



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:38 am BST

PDB ID : 2F6I  
Title : Crystal structure of the ClpP protease catalytic domain from Plasmodium falciparum  
Authors : Mulichak, A.; Loppnau, P.; Bray, J.; Amani, M.; Vedadi, M.; Wasney, G.; Finerty, P.; Sundstrom, M.; Weigelt, J.; Edwards, A.; Arrowsmith, C.; Hui, R.; Plotnikova, O.; Structural Genomics Consortium (SGC)  
Deposited on : 2005-11-29  
Resolution : 2.45 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

<https://www.wwpdb.org/validation/2017/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:

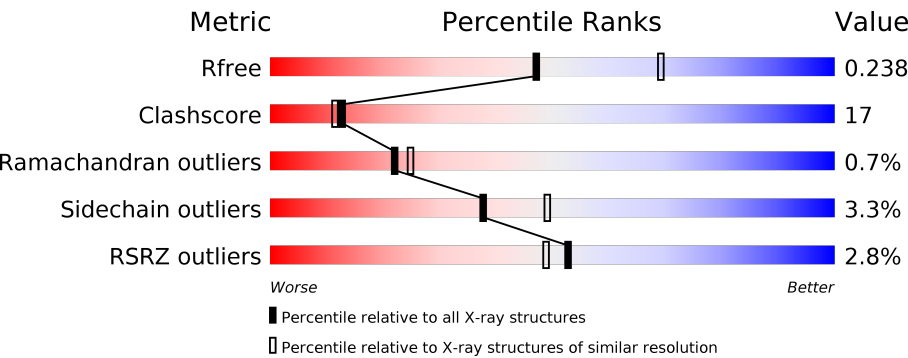
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.45 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))
$R_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\leq 5\%$ . 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	215	<div><div>3%</div><div><div></div><div>64%</div><div>20%</div><div>•</div><div>15%</div></div></div>
1	B	215	<div><div>%</div><div><div></div><div>55%</div><div>23%</div><div>•</div><div>19%</div></div></div>
1	C	215	<div><div>4%</div><div><div></div><div>61%</div><div>22%</div><div>•</div><div>15%</div></div></div>
1	D	215	<div><div>%</div><div><div></div><div>53%</div><div>31%</div><div>•</div><div>15%</div></div></div>
1	E	215	<div><div>2%</div><div><div></div><div>57%</div><div>23%</div><div>•</div><div>19%</div></div></div>
1	F	215	<div><div>2%</div><div><div></div><div>59%</div><div>24%</div><div>•</div><div>16%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	215	<div><div></div><div>2%</div><div>56%</div><div>24%</div><div>•</div><div>17%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10189 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 ATP-dependent CLP protease, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1447	936	234	271	6			
1	B	174	Total	C	N	O	S	0	0	0
			1387	898	223	260	6			
1	C	183	Total	C	N	O	S	0	0	0
			1450	938	235	271	6			
1	D	182	Total	C	N	O	S	0	0	0
			1434	927	233	269	5			
1	E	175	Total	C	N	O	S	0	0	0
			1391	900	224	261	6			
1	F	181	Total	C	N	O	S	0	0	0
			1434	927	232	270	5			
1	G	178	Total	C	N	O	S	0	0	0
			1398	904	226	263	5			

There are 161 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	MET	-	CLONING ARTIFACT	UNP O97252
A	157	GLY	-	CLONING ARTIFACT	UNP O97252
A	158	SER	-	CLONING ARTIFACT	UNP O97252
A	159	SER	-	CLONING ARTIFACT	UNP O97252
A	160	HIS	-	EXPRESSION TAG	UNP O97252
A	161	HIS	-	EXPRESSION TAG	UNP O97252
A	162	HIS	-	EXPRESSION TAG	UNP O97252
A	163	HIS	-	EXPRESSION TAG	UNP O97252
A	164	HIS	-	EXPRESSION TAG	UNP O97252
A	165	HIS	-	EXPRESSION TAG	UNP O97252
A	166	SER	-	CLONING ARTIFACT	UNP O97252
A	167	SER	-	CLONING ARTIFACT	UNP O97252
A	168	GLY	-	CLONING ARTIFACT	UNP O97252
A	169	ARG	-	CLONING ARTIFACT	UNP O97252
A	170	GLU	-	CLONING ARTIFACT	UNP O97252

