



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:10 AM GMT

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 Full wwPDB X-ray Structure Validation 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

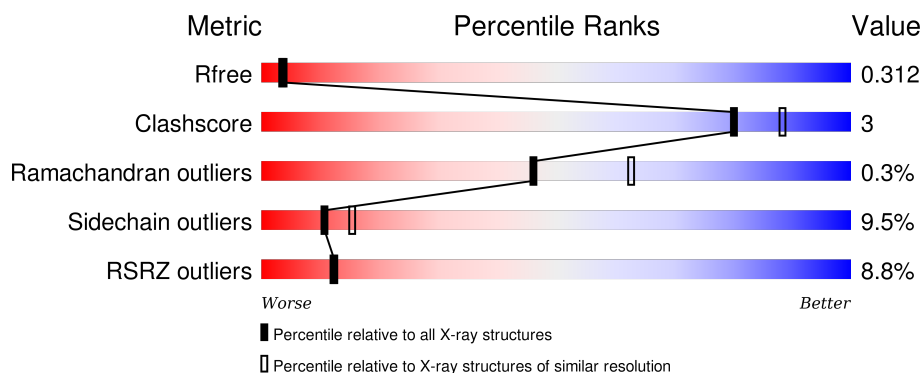
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 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	266	<div> <div>5%</div> <div>75%</div> <div>18%</div> <div>• •</div> </div>
1	B	266	<div> <div>3%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	C	266	<div> <div>5%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	D	266	<div> <div>4%</div> <div>82%</div> <div>11%</div> <div>• 5%</div> </div>
1	E	266	<div> <div>6%</div> <div>80%</div> <div>12%</div> <div>• 5%</div> </div>

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

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	265	-	-	-	X

## 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

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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

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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

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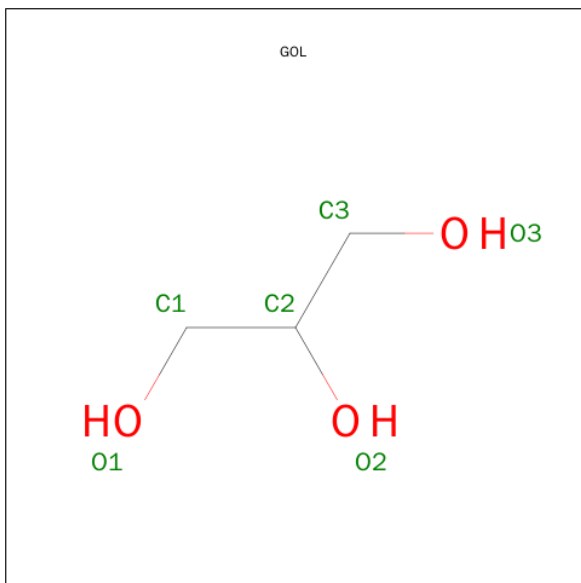
Chain	Residue	Modelled	Actual	Comment	Reference
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I	1	LEU	-	expression tag	UNP Q5ZX22
I	257	GLU	-	expression tag	UNP Q5ZX22
I	258	GLY	-	expression tag	UNP Q5ZX22
I	259	HIS	-	expression tag	UNP Q5ZX22
I	260	HIS	-	expression tag	UNP Q5ZX22
I	261	HIS	-	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

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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		



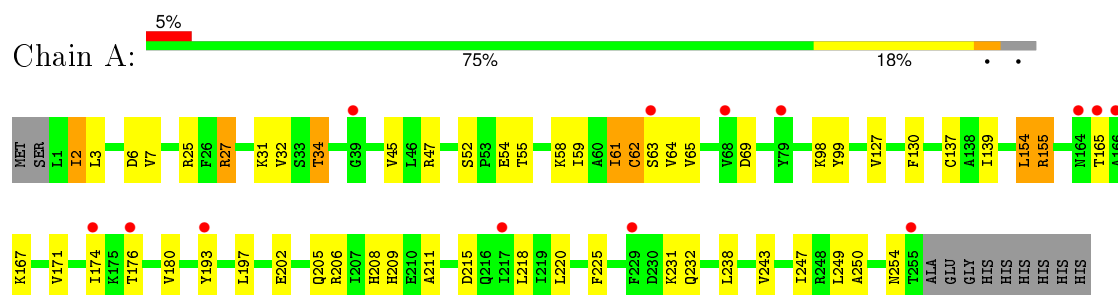
- Molecule 3 is water.

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

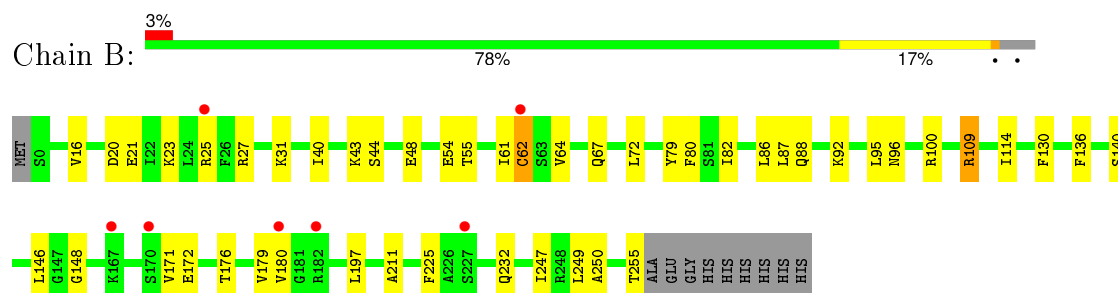
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

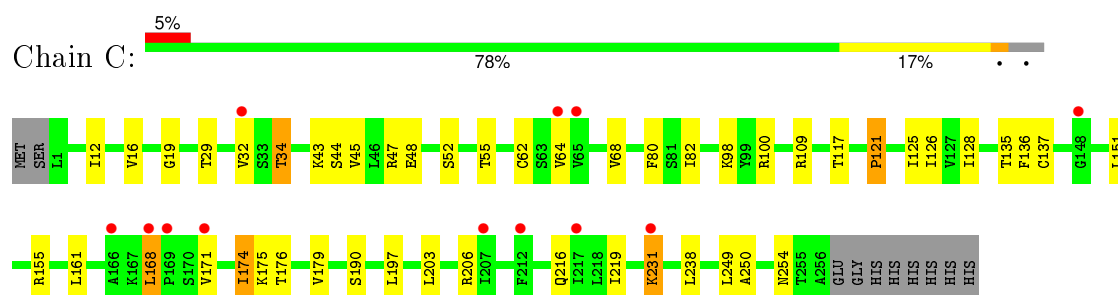
- Molecule 1: Type III pantothenate kinase



