP Q5ZX22
F	257	GLU	-	expression tag	UNP Q5ZX22
F	258	GLY	-	expression tag	UNP Q5ZX22
F	259	HIS	-	expression tag	UNP Q5ZX22
F	260	HIS	-	expression tag	UNP Q5ZX22
F	261	HIS	-	expression tag	UNP Q5ZX22
F	262	HIS	-	expression tag	UNP Q5ZX22
F	263	HIS	-	expression tag	UNP Q5ZX22
F	264	HIS	-	expression tag	UNP Q5ZX22
G	-1	MET	-	expression tag	UNP Q5ZX22
G	0	SER	-	expression tag	UNP Q5ZX22
G	1	LEU	-	expression tag	UNP Q5ZX22
G	257	GLU	-	expression tag	UNP Q5ZX22
G	258	GLY	-	expression tag	UNP Q5ZX22
G	259	HIS	-	expression tag	UNP Q5ZX22
G	260	HIS	-	expression tag	UNP Q5ZX22
G	261	HIS	-	expression tag	UNP Q5ZX22
G	262	HIS	-	expression tag	UNP Q5ZX22
G	263	HIS	-	expression tag	UNP Q5ZX22
G	264	HIS	-	expression tag	UNP Q5ZX22
H	-1	MET	-	expression tag	UNP Q5ZX22
H	0	SER	-	expression tag	UNP Q5ZX22
H	1	LEU	-	expression tag	UNP Q5ZX22
H	257	GLU	-	expression tag	UNP Q5ZX22
H	258	GLY	-	expression tag	UNP Q5ZX22
H	259	HIS	-	expression tag	UNP Q5ZX22
H	260	HIS	-	expression tag	UNP Q5ZX22
H	261	HIS	-	expression tag	UNP Q5ZX22
H	262	HIS	-	expression tag	UNP Q5ZX22
H	263	HIS	-	expression tag	UNP Q5ZX22
H	264	HIS	-	expression tag	UNP Q5ZX22
I	-1	MET	-	expression tag	UNP Q5ZX22

Continued on next page...

Continued from previous page...

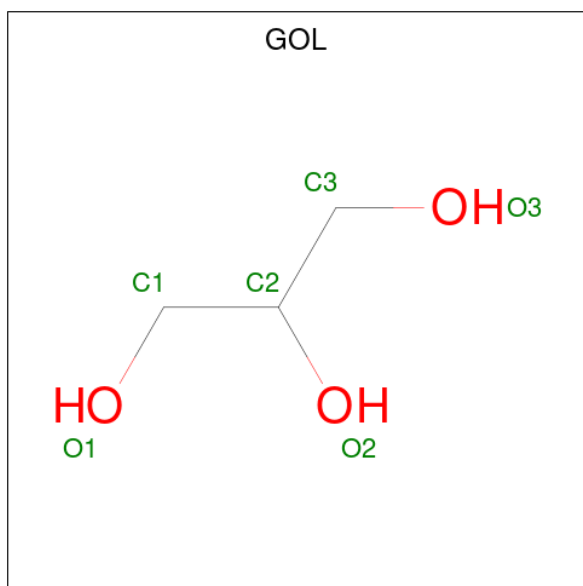
Chain	Residue	Modelled	Actual	Comment	Reference
I	0	SER	-	expression tag	UNP Q5ZX22
I	1	LEU	-	expression tag	UNP Q5ZX22
I	257	GLU	-	expression tag	UNP Q5ZX22
I	258	GLY	-	expression tag	UNP Q5ZX22
I	259	HIS	-	expression tag	UNP Q5ZX22
I	260	HIS	-	expression tag	UNP Q5ZX22
I	261	HIS	-	expression tag	UNP Q5ZX22
I	262	HIS	-	expression tag	UNP Q5ZX22
I	263	HIS	-	expression tag	UNP Q5ZX22
I	264	HIS	-	expression tag	UNP Q5ZX22
J	-1	MET	-	expression tag	UNP Q5ZX22
J	0	SER	-	expression tag	UNP Q5ZX22
J	1	LEU	-	expression tag	UNP Q5ZX22
J	257	GLU	-	expression tag	UNP Q5ZX22
J	258	GLY	-	expression tag	UNP Q5ZX22
J	259	HIS	-	expression tag	UNP Q5ZX22
J	260	HIS	-	expression tag	UNP Q5ZX22
J	261	HIS	-	expression tag	UNP Q5ZX22
J	262	HIS	-	expression tag	UNP Q5ZX22
J	263	HIS	-	expression tag	UNP Q5ZX22
J	264	HIS	-	expression tag	UNP Q5ZX22
K	-1	MET	-	expression tag	UNP Q5ZX22
K	0	SER	-	expression tag	UNP Q5ZX22
K	1	LEU	-	expression tag	UNP Q5ZX22
K	257	GLU	-	expression tag	UNP Q5ZX22
K	258	GLY	-	expression tag	UNP Q5ZX22
K	259	HIS	-	expression tag	UNP Q5ZX22
K	260	HIS	-	expression tag	UNP Q5ZX22
K	261	HIS	-	expression tag	UNP Q5ZX22
K	262	HIS	-	expression tag	UNP Q5ZX22
K	263	HIS	-	expression tag	UNP Q5ZX22
K	264	HIS	-	expression tag	UNP Q5ZX22
L	-1	MET	-	expression tag	UNP Q5ZX22
L	0	SER	-	expression tag	UNP Q5ZX22
L	1	LEU	-	expression tag	UNP Q5ZX22
L	257	GLU	-	expression tag	UNP Q5ZX22
L	258	GLY	-	expression tag	UNP Q5ZX22
L	259	HIS	-	expression tag	UNP Q5ZX22
L	260	HIS	-	expression tag	UNP Q5ZX22
L	261	HIS	-	expression tag	UNP Q5ZX22
L	262	HIS	-	expression tag	UNP Q5ZX22
L	263	HIS	-	expression tag	UNP Q5ZX22