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Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ASN	-	CLONING ARTIFACT	UNP 097252
A	172	LEU	-	CLONING ARTIFACT	UNP 097252
A	173	TYR	-	CLONING ARTIFACT	UNP 097252
A	174	PHE	-	CLONING ARTIFACT	UNP 097252
A	175	GLN	-	CLONING ARTIFACT	UNP 097252
A	176	GLY	-	CLONING ARTIFACT	UNP 097252
A	177	HIS	-	CLONING ARTIFACT	UNP 097252
A	178	MET	-	CLONING ARTIFACT	UNP 097252
B	156	MET	-	CLONING ARTIFACT	UNP 097252
B	157	GLY	-	CLONING ARTIFACT	UNP 097252
B	158	SER	-	CLONING ARTIFACT	UNP 097252
B	159	SER	-	CLONING ARTIFACT	UNP 097252
B	160	HIS	-	EXPRESSION TAG	UNP 097252
B	161	HIS	-	EXPRESSION TAG	UNP 097252
B	162	HIS	-	EXPRESSION TAG	UNP 097252
B	163	HIS	-	EXPRESSION TAG	UNP 097252
B	164	HIS	-	EXPRESSION TAG	UNP 097252
B	165	HIS	-	EXPRESSION TAG	UNP 097252
B	166	SER	-	CLONING ARTIFACT	UNP 097252
B	167	SER	-	CLONING ARTIFACT	UNP 097252
B	168	GLY	-	CLONING ARTIFACT	UNP 097252
B	169	ARG	-	CLONING ARTIFACT	UNP 097252
B	170	GLU	-	CLONING ARTIFACT	UNP 097252
B	171	ASN	-	CLONING ARTIFACT	UNP 097252
B	172	LEU	-	CLONING ARTIFACT	UNP 097252
B	173	TYR	-	CLONING ARTIFACT	UNP 097252
B	174	PHE	-	CLONING ARTIFACT	UNP 097252
B	175	GLN	-	CLONING ARTIFACT	UNP 097252
B	176	GLY	-	CLONING ARTIFACT	UNP 097252
B	177	HIS	-	CLONING ARTIFACT	UNP 097252
B	178	MET	-	CLONING ARTIFACT	UNP 097252
C	156	MET	-	CLONING ARTIFACT	UNP 097252
C	157	GLY	-	CLONING ARTIFACT	UNP 097252
C	158	SER	-	CLONING ARTIFACT	UNP 097252
C	159	SER	-	CLONING ARTIFACT	UNP 097252
C	160	HIS	-	EXPRESSION TAG	UNP 097252
C	161	HIS	-	EXPRESSION TAG	UNP 097252
C	162	HIS	-	EXPRESSION TAG	UNP 097252
C	163	HIS	-	EXPRESSION TAG	UNP 097252
C	164	HIS	-	EXPRESSION TAG	UNP 097252
C	165	HIS	-	EXPRESSION TAG	UNP 097252
C	166	SER	-	CLONING ARTIFACT	UNP 097252