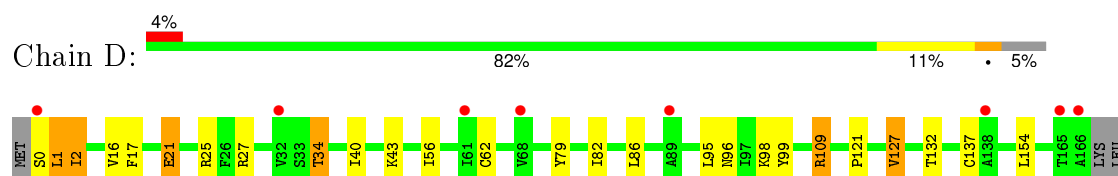
- Molecule 1: Type III pantothenate kinase

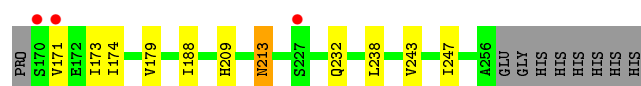


- Molecule 1: Type III pantothenate kinase

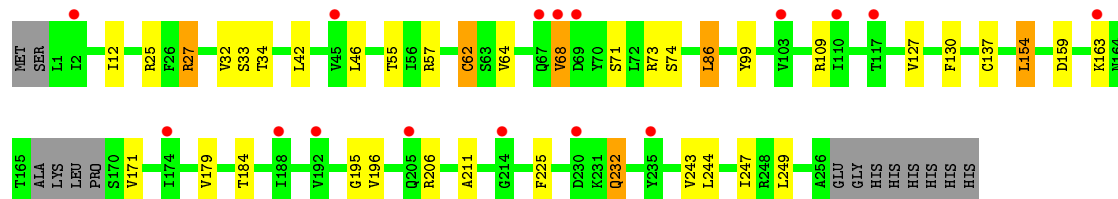
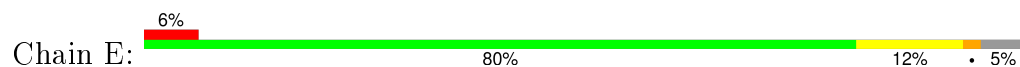


- Molecule 1: Type III pantothenate kinase

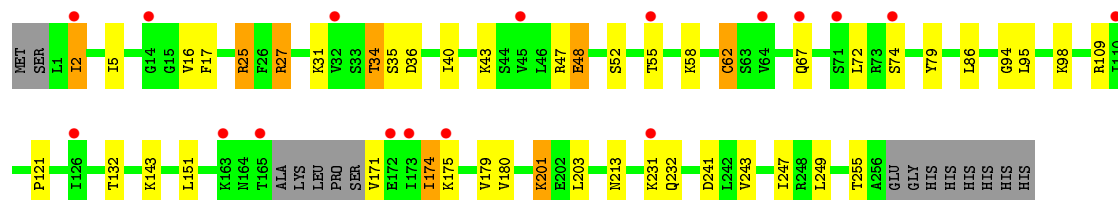
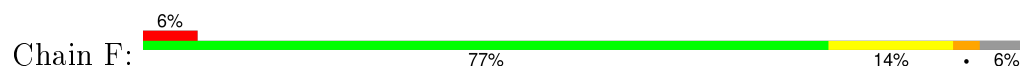




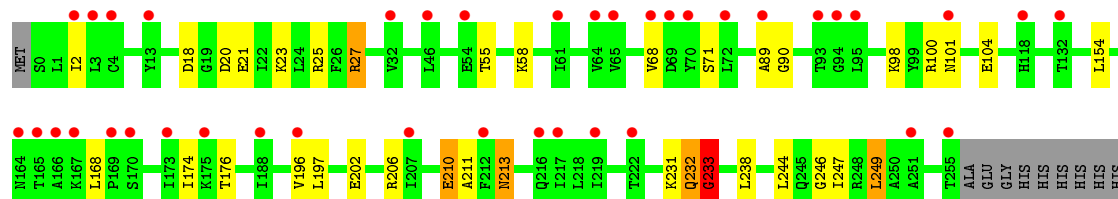
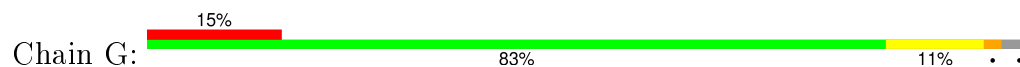
- Molecule 1: Type III pantothenate kinase



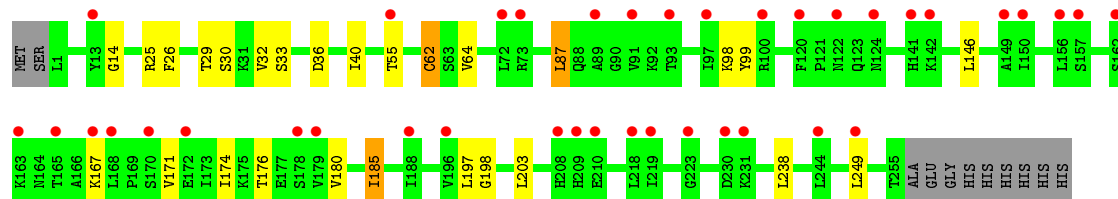
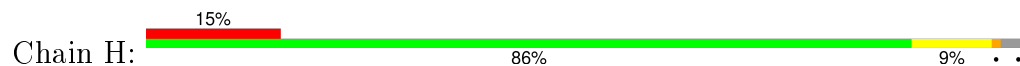
- Molecule 1: Type III pantothenate kinase



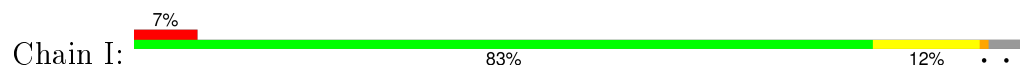
- Molecule 1: Type III pantothenate kinase

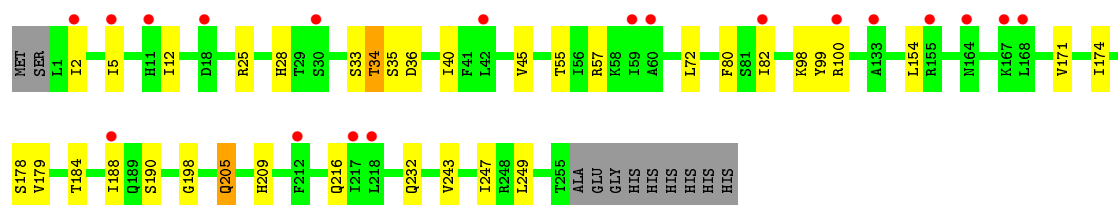


- Molecule 1: Type III pantothenate kinase

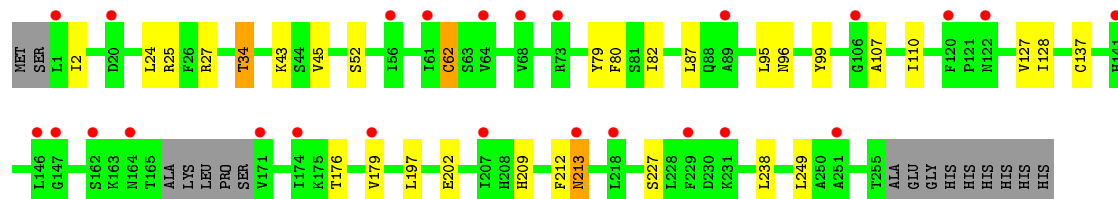
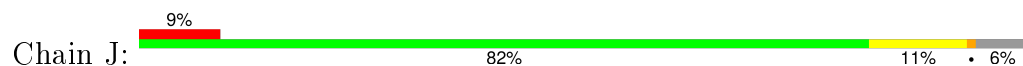


