



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2016 – 02:07 PM EDT

PDB ID : 4N1A  
Title : Thermomonospora curvata EccC (ATPases 2 and 3) in complex with a signal sequence peptide  
Authors : Dovala, D.L.; Bendebury, A.; Cox, J.S.; Stroud, R.M.; Rosenberg, O.S.  
Deposited on : 2013-10-03  
Resolution : 3.24 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

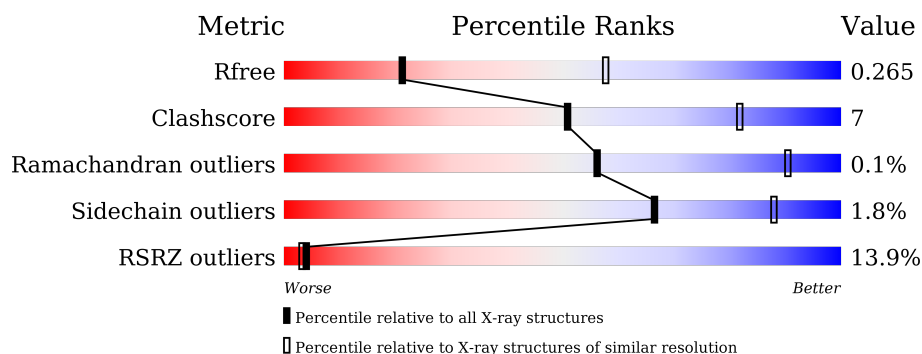
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.24 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	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)

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	589	<div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	B	589	<div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	C	589	<div> <div>79%</div> <div>14%</div> <div>6%</div> </div>
1	E	589	<div> <div>51%</div> <div>78%</div> <div>16%</div> <div>6%</div> </div>
2	G	23	<div> <div>17%</div> <div>13%</div> <div>70%</div> </div>
2	H	23	<div> <div>17%</div> <div>74%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	23	<div><div><div></div><div></div><div></div></div><div>17%9%.</div><div>70%</div></div>
2	K	23	<div><div><div></div><div></div><div></div></div><div>9%22%.</div><div>74%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17460 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 Cell divisionFtsK/SpoIIIE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4298	2712	762	814	10			
1	B	553	Total	C	N	O	S	0	0	0
			4229	2671	738	810	10			
1	C	554	Total	C	N	O	S	0	0	0
			4247	2682	744	811	10			
1	E	555	Total	C	N	O	S	0	0	0
			4292	2709	759	814	10			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	MET	-	EXPRESSION TAG	UNP D1A4G7
A	728	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	729	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	730	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	731	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	732	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	733	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	734	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	735	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	736	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	737	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	738	SER	-	EXPRESSION TAG	UNP D1A4G7
A	739	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	740	PHE	-	EXPRESSION TAG	UNP D1A4G7
A	741	SER	-	EXPRESSION TAG	UNP D1A4G7
A	742	ILE	-	EXPRESSION TAG	UNP D1A4G7
A	743	ASP	-	EXPRESSION TAG	UNP D1A4G7
A	744	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	745	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	746	SER	-	EXPRESSION TAG	UNP D1A4G7
A	747	LEU	-	EXPRESSION TAG	UNP D1A4G7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	748	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	749	VAL	-	EXPRESSION TAG	UNP D1A4G7
A	750	LEU	-	EXPRESSION TAG	UNP D1A4G7
A	751	PHE	-	EXPRESSION TAG	UNP D1A4G7
A	752	GLN	-	EXPRESSION TAG	UNP D1A4G7
A	753	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	754	PRO	-	EXPRESSION TAG	UNP D1A4G7
A	755	SER	-	EXPRESSION TAG	UNP D1A4G7
A	756	SER	-	EXPRESSION TAG	UNP D1A4G7
A	757	PRO	-	EXPRESSION TAG	UNP D1A4G7
A	758	SER	-	EXPRESSION TAG	UNP D1A4G7
B	727	MET	-	EXPRESSION TAG	UNP D1A4G7
B	728	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	729	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	730	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	731	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	732	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	733	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	734	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	735	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	736	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	737	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	738	SER	-	EXPRESSION TAG	UNP D1A4G7
B	739	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	740	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	741	SER	-	EXPRESSION TAG	UNP D1A4G7
B	742	ILE	-	EXPRESSION TAG	UNP D1A4G7
B	743	ASP	-	EXPRESSION TAG	UNP D1A4G7
B	744	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	745	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	746	SER	-	EXPRESSION TAG	UNP D1A4G7
B	747	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	748	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	749	VAL	-	EXPRESSION TAG	UNP D1A4G7
B	750	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	751	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	752	GLN	-	EXPRESSION TAG	UNP D1A4G7
B	753	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	754	PRO	-	EXPRESSION TAG	UNP D1A4G7
B	755	SER	-	EXPRESSION TAG	UNP D1A4G7
B	756	SER	-	EXPRESSION TAG	UNP D1A4G7
B	757	PRO	-	EXPRESSION TAG	UNP D1A4G7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	758	SER	-	EXPRESSION TAG	UNP D1A4G7
C	727	MET	-	EXPRESSION TAG	UNP D1A4G7
C	728	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	729	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	730	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	731	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	732	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	733	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	734	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	735	HIS	-	EXPRESSION TAG	UNP D1A4G7
C	736	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	737	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	738	SER	-	EXPRESSION TAG	UNP D1A4G7
C	739	GLU	-	EXPRESSION TAG	UNP D1A4G7
C	740	PHE	-	EXPRESSION TAG	UNP D1A4G7
C	741	SER	-	EXPRESSION TAG	UNP D1A4G7
C	742	ILE	-	EXPRESSION TAG	UNP D1A4G7
C	743	ASP	-	EXPRESSION TAG	UNP D1A4G7
C	744	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	745	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	746	SER	-	EXPRESSION TAG	UNP D1A4G7
C	747	LEU	-	EXPRESSION TAG	UNP D1A4G7
C	748	GLU	-	EXPRESSION TAG	UNP D1A4G7
C	749	VAL	-	EXPRESSION TAG	UNP D1A4G7
C	750	LEU	-	EXPRESSION TAG	UNP D1A4G7
C	751	PHE	-	EXPRESSION TAG	UNP D1A4G7
C	752	GLN	-	EXPRESSION TAG	UNP D1A4G7
C	753	GLY	-	EXPRESSION TAG	UNP D1A4G7
C	754	PRO	-	EXPRESSION TAG	UNP D1A4G7
C	755	SER	-	EXPRESSION TAG	UNP D1A4G7
C	756	SER	-	EXPRESSION TAG	UNP D1A4G7
C	757	PRO	-	EXPRESSION TAG	UNP D1A4G7
C	758	SER	-	EXPRESSION TAG	UNP D1A4G7
E	727	MET	-	EXPRESSION TAG	UNP D1A4G7
E	728	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	729	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	730	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	731	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	732	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	733	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	734	HIS	-	EXPRESSION TAG	UNP D1A4G7
E	735	HIS	-	EXPRESSION TAG	UNP D1A4G7

