

# Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 06:57 am BST

PDB ID : 5LON

Title: Structure of /K. lactis/ Dcp1-Dcp2 decapping complex.

Authors: Charenton, C.; Taverniti, V.; Gaudon-Plesse, C.; Back, R.; Seraphin, B.;

Graille, M.

Deposited on : 2016-08-09

Resolution : 3.50 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

EDS : 2.11

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)

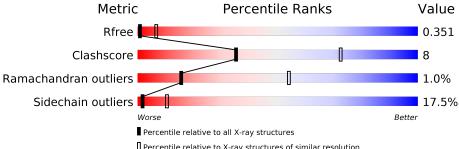
Validation Pipeline (wwPDB-VP) : 2.11

#### Overall quality at a glance (i) 1

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



Percentile relative to X-ray structures of similar resolution

Metric	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 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  $\leq 5\%$ 

Mol	Chain	Length	Quality of chain				
1	A	281	58%	18% •	21%		
2	В	188	55%	34%	• 7%		



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3242 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 KLLA0F23980p.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	${f AltConf}$	Trace		
1	A	221	Total 1807	C 1177	N 298	O 326	S 6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	HIS	_	expression tag	UNP Q6CIU1
A	277	HIS	-	expression tag	UNP Q6CIU1
A	278	HIS	_	expression tag	UNP Q6CIU1
A	279	HIS	-	expression tag	UNP Q6CIU1
A	280	HIS	_	expression tag	UNP Q6CIU1
A	281	HIS	-	expression tag	UNP Q6CIU1

• Molecule 2 is a protein called KLLA0E01827p.

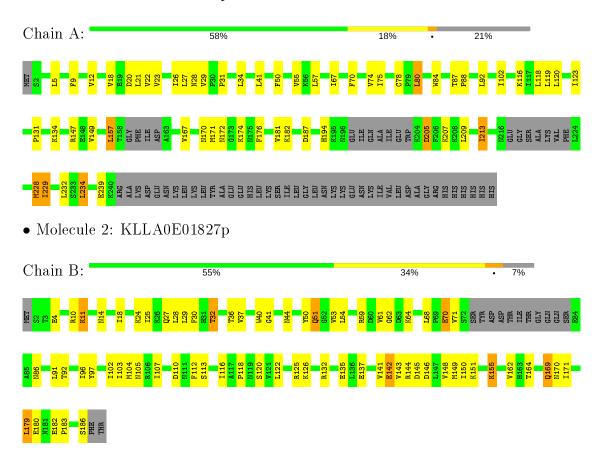
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	174	Total	С	N	О	S	0	0	0
		114	1435	923	241	268	3			U



## 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: KLLA0F23980p





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants	216.69Å 216.69Å 216.69Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.45 - 3.50	Depositor
Resolution (A)	46.20 - 3.50	EDS
% Data completeness	100.0 (48.45-3.50)	Depositor
(in resolution range)	100.0 (46.20-3.50)	EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.26	Depositor
$< I/\sigma(I) > 1$	1.20 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
P. P.	0.250 , 0.312	Depositor
$R, R_{free}$	0.299 , $0.351$	DCC
$R_{free}$ test set	543 reflections $(4.82%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	147.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 268.5	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.43, < L^2>=0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3242	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.

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



 $<sup>^{1}</sup>$ Intensities estimated from amplitudes.