- Molecule 1: Type III pantothenate kinase

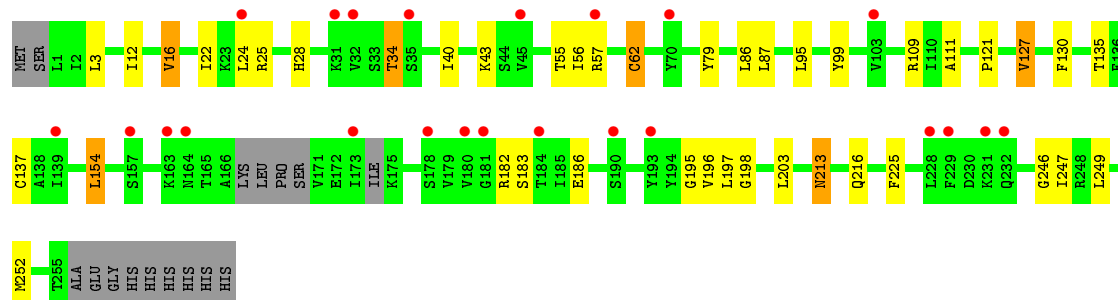
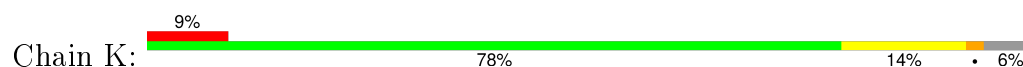




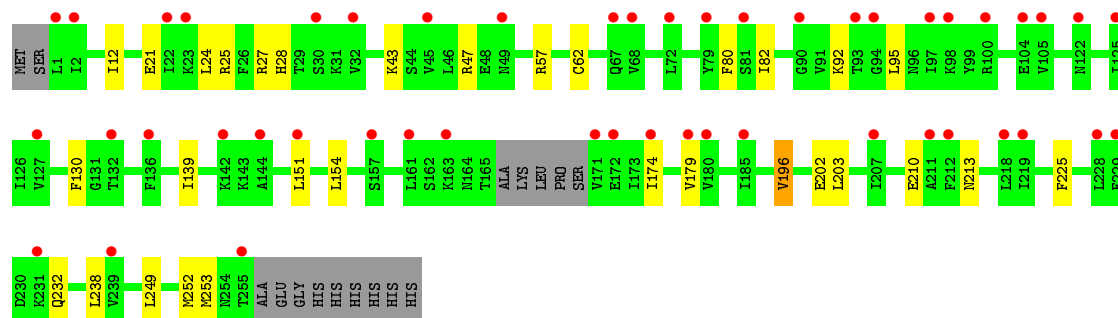
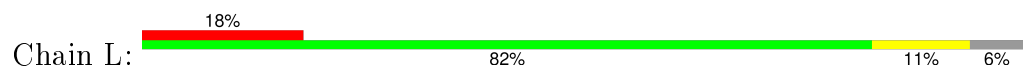
- Molecule 1: Type III pantothenate kinase



- 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, $\alpha$ , $\beta$ , $\gamma$	95.39 Å   134.57 Å   134.40 Å 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) 81.7 (32.01-2.35)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.36 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.259 , 0.313 0.259 , 0.312	Depositor DCC
$R_{free}$ test set	3908 reflections (3.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 135121 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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

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

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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.