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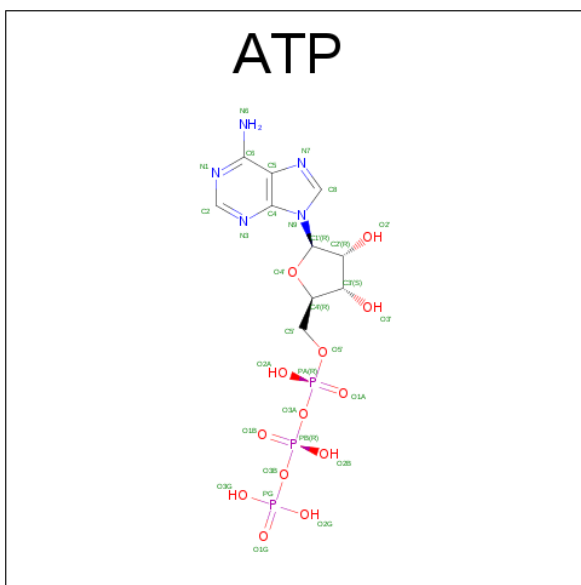
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Chain	Residue	Modelled	Actual	Comment	Reference
E	736	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	737	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	738	SER	-	EXPRESSION TAG	UNP D1A4G7
E	739	GLU	-	EXPRESSION TAG	UNP D1A4G7
E	740	PHE	-	EXPRESSION TAG	UNP D1A4G7
E	741	SER	-	EXPRESSION TAG	UNP D1A4G7
E	742	ILE	-	EXPRESSION TAG	UNP D1A4G7
E	743	ASP	-	EXPRESSION TAG	UNP D1A4G7
E	744	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	745	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	746	SER	-	EXPRESSION TAG	UNP D1A4G7
E	747	LEU	-	EXPRESSION TAG	UNP D1A4G7
E	748	GLU	-	EXPRESSION TAG	UNP D1A4G7
E	749	VAL	-	EXPRESSION TAG	UNP D1A4G7
E	750	LEU	-	EXPRESSION TAG	UNP D1A4G7
E	751	PHE	-	EXPRESSION TAG	UNP D1A4G7
E	752	GLN	-	EXPRESSION TAG	UNP D1A4G7
E	753	GLY	-	EXPRESSION TAG	UNP D1A4G7
E	754	PRO	-	EXPRESSION TAG	UNP D1A4G7
E	755	SER	-	EXPRESSION TAG	UNP D1A4G7
E	756	SER	-	EXPRESSION TAG	UNP D1A4G7
E	757	PRO	-	EXPRESSION TAG	UNP D1A4G7
E	758	SER	-	EXPRESSION TAG	UNP D1A4G7

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	0	0	0
			56	35	12	9			
2	H	6	Total	C	N	O	0	0	0
			48	31	10	7			
2	J	7	Total	C	N	O	0	0	0
			50	32	9	9			
2	K	6	Total	C	N	O	0	0	0
			45	29	8	8			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



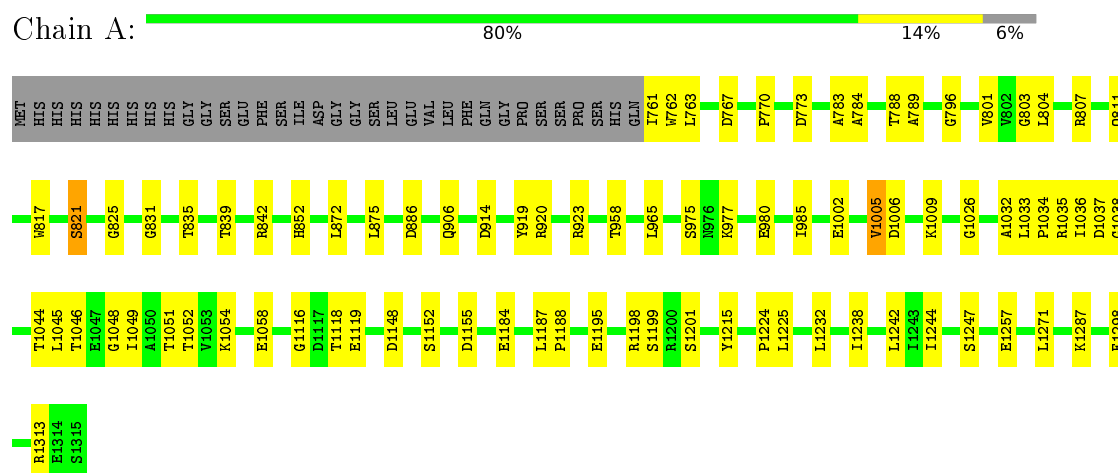


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		

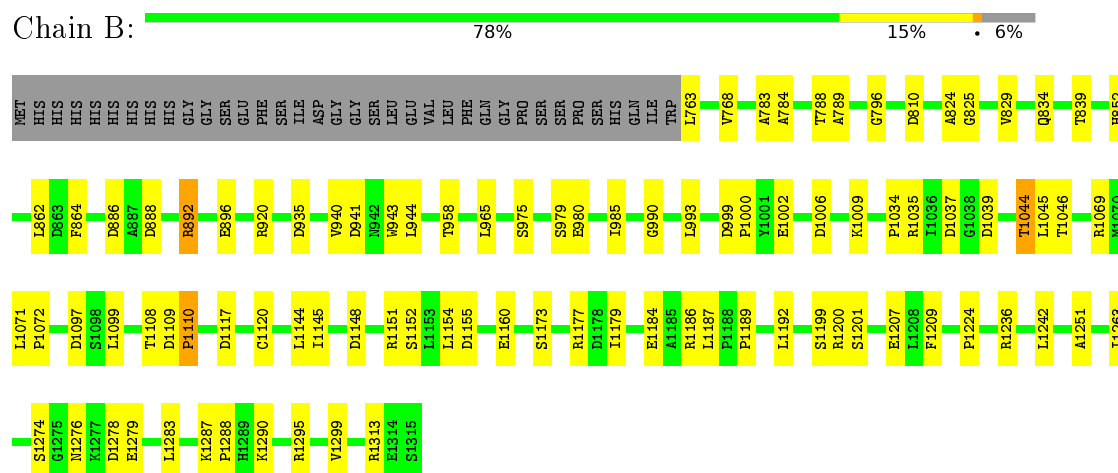
### 3 Residue-property plots

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

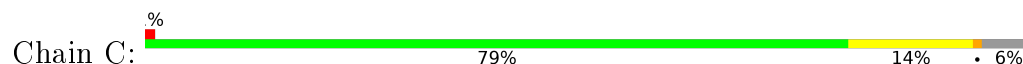
#### • Molecule 1: Cell divisionFtsK/SpoIIIE