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Chain	Residue	Modelled	Actual	Comment	Reference
C	167	SER	-	CLONING ARTIFACT	UNP 097252
C	168	GLY	-	CLONING ARTIFACT	UNP 097252
C	169	ARG	-	CLONING ARTIFACT	UNP 097252
C	170	GLU	-	CLONING ARTIFACT	UNP 097252
C	171	ASN	-	CLONING ARTIFACT	UNP 097252
C	172	LEU	-	CLONING ARTIFACT	UNP 097252
C	173	TYR	-	CLONING ARTIFACT	UNP 097252
C	174	PHE	-	CLONING ARTIFACT	UNP 097252
C	175	GLN	-	CLONING ARTIFACT	UNP 097252
C	176	GLY	-	CLONING ARTIFACT	UNP 097252
C	177	HIS	-	CLONING ARTIFACT	UNP 097252
C	178	MET	-	CLONING ARTIFACT	UNP 097252
D	156	MET	-	CLONING ARTIFACT	UNP 097252
D	157	GLY	-	CLONING ARTIFACT	UNP 097252
D	158	SER	-	CLONING ARTIFACT	UNP 097252
D	159	SER	-	CLONING ARTIFACT	UNP 097252
D	160	HIS	-	EXPRESSION TAG	UNP 097252
D	161	HIS	-	EXPRESSION TAG	UNP 097252
D	162	HIS	-	EXPRESSION TAG	UNP 097252
D	163	HIS	-	EXPRESSION TAG	UNP 097252
D	164	HIS	-	EXPRESSION TAG	UNP 097252
D	165	HIS	-	EXPRESSION TAG	UNP 097252
D	166	SER	-	CLONING ARTIFACT	UNP 097252
D	167	SER	-	CLONING ARTIFACT	UNP 097252
D	168	GLY	-	CLONING ARTIFACT	UNP 097252
D	169	ARG	-	CLONING ARTIFACT	UNP 097252
D	170	GLU	-	CLONING ARTIFACT	UNP 097252
D	171	ASN	-	CLONING ARTIFACT	UNP 097252
D	172	LEU	-	CLONING ARTIFACT	UNP 097252
D	173	TYR	-	CLONING ARTIFACT	UNP 097252
D	174	PHE	-	CLONING ARTIFACT	UNP 097252
D	175	GLN	-	CLONING ARTIFACT	UNP 097252
D	176	GLY	-	CLONING ARTIFACT	UNP 097252
D	177	HIS	-	CLONING ARTIFACT	UNP 097252
D	178	MET	-	CLONING ARTIFACT	UNP 097252
E	156	MET	-	CLONING ARTIFACT	UNP 097252
E	157	GLY	-	CLONING ARTIFACT	UNP 097252
E	158	SER	-	CLONING ARTIFACT	UNP 097252
E	159	SER	-	CLONING ARTIFACT	UNP 097252
E	160	HIS	-	EXPRESSION TAG	UNP 097252
E	161	HIS	-	EXPRESSION TAG	UNP 097252
E	162	HIS	-	EXPRESSION TAG	UNP 097252

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Chain	Residue	Modelled	Actual	Comment	Reference
E	163	HIS	-	EXPRESSION TAG	UNP 097252
E	164	HIS	-	EXPRESSION TAG	UNP 097252
E	165	HIS	-	EXPRESSION TAG	UNP 097252
E	166	SER	-	CLONING ARTIFACT	UNP 097252
E	167	SER	-	CLONING ARTIFACT	UNP 097252
E	168	GLY	-	CLONING ARTIFACT	UNP 097252
E	169	ARG	-	CLONING ARTIFACT	UNP 097252
E	170	GLU	-	CLONING ARTIFACT	UNP 097252
E	171	ASN	-	CLONING ARTIFACT	UNP 097252
E	172	LEU	-	CLONING ARTIFACT	UNP 097252
E	173	TYR	-	CLONING ARTIFACT	UNP 097252
E	174	PHE	-	CLONING ARTIFACT	UNP 097252
E	175	GLN	-	CLONING ARTIFACT	UNP 097252
E	176	GLY	-	CLONING ARTIFACT	UNP 097252
E	177	HIS	-	CLONING ARTIFACT	UNP 097252
E	178	MET	-	CLONING ARTIFACT	UNP 097252
F	156	MET	-	CLONING ARTIFACT	UNP 097252
F	157	GLY	-	CLONING ARTIFACT	UNP 097252
F	158	SER	-	CLONING ARTIFACT	UNP 097252
F	159	SER	-	CLONING ARTIFACT	UNP 097252
F	160	HIS	-	EXPRESSION TAG	UNP 097252
F	161	HIS	-	EXPRESSION TAG	UNP 097252
F	162	HIS	-	EXPRESSION TAG	UNP 097252
F	163	HIS	-	EXPRESSION TAG	UNP 097252
F	164	HIS	-	EXPRESSION TAG	UNP 097252
F	165	HIS	-	EXPRESSION TAG	UNP 097252
F	166	SER	-	CLONING ARTIFACT	UNP 097252
F	167	SER	-	CLONING ARTIFACT	UNP 097252
F	168	GLY	-	CLONING ARTIFACT	UNP 097252
F	169	ARG	-	CLONING ARTIFACT	UNP 097252
F	170	GLU	-	CLONING ARTIFACT	UNP 097252
F	171	ASN	-	CLONING ARTIFACT	UNP 097252
F	172	LEU	-	CLONING ARTIFACT	UNP 097252
F	173	TYR	-	CLONING ARTIFACT	UNP 097252
F	174	PHE	-	CLONING ARTIFACT	UNP 097252
F	175	GLN	-	CLONING ARTIFACT	UNP 097252
F	176	GLY	-	CLONING ARTIFACT	UNP 097252
F	177	HIS	-	CLONING ARTIFACT	UNP 097252
F	178	MET	-	CLONING ARTIFACT	UNP 097252
G	156	MET	-	CLONING ARTIFACT	UNP 097252
G	157	GLY	-	CLONING ARTIFACT	UNP 097252
G	158	SER	-	CLONING ARTIFACT	UNP 097252

