



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:01 am GMT

PDB ID : 2IMO  
Title : Crystal structure of allantoate amidohydrolase from Escherichia coli at pH 4.6  
Authors : Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center  
for Structural Genomics (NYSGXRC)  
Deposited on : 2006-10-04  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

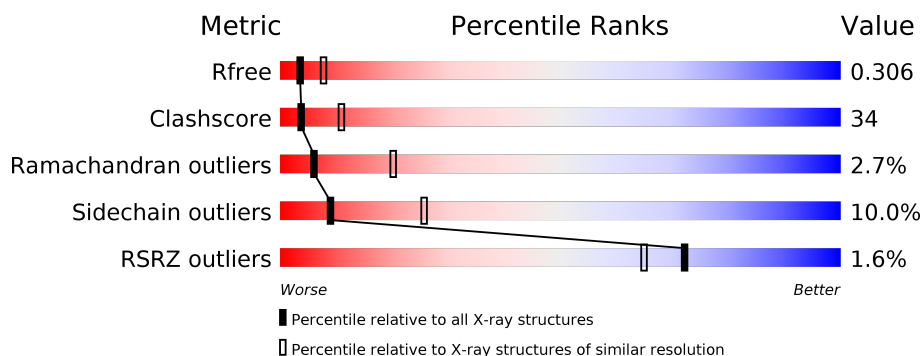
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	423	<div> <div> <div></div> <div>50%</div> <div>37%</div> <div>7%</div> <div>6%</div> </div> <div> <div></div> </div> </div>
1	B	423	<div> <div> <div></div> <div>39%</div> <div>44%</div> <div>9%</div> <div>7%</div> </div> <div> <div></div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6265 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 Allantoate amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	Se	0	0	0
			3128	1975	541	592	7	13			
1	B	394	Total	C	N	O	S	Se	0	0	0
			3080	1946	535	579	7	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CLONING ARTIFACT	UNP P77425
A	2	SER	-	CLONING ARTIFACT	UNP P77425
A	3	LEU	-	CLONING ARTIFACT	UNP P77425
A	29	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	49	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	125	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	167	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	234	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	258	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	308	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	315	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	325	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	332	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	354	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	373	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	405	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	414	GLU	-	EXPRESSION TAG	UNP P77425
A	415	GLY	-	EXPRESSION TAG	UNP P77425
A	416	GLY	-	EXPRESSION TAG	UNP P77425
A	417	SER	-	EXPRESSION TAG	UNP P77425
A	418	HIS	-	EXPRESSION TAG	UNP P77425
A	419	HIS	-	EXPRESSION TAG	UNP P77425
A	420	HIS	-	EXPRESSION TAG	UNP P77425
A	421	HIS	-	EXPRESSION TAG	UNP P77425
A	422	HIS	-	EXPRESSION TAG	UNP P77425

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	HIS	-	EXPRESSION TAG	UNP P77425
B	1	MSE	-	CLONING ARTIFACT	UNP P77425
B	2	SER	-	CLONING ARTIFACT	UNP P77425
B	3	LEU	-	CLONING ARTIFACT	UNP P77425
B	29	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	49	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	125	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	167	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	234	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	258	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	308	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	315	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	325	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	332	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	354	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	373	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	405	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	414	GLU	-	EXPRESSION TAG	UNP P77425
B	415	GLY	-	EXPRESSION TAG	UNP P77425
B	416	GLY	-	EXPRESSION TAG	UNP P77425
B	417	SER	-	EXPRESSION TAG	UNP P77425
B	418	HIS	-	EXPRESSION TAG	UNP P77425
B	419	HIS	-	EXPRESSION TAG	UNP P77425
B	420	HIS	-	EXPRESSION TAG	UNP P77425
B	421	HIS	-	EXPRESSION TAG	UNP P77425
B	422	HIS	-	EXPRESSION TAG	UNP P77425
B	423	HIS	-	EXPRESSION TAG	UNP P77425