### 5 Model quality (i)

### 5.1 Standard geometry (i)

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		
10101	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	Α	0.51	0/1848	0.70	0/2495	
2	В	0.52	0/1468	0.75	1/1994 (0.1%)	
All	All	0.51	0/3316	0.72	1/4489 (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
2	В	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	146	ASP	CB-CG-OD2	5.23	123.00	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Group
2	В	70	GLU	Peptide

#### 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	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	A	1807	0	1836	22	0
2	В	1435	0	1429	32	0
All	All	3242	0	3265	53	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 8.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

2:B:61:VAL:HG21	Atom-1	Atom-2	Interatomic	Clash
2:B:50:TYR:HA         2:B:105:ASN:HD21         1.55         0.71           1:A:102:ILE:HB         1:A:174:LYS:HG2         1.73         0.68           1:A:21:LEU:HD21         1:A:50:PHE:HD1         1.58         0.66           1:A:41:LEU:HD22         1:A:92:LEU:HB3         1.79         0.63           2:B:30:PHE:CE2         2:B:171:ILE:HG22         2.33         0.63           2:B:32:THR:HG22         2:B:51-ILE:HD11         1.82         0.62           2:B:51:GLN:HB3         2:B:107:ILE:HD11         1.82         0.61           2:B:53:VAL:HG13         2:B:104:MET:HB2         1.83         0.60           2:B:137:GLU:OE2         2:B:155:LYS:HG2         2.00         0.60           2:B:137:GLU:OE2         2:B:155:LYS:HB2         2.01         0.60           2:B:182:GLU:HG3         2:B:183:PRO:HD2         1.85         0.58           2:B:32:THR:O         2:B:50:ASN:ND2         2.19         0.57           2:B:32:THR:O         2:B:53:VS:CE         2.55         0.56           2:B:137:GLU:OE2         2:B:155:LYS:CE         2.55         0.55           1:A:27:LEU:HD23         1:A:28:HB3         1.88         0.55           2:B:19:LEU:HD23         2:B:155:LYS:CG         2.56         0.54	0 D 01 1141 11C01		distance (Å)	overlap (Å)
1:A:102:ILE:HB       1:A:174:LYS:HG2       1.73       0.68         1:A:21:LEU:HD21       1:A:50:PHE:HD1       1.58       0.66         1:A:41:LEU:HD22       1:A:92:LEU:HB3       1.79       0.63         2:B:30:PHE:CE2       2:B:54:LEU:HB3       1.79       0.63         2:B:32:THR:HG22       2:B:54:LEU:HB3       1.82       0.62         2:B:51:GLN:HB3       2:B:107:ILE:HD11       1.82       0.61         2:B:53:VAL:HG13       2:B:104:MET:HB2       1.83       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HG2       2.00       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HG2       2.00       0.60         2:B:182:GLU:HG3       2:B:183:PRO:HD2       1.85       0.58         2:B:182:GLU:HG3       2:B:183:PRO:HD2       1.85       0.58         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:127:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:149:MET:HB2       1.90       0.53				
1:A:21:LEU:HD21       1:A:50:PHE:HD1       1.58       0.66         1:A:41:LEU:HD22       1:A:92:LEU:HB3       1.79       0.63         2:B:30:PHE:CE2       2:B:171:ILE:HG22       2.33       0.63         2:B:52:THR:HG22       2:B:54:LEU:HB3       1.82       0.62         2:B:51:GLN:HB3       2:B:107:ILE:HD11       1.82       0.61         2:B:53:VAL:HG13       2:B:104:MET:HB2       1.83       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HG2       2.00       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HE2       2.01       0.60         2:B:182:GLU:HG3       2:B:183:PRO:HD2       1.85       0.58         2:B:30:TYR:HA       2:B:105:ASN:ND2       2.19       0.57         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:137:GLU:OE2       2:B:174:RCZ       2.42       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:10:CCZ       2:B:32:THR:HB       2.43       0.54				
1:A:41:LEU:HD22       1:A:92:LEU:HB3       1.79       0.63         2:B:30:PHE:CE2       2:B:171:ILE:HG22       2.33       0.63         2:B:32:THR:HG22       2:B:54:LEU:HB3       1.82       0.62         2:B:51:GLN:HB3       2:B:107:ILE:HD11       1.82       0.61         2:B:53:VAL:HG13       2:B:104:MET:HB2       1.83       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HG2       2.00       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HE2       2.01       0.60         2:B:182:GLU:HG3       2:B:183:PRO:HD2       1.85       0.58         2:B:50:TYR:HA       2:B:105:ASN:ND2       2.19       0.57         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:17:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:155:LYS:CG       2.56       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:16:LE:HB       1.56       0.53				
2:B:30:PHE:CE2       2:B:171:ILE:HG22       2:33       0.63         2:B:32:THR:HG22       2:B:54:LEU:HB3       1.82       0.62         2:B:51:GLN:HB3       2:B:107:ILE:HD11       1.82       0.61         2:B:53:VAL:HG13       2:B:104:MET:HB2       1.83       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HG2       2.00       0.60         2:B:182:GLU:HG3       2:B:155:LYS:HE2       2.01       0.60         2:B:50:TYR:HA       2:B:105:ASN:ND2       2.19       0.57         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:17:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:30:PHE:CZ       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:149:MET:HB2       1.90       0.53         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:18:ILE:HB       2:B:125:LE:HD11       1.90       0.52         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53				