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	264	HIS	-	expression tag	UNP Q5ZX22

- 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	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		

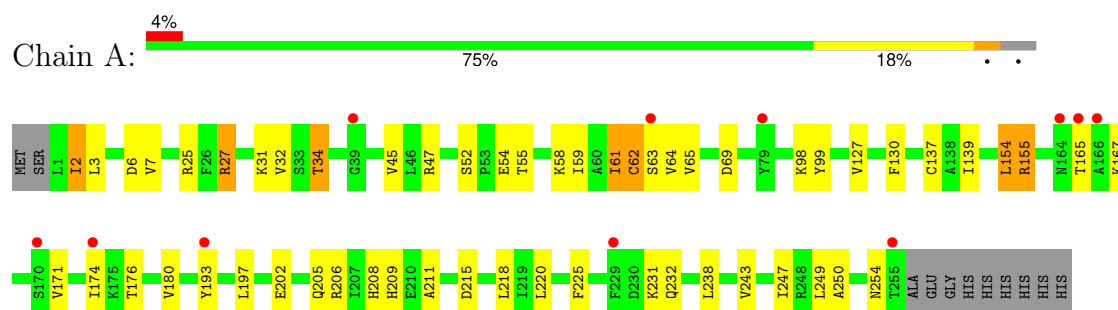
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	39	Total O 39 39	0	0
3	B	37	Total O 37 37	0	0
3	C	33	Total O 33 33	0	0
3	D	28	Total O 28 28	0	0
3	E	30	Total O 30 30	0	0
3	F	27	Total O 27 27	0	0
3	G	18	Total O 18 18	0	0
3	H	10	Total O 10 10	0	0
3	I	27	Total O 27 27	0	0
3	J	12	Total O 12 12	0	0
3	K	15	Total O 15 15	0	0
3	L	9	Total O 9 9	0	0