All (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
1:A:62:CYS:HB2	1:A:247:ILE:HG12	1.70	0.72
1:A:64:VAL:HG23	1:A:64:VAL:O	1.90	0.70
1:C:231:LYS:H	1:C:231:LYS:HD2	1.57	0.69
1:G:232:GLN:O	1:G:233:GLY:C	2.30	0.69
1:H:171:VAL:HG23	1:H:185:ILE:HG13	1.74	0.69
1:A:155:ARG:HD2	3:A:302:HOH:O	1.96	0.64
1:F:2:ILE:HG22	1:F:17:PHE:HB2	1.79	0.64
1:B:27:ARG:HB3	1:F:34[A]:THR:HG21	1.79	0.63
1:A:32:VAL:O	1:A:32:VAL:HG13	1.99	0.60
1:A:61:ILE:O	1:A:61:ILE:HG22	2.00	0.60
1:E:62:CYS:HB3	1:E:247:ILE:HG12	1.84	0.59
1:A:2:ILE:HG12	1:A:58:LYS:HB2	1.85	0.58
1:F:36:ASP:O	1:F:40:ILE:HG12	2.03	0.58
1:D:109:ARG:HA	1:D:109:ARG:HE	1.68	0.58
1:E:244:LEU:HA	1:E:247:ILE:HD12	1.87	0.57
1:J:27:ARG:HB3	1:K:34[A]:THR:HG21	1.87	0.57
1:A:27:ARG:HB3	1:D:34[A]:THR:HG21	1.87	0.56
1:I:80:PHE:HB3	1:I:82:ILE:HD12	1.90	0.54
1:D:43:LYS:HD2	1:D:79:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:ARG:O	1:G:210:GLU:HB2	2.08	0.54
1:D:2:ILE:HG23	1:D:17:PHE:HB2	1.89	0.53
1:A:130:PHE:HB3	1:A:225:PHE:HB2	1.90	0.53
1:J:43:LYS:HD2	1:J:79:TYR:HB3	1.90	0.53
1:F:5:ILE:HG21	1:F:72:LEU:HD21	1.91	0.53
1:K:183:SER:HB3	1:K:186:GLU:HB2	1.91	0.53
1:K:195:GLY:HA3	1:L:151:LEU:HD21	1.91	0.53
1:F:35:SER:HB3	1:F:74:SER:HB3	1.90	0.53
1:J:45:VAL:HB	1:K:40:ILE:HD11	1.90	0.53
1:G:211:ALA:HB2	1:H:180:VAL:HG21	1.91	0.52
1:A:6:ASP:HA	1:A:62:CYS:O	2.09	0.52
1:F:243:VAL:O	1:F:247:ILE:HG13	2.10	0.52
1:A:208:HIS:NE2	1:A:215:ASP:O	2.28	0.52
1:E:195:GLY:HA3	1:F:151:LEU:HD21	1.91	0.52
1:L:154:LEU:HD21	1:L:196:VAL:HG11	1.93	0.51
1:K:130:PHE:HB3	1:K:225:PHE:HB2	1.93	0.51
1:A:205:GLN:O	1:A:209:HIS:ND1	2.40	0.51
1:B:62:CYS:HB2	1:B:87:LEU:HD23	1.93	0.50
1:K:43:LYS:HD2	1:K:79:TYR:HB3	1.92	0.50
1:J:209:HIS:O	1:J:213:ASN:ND2	2.45	0.50
1:A:127:VAL:HG13	1:A:137:CYS:HB2	1.92	0.50
1:B:40:ILE:HD11	1:C:45:VAL:HA	1.92	0.50
1:G:246:GLY:HA2	1:G:249:LEU:HB2	1.93	0.49
1:I:179:VAL:HA	1:I:190:SER:HB3	1.94	0.49
1:F:43:LYS:HD2	1:F:79:TYR:HB3	1.93	0.49
1:I:12:ILE:HB	1:I:28:HIS:HB3	1.92	0.49
1:A:193:TYR:OH	1:A:232:GLN:NE2	2.46	0.49
1:A:243:VAL:O	1:A:247:ILE:HG13	2.12	0.48
1:C:80:PHE:HB3	1:C:82:ILE:HD12	1.95	0.48
1:G:2:ILE:HG13	1:G:58:LYS:HB3	1.95	0.48
1:F:174:ILE:CG1	1:F:175:LYS:N	2.70	0.48
1:C:12:ILE:HD11	1:C:68:VAL:HG11	1.96	0.48
1:A:165:THR:HG22	1:A:167:LYS:H	1.78	0.48
1:I:36:ASP:O	1:I:40:ILE:HG12	2.14	0.47
1:C:206:ARG:HB3	1:D:179:VAL:HG11	1.95	0.47
1:H:62:CYS:HB2	1:H:87:LEU:HD13	1.97	0.47
1:B:109:ARG:NH1	3:B:279:HOH:O	2.47	0.47
1:G:101:ASN:HD22	1:G:104:GLU:HG3	1.79	0.47
1:B:86:LEU:HB3	1:B:88:GLN:HG3	1.96	0.46
1:B:140:SER:HB3	1:B:146:LEU:HD11	1.96	0.46
1:A:180:VAL:HG21	1:B:211:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:LEU:HB2	1:K:56:ILE:HD12	1.98	0.46
1:D:243:VAL:O	1:D:247:ILE:HG13	2.15	0.46
1:K:111:ALA:O	1:K:246:GLY:HA3	2.16	0.46
1:B:48:GLU:OE1	1:F:47:ARG:NH1	2.48	0.46
1:E:211:ALA:HB2	1:F:180:VAL:HG21	1.97	0.46
1:I:184:THR:O	1:I:188:ILE:HG22	2.15	0.46
1:A:211:ALA:HB2	1:B:180:VAL:HG21	1.98	0.46
1:A:61:ILE:HG23	1:A:63:SER:HB3	1.98	0.46
1:K:16:VAL:HG13	1:K:24:LEU:HB3	1.98	0.45
1:K:62:CYS:HB3	1:K:247:ILE:HG12	1.98	0.45
1:A:202:GLU:OE1	1:A:206:ARG:NE	2.49	0.45
1:F:62:CYS:HB3	1:F:247:ILE:HG12	1.98	0.45
1:C:250:ALA:O	1:C:254:ASN:ND2	2.43	0.45
1:F:2:ILE:HG12	1:F:58:LYS:HB2	1.99	0.45
1:F:121:PRO:HG2	1:I:178[B]:SER:HB2	1.98	0.45
1:F:121:PRO:HG2	1:I:178[A]:SER:HB2	1.98	0.45
1:F:25:ARG:NH1	1:F:241:ASP:OD1	2.50	0.45
1:D:127:VAL:HG13	1:D:137:CYS:HB2	1.99	0.45
1:C:117:THR:O	1:C:121:PRO:HA	2.17	0.45
1:G:232:GLN:HE21	1:G:232:GLN:HB2	1.48	0.44
1:B:40:ILE:HD12	1:C:48:GLU:HG3	1.97	0.44
1:A:45:VAL:HB	1:D:40:ILE:HD11	2.00	0.44
1:C:161:LEU:HB3	1:C:168:LEU:HD22	1.99	0.44
1:H:36:ASP:O	1:H:40:ILE:HG12	2.17	0.44
1:B:62:CYS:HB3	1:B:247:ILE:HG12	2.00	0.44
1:G:18:ASP:HB2	1:G:23:LYS:HE2	2.00	0.44
1:I:243:VAL:O	1:I:247:ILE:HG13	2.18	0.44
1:K:198:GLY:HA3	1:L:202:GLU:HB2	1.98	0.44
1:A:250:ALA:O	1:A:254:ASN:ND2	2.33	0.44
1:K:62:CYS:HB2	1:K:87:LEU:HD23	2.00	0.44
1:F:94:GLY:O	1:F:143[B]:LYS:HE3	2.18	0.43
1:E:154:LEU:HD22	1:E:196:VAL:HG11	2.00	0.43
1:E:12:ILE:HD11	1:E:68:VAL:HG11	1.99	0.43
1:B:130:PHE:HB3	1:B:225:PHE:HB2	2.01	0.43
1:B:136:PHE:O	1:B:148:GLY:HA3	2.18	0.43
1:K:154:LEU:HD22	1:K:196:VAL:HG11	1.98	0.43
1:E:130:PHE:HB3	1:E:225:PHE:HB2	2.01	0.43
1:J:62:CYS:HB2	1:J:87:LEU:HD23	2.01	0.43
1:E:73:ARG:HD3	1:E:86:LEU:HD21	1.99	0.43
1:A:7:VAL:O	1:A:64:VAL:HG13	2.19	0.43
1:B:43:LYS:HD2	1:B:79:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ARG:HB2	1:E:27:ARG:HE	1.57	0.43
1:B:114:ILE:HD13	1:B:250:ALA:HB2	2.00	0.43
1:C:136:PHE:HE1	1:C:151:LEU:HD12	1.84	0.43
1:C:52:SER:HB3	1:C:55:THR:HG23	2.00	0.43
1:A:64:VAL:HG22	1:A:65:VAL:HG23	2.01	0.42
1:K:12:ILE:HB	1:K:28:HIS:HB3	2.00	0.42
1:J:212:PHE:O	1:J:213:ASN:CB	2.66	0.42
1:L:130:PHE:HB3	1:L:225:PHE:HB2	2.01	0.42
1:C:126:ILE:HA	1:C:137:CYS:O	2.20	0.42
1:A:64:VAL:O	1:A:64:VAL:CG2	2.58	0.42
1:E:232:GLN:HE21	1:E:232:GLN:HB2	1.69	0.42
1:B:61:ILE:HD13	1:B:72:LEU:HG	2.02	0.42
1:I:205:GLN:HG2	1:I:209:HIS:HE1	1.84	0.42
1:H:40:ILE:HD11	1:I:45:VAL:HA	2.02	0.42
1:L:92:LYS:HD3	1:L:253:MET:HB3	2.02	0.42
1:E:127:VAL:HG13	1:E:137:CYS:HB2	2.01	0.42
1:G:244:LEU:HA	1:G:247:ILE:HD12	2.02	0.42
1:L:12:ILE:N	1:L:28:HIS:O	2.50	0.42
1:C:109:ARG:HD3	1:C:109:ARG:HA	1.79	0.41
1:C:179:VAL:HA	1:C:190:SER:HB3	2.02	0.41
1:A:63:SER:HB2	1:A:69:ASP:OD1	2.20	0.41
1:D:21:GLU:H	1:D:21:GLU:HG2	1.68	0.41
1:D:27:ARG:HB2	1:D:27:ARG:HE	1.58	0.41
1:B:80:PHE:HB3	1:B:82:ILE:HD12	2.01	0.41
1:J:107:ALA:HA	1:J:110:ILE:HD12	2.01	0.41
1:E:243:VAL:O	1:E:247:ILE:HG13	2.20	0.41
1:I:205:GLN:HG2	1:I:209:HIS:CE1	2.55	0.41
1:K:127:VAL:HG13	1:K:137:CYS:HB2	2.02	0.41
1:G:154:LEU:HA	1:G:154:LEU:HD23	1.76	0.41
1:G:89:ALA:HA	1:G:90:GLY:HA2	1.59	0.41
1:E:42:LEU:O	1:E:46:LEU:HG	2.20	0.41
1:C:174:ILE:HG12	1:C:175:LYS:N	2.36	0.41
1:I:34[A]:THR:HG21	1:L:27:ARG:HB3	2.01	0.41
1:J:80:PHE:HB3	1:J:82:ILE:HD12	2.02	0.41
1:D:109:ARG:HA	1:D:109:ARG:NE	2.32	0.41
1:D:154:LEU:HD23	1:D:173:ILE:CG2	2.50	0.41
1:C:43:LYS:NZ	1:F:48:GLU:HG3	2.36	0.41
1:C:43:LYS:HE2	1:C:47:ARG:HH12	1.85	0.41
1:G:202:GLU:HB2	1:H:198:GLY:HA3	2.02	0.41
1:H:14:GLY:HA3	1:H:26:PHE:CZ	2.55	0.41
1:A:34[A]:THR:HG21	1:E:27:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD23	1:A:59:ILE:HG12	2.03	0.41
1:G:154:LEU:HD21	1:G:196:VAL:HG11	2.02	0.40
1:L:80:PHE:HB3	1:L:82:ILE:HD12	2.03	0.40
1:E:159:ASP:O	1:E:163:LYS:HB2	2.21	0.40
1:I:198:GLY:HA3	1:J:202:GLU:HB2	2.02	0.40
1:G:27:ARG:HB3	1:J:34[A]:THR:HG21	2.02	0.40
1:L:43:LYS:HE2	1:L:47:ARG:HH22	1.86	0.40
1:F:201:LYS:HE2	1:F:201:LYS:HB3	1.68	0.40
1:L:203:LEU:HD13	1:L:203:LEU:HA	2.00	0.40
1:I:5:ILE:HG21	1:I:72:LEU:HD21	2.03	0.40
1:H:98:LYS:HB2	1:H:146:LEU:HA	2.04	0.40
1:D:209:HIS:HA	1:D:213:ASN:HA	2.02	0.40
1:J:127:VAL:HG13	1:J:137:CYS:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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
1	C	259/266 (97%)	248 (96%)	9 (4%)	2 (1%)	24	35
1	D	256/266 (96%)	250 (98%)	5 (2%)	1 (0%)	39	56
1	E	252/266 (95%)	245 (97%)	7 (3%)	0	100	100
1	F	251/266 (94%)	238 (95%)	12 (5%)	1 (0%)	39	56
1	G	256/266 (96%)	244 (95%)	10 (4%)	2 (1%)	24	35
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%)	39	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	250/266 (94%)	244 (98%)	4 (2%)	2 (1%)	24	35
1	L	250/266 (94%)	240 (96%)	9 (4%)	1 (0%)	39	56
All	All	3060/3192 (96%)	2943 (96%)	107 (4%)	10 (0%)	46	63