2:B:32:THR:HG22       2:B:54:LEU:HB3       1.82       0.62         2:B:51:GLN:HB3       2:B:107:ILE:HD11       1.82       0.61         2:B:53:VAL:HG13       2:B:104:MET:HB2       1.83       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HG2       2.00       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HE2       2.01       0.60         2:B:182:GLU:HG3       2:B:183:PRO:HD2       1.85       0.58         2:B:50:TYR:HA       2:B:105:ASN:ND2       2.19       0.57         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:16:LE:HD11       1.90       0.52         1:A:28:ASN:HD21       2:B:16:LE:HD11       1.90       0.52     <				
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2:B:53:VAL:HG13       2:B:104:MET:HB2       1.83       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HG2       2.00       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HE2       2.01       0.60         2:B:182:GLU:HG3       2:B:183:PRO:HD2       1.85       0.58         2:B:50:TYR:HA       2:B:105:ASN:ND2       2.19       0.57         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:99:TYR:CZ       2.42       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:149:MET:HB2       1.90       0.53         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52				
2:B:137:GLU:OE2       2:B:155:LYS:HG2       2.00       0.60         2:B:137:GLU:OE2       2:B:155:LYS:HE2       2.01       0.60         2:B:182:GLU:HG3       2:B:183:PRO:HD2       1.85       0.58         2:B:50:TYR:HA       2:B:105:ASN:ND2       2.19       0.57         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:349:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:74:VAL:HG23       2.12       0.48 <td>2:B:51:GLN:HB3</td> <td>2:B:107:ILE:HD11</td> <td>1.82</td> <td>0.61</td>	2:B:51:GLN:HB3	2:B:107:ILE:HD11	1.82	0.61
2:B:137:GLU:OE2       2:B:155:LYS:HE2       2.01       0.60         2:B:182:GLU:HG3       2:B:183:PRO:HD2       1.85       0.58         2:B:50:TYR:HA       2:B:105:ASN:ND2       2.19       0.57         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:28:LEU:HD23       1.78       0.47	2:B:53:VAL:HG13	2:B:104:MET:HB2	1.83	0.60
2:B:182:GLU:HG3       2:B:183:PRO:HD2       1.85       0.58         2:B:50:TYR:HA       2:B:105:ASN:ND2       2.19       0.57         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.47	2:B:137:GLU:OE2	2:B:155:LYS:HG2	2.00	0.60
2:B:50:TYR:HA       2:B:105:ASN:ND2       2.19       0.57         2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD23       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47 </td <td>2:B:137:GLU:OE2</td> <td>2:B:155:LYS:HE2</td> <td>2.01</td> <td>0.60</td>	2:B:137:GLU:OE2	2:B:155:LYS:HE2	2.01	0.60
2:B:32:THR:O       2:B:53:VAL:HG23       2.05       0.56         2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:182:GLU:HG3	2:B:183:PRO:HD2	1.85	0.58
2:B:137:GLU:OE2       2:B:155:LYS:CE       2.55       0.55         1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:50:TYR:HA	2:B:105:ASN:ND2	2.19	0.57
1:A:57:LEU:HD23       1:A:234:LEU:HB3       1.88       0.55         2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:32:THR:O	2:B:53:VAL:HG23	2.05	0.56
2:B:27:GLN:HE22       2:B:186:SER:HB2       1.73       0.54         2:B:91:LEU:HD23       2:B:97:TYR:CZ       2.42       0.54         2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:137:GLU:OE2	2:B:155:LYS:CE	2.55	0.55
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2:B:137:GLU:OE2       2:B:155:LYS:CG       2.56       0.54         2:B:30:PHE:CZ       2:B:32:THR:HB       2.43       0.54         2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:27:GLN:HE22	2:B:186:SER:HB2	1.73	0.54
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2:B:142:GLU:HG2       2:B:149:MET:HB2       1.90       0.53         2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:137:GLU:OE2	2:B:155:LYS:CG	2.56	0.54
2:B:125:ARG:HH21       2:B:126:LYS:HE2       1.74       0.53         1:A:28:ASN:HD21       2:B:14:ASN:HD21       1.56       0.53         2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:30:PHE:CZ	2:B:32:THR:HB	2.43	0.54
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2:B:18:ILE:HB       2:B:25:ILE:HD11       1.90       0.52         1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:125:ARG:HH21	2:B:126:LYS:HE2	1.74	0.53
1:A:21:LEU:HD11       1:A:55:VAL:HG21       1.92       0.52         1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	1:A:28:ASN:HD21	2:B:14:ASN:HD21	1.56	0.53
1:A:88:PRO:O       1:A:92:LEU:HG       2.13       0.49         1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:18:ILE:HB	2:B:25:ILE:HD11	1.90	0.52
1:A:70:PHE:O       1:A:74:VAL:HG23       2.12       0.48         2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	1:A:21:LEU:HD11	1:A:55:VAL:HG21	1.92	0.52
2:B:11:LYS:HZ2       2:B:28:LEU:HD23       1.78       0.48         1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	1:A:88:PRO:O	1:A:92:LEU:HG	2.13	0.49
1:A:80:LEU:H       1:A:80:LEU:HD22       1.78       0.47         1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	1:A:70:PHE:O	1:A:74:VAL:HG23	2.12	0.48
1:A:157:LEU:HD13       1:A:181:VAL:HG21       1.95       0.47         1:A:18:VAL:O       1:A:22:VAL:HG23       2.14       0.47	2:B:11:LYS:HZ2	2:B:28:LEU:HD23	1.78	0.48
1:A:18:VAL:O 1:A:22:VAL:HG23 2.14 0.47	1:A:80:LEU:H	1:A:80:LEU:HD22	1.78	0.47
1:A:18:VAL:O 1:A:22:VAL:HG23 2.14 0.47	1:A:157:LEU:HD13	1:A:181:VAL:HG21	1.95	0.47
1:A:116:LYS:HG2	1:A:18:VAL:O	1:A:22:VAL:HG23	2.14	
	1:A:116:LYS:HG2	1:A:205:ASP:HA		