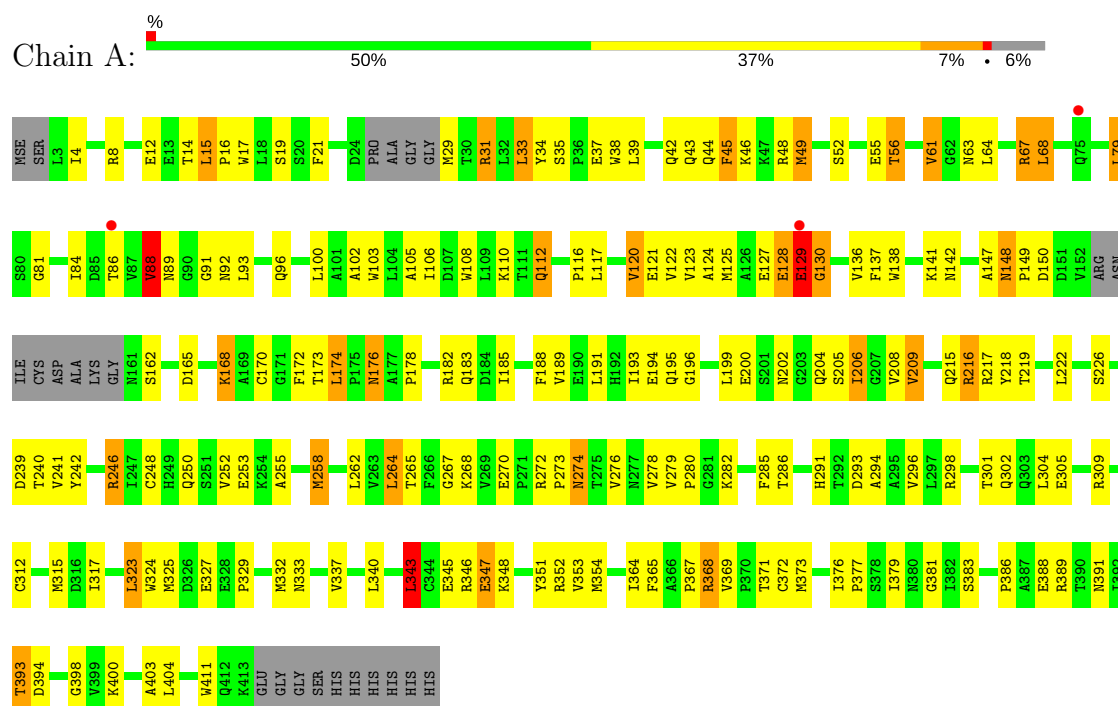
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	37	Total O 37 37	0	0
2	B	20	Total O 20 20	0	0