All (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
1	D	121	PRO
1	G	213	ASN
1	C	121	PRO
1	K	121	PRO
1	C	19	GLY

### 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%)	6	8
1	B	221/222 (100%)	193 (87%)	28 (13%)	5	6
1	C	218/222 (98%)	195 (89%)	23 (11%)	8	12
1	D	217/222 (98%)	194 (89%)	23 (11%)	8	12
1	E	214/222 (96%)	192 (90%)	22 (10%)	9	13
1	F	213/222 (96%)	188 (88%)	25 (12%)	7	8
1	G	216/222 (97%)	198 (92%)	18 (8%)	14	21
1	H	217/222 (98%)	200 (92%)	17 (8%)	16	24
1	I	219/222 (99%)	201 (92%)	18 (8%)	14	21
1	J	214/222 (96%)	197 (92%)	17 (8%)	15	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	214/222 (96%)	191 (89%)	23 (11%)	8	11
1	L	213/222 (96%)	198 (93%)	15 (7%)	19	29
All	All	2594/2664 (97%)	2339 (90%)	255 (10%)	11	14

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	25	ARG
1	A	27	ARG
1	A	31	LYS
1	A	34[A]	THR
1	A	34[B]	THR
1	A	47	ARG
1	A	52	SER
1	A	54[A]	GLU
1	A	54[B]	GLU
1	A	55	THR
1	A	61	ILE
1	A	98	LYS
1	A	99	TYR
1	A	139	ILE
1	A	154	LEU
1	A	155	ARG
1	A	171	VAL
1	A	174	ILE
1	A	176	THR
1	A	197	LEU
1	A	218	LEU
1	A	220	LEU
1	A	231	LYS
1	A	238	LEU
1	A	249	LEU
1	B	16	VAL
1	B	20	ASP
1	B	21	GLU
1	B	23	LYS
1	B	25	ARG
1	B	31	LYS
1	B	44	SER
1	B	54	GLU