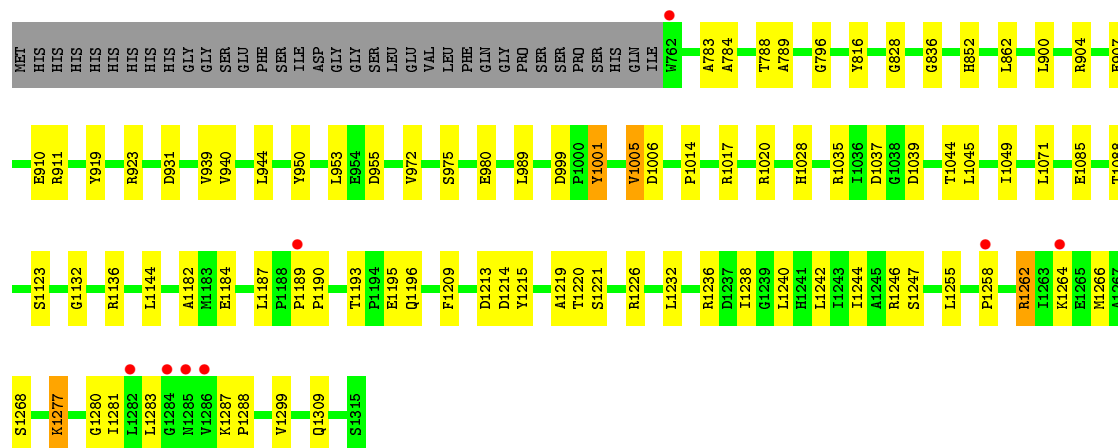


#### • Molecule 1: Cell divisionFtsK/SpoIIIE

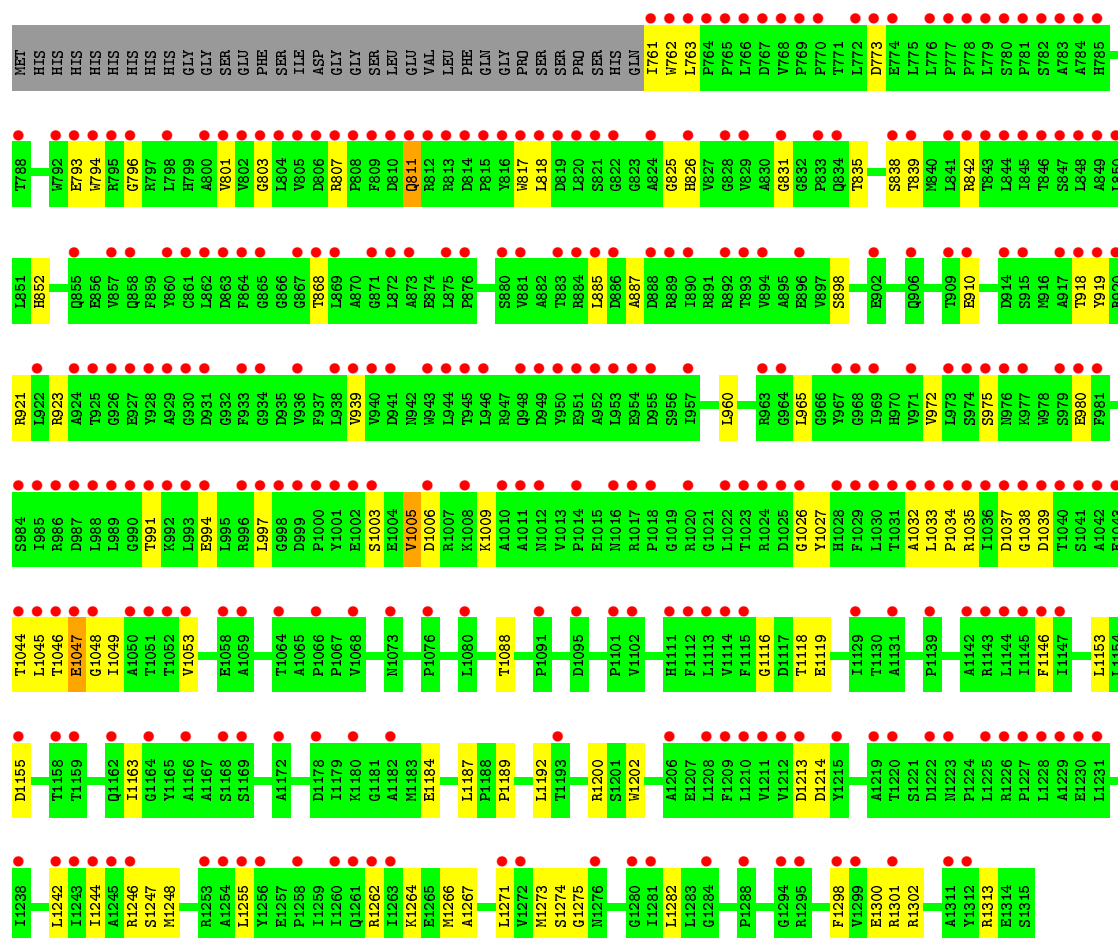


#### • Molecule 1: Cell divisionFtsK/SpoIIIE





• Molecule 1: Cell divisionFtsK/SpoIIIE



• Molecule 2: Uncharacterized protein

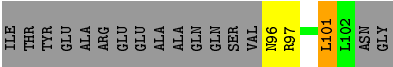




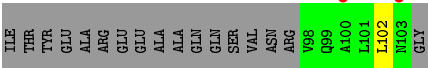
● Molecule 2: Uncharacterized protein



● Molecule 2: Uncharacterized protein



● Molecule 2: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.15Å 216.15Å 186.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 3.24 48.33 – 3.24	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.15-3.24) 100.0 (48.33-3.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.226 , 0.266 0.226 , 0.265	Depositor DCC
$R_{free}$ test set	2000 reflections (2.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17460	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	0.25	0/4395	0.40	0/5984
1	B	0.26	0/4324	0.43	1/5895 (0.0%)
1	C	0.20	0/4344	0.40	0/5924
1	E	0.28	0/4389	0.47	1/5977 (0.0%)
2	G	0.22	0/55	0.41	0/73
2	H	0.21	0/47	0.39	0/62
2	J	0.22	0/49	0.38	0/66
2	K	0.28	0/44	0.54	0/59
All	All	0.25	0/17647	0.43	2/24040 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	768	VAL	C-N-CD	5.94	140.87	128.40
1	E	1033	LEU	C-N-CD	5.73	140.44	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4298	0	4268	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4229	0	4164	57	0
1	C	4247	0	4175	60	0
1	E	4292	0	4257	73	0
2	G	56	0	62	2	0
2	H	48	0	56	2	0
2	J	50	0	51	3	0
2	K	45	0	49	1	0
3	A	62	0	24	1	0
3	B	62	0	24	3	0
3	C	62	0	24	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
5	B	1	0	0	0	0
All	All	17460	0	17154	238	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 7.