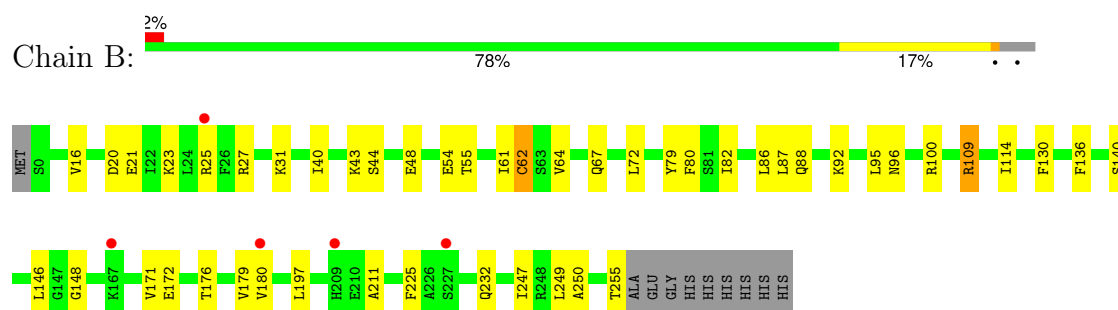
3 Residue-property plots [i](#)

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 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.

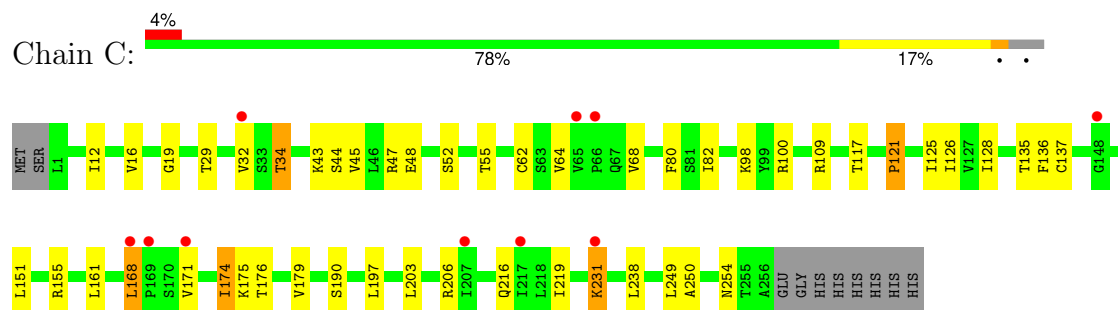
- Molecule 1: Type III pantothenate kinase



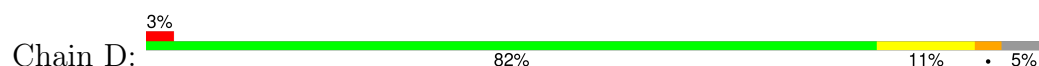
- Molecule 1: Type III pantothenate kinase



- Molecule 1: Type III pantothenate kinase

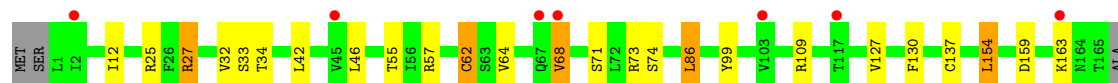
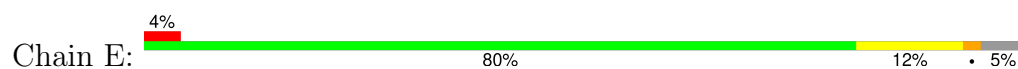


- Molecule 1: Type III pantothenate kinase

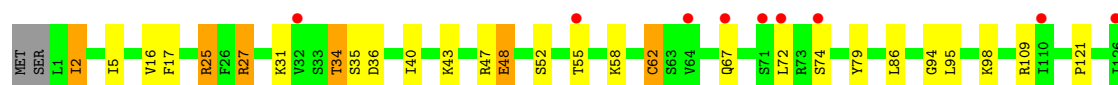
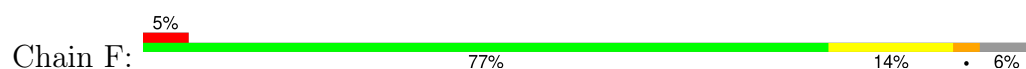




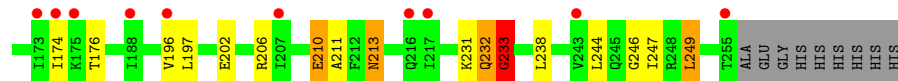
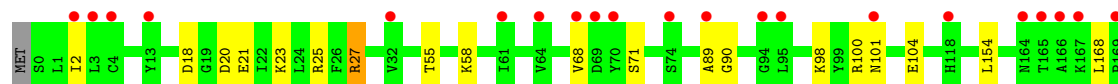
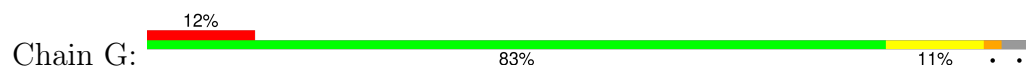
• Molecule 1: Type III pantothenate kinase



