



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 08:15 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

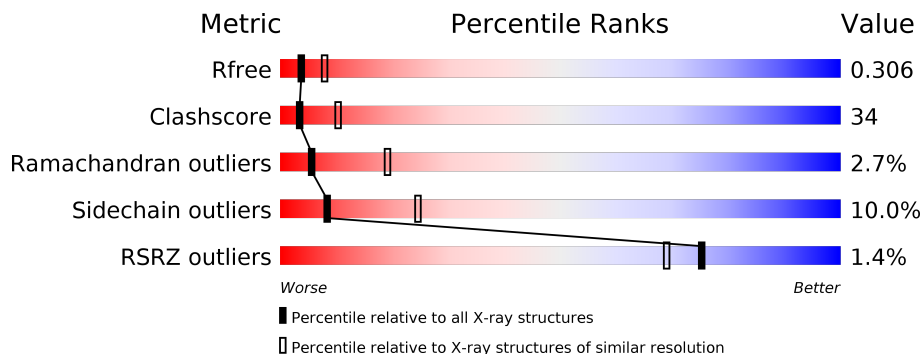
1 Overall quality at a glance

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}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (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 ≥ 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	
1	B	423	

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

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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

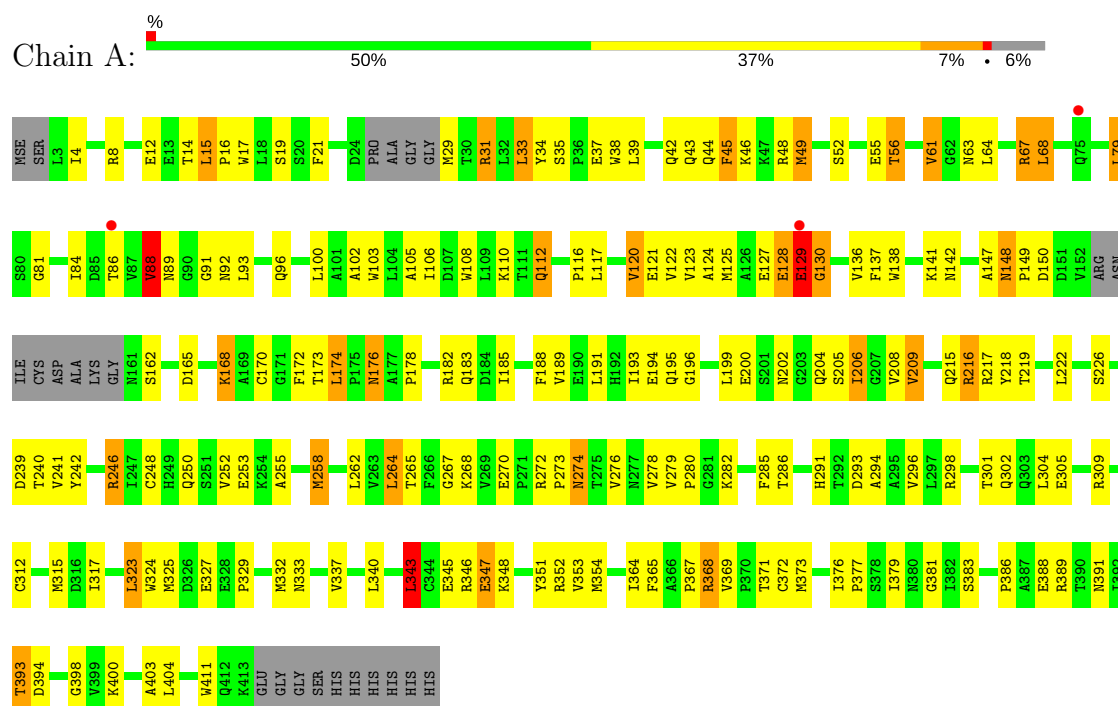
- Molecule 2 is water.