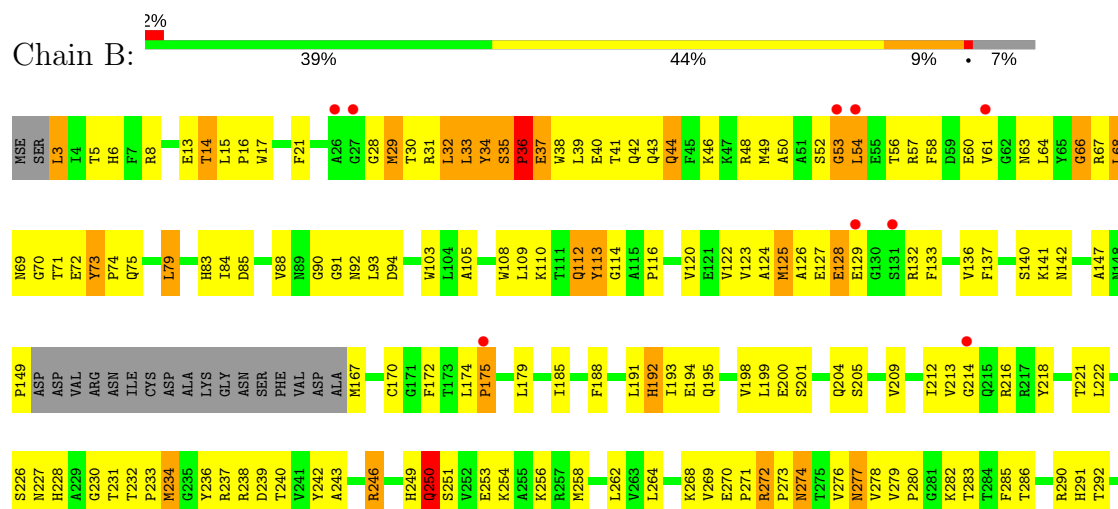
### 3 Residue-property plots

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

#### • Molecule 1: Allantoate amidohydrolase



#### • Molecule 1: Allantoate amidohydrolase



P370	L297	M308	M315	L323	P329	M332	M333	M334	E347	M348	L349	P350	P351	P352	P353	M354	H355	P356	H360	Q363	L364	P365	P367	P368	P369
C371	R298	M309	D316	E324	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
M373			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
L374			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
F375			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
L376			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
P377			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
S378			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
L379			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
M380			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
G381			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
L382			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
S383			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
H384			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
M385			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
P386			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
A387			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
E388			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
R389			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
T390			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
L395			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
A396			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
E397			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
G398			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
V399			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
K400			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
A403			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
L404			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
M405			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
L406			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
Y407			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
Q408			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
L409			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
A410			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
W411			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
Q412			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
K413			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLJ			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
CLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L350	P351	P352	P353	P354	H355	P356	P357	H360	Q363	L364	P365	P367	P368	P369
GLY			L317	M325	V330	P331	M332	M333	E348	E349	L35														

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.75Å 183.92Å 48.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.80 48.78 – 2.77	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.78-2.80) 88.5 (48.78-2.77)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.245 , 0.302 0.264 , 0.306	Depositor DCC
$R_{free}$ test set	578 reflections (2.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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

### 5.1 Standard geometry

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	0.55	2/3183 (0.1%)	0.74	3/4302 (0.1%)
1	B	0.54	4/3136 (0.1%)	0.71	1/4239 (0.0%)
All	All	0.55	6/6319 (0.1%)	0.72	4/8541 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	MSE	CG-SE	-5.50	1.76	1.95
1	B	29	MSE	CG-SE	-5.45	1.76	1.95
1	B	354	MSE	CG-SE	-5.08	1.78	1.95
1	B	125	MSE	CG-SE	-5.07	1.78	1.95
1	A	49	MSE	CG-SE	-5.05	1.78	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	LEU	CA-CB-CG	6.11	129.36	115.30
1	B	66	GLY	N-CA-C	-5.41	99.57	113.10
1	A	343	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	68	LEU	N-CA-C	-5.30	96.69	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3128	0	3064	180	0
1	B	3080	0	3028	247	0
2	A	37	0	0	6	0
2	B	20	0	0	3	0
All	All	6265	0	6092	419	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 34.

The worst 5 of 419 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:B:344:CYS:HA	1:B:349:LEU:HD12	1.42	1.02
1:A:365:PHE:HB3	1:A:371:THR:HG21	1.49	0.94
1:A:379:ILE:HD11	1:A:389:ARG:HB2	1.49	0.94
1:B:209:VAL:HG11	1:B:373:MSE:HE3	1.49	0.93
1:A:208:VAL:HG13	1:A:340:LEU:HD23	1.51	0.92

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	393/423 (93%)	350 (89%)	35 (9%)	8 (2%)	9	28
1	B	390/423 (92%)	328 (84%)	49 (13%)	13 (3%)	4	15
All	All	783/846 (93%)	678 (87%)	84 (11%)	21 (3%)	6	20

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	36	PRO
1	B	320	ASP
1	B	379	ILE
1	A	129	GLU

### 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	338/341 (99%)	306 (90%)	32 (10%)	10	28
1	B	331/341 (97%)	296 (89%)	35 (11%)	8	23
All	All	669/682 (98%)	602 (90%)	67 (10%)	9	26

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	ARG
1	B	44	GLN
1	B	378	SER
1	A	393	THR
1	B	14	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	ASN
1	B	92	ASN
1	B	384	HIS
1	B	75	GLN
1	A	202	ASN

### 5.3.3 RNA ⓘ

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](#)

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	386/423 (91%)	-0.15	3 (0%) 86 81	26, 45, 66, 84	0
1	B	381/423 (90%)	0.11	9 (2%) 59 49	32, 59, 91, 99	0
All	All	767/846 (90%)	-0.02	12 (1%) 72 65	26, 51, 84, 99	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	GLY	5.6
1	B	26	ALA	5.2
1	B	175	PRO	3.9
1	B	27	GLY	3.1
1	B	129	GLU	2.9

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.