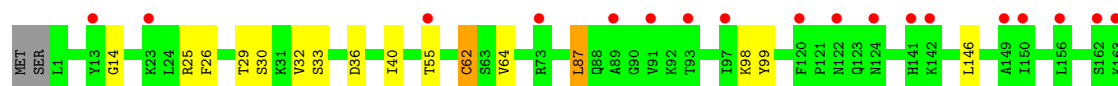
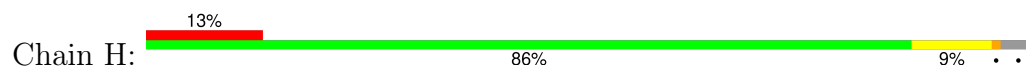
• Molecule 1: Type III pantothenate kinase



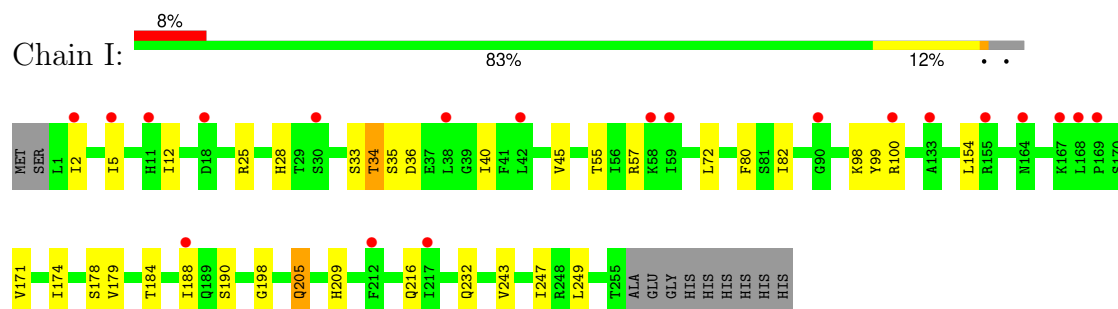
• Molecule 1: Type III pantothenate kinase



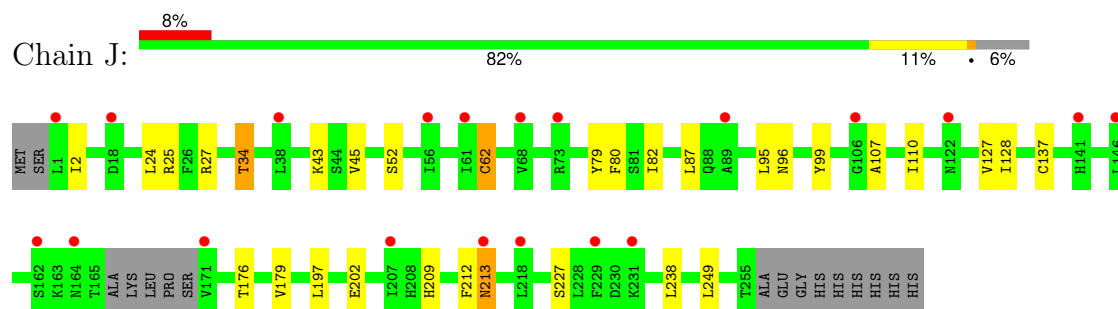
• Molecule 1: Type III pantothenate kinase