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Mol	Chain	Res	Type
1	B	55	THR
1	B	62	CYS
1	B	64	VAL
1	B	67[A]	GLN
1	B	67[B]	GLN
1	B	92	LYS
1	B	95	LEU
1	B	96	ASN
1	B	100[A]	ARG
1	B	100[B]	ARG
1	B	109	ARG
1	B	171	VAL
1	B	172[A]	GLU
1	B	172[B]	GLU
1	B	176	THR
1	B	179	VAL
1	B	197	LEU
1	B	232	GLN
1	B	249	LEU
1	B	255	THR
1	C	16	VAL
1	C	29	THR
1	C	32	VAL
1	C	34[A]	THR
1	C	34[B]	THR
1	C	44	SER
1	C	62	CYS
1	C	64	VAL
1	C	98	LYS
1	C	100	ARG
1	C	125	ILE
1	C	135	THR
1	C	155	ARG
1	C	168	LEU
1	C	171	VAL
1	C	174	ILE
1	C	176	THR
1	C	197	LEU
1	C	203	LEU
1	C	216	GLN
1	C	231	LYS
1	C	238	LEU

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Mol	Chain	Res	Type
1	C	249	LEU
1	D	1	LEU
1	D	2	ILE
1	D	16	VAL
1	D	21	GLU
1	D	25	ARG
1	D	34[A]	THR
1	D	34[B]	THR
1	D	62	CYS
1	D	82	ILE
1	D	86	LEU
1	D	95	LEU
1	D	96	ASN
1	D	98	LYS
1	D	99	TYR
1	D	109	ARG
1	D	127	VAL
1	D	132	THR
1	D	171	VAL
1	D	174	ILE
1	D	188	ILE
1	D	213	ASN
1	D	232	GLN
1	D	238	LEU
1	E	25	ARG
1	E	27	ARG
1	E	32	VAL
1	E	33	SER
1	E	34[A]	THR
1	E	34[B]	THR
1	E	55	THR
1	E	57	ARG
1	E	62	CYS
1	E	64	VAL
1	E	68	VAL
1	E	71	SER
1	E	74	SER
1	E	86	LEU
1	E	99	TYR
1	E	109	ARG
1	E	154	LEU
1	E	171	VAL

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Mol	Chain	Res	Type
1	E	179	VAL
1	E	184	THR
1	E	232	GLN
1	E	249	LEU
1	F	2	ILE
1	F	16	VAL
1	F	25	ARG
1	F	27	ARG
1	F	31	LYS
1	F	34[A]	THR
1	F	34[B]	THR
1	F	48	GLU
1	F	52	SER
1	F	55	THR
1	F	62	CYS
1	F	67	GLN
1	F	86	LEU
1	F	95	LEU
1	F	98	LYS
1	F	109	ARG
1	F	132	THR
1	F	171	VAL
1	F	174	ILE
1	F	201	LYS
1	F	203	LEU
1	F	231	LYS
1	F	232	GLN
1	F	249	LEU
1	F	255	THR
1	G	20	ASP
1	G	21	GLU
1	G	25	ARG
1	G	27	ARG
1	G	55	THR
1	G	68	VAL
1	G	71	SER
1	G	98	LYS
1	G	100	ARG
1	G	168	LEU
1	G	174	ILE
1	G	176	THR
1	G	197	LEU

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Mol	Chain	Res	Type
1	G	210	GLU
1	G	213	ASN
1	G	232	GLN
1	G	238	LEU
1	G	249	LEU
1	H	25	ARG
1	H	29	THR
1	H	30	SER
1	H	33	SER
1	H	55	THR
1	H	62	CYS
1	H	64	VAL
1	H	87	LEU
1	H	99	TYR
1	H	167	LYS
1	H	174	ILE
1	H	176	THR
1	H	185	ILE
1	H	197	LEU
1	H	203	LEU
1	H	238	LEU
1	H	249	LEU
1	I	2	ILE
1	I	25	ARG
1	I	33	SER
1	I	34[A]	THR
1	I	34[B]	THR
1	I	35	SER
1	I	55	THR
1	I	57	ARG
1	I	98	LYS
1	I	99	TYR
1	I	100	ARG
1	I	154	LEU
1	I	171	VAL
1	I	174	ILE
1	I	205	GLN
1	I	216	GLN
1	I	232	GLN
1	I	249	LEU
1	J	2	ILE
1	J	24	LEU

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Mol	Chain	Res	Type
1	J	25	ARG
1	J	34[A]	THR
1	J	34[B]	THR
1	J	52	SER
1	J	62	CYS
1	J	95	LEU
1	J	96	ASN
1	J	99	TYR
1	J	128	ILE
1	J	176	THR
1	J	179	VAL
1	J	197	LEU
1	J	227	SER
1	J	238	LEU
1	J	249	LEU
1	K	16	VAL
1	K	22	ILE
1	K	25	ARG
1	K	34[A]	THR
1	K	34[B]	THR
1	K	55	THR
1	K	57	ARG
1	K	62	CYS
1	K	86	LEU
1	K	95	LEU
1	K	99	TYR
1	K	109	ARG
1	K	127	VAL
1	K	135[A]	THR
1	K	135[B]	THR
1	K	154	LEU
1	K	182	ARG
1	K	197	LEU
1	K	203	LEU
1	K	213	ASN
1	K	216	GLN
1	K	249	LEU
1	K	252	MET
1	L	21	GLU
1	L	24	LEU
1	L	25	ARG
1	L	57	ARG

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Mol	Chain	Res	Type
1	L	62	CYS
1	L	95	LEU
1	L	139	ILE
1	L	174	ILE
1	L	179	VAL
1	L	196	VAL
1	L	210	GLU
1	L	232	GLN
1	L	238	LEU
1	L	249	LEU
1	L	252	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	216	GLN
1	A	232	GLN
1	A	245	GLN
1	B	123	GLN
1	B	216	GLN
1	B	232	GLN
1	B	245	GLN
1	C	67	GLN
1	C	112	ASN
1	C	245	GLN
1	D	50	ASN
1	D	88	GLN
1	D	122	ASN
1	D	232	GLN
1	E	216	GLN
1	E	232	GLN
1	E	245	GLN
1	F	67	GLN
1	F	96	ASN
1	F	232	GLN
1	G	101	ASN
1	G	112	ASN
1	G	164	ASN
1	G	213	ASN
1	G	232	GLN
1	G	245	GLN