All (238) 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:E:1035:ARG:NH2	1:E:1037:ASP:OD2	1.80	1.13
1:E:1044:THR:HA	1:E:1047:GLU:OE2	1.56	0.98
1:C:1264:LYS:NZ	1:C:1268:SER:O	2.01	0.93
1:E:763:LEU:HD21	1:E:811:GLN:HA	1.57	0.86
1:E:1044:THR:CA	1:E:1047:GLU:OE2	2.24	0.85
1:E:1035:ARG:NH2	1:E:1039:ASP:HB3	1.94	0.82
1:C:1001:TYR:HD1	1:C:1001:TYR:H	1.29	0.81
1:B:1035:ARG:NH1	1:B:1039:ASP:HB3	1.94	0.81
1:E:1006:ASP:HB3	1:E:1009:LYS:HG3	1.61	0.81
1:E:1300:GLU:OE2	1:E:1302:ARG:NE	2.14	0.80
1:C:1277:LYS:HZ2	1:C:1280:GLY:H	1.29	0.79
1:E:997:LEU:HD12	1:E:1003:SER:HB2	1.63	0.79
1:C:1226:ARG:HG3	1:C:1226:ARG:HH11	1.48	0.78
1:B:975:SER:OG	1:B:980:GLU:OE2	2.01	0.77
1:E:1184:GLU:HA	1:E:1187:LEU:HD23	1.68	0.75
2:G:97:ARG:NH1	2:G:100:ALA:HB2	2.03	0.74
1:A:1035:ARG:NH1	1:A:1044:THR:O	2.21	0.73
1:E:1009:LYS:NZ	1:E:1026:GLY:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1148:ASP:OD2	1:B:1152:SER:N	2.22	0.72
1:E:761:ILE:HG23	1:E:762:TRP:H	1.55	0.72
1:E:1035:ARG:NH2	1:E:1037:ASP:CG	2.43	0.70
1:E:994:GLU:OE2	1:E:1003:SER:OG	2.07	0.69
1:E:1035:ARG:NH2	1:E:1039:ASP:CB	2.55	0.68
1:E:1242:LEU:HD23	1:E:1244:ILE:HD11	1.76	0.67
1:C:1035:ARG:HH11	1:C:1037:ASP:HB3	1.59	0.67
1:E:1035:ARG:CZ	1:E:1039:ASP:HB3	2.25	0.66
1:E:825:GLY:HA3	1:E:965:LEU:HD11	1.78	0.66
1:A:1184:GLU:HA	1:A:1187:LEU:HD23	1.78	0.65
1:E:839:THR:HG22	1:E:842:ARG:HH21	1.61	0.64
1:A:839:THR:HG22	1:A:842:ARG:HH21	1.60	0.64
1:C:950:TYR:HB3	1:C:953:LEU:HD13	1.79	0.64
1:E:1035:ARG:CZ	1:E:1037:ASP:OD2	2.46	0.63
1:A:1009:LYS:NZ	1:A:1026:GLY:O	2.29	0.63
2:G:97:ARG:HH11	2:G:100:ALA:HB2	1.62	0.63
1:E:975:SER:OG	1:E:980:GLU:OE1	2.17	0.62
1:B:1035:ARG:NH2	1:B:1044:THR:O	2.32	0.62
1:E:1035:ARG:HH21	1:E:1037:ASP:CG	2.03	0.61
1:A:977:LYS:HB3	1:A:1002:GLU:OE2	1.99	0.61
1:A:1242:LEU:HD23	1:A:1244:ILE:HD11	1.81	0.61
1:C:1232:LEU:HD11	1:C:1262:ARG:HB2	1.83	0.61
1:E:1006:ASP:CB	1:E:1009:LYS:HG3	2.30	0.61
1:E:997:LEU:CD1	1:E:1003:SER:HB2	2.30	0.61
1:B:1184:GLU:HA	1:B:1187:LEU:HD23	1.84	0.60
1:A:1006:ASP:OD2	1:A:1009:LYS:HG3	2.02	0.60
1:A:825:GLY:HA3	1:A:965:LEU:HD11	1.82	0.59
1:C:1035:ARG:NH1	1:C:1039:ASP:HB3	2.17	0.59
1:C:1226:ARG:NH1	1:C:1258:PRO:HG2	2.18	0.59
1:B:824:ALA:HA	1:B:990:GLY:HA3	1.83	0.58
1:C:910:GLU:HB2	1:E:1266:MET:HG2	1.84	0.58
1:B:1034:PRO:HD2	1:B:1045:LEU:HD11	1.85	0.58
1:B:1108:THR:O	1:B:1236:ARG:NH1	2.35	0.58
1:E:919:TYR:CZ	1:E:923:ARG:HD2	2.39	0.58
1:A:831:GLY:HA3	1:A:835:THR:HG21	1.85	0.57
1:E:1035:ARG:HH21	1:E:1039:ASP:CB	2.17	0.57
1:E:1044:THR:CB	1:E:1047:GLU:OE2	2.52	0.57
1:A:1036:ILE:HG12	1:A:1052:THR:HG23	1.85	0.57
1:A:761:ILE:HG23	1:A:762:TRP:H	1.69	0.56
1:E:1005:VAL:HG13	1:E:1006:ASP:H	1.70	0.56
1:A:975:SER:OG	1:A:980:GLU:OE1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1049:ILE:O	1:E:1053:VAL:HG23	2.04	0.56
1:C:1264:LYS:HD2	1:C:1283:LEU:HD22	1.86	0.56
1:B:839:THR:HG21	3:B:1401:ATP:N7	2.20	0.56
1:C:1226:ARG:HH12	1:C:1258:PRO:HG2	1.70	0.56
1:A:919:TYR:CZ	1:A:923:ARG:HD2	2.41	0.55
1:A:839:THR:HG23	3:A:1401:ATP:O1A	2.07	0.54
1:B:1035:ARG:HH12	1:B:1039:ASP:HB3	1.72	0.54
1:C:1266:MET:HA	1:E:910:GLU:HG2	1.89	0.54
1:E:1155:ASP:OD2	1:E:1313:ARG:NH2	2.40	0.54
1:E:831:GLY:HA3	1:E:835:THR:HG21	1.88	0.54
1:C:1035:ARG:NH2	1:C:1044:THR:O	2.40	0.54
1:C:1220:THR:OG1	1:C:1221:SER:N	2.40	0.54
1:E:1248:MET:HG3	1:E:1275:GLY:HA2	1.90	0.54
1:E:1118:THR:HG22	1:E:1119:GLU:HG3	1.90	0.53
1:E:796:GLY:HA2	1:E:852:HIS:CD2	2.44	0.53
1:C:1277:LYS:HZ2	1:C:1280:GLY:N	2.02	0.53
1:E:1035:ARG:NH1	1:E:1048:GLY:HA3	2.24	0.53
1:B:1199:SER:HG	1:B:1201:SER:HG	1.56	0.53
1:C:919:TYR:CZ	1:C:923:ARG:HD2	2.45	0.52
1:C:1071:LEU:HD13	1:C:1309:GLN:HB2	1.92	0.51
1:C:1277:LYS:NZ	1:C:1280:GLY:H	2.04	0.51
1:A:1045:LEU:O	1:A:1049:ILE:HG13	2.11	0.51
1:B:1283:LEU:HB3	1:B:1299:VAL:HG21	1.92	0.51
1:A:1155:ASP:OD1	1:A:1313:ARG:NH2	2.44	0.51
1:E:1271:LEU:HB3	1:E:1298:PHE:HA	1.93	0.51
1:B:1200:ARG:NH2	1:B:1207:GLU:OE1	2.41	0.50
1:E:773:ASP:OD1	1:E:773:ASP:N	2.44	0.50
1:C:1246:ARG:NH1	1:C:1247:SER:O	2.45	0.50
1:C:1144:LEU:HD23	1:C:1209:PHE:HB2	1.93	0.50
1:C:1236:ARG:NH2	1:E:910:GLU:OE2	2.41	0.50
1:B:796:GLY:HA2	1:B:852:HIS:CD2	2.47	0.49
1:C:1014:PRO:HB2	1:C:1017:ARG:HB3	1.92	0.49
1:B:862:LEU:HB2	1:B:940:VAL:HG12	1.94	0.49
1:E:1267:ALA:HB1	1:E:1301:ARG:HD2	1.93	0.49
1:C:1005:VAL:HG13	1:C:1006:ASP:H	1.78	0.49
1:C:1017:ARG:HB2	1:C:1017:ARG:NH1	2.27	0.49
1:B:1144:LEU:HD23	1:B:1209:PHE:HB2	1.93	0.49
1:E:1037:ASP:OD1	1:E:1038:GLY:N	2.45	0.49
1:B:1189:PRO:HD2	1:B:1192:LEU:HD11	1.94	0.49
1:B:920:ARG:NH1	1:B:935:ASP:OD2	2.45	0.49
1:B:1276:ASN:ND2	1:B:1278:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1246:ARG:HH11	1:E:1246:ARG:HG2	1.78	0.49
1:E:838:SER:HB3	1:E:868:THR:HG21	1.95	0.48
1:C:939:VAL:HG22	1:C:972:VAL:HB	1.95	0.48
1:E:839:THR:HG22	1:E:842:ARG:NH2	2.29	0.48
1:A:821:SER:HB3	1:A:920:ARG:HH12	1.78	0.48
1:A:1271:LEU:HB3	1:A:1298:PHE:HA	1.96	0.48
1:B:1035:ARG:HH11	1:B:1039:ASP:HB3	1.74	0.48
1:B:864:PHE:H	1:B:941:ASP:HB3	1.78	0.48
1:C:783:ALA:HA	1:C:784:ALA:HA	1.51	0.48
1:E:1035:ARG:HH21	1:E:1039:ASP:HB2	1.78	0.48
1:A:1118:THR:HG22	1:A:1119:GLU:HG3	1.96	0.48
1:A:1195:GLU:OE1	1:A:1198:ARG:NH1	2.46	0.48
1:B:1155:ASP:OD2	1:B:1313:ARG:NH2	2.47	0.47
1:B:825:GLY:H	1:B:965:LEU:HD21	1.79	0.47
1:B:958:THR:HG23	1:B:985:ILE:HB	1.95	0.47
1:E:1009:LYS:HE2	1:E:1009:LYS:HB3	1.62	0.47
1:A:886:ASP:OD1	1:A:886:ASP:N	2.47	0.47
1:A:1224:PRO:HG2	1:A:1225:LEU:HD12	1.96	0.47
1:E:1146:PHE:HD2	1:E:1153:LEU:HD23	1.79	0.47
1:A:788:THR:OG1	1:A:789:ALA:N	2.48	0.47
1:B:783:ALA:HA	1:B:784:ALA:HA	1.55	0.47
1:C:828:GLY:HA3	1:C:989:LEU:HD23	1.97	0.47
1:A:763:LEU:HD21	1:A:811:GLN:HA	1.97	0.47
1:C:836:GLY:HA2	3:C:1401:ATP:O1A	2.15	0.47