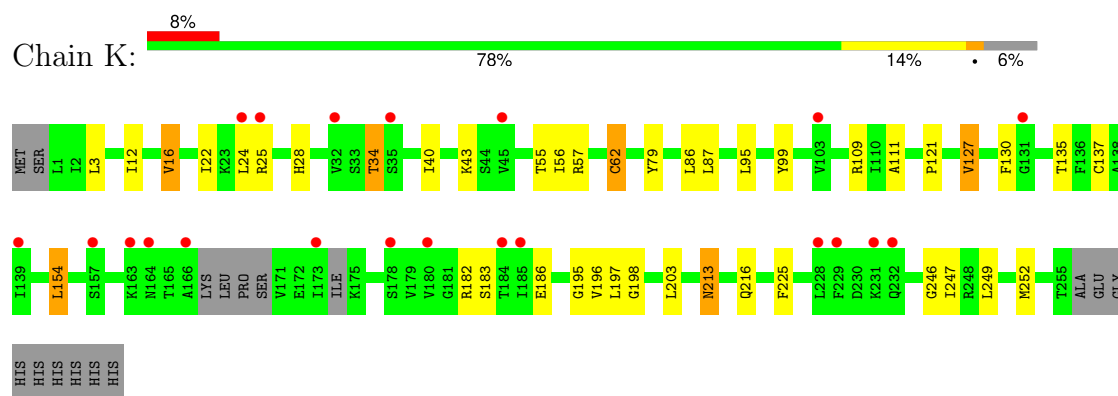
- Molecule 1: Type III pantothenate kinase



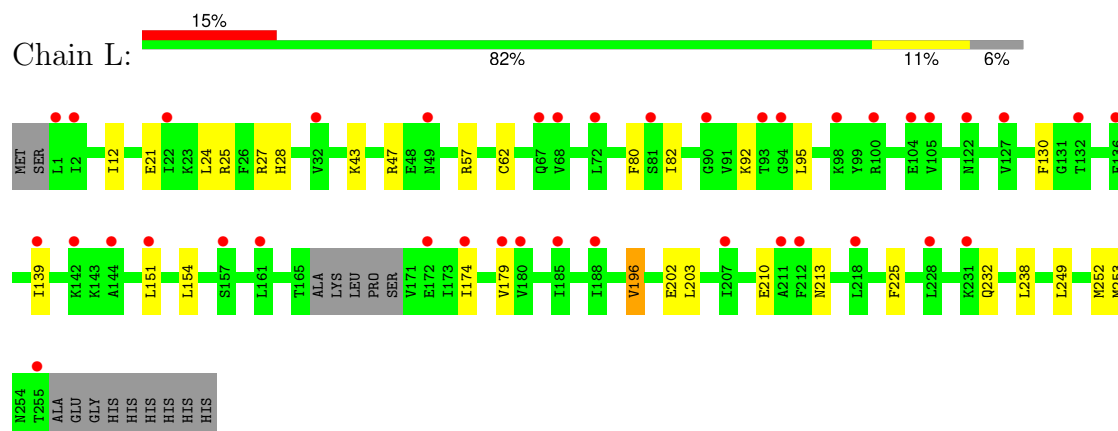
- Molecule 1: Type III pantothenate kinase



- Molecule 1: Type III pantothenate kinase



- Molecule 1: Type III pantothenate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.39Å 134.57Å 134.40Å 90.00° 93.24° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 32.01 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.40) 88.4 (32.01-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.259 , 0.313 0.260 , 0.312	Depositor DCC
R_{free} test set	4086 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23826	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.41	0/2015	0.61	1/2728 (0.0%)
1	B	0.43	0/2047	0.67	0/2768
1	C	0.44	0/2021	0.62	0/2736
1	D	0.43	0/2011	0.63	0/2719
1	E	0.41	0/1982	0.61	0/2682
1	F	0.40	0/1974	0.61	0/2670
1	G	0.45	0/1999	0.59	0/2707
1	H	0.39	0/2012	0.57	0/2723
1	I	0.39	0/2022	0.59	0/2737
1	J	0.38	0/1987	0.58	0/2687
1	K	0.39	0/1989	0.59	0/2690
1	L	0.39	0/1974	0.56	0/2668
All	All	0.41	0/24033	0.60	1/32515 (0.0%)

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	A	0	1
1	D	0	1
1	G	0	2
1	H	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	LEU	CA-CB-CG	5.36	127.62	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	CYS	Peptide
1	D	0	SER	Peptide
1	G	231	LYS	Peptide
1	G	233	GLY	Peptide
1	H	32	VAL	Peptide