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Mol	Chain	Res	Type
1	H	9	ASN
1	H	245	GLN
1	I	9	ASN
1	I	28	HIS
1	I	88	GLN
1	I	208	HIS
1	I	216	GLN
1	I	232	GLN
1	J	122	ASN
1	J	213	ASN
1	J	232	GLN
1	J	245	GLN
1	K	189	GLN
1	K	216	GLN
1	K	245	GLN
1	L	9	ASN
1	L	232	GLN
1	L	245	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	A	265	-	5,5,5	0.38	0	5,5,5	0.17	0
2	GOL	A	266	-	5,5,5	0.32	0	5,5,5	0.32	0
2	GOL	B	265	-	5,5,5	0.35	0	5,5,5	0.32	0
2	GOL	C	265	-	5,5,5	0.34	0	5,5,5	0.25	0
2	GOL	C	266	-	5,5,5	0.34	0	5,5,5	0.31	0
2	GOL	E	265	-	5,5,5	0.33	0	5,5,5	0.25	0
2	GOL	E	266	-	5,5,5	0.28	0	5,5,5	0.44	0
2	GOL	H	265	-	5,5,5	0.35	0	5,5,5	0.18	0
2	GOL	H	266	-	5,5,5	0.33	0	5,5,5	0.25	0
2	GOL	J	265	-	5,5,5	0.36	0	5,5,5	0.32	0
2	GOL	L	265	-	5,5,5	0.34	0	5,5,5	0.38	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	A	265	-	-	0/4/4/4	0/0/0/0
2	GOL	A	266	-	-	0/4/4/4	0/0/0/0
2	GOL	B	265	-	-	0/4/4/4	0/0/0/0
2	GOL	C	265	-	-	0/4/4/4	0/0/0/0
2	GOL	C	266	-	-	0/4/4/4	0/0/0/0
2	GOL	E	265	-	-	0/4/4/4	0/0/0/0
2	GOL	E	266	-	-	0/4/4/4	0/0/0/0
2	GOL	H	265	-	-	0/4/4/4	0/0/0/0
2	GOL	H	266	-	-	0/4/4/4	0/0/0/0
2	GOL	J	265	-	-	0/4/4/4	0/0/0/0
2	GOL	L	265	-	-	0/4/4/4	0/0/0/0

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

### 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	255/266 (95%)	0.37	13 (5%) 32 32	28, 54, 79, 87	0
1	B	256/266 (96%)	0.34	7 (2%) 58 57	29, 52, 74, 82	0
1	C	256/266 (96%)	0.39	12 (4%) 35 36	34, 55, 73, 94	0
1	D	254/266 (95%)	0.36	11 (4%) 39 40	38, 54, 78, 111	0
1	E	252/266 (94%)	0.47	16 (6%) 23 24	32, 52, 78, 102	0
1	F	251/266 (94%)	0.51	17 (6%) 20 20	39, 58, 83, 100	0
1	G	256/266 (96%)	0.97	39 (15%) 3 3	45, 69, 92, 135	0
1	H	255/266 (95%)	0.90	39 (15%) 3 3	44, 68, 96, 113	0
1	I	255/266 (95%)	0.62	19 (7%) 17 17	46, 65, 90, 104	0
1	J	250/266 (93%)	0.74	25 (10%) 9 9	47, 67, 90, 99	0
1	K	250/266 (93%)	0.64	23 (9%) 11 11	39, 63, 99, 115	0
1	L	250/266 (93%)	1.11	48 (19%) 2 1	50, 75, 102, 120	0
All	All	3040/3192 (95%)	0.62	269 (8%) 12 12	28, 61, 90, 135	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	167	LYS	14.6
1	L	94	GLY	13.5
1	I	167	LYS	11.6
1	G	169	PRO	10.5
1	G	166	ALA	9.6
1	K	180	VAL	8.5
1	H	231	LYS	8.5
1	C	32	VAL	8.2
1	G	165	THR	8.1
1	G	3	LEU	7.7
1	H	167	LYS	7.4