1:A:803:GLY:HA2	1:A:1032:ALA:HB2	1.95	0.47
1:C:788:THR:OG1	1:C:789:ALA:N	2.48	0.47
1:B:825:GLY:HA3	1:B:965:LEU:HD11	1.97	0.47
1:C:900:LEU:HD11	1:C:931:ASP:OD2	2.14	0.47
1:B:1035:ARG:NH1	1:B:1037:ASP:OD1	2.48	0.46
1:B:944:LEU:HB2	1:B:980:GLU:OE2	2.15	0.46
1:C:1283:LEU:HB3	1:C:1299:VAL:HG21	1.96	0.46
1:C:1123:SER:OG	3:C:1402:ATP:O1B	2.34	0.46
1:C:1226:ARG:NH1	1:C:1226:ARG:HG3	2.24	0.46
1:B:1290:LYS:H	1:B:1290:LYS:HD2	1.80	0.46
1:C:1277:LYS:HZ3	1:C:1280:GLY:HA2	1.81	0.46
1:B:1251:ALA:N	1:B:1279:GLU:OE2	2.46	0.46
1:B:999:ASP:N	1:B:1000:PRO:HD3	2.31	0.46
1:B:958:THR:HA	1:B:985:ILE:HD12	1.97	0.46
1:C:862:LEU:HB2	1:C:940:VAL:HG12	1.97	0.46
1:E:1163:ILE:HB	2:K:102:LEU:HD21	1.98	0.46
1:E:1116:GLY:O	1:E:1247:SER:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:803:GLY:HA2	1:E:1032:ALA:HB2	1.98	0.45
1:C:1213:ASP:OD1	1:C:1214:ASP:N	2.49	0.45
1:A:796:GLY:HA2	1:A:852:HIS:CD2	2.52	0.45
1:B:839:THR:HG22	3:B:1401:ATP:O1A	2.15	0.45
1:B:888:ASP:OD2	1:B:1295:ARG:NH1	2.49	0.45
1:A:767:ASP:N	1:A:767:ASP:OD1	2.36	0.45
1:C:1017:ARG:HH11	1:C:1017:ARG:HB2	1.81	0.45
1:C:1132:GLY:O	1:C:1136:ARG:HD3	2.17	0.45
1:B:1186:ARG:HH22	2:H:98:VAL:HG22	1.81	0.45
1:E:1262:ARG:O	1:E:1266:MET:HG3	2.16	0.45
1:B:1242:LEU:HD23	1:B:1263:ILE:HD11	1.99	0.45
1:B:834:GLN:NE2	3:B:1401:ATP:O3G	2.50	0.45
1:C:1215:TYR:CZ	1:C:1219:ALA:HB2	2.51	0.45
1:A:783:ALA:HA	1:A:784:ALA:HA	1.65	0.45
1:B:1186:ARG:NH2	2:H:98:VAL:HG22	2.32	0.44
1:A:773:ASP:N	1:A:773:ASP:OD1	2.46	0.44
1:C:1045:LEU:O	1:C:1049:ILE:HG13	2.18	0.44
1:B:979:SER:CB	1:B:1002:GLU:OE2	2.66	0.44
1:E:1035:ARG:NH2	1:E:1039:ASP:HB2	2.33	0.44
1:A:770:PRO:HG3	1:A:804:LEU:HG	2.00	0.44
1:B:892:ARG:NH2	1:B:1099:LEU:HG	2.32	0.44
1:B:1117:ASP:OD1	1:B:1120:CYS:HB3	2.18	0.43
1:E:918:THR:HG23	1:E:921:ARG:HH22	1.82	0.43
1:A:1187:LEU:HD13	1:A:1188:PRO:HD2	2.00	0.43
1:B:1145:ILE:HD12	1:B:1179:ILE:HD11	1.99	0.43
1:E:793:GLU:HG3	1:E:794:TRP:CD1	2.53	0.43
1:E:898:SER:HA	1:E:960:LEU:HD11	1.99	0.43
1:A:1215:TYR:HE2	1:A:1257:GLU:OE2	2.01	0.43
1:C:1226:ARG:NH1	1:C:1226:ARG:CG	2.81	0.43
1:B:999:ASP:N	1:B:1000:PRO:CD	2.81	0.43
1:A:1037:ASP:OD1	1:A:1038:GLY:N	2.52	0.43
1:C:1182:ALA:HB2	2:J:101:LEU:HD13	2.00	0.43
2:J:96:ASN:OD1	2:J:97:ARG:N	2.41	0.43
1:A:1035:ARG:NH1	1:A:1048:GLY:HA3	2.34	0.43
1:A:872:LEU:HB3	1:A:875:LEU:HD12	2.00	0.43
1:B:1006:ASP:HB3	1:B:1009:LYS:HB2	2.01	0.42
1:E:1044:THR:OG1	1:E:1047:GLU:OE2	2.36	0.42
1:B:788:THR:OG1	1:B:789:ALA:N	2.52	0.42
1:E:763:LEU:HD23	1:E:763:LEU:HA	1.82	0.42
1:A:807:ARG:NH2	1:B:810:ASP:OD1	2.52	0.42
1:C:1035:ARG:HH21	1:C:1045:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:VAL:HG21	1:B:943:TRP:HE3	1.84	0.42
1:C:1277:LYS:NZ	1:C:1280:GLY:N	2.63	0.42
1:C:796:GLY:HA2	1:C:852:HIS:CD2	2.54	0.42
1:E:1264:LYS:HD2	1:E:1282:LEU:O	2.20	0.42
1:A:1187:LEU:HD22	1:A:1238:ILE:HG21	1.99	0.42
1:C:1242:LEU:HD23	1:C:1244:ILE:HD11	2.02	0.42
1:E:939:VAL:HG22	1:E:972:VAL:HB	2.00	0.42
1:C:904:ARG:HA	1:C:907:GLU:HB3	2.00	0.42
1:E:1213:ASP:OD1	1:E:1214:ASP:N	2.53	0.42
2:J:97:ARG:O	2:J:101:LEU:HB2	2.20	0.42
1:B:892:ARG:NH1	1:B:896:GLU:OE1	2.53	0.42
1:B:979:SER:HB3	1:B:1002:GLU:OE2	2.19	0.42
1:E:1189:PRO:HD2	1:E:1192:LEU:HD11	2.02	0.42
1:E:818:LEU:HD13	1:E:991:THR:HG21	2.01	0.42
1:A:1005:VAL:HG13	1:A:1006:ASP:H	1.84	0.42
1:A:1054:LYS:HE3	1:A:1058:GLU:OE2	2.20	0.42
1:B:1287:LYS:HA	1:B:1288:PRO:HD3	1.84	0.42
1:C:1238:ILE:HG13	1:C:1240:LEU:H	1.85	0.42
1:A:914:ASP:N	1:A:914:ASP:OD1	2.53	0.41
1:C:1184:GLU:HA	1:C:1187:LEU:HG	2.02	0.41
1:E:807:ARG:HG2	1:E:1027:TYR:CD1	2.55	0.41
1:A:1033:LEU:HA	1:A:1034:PRO:HD3	1.83	0.41
1:E:1200:ARG:HA	1:E:1202:TRP:CZ3	2.54	0.41
1:E:918:THR:HG23	1:E:921:ARG:NH2	2.35	0.41
1:A:1287:LYS:HE3	1:A:1287:LYS:HB2	1.96	0.41
1:B:892:ARG:O	1:B:892:ARG:HD3	2.20	0.41
1:A:1232:LEU:HA	1:A:1232:LEU:HD23	1.91	0.41
1:B:1071:LEU:HA	1:B:1072:PRO:HD3	1.93	0.41
1:B:1173:SER:HB2	1:B:1224:PRO:HB3	2.02	0.41
1:C:1020:ARG:HH21	1:C:1028:HIS:HB3	1.85	0.41
1:C:919:TYR:OH	1:C:931:ASP:OD1	2.28	0.41
1:E:885:LEU:O	1:E:887:ALA:N	2.54	0.41
1:A:1116:GLY:O	1:A:1247:SER:HA	2.20	0.41
1:C:1193:THR:HG22	1:C:1195:GLU:H	1.85	0.41
1:C:1085:GLU:HA	1:E:1088:THR:HG23	2.03	0.41
1:A:958:THR:HG23	1:A:985:ILE:HB	2.02	0.41
1:C:944:LEU:HD22	1:C:980:GLU:OE2	2.21	0.41
1:E:826:HIS:CE1	1:E:965:LEU:HD13	2.56	0.41
1:E:1271:LEU:HD11	1:E:1273:MET:CE	2.51	0.41
1:C:975:SER:OG	1:C:980:GLU:OE1	2.36	0.41
1:A:1199:SER:OG	1:A:1201:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1035:ARG:HD3	1:C:1037:ASP:HB3	2.03	0.41
1:C:1287:LYS:HA	1:C:1288:PRO:HD3	1.94	0.41
1:A:801:VAL:HB	1:A:817:TRP:CE2	2.56	0.40
1:C:904:ARG:NE	1:C:931:ASP:OD2	2.49	0.40
1:E:1255:LEU:HD13	1:E:1264:LYS:HE2	2.03	0.40
1:A:1148:ASP:OD2	1:A:1152:SER:N	2.54	0.40
1:B:1109:ASP:HA	1:B:1110:PRO:HD3	1.88	0.40
1:E:1273:MET:O	1:E:1274:SER:C	2.59	0.40
1:E:801:VAL:HB	1:E:817:TRP:CE2	2.56	0.40
1:B:1151:ARG:HB3	1:B:1154:LEU:HD21	2.04	0.40
1:B:829:VAL:HG22	1:B:993:LEU:HB2	2.04	0.40
1:B:892:ARG:HD2	1:B:1069:ARG:O	2.21	0.40
1:A:1035:ARG:CZ	1:A:1048:GLY:HA3	2.51	0.40
1:C:1189:PRO:HA	1:C:1190:PRO:HD3	1.89	0.40
1:E:1034:PRO:HD2	1:E:1045:LEU:HD11	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	553/589 (94%)	535 (97%)	18 (3%)	0	100	100
1	B	551/589 (94%)	524 (95%)	26 (5%)	1 (0%)	52	87
1	C	552/589 (94%)	515 (93%)	37 (7%)	0	100	100
1	E	553/589 (94%)	536 (97%)	16 (3%)	1 (0%)	52	87
2	G	5/23 (22%)	5 (100%)	0	0	100	100
2	H	4/23 (17%)	4 (100%)	0	0	100	100
2	J	5/23 (22%)	5 (100%)	0	0	100	100
2	K	4/23 (17%)	2 (50%)	2 (50%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2227/2448 (91%)	2126 (96%)	99 (4%)	2 (0%)	56 90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	886	ASP
1	E	1005	VAL