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A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	overlap (Å)
2:B:24:LYS:HB2	2:B:59:ARG:HH21	1.79	0.46
1:A:213:ILE:HG21	1:A:229:ILE:HG12	1.97	0.46
1:A:21:LEU:HD21	1:A:50:PHE:CD1	2.46	0.46
2:B:143:VAL:HG21	2:B:169:GLN:HG3	1.98	0.45
2:B:144:ARG:HD2	2:B:149:MET:SD	2.57	0.45
2:B:141:VAL:HA	2:B:149:MET:O	2.17	0.45
1:A:131:PRO:HG2	1:A:149:VAL:HG23	1.99	0.44
1:A:171:MET:HB2	1:A:176:PHE:CE2	2.52	0.44
1:A:228:MET:O	1:A:232:LEU:HB2	2.18	0.44
1:A:22:VAL:HA	1:A:26:ILE:HD12	2.00	0.44
1:A:22:VAL:HG21	1:A:78:CYS:SG	2.57	0.44
2:B:18:ILE:HG23	2:B:102:ILE:HD13	1.99	0.44
1:A:171:MET:HB2	1:A:176:PHE:HE2	1.82	0.44
2:B:103:ILE:HB	2:B:112:PHE:HB3	1.99	0.43
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.80	0.42
1:A:57:LEU:HB3	1:A:234:LEU:HD22	2.00	0.42
2:B:141:VAL:HG12	2:B:150:ILE:HG12	2.01	0.42
1:A:229:ILE:H	1:A:229:ILE:HG13	1.55	0.42
2:B:61:VAL:HA	2:B:62:GLY:HA3	1.67	0.41
2:B:148:VAL:HG21	2:B:171:ILE:HD11	2.02	0.41
2:B:118:PRO:HA	2:B:179:LEU:HA	2.04	0.40