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	1967	0	2026	27	0
1	B	1993	0	2063	17	0
1	C	1973	0	2034	19	0
1	D	1962	0	2024	14	0
1	E	1938	0	1987	16	0
1	F	1931	0	1988	22	0
1	G	1960	0	2013	14	0
1	H	1967	0	2025	8	0
1	I	1971	0	2034	14	0
1	J	1941	0	1996	11	0
1	K	1941	0	1996	15	0
1	L	1931	0	1990	10	0
2	A	12	0	16	0	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
2	E	12	0	16	0	0
2	H	12	0	16	0	0
2	J	6	0	8	0	0
2	L	6	0	8	0	0
3	A	39	0	0	1	0
3	B	37	0	0	1	0
3	C	33	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	0	0	0
3	E	30	0	0	0	0
3	F	27	0	0	0	0
3	G	18	0	0	0	0
3	H	10	0	0	0	0
3	I	27	0	0	0	0
3	J	12	0	0	0	0
3	K	15	0	0	0	0
3	L	9	0	0	0	0
All	All	23826	0	24264	160	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 3.

The worst 5 of 160 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:F:174:ILE:HG13	1:F:175:LYS:N	1.94	0.79
1:D:1:LEU:HB3	1:D:56:ILE:HD13	1.67	0.75
1:C:128:ILE:HD11	1:C:219:ILE:HD11	1.67	0.75
1:C:34[A]:THR:HG21	1:F:27:ARG:HB3	1.71	0.73
1:E:206:ARG:HB3	1:F:179:VAL:HG21	1.71	0.73

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	258/266 (97%)	249 (96%)	9 (4%)	0	100	100
1	B	261/266 (98%)	252 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	259/266 (97%)	248 (96%)	9 (4%)	2 (1%)	19	29
1	D	256/266 (96%)	250 (98%)	5 (2%)	1 (0%)	34	48
1	E	252/266 (95%)	245 (97%)	7 (3%)	0	100	100
1	F	251/266 (94%)	238 (95%)	12 (5%)	1 (0%)	34	48
1	G	256/266 (96%)	244 (95%)	10 (4%)	2 (1%)	19	29
1	H	257/266 (97%)	246 (96%)	11 (4%)	0	100	100
1	I	259/266 (97%)	244 (94%)	15 (6%)	0	100	100
1	J	251/266 (94%)	243 (97%)	7 (3%)	1 (0%)	34	48
1	K	250/266 (94%)	244 (98%)	4 (2%)	2 (1%)	19	29
1	L	250/266 (94%)	240 (96%)	9 (4%)	1 (0%)	34	48
All	All	3060/3192 (96%)	2943 (96%)	107 (4%)	10 (0%)	41	55

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	233	GLY
1	J	213	ASN
1	F	213	ASN
1	K	213	ASN
1	L	213	ASN

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	218/222 (98%)	192 (88%)	26 (12%)	5	6
1	B	221/222 (100%)	193 (87%)	28 (13%)	4	5
1	C	218/222 (98%)	195 (89%)	23 (11%)	6	9
1	D	217/222 (98%)	194 (89%)	23 (11%)	6	9
1	E	214/222 (96%)	192 (90%)	22 (10%)	7	10
1	F	213/222 (96%)	188 (88%)	25 (12%)	5	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	216/222 (97%)	198 (92%)	18 (8%)	11	17
1	H	217/222 (98%)	200 (92%)	17 (8%)	12	19
1	I	219/222 (99%)	201 (92%)	18 (8%)	11	17
1	J	214/222 (96%)	197 (92%)	17 (8%)	12	19
1	K	214/222 (96%)	191 (89%)	23 (11%)	6	9
1	L	213/222 (96%)	198 (93%)	15 (7%)	15	24
All	All	2594/2664 (97%)	2339 (90%)	255 (10%)	8	11

5 of 255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	109	ARG
1	K	34[B]	THR
1	F	231	LYS
1	K	25	ARG
1	K	213	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	245	GLN
1	J	122	ASN
1	I	9	ASN
1	I	208	HIS
1	J	232	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

11 ligands are modelled in this entry.