### 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	455/485 (94%)	450 (99%)	5 (1%)	80 93
1	B	445/485 (92%)	436 (98%)	9 (2%)	63 87
1	C	446/485 (92%)	434 (97%)	12 (3%)	52 83
1	E	454/485 (94%)	451 (99%)	3 (1%)	88 96
2	G	6/18 (33%)	5 (83%)	1 (17%)	3 13
2	H	5/18 (28%)	3 (60%)	2 (40%)	0 0
2	J	5/18 (28%)	4 (80%)	1 (20%)	1 7
2	K	5/18 (28%)	5 (100%)	0	100 100
All	All	1821/2012 (90%)	1788 (98%)	33 (2%)	66 88

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	821	SER
1	A	906	GLN
1	A	1005	VAL
1	A	1046	THR
1	A	1051	THR
1	B	763	LEU
1	B	892	ARG
1	B	1044	THR

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Mol	Chain	Res	Type
1	B	1046	THR
1	B	1097	ASP
1	B	1110	PRO
1	B	1160	GLU
1	B	1177	ARG
1	B	1274	SER
1	C	816	TYR
1	C	911	ARG
1	C	955	ASP
1	C	999	ASP
1	C	1001	TYR
1	C	1005	VAL
1	C	1088	THR
1	C	1196	GLN
1	C	1255	LEU
1	C	1262	ARG
1	C	1277	LYS
1	C	1281	ILE
2	G	98	VAL
2	H	98	VAL
2	H	101	LEU
2	J	101	LEU
1	E	811	GLN
1	E	1046	THR
1	E	1047	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	99	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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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
3	ATP	A	1401	4	26,33,33	0.97	1 (3%)	26,52,52	1.61	1 (3%)
3	ATP	A	1402	4	26,33,33	0.97	1 (3%)	26,52,52	1.61	1 (3%)
3	ATP	B	1401	4	26,33,33	0.97	1 (3%)	26,52,52	1.59	1 (3%)
3	ATP	B	1402	4	26,33,33	0.97	1 (3%)	26,52,52	1.61	1 (3%)
3	ATP	C	1401	4	26,33,33	0.97	1 (3%)	26,52,52	1.64	1 (3%)
3	ATP	C	1402	4	26,33,33	0.96	1 (3%)	26,52,52	1.60	1 (3%)