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

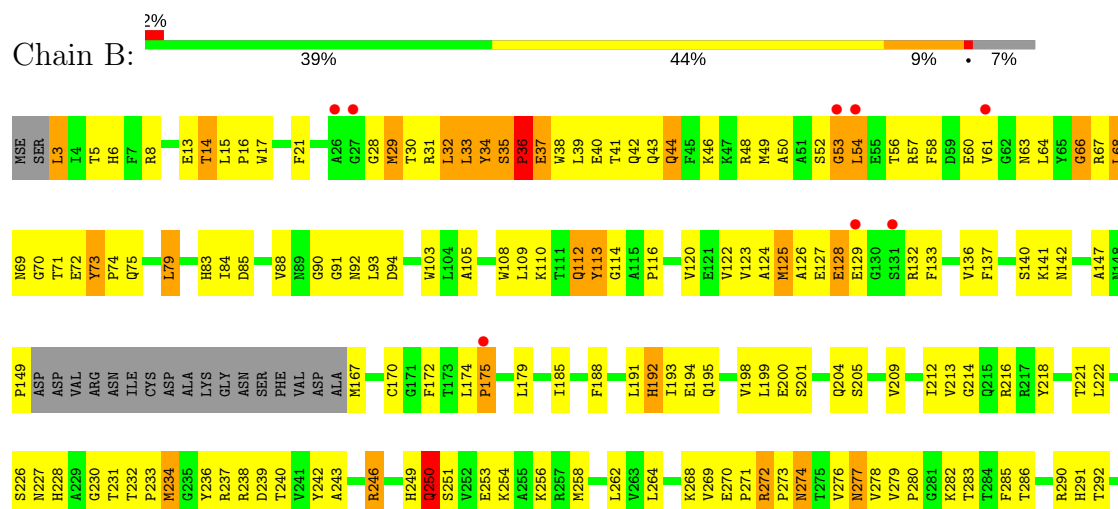
3 Residue-property plots

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	P339	M335	L343	P349	G348	G349	P350	P351	P352	P353	P354	P355	P356	P357	P358	P359
C372	R298	M309	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
M373	T301	M310	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
L374	G302	M311	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
F375	M308	M312	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
L376	M309	M313	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
P377	M310	M314	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
S378	M311	M315	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
L379	M312	M316	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
M380	G302	M317	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
G381	M308	M318	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
R382	M309	M319	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
S383	M310	M320	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
G384	M311	M321	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
M385	M312	M322	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
P386	M313	M323	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
A387	M314	M324	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
E388	M315	M325	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
R389	M316	M326	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
T390	M317	M327	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
L395	M318	M328	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
A396	M319	M329	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
E397	M320	M330	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
G398	M321	M331	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
P399	M322	M332	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
V399	M323	M333	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
R399	M324	M334	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
V399	M325	M335	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
G400	M326	M336	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
K400	M327	M337	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
A403	M328	M338	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
L404	M329	M339	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
M405	M330	M340	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
L406	M331	M341	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
L407	M332	M342	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
Y407	M333	M343	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
Q408	M334	M344	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
L409	M335	M345	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
A410	M336	M346	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
L411	M337	M347	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
Q412	M338	M348	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
K413	M339	M349	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GL1J	M340	M350	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
GL1J	M341	M351	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
CLY	M342	M352	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M343	M353	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M344	M354	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
GLY	M345	M355	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
GLY	M346	M356	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M347	M357	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M348	M358	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
GLY	M349	M359	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
GLY	M350	M360	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M351	M361	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M352	M362	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
GLY	M353	M363	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
GLY	M354	M364	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M355	M365	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M356	M366	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
GLY	M357	M367	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
GLY	M358	M368	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M359	M369	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M360	M370	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
GLY	M361	M371	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
GLY	M362	M372	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M363	M373	D316	G324	V330	V331	M332	L336	V337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R358	R359
GLY	M364	M374	G318	M325	M332	M333	M334	L337	M337	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351
GLY	M365	M375	R319	D320	M338	M339	M340	L340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353
GLY	M366	M376	L315	L323	P329	P330	M335	L336	P337	L346	L349	L350	R351	R352	R353	R354	R355	R356	R357	R	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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%)	8	27
1	B	390/423 (92%)	328 (84%)	49 (13%)	13 (3%)	4	14
All	All	783/846 (93%)	678 (87%)	84 (11%)	21 (3%)	5	19

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	TYR

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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%)	9	27
1	B	331/341 (97%)	296 (89%)	35 (11%)	7	22
All	All	669/682 (98%)	602 (90%)	67 (10%)	8	24

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/423 (91%)	-0.15	3 (0%) 86 81	26, 45, 66, 84	0
1	B	381/423 (90%)	0.11	8 (2%) 63 54	32, 59, 91, 99	0
All	All	767/846 (90%)	-0.02	11 (1%) 75 69	26, 51, 84, 99	0

The worst 5 of 11 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.