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	213/281 (76%)	185 (87%)	27 (13%)	1 (0%)	29 68
2	В	170/188 (90%)	151 (89%)	16 (9%)	3 (2%)	8 41
All	All	383/469 (82%)	336 (88%)	43 (11%)	4 (1%)	15 54



All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	71	VAL
2	В	155	LYS
2	В	41	GLY
1	A	31	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	$206/257 \; (80\%)$	172 (84%)	34 (16%)	2 13
2	В	$159/172 \ (92\%)$	129 (81%)	30 (19%)	1 8
All	All	$365/429 \ (85\%)$	301 (82%)	64 (18%)	2 10

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	PHE
1	A	12	VAL
1	A	20	ASP
1	A	23	VAL
1	A	27	LEU
1	A	29	VAL
1	A	34	LEU
1	A	67	ILE
1	A	75	ILE
1	A	80	LEU
1	A	84	TRP
1	A	87	THR
1	A	118	LEU
1	A	119	LEU
1	A	120	LEU
1	A	123	ILE
1	A	134	LYS
1	A	147	ARG

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Mol	$\mathbf{Chain}$	Dag	
		Res	Type
1	Α	157	LEU
1	Α	167	VAL
1	A	170	ASN
1	A A	172	ASN
1	A	182	LYS
1	A	187	ASP
1	A A A A	194	HIS
1	Α	205	ASP
1	Α	207	LYS
1	A	209	LEU
1	A	213	ILE
1	A	228	MET
1	A	229	ILE
1	A A A A A	234	ILE LEU
1	A	239	GLU
2	В	4	GLU
2	В	10	ARG
2 2 2 2	В	11	ARG LYS
2	В	29	LEU
2	В	32	THR
2	В	36	THR
2	В	37	VAL
2	В	40	TRP
2	В	44	ASN
2	В	51	GLN
2	В	64	LYS
2 2	В	70	GLU
	В	86	ASN
2 2	В	92	THR
2	В	110	ASP
2	В	113	SER
2	В	116	ILE
2	В	120	SER
2 2	В	122	LEU
2	В	132	ARG
2	В	135	GLU
2	В	142	GLU
2 2 2 2 2 2	В	145	ASP
2	В	151	LYS
2	В	162	VAL
2	В	164	THR
2	В	169	GLN

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Mol	Chain	Res	Type
2	В	170	ASN
2	В	179	LEU
2	В	180	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	28	ASN
1	A	64	ASN
1	A	170	ASN
1	A	175	ASN
2	В	27	GLN
2	В	51	GLN
2	В	169	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)

There are no ligands in this entry.

#### 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)

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

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

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

### 6.3 Carbohydrates (i)

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

#### 6.4 Ligands (i)

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

#### 6.5 Other polymers (i)

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