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
3	ATP	A	1401	4	-	0/18/38/38	0/3/3/3
3	ATP	A	1402	4	-	0/18/38/38	0/3/3/3
3	ATP	B	1401	4	-	0/18/38/38	0/3/3/3
3	ATP	B	1402	4	-	0/18/38/38	0/3/3/3
3	ATP	C	1401	4	-	0/18/38/38	0/3/3/3
3	ATP	C	1402	4	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1402	ATP	C5-C4	3.11	1.47	1.40
3	B	1401	ATP	C5-C4	3.12	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1401	ATP	C5-C4	3.14	1.47	1.40
3	A	1402	ATP	C5-C4	3.14	1.47	1.40
3	B	1402	ATP	C5-C4	3.14	1.47	1.40
3	A	1401	ATP	C5-C4	3.14	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1401	ATP	N3-C2-N1	-6.47	123.79	128.87
3	B	1402	ATP	N3-C2-N1	-6.43	123.82	128.87
3	A	1401	ATP	N3-C2-N1	-6.42	123.82	128.87
3	C	1402	ATP	N3-C2-N1	-6.36	123.88	128.87
3	A	1402	ATP	N3-C2-N1	-6.26	123.95	128.87
3	B	1401	ATP	N3-C2-N1	-6.25	123.96	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1401	ATP	1	0
3	B	1401	ATP	3	0
3	C	1401	ATP	1	0
3	C	1402	ATP	1	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 ⓘ

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	555/589 (94%)	-0.35	0 100 100	25, 48, 78, 103	0
1	B	553/589 (93%)	-0.33	0 100 100	29, 55, 90, 122	0
1	C	554/589 (94%)	-0.08	8 (1%) 78 67	43, 84, 137, 177	0
1	E	555/589 (94%)	2.40	301 (54%) 0 0	122, 187, 222, 279	0
2	G	7/23 (30%)	-0.30	0 100 100	64, 66, 92, 95	0
2	H	6/23 (26%)	-0.03	0 100 100	96, 102, 122, 128	0
2	J	7/23 (30%)	0.01	0 100 100	102, 110, 118, 124	0
2	K	6/23 (26%)	1.55	2 (33%) 0 1	136, 159, 170, 175	0
All	All	2243/2448 (91%)	0.41	311 (13%) 4 3	25, 72, 205, 279	0