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Mol	Chain	Res	Type	RSRZ
1	H	141	HIS	7.1
1	G	70	TYR	6.7
1	H	249	LEU	6.5
1	H	156	LEU	6.4
1	J	229	PHE	6.3
1	L	2	ILE	6.3
1	J	231	LYS	6.3
1	H	168	LEU	5.9
1	L	151	LEU	5.8
1	E	214	GLY	5.7
1	L	180	VAL	5.7
1	G	188	ILE	5.7
1	K	163	LYS	5.7
1	G	217	ILE	5.7
1	G	2	ILE	5.6
1	L	67	GLN	5.6
1	H	142	LYS	5.6
1	I	2	ILE	5.5
1	I	133	ALA	5.3
1	L	127	VAL	5.2
1	K	32	VAL	5.1
1	L	142	LYS	5.1
1	L	231	LYS	5.1
1	G	164	ASN	5.0
1	E	68	VAL	5.0
1	G	4	CYS	4.8
1	G	175	LYS	4.8
1	C	217	ILE	4.7
1	I	100	ARG	4.7
1	J	73	ARG	4.7
1	H	218	LEU	4.7
1	L	144	ALA	4.7
1	J	122	ASN	4.7
1	G	61	ILE	4.7
1	J	68	VAL	4.7
1	F	172	GLU	4.6
1	L	81	SER	4.6
1	K	164	ASN	4.6
1	K	231	LYS	4.5
1	F	64	VAL	4.5
1	L	122	ASN	4.4
1	I	42	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	45	VAL	4.3
1	L	179	VAL	4.3
1	H	120	PHE	4.3
1	K	157	SER	4.3
1	A	174	ILE	4.3
1	L	174	ILE	4.2
1	L	211	ALA	4.2
1	E	192	VAL	4.1
1	F	71	SER	4.1
1	H	170	SER	4.1
1	F	67	GLN	4.0
1	I	212	PHE	4.0
1	D	165	THR	4.0
1	I	11	HIS	4.0
1	B	167	LYS	4.0
1	K	229	PHE	4.0
1	L	104	GLU	3.9
1	H	97	ILE	3.8
1	J	56	ILE	3.8
1	J	164	ASN	3.8
1	L	93	THR	3.7
1	L	68	VAL	3.7
1	I	18	ASP	3.7
1	L	105	VAL	3.6
1	J	106	GLY	3.6
1	H	162	SER	3.6
1	E	103	VAL	3.6
1	L	185	ILE	3.6
1	J	207	ILE	3.6
1	L	218	LEU	3.6
1	G	255	THR	3.5
1	I	5	ILE	3.5
1	B	227	SER	3.5
1	G	95	LEU	3.5
1	L	207	ILE	3.5
1	E	205	GLN	3.4
1	L	228	LEU	3.4
1	A	164	ASN	3.4
1	K	228	LEU	3.4
1	B	25	ARG	3.4
1	I	168	LEU	3.4
1	G	68	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	101	ASN	3.3
1	G	64	VAL	3.3
1	K	24	LEU	3.3
1	D	32	VAL	3.3
1	K	232	GLN	3.3
1	J	141	HIS	3.3
1	H	196	VAL	3.2
1	H	13	TYR	3.2
1	G	69	ASP	3.2
1	F	74	SER	3.2
1	I	188	ILE	3.2
1	K	173	ILE	3.2
1	G	173	ILE	3.2
1	L	98	LYS	3.1
1	H	165	THR	3.1
1	F	231	LYS	3.1
1	H	150	ILE	3.1
1	I	59	ILE	3.1
1	I	155[A]	ARG	3.1
1	J	171	VAL	3.1
1	L	136	PHE	3.1
1	A	165	THR	3.1
1	G	118	HIS	3.1
1	C	231	LYS	3.1
1	H	219	ILE	3.0
1	A	229	PHE	3.0
1	A	166	ALA	3.0
1	K	35	SER	3.0
1	H	172	GLU	3.0
1	L	1	LEU	3.0
1	H	149	ALA	3.0
1	J	89	ALA	3.0
1	I	164	ASN	3.0
1	L	229	PHE	3.0
1	D	171	VAL	3.0
1	G	196	VAL	3.0
1	K	70	TYR	3.0
1	G	207	ILE	3.0
1	D	166	ALA	2.9
1	L	172	GLU	2.9
1	C	171	VAL	2.9
1	K	139	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	94	GLY	2.9
1	G	170	SER	2.9
1	D	89	ALA	2.9
1	J	61	ILE	2.9
1	F	2	ILE	2.9
1	A	63	SER	2.8
1	L	49	ASN	2.8
1	G	32	VAL	2.8
1	H	209	HIS	2.8
1	H	244	LEU	2.8
1	C	65	VAL	2.8
1	K	190	SER	2.8
1	L	157	SER	2.8
1	E	69	ASP	2.8
1	D	0	SER	2.8
1	G	216	GLN	2.8
1	L	132	THR	2.8
1	L	90	GLY	2.8
1	F	165	THR	2.8
1	A	39	GLY	2.7
1	H	223	GLY	2.7
1	J	1	LEU	2.7
1	L	72	LEU	2.7
1	I	30	SER	2.7
1	J	120	PHE	2.7
1	C	166	ALA	2.7
1	F	163	LYS	2.7
1	C	148	GLY	2.6
1	G	89	ALA	2.6
1	E	230	ASP	2.6
1	F	126	ILE	2.6
1	D	170	SER	2.6
1	E	117	THR	2.6
1	H	55	THR	2.6
1	G	251	ALA	2.6
1	L	255	THR	2.6
1	G	54	GLU	2.6
1	C	169	PRO	2.6
1	H	179	VAL	2.6
1	E	235	TYR	2.6
1	C	64	VAL	2.5
1	I	218	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	188	ILE	2.5
1	C	168	LEU	2.5
1	F	173	ILE	2.5
1	L	125	ILE	2.5
1	L	32	VAL	2.5
1	A	79	TYR	2.5
1	A	176	THR	2.5
1	H	93	THR	2.5
1	F	175	LYS	2.5
1	L	23	LYS	2.5
1	L	30	SER	2.5
1	D	68	VAL	2.5
1	J	64	VAL	2.5
1	G	132	THR	2.5
1	L	97	ILE	2.5
1	A	68	VAL	2.5
1	B	180	VAL	2.5
1	H	91	VAL	2.5
1	G	72	LEU	2.5
1	F	110	ILE	2.5
1	D	138	ALA	2.5
1	K	103	VAL	2.4
1	K	181	GLY	2.4
1	D	61	ILE	2.4
1	I	82	ILE	2.4
1	L	22	ILE	2.4
1	B	170	SER	2.4
1	H	163	LYS	2.4
1	H	124	ASN	2.4
1	B	182	ARG	2.4
1	H	178	SER	2.4
1	L	163	LYS	2.4
1	G	13	TYR	2.4
1	K	193	TYR	2.4
1	J	218	LEU	2.4
1	K	184	THR	2.3
1	K	178	SER	2.3
1	G	93	THR	2.3
1	B	62	CYS	2.3
1	J	213	ASN	2.3
1	E	67	GLN	2.3
1	H	210	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	161	LEU	2.3
1	A	217	ILE	2.3
1	E	2	ILE	2.3
1	E	163	LYS	2.3
1	E	110	ILE	2.3
1	G	46	LEU	2.3
1	J	20	ASP	2.3
1	L	239	VAL	2.3
1	H	122	ASN	2.2
1	A	255	THR	2.2
1	H	73	ARG	2.2
1	K	31	LYS	2.2
1	E	174	ILE	2.2
1	F	55	THR	2.2
1	K	45	VAL	2.2
1	H	89	ALA	2.2
1	C	207	ILE	2.2
1	D	227	SER	2.2
1	J	162	SER	2.2
1	J	147	GLY	2.2
1	L	100	ARG	2.2
1	E	188	ILE	2.2
1	H	230	ASP	2.2
1	F	14	GLY	2.2
1	G	212	PHE	2.2
1	G	219	ILE	2.2
1	A	193	TYR	2.2
1	H	157	SER	2.2
1	L	219	ILE	2.2
1	J	251	ALA	2.1
1	H	72	LEU	2.1
1	H	208	HIS	2.1
1	L	45	VAL	2.1
1	I	217	ILE	2.1
1	J	146	LEU	2.1
1	G	222	THR	2.1
1	F	32	VAL	2.1
1	F	45	VAL	2.1
1	J	174	ILE	2.1
1	J	179	VAL	2.1
1	L	212	PHE	2.1
1	I	60	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	57	ARG	2.0
1	H	100	ARG	2.0
1	G	65	VAL	2.0
1	L	171	VAL	2.0
1	C	212	PHE	2.0
1	L	79	TYR	2.0

## 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 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
2	GOL	A	265	6/6	0.94	0.22	2.23	57,74,86,98	0
2	GOL	H	266	6/6	0.81	0.28	0.52	69,76,85,96	0
2	GOL	L	265	6/6	0.89	0.20	-0.14	72,83,91,96	0
2	GOL	H	265	6/6	0.91	0.18	-0.23	76,84,104,108	0
2	GOL	B	265	6/6	0.95	0.13	-0.66	34,58,64,66	0
2	GOL	E	265	6/6	0.95	0.13	-0.70	39,43,46,55	0
2	GOL	E	266	6/6	0.96	0.12	-1.20	46,67,71,86	0
2	GOL	A	266	6/6	0.85	0.15	-1.41	60,68,70,71	0
2	GOL	C	265	6/6	0.74	0.18	-	47,55,76,79	0
2	GOL	J	265	6/6	0.76	0.31	-	61,84,87,91	0
2	GOL	C	266	6/6	0.90	0.14	-	51,62,70,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.