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	E	265	-	5,5,5	0.36	0	5,5,5	0.31	0
2	GOL	J	265	-	5,5,5	0.40	0	5,5,5	0.31	0
2	GOL	C	266	-	5,5,5	0.37	0	5,5,5	0.39	0
2	GOL	A	266	-	5,5,5	0.35	0	5,5,5	0.37	0
2	GOL	A	265	-	5,5,5	0.41	0	5,5,5	0.21	0
2	GOL	L	265	-	5,5,5	0.38	0	5,5,5	0.35	0
2	GOL	E	266	-	5,5,5	0.33	0	5,5,5	0.47	0
2	GOL	B	265	-	5,5,5	0.38	0	5,5,5	0.32	0
2	GOL	H	265	-	5,5,5	0.38	0	5,5,5	0.27	0
2	GOL	H	266	-	5,5,5	0.36	0	5,5,5	0.31	0
2	GOL	C	265	-	5,5,5	0.37	0	5,5,5	0.29	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
2	GOL	E	265	-	-	2/4/4/4	-
2	GOL	J	265	-	-	0/4/4/4	-
2	GOL	C	266	-	-	3/4/4/4	-
2	GOL	A	266	-	-	4/4/4/4	-
2	GOL	A	265	-	-	1/4/4/4	-
2	GOL	L	265	-	-	2/4/4/4	-
2	GOL	E	266	-	-	4/4/4/4	-
2	GOL	B	265	-	-	2/4/4/4	-
2	GOL	H	265	-	-	2/4/4/4	-
2	GOL	H	266	-	-	2/4/4/4	-
2	GOL	C	265	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	266	GOL	O1-C1-C2-O2
2	A	266	GOL	C1-C2-C3-O3
2	B	265	GOL	O1-C1-C2-C3
2	C	265	GOL	C1-C2-C3-O3
2	C	265	GOL	O2-C2-C3-O3

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, 95th 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 ²)	Q<0.9
1	A	255/266 (95%)	0.24	11 (4%) 35 33	28, 54, 79, 87	0
1	B	256/266 (96%)	0.18	5 (1%) 65 63	29, 52, 74, 82	0
1	C	256/266 (96%)	0.27	10 (3%) 39 38	34, 55, 73, 94	0
1	D	254/266 (95%)	0.24	9 (3%) 44 43	38, 54, 78, 111	0
1	E	252/266 (94%)	0.36	11 (4%) 34 33	32, 52, 78, 102	0
1	F	251/266 (94%)	0.36	14 (5%) 24 23	39, 58, 83, 100	0
1	G	256/266 (96%)	0.77	31 (12%) 4 3	45, 69, 92, 135	0
1	H	255/266 (95%)	0.73	35 (13%) 3 2	44, 68, 96, 113	0
1	I	255/266 (95%)	0.47	20 (7%) 13 11	46, 65, 90, 104	0
1	J	250/266 (93%)	0.56	20 (8%) 12 11	47, 67, 90, 99	0
1	K	250/266 (93%)	0.43	21 (8%) 11 10	39, 63, 99, 115	0
1	L	250/266 (93%)	0.97	39 (15%) 2 1	50, 75, 102, 120	0
All	All	3040/3192 (95%)	0.46	226 (7%) 14 13	28, 61, 90, 135	0

The worst 5 of 226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	167	LYS	14.0
1	L	94	GLY	12.2
1	I	167	LYS	10.1
1	G	169	PRO	8.4
1	G	166	ALA	8.4

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, 95th 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(\AA^2)	Q<0.9
2	GOL	C	265	6/6	0.71	0.19	47,55,76,79	0
2	GOL	J	265	6/6	0.77	0.26	61,84,87,91	0
2	GOL	A	266	6/6	0.82	0.16	60,68,70,71	0
2	GOL	C	266	6/6	0.87	0.14	51,62,70,74	0
2	GOL	H	266	6/6	0.88	0.26	69,76,85,96	0
2	GOL	L	265	6/6	0.89	0.18	72,83,91,96	0
2	GOL	H	265	6/6	0.94	0.17	76,84,104,108	0
2	GOL	E	265	6/6	0.94	0.13	39,43,46,55	0
2	GOL	A	265	6/6	0.95	0.19	57,74,86,98	0
2	GOL	E	266	6/6	0.95	0.11	46,67,71,86	0
2	GOL	B	265	6/6	0.97	0.11	34,58,64,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.