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	767	ASP	10.2
1	E	801	VAL	9.2
1	E	934	GLY	8.3
1	E	816	TYR	8.3
1	E	988	LEU	7.7
1	E	841	LEU	7.4
1	E	817	TRP	7.2
1	E	794	TRP	7.0
1	E	784	ALA	6.9
1	E	761	ILE	6.8
1	E	769	PRO	6.8
1	E	762	TRP	6.7
1	E	975	SER	6.7
1	E	950	TYR	6.6
1	E	850	LEU	6.6
1	E	768	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
1	E	808	PRO	6.5
1	E	829	VAL	6.5
1	E	818	LEU	6.4
1	E	764	PRO	6.3
1	E	998	GLY	6.3
1	E	999	ASP	5.9
1	E	914	ASP	5.9
1	E	1228	LEU	5.9
1	E	927	GLU	5.9
1	E	848	LEU	5.8
1	E	953	LEU	5.8
1	E	946	LEU	5.8
1	E	806	ASP	5.7
1	E	1031	THR	5.7
1	E	814	ASP	5.7
1	E	765	PRO	5.6
1	E	819	ASP	5.6
1	E	802	VAL	5.5
1	E	1003	SER	5.5
1	E	1053	VAL	5.5
1	E	783	ALA	5.5
1	E	811	GLN	5.5
1	E	863	ASP	5.4
1	E	1018	PRO	5.3
1	E	1215	TYR	5.3
1	E	940	VAL	5.3
1	E	1046	THR	5.2
1	E	922	LEU	5.1
1	E	1145	ILE	5.1
1	E	843	THR	5.1
1	E	1002	GLU	5.1
1	E	855	GLN	4.9
1	E	1051	THR	4.9
1	E	1039	ASP	4.9
1	E	881	VAL	4.9
1	E	1026	GLY	4.9
1	E	1032	ALA	4.9
1	E	763	LEU	4.8
1	E	777	PRO	4.8
1	E	1029	PHE	4.8
1	E	949	ASP	4.7
1	E	792	TRP	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	845	ILE	4.7
1	E	766	LEU	4.7
1	E	772	LEU	4.6
1	E	1255	LEU	4.6
1	E	928	TYR	4.6
1	E	773	ASP	4.6
1	E	1017	ARG	4.6
1	E	1144	LEU	4.6
1	E	994	GLU	4.6
1	E	807	ARG	4.6
1	E	820	LEU	4.6
1	E	844	LEU	4.5
1	E	973	LEU	4.5
1	E	804	LEU	4.5
2	K	103	ASN	4.5
1	E	1052	THR	4.5
1	E	774	GLU	4.4
1	E	1112	PHE	4.4
1	E	930	GLY	4.4
1	E	828	GLY	4.4
1	E	810	ASP	4.4
1	E	1091	PRO	4.4
1	E	834	GLN	4.3
1	E	926	GLY	4.3
1	E	954	GLU	4.2
1	E	991	THR	4.2
1	E	880	SER	4.2
1	E	945	THR	4.2
1	E	993	LEU	4.2
1	E	1115	PHE	4.2
1	E	948	GLN	4.2
1	E	1162	GLN	4.2
1	E	1011	ALA	4.1
1	E	776	LEU	4.1
1	E	778	PRO	4.1
1	E	1012	ASN	4.1
1	E	979	SER	4.1
1	E	976	ASN	4.1
1	E	805	VAL	4.0
1	E	800	ALA	4.0
1	E	809	PHE	4.0
1	E	1146	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	871	GLY	3.9
1	E	919	TYR	3.9
1	E	1281	ILE	3.9
1	E	849	ALA	3.9
1	E	1242	LEU	3.9
1	E	974	SER	3.9
1	E	933	PHE	3.8
1	E	894	VAL	3.8
1	E	864	PHE	3.8
1	E	1045	LEU	3.8
1	E	1068	VAL	3.8
1	E	1231	LEU	3.8
1	E	893	THR	3.8
1	E	925	THR	3.8
1	E	1223	ASN	3.8
1	E	989	LEU	3.7
1	E	1044	THR	3.7
1	E	1271	LEU	3.7
1	E	1006	ASP	3.7
1	E	858	GLN	3.7
1	E	1113	LEU	3.7
1	C	1285	ASN	3.6
1	E	846	THR	3.6
1	E	1280	GLY	3.6
1	E	1288	PRO	3.6
1	E	1258	PRO	3.6
1	E	1256	TYR	3.6
1	E	917	ALA	3.6
1	E	1155	ASP	3.6
1	E	1001	TYR	3.6
1	E	1000	PRO	3.5
1	E	1299	VAL	3.5
1	E	1010	ALA	3.5
1	E	1276	ASN	3.5
1	E	798	LEU	3.5
1	E	1260	ILE	3.5
1	E	813	ARG	3.5
1	E	971	VAL	3.5
1	E	890	ILE	3.5
1	E	847	SER	3.5
1	E	788	THR	3.4
1	E	812	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	780	SER	3.4
1	E	860	TYR	3.4
1	E	1014	PRO	3.4
1	E	1147	ILE	3.4
1	C	1282	LEU	3.4
1	E	1111	HIS	3.3
1	C	1258	PRO	3.3
1	E	1038	GLY	3.3
1	E	1143	ARG	3.3
1	E	1166	ALA	3.3
1	E	803	GLY	3.3
1	E	918	THR	3.2
1	E	793	GLU	3.2
1	E	1244	ILE	3.2
1	E	984	SER	3.2
1	E	839	THR	3.2
1	E	795	ARG	3.2
1	E	1226	ARG	3.2
1	E	992	LYS	3.2
1	E	865	GLY	3.2
1	E	1208	LEU	3.2
1	E	1037	ASP	3.2
1	E	944	LEU	3.2
1	E	892	ARG	3.1
1	E	1030	LEU	3.1
1	E	1213	ASP	3.1
1	E	867	GLY	3.1
1	E	1311	ALA	3.1
1	E	969	ILE	3.1
1	E	1229	ALA	3.1
1	E	987	ASP	3.0
1	E	884	ARG	3.0
1	E	869	LEU	3.0
1	E	872	LEU	3.0
1	E	796	GLY	3.0
1	E	876	PRO	3.0
1	E	1034	PRO	3.0
1	E	861	CYS	3.0
1	E	1243	ILE	2.9
1	E	929	ALA	2.9
1	E	1253	ARG	2.9
1	E	1080	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	1129	ILE	2.9
1	E	1101	PRO	2.9
1	E	943	TRP	2.9
1	E	1047	GLU	2.9
1	E	868	THR	2.9
1	E	1114	VAL	2.9
1	E	1225	LEU	2.9
1	E	967	TYR	2.9
1	E	957	ILE	2.9
1	E	1211	VAL	2.8
1	C	1284	GLY	2.8
1	E	1066	PRO	2.8
1	E	1022	LEU	2.8
1	E	1210	LEU	2.8
1	E	931	ASP	2.8
1	E	941	ASP	2.8
1	E	1028	HIS	2.8
1	E	1180	LYS	2.8
1	E	1041	SER	2.8
1	E	1036	ILE	2.8
1	E	1219	ALA	2.8
1	E	951	GLU	2.8
1	E	939	VAL	2.8
1	C	1189	PRO	2.8
1	E	924	ALA	2.8
1	E	888	ASP	2.8
1	E	1048	GLY	2.8
1	E	980	GLU	2.7
1	E	915	SER	2.7
1	E	883	THR	2.7
1	E	1246	ARG	2.7
1	E	1164	GLY	2.7
1	E	1064	THR	2.7
1	E	985	ILE	2.7
1	E	1020	ARG	2.7
1	E	1230	GLU	2.7
1	E	1227	PRO	2.7
1	E	1254	ALA	2.7
1	E	886	ASP	2.7
1	E	781	PRO	2.7
1	E	821	SER	2.7
1	E	1042	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	955	ASP	2.7
1	E	1035	ARG	2.7
1	E	1158	THR	2.6
1	E	833	PRO	2.6
1	E	1262	ARG	2.6
1	E	1168	SER	2.6
2	K	100	ALA	2.6
1	E	779	LEU	2.6
1	E	963	ARG	2.6
1	E	1212	VAL	2.6
1	E	952	ALA	2.6
1	E	906	GLN	2.5
1	E	1182	ALA	2.5
1	E	1142	ALA	2.5
1	E	1095	ASP	2.5
1	E	815	PRO	2.5
1	E	1139	PRO	2.5
1	E	1220	THR	2.5
1	E	1261	GLN	2.5
1	E	1159	THR	2.5
1	E	1238	ILE	2.5
1	E	1222	ASP	2.5
1	E	842	ARG	2.5
1	E	997	LEU	2.4
1	E	1294	GLY	2.4
1	E	1023	THR	2.4
1	E	1178	ASP	2.4
1	E	873	ALA	2.4
1	E	902	GLU	2.4
1	E	1131	ALA	2.4
1	E	1298	PHE	2.4
1	E	910	GLU	2.4
1	E	831	GLY	2.4
1	E	824	ALA	2.4
1	E	1172	ALA	2.4
1	E	770	PRO	2.4
1	E	1040	THR	2.4
1	E	1043	GLU	2.3
1	E	1058	GLU	2.3
1	C	1286	VAL	2.3
1	E	1284	GLY	2.3
1	E	1076	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	1024	ARG	2.3
1	C	762	TRP	2.3
1	E	909	THR	2.3
1	E	1016	ASN	2.3
1	E	977	LYS	2.3
1	E	822	GLY	2.3
1	E	981	PHE	2.2
1	E	1272	VAL	2.2
1	E	889	ARG	2.2
1	E	875	LEU	2.2
1	E	857	VAL	2.2
1	E	1059	ALA	2.2
1	E	826	HIS	2.2
1	C	1264	LYS	2.2
1	E	990	GLY	2.2
1	E	1206	ALA	2.2
1	E	1301	ARG	2.2
1	E	1169	SER	2.2
1	E	1033	LEU	2.2
1	E	1073	ASN	2.2
1	E	1295	ARG	2.2
1	E	968	GLY	2.1
1	E	782	SER	2.1
1	E	885	LEU	2.1
1	E	1209	PHE	2.1
1	E	938	LEU	2.1
1	E	785	HIS	2.1
1	E	838	SER	2.1
1	E	996	ARG	2.1
1	E	1263	ILE	2.1
1	E	920	ARG	2.1
1	E	986	ARG	2.1
1	E	1245	ALA	2.1
1	E	1312	TYR	2.1
1	E	964	GLY	2.1
1	E	1008	LYS	2.0
1	E	896	GLU	2.0
1	E	936	VAL	2.0
1	E	1025	ASP	2.0
1	E	1050	ALA	2.0
1	E	1193	THR	2.0
1	E	862	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	1102	VAL	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
3	ATP	B	1402	31/31	0.94	0.19	0.09	43,58,78,120	0
3	ATP	C	1402	31/31	0.95	0.17	0.07	54,68,77,83	0
3	ATP	B	1401	31/31	0.96	0.19	0.06	28,44,68,79	0
3	ATP	C	1401	31/31	0.96	0.17	-0.43	35,60,79,88	0
3	ATP	A	1402	31/31	0.97	0.17	-0.61	24,39,57,88	0
3	ATP	A	1401	31/31	0.97	0.17	-0.64	38,62,77,82	0
4	MG	B	1404	1/1	0.99	0.19	-	34,34,34,34	0
4	MG	E	1402	1/1	-0.27	0.64	-	286,286,286,286	0
4	MG	C	1404	1/1	0.97	0.22	-	45,45,45,45	0
4	MG	E	1401	1/1	0.06	0.40	-	204,204,204,204	0
4	MG	A	1404	1/1	0.97	0.23	-	45,45,45,45	0
4	MG	C	1403	1/1	0.96	0.19	-	55,55,55,55	0
4	MG	A	1403	1/1	0.97	0.40	-	43,43,43,43	0
4	MG	B	1403	1/1	0.96	0.21	-	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.