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Chain	Residue	Modelled	Actual	Comment	Reference
G	159	SER	-	CLONING ARTIFACT	UNP O97252
G	160	HIS	-	EXPRESSION TAG	UNP O97252
G	161	HIS	-	EXPRESSION TAG	UNP O97252
G	162	HIS	-	EXPRESSION TAG	UNP O97252
G	163	HIS	-	EXPRESSION TAG	UNP O97252
G	164	HIS	-	EXPRESSION TAG	UNP O97252
G	165	HIS	-	EXPRESSION TAG	UNP O97252
G	166	SER	-	CLONING ARTIFACT	UNP O97252
G	167	SER	-	CLONING ARTIFACT	UNP O97252
G	168	GLY	-	CLONING ARTIFACT	UNP O97252
G	169	ARG	-	CLONING ARTIFACT	UNP O97252
G	170	GLU	-	CLONING ARTIFACT	UNP O97252
G	171	ASN	-	CLONING ARTIFACT	UNP O97252
G	172	LEU	-	CLONING ARTIFACT	UNP O97252
G	173	TYR	-	CLONING ARTIFACT	UNP O97252
G	174	PHE	-	CLONING ARTIFACT	UNP O97252
G	175	GLN	-	CLONING ARTIFACT	UNP O97252
G	176	GLY	-	CLONING ARTIFACT	UNP O97252
G	177	HIS	-	CLONING ARTIFACT	UNP O97252
G	178	MET	-	CLONING ARTIFACT	UNP O97252

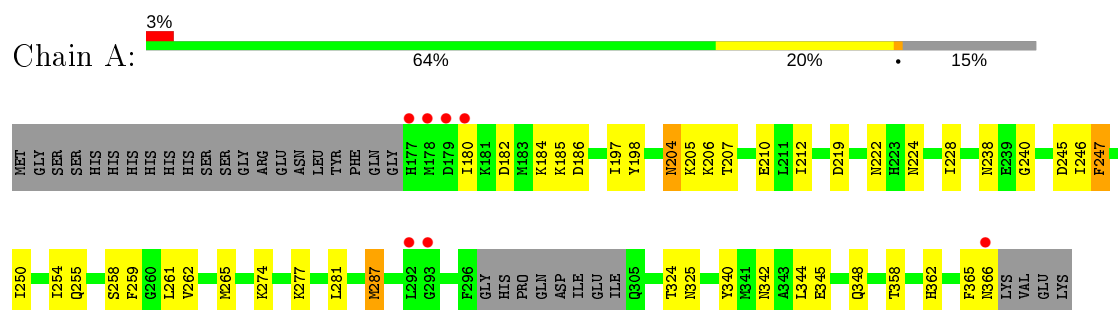
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	55	Total O 55 55	0	0
2	B	41	Total O 41 41	0	0
2	C	33	Total O 33 33	0	0
2	D	23	Total O 23 23	0	0
2	E	27	Total O 27 27	0	0
2	F	35	Total O 35 35	0	0
2	G	34	Total O 34 34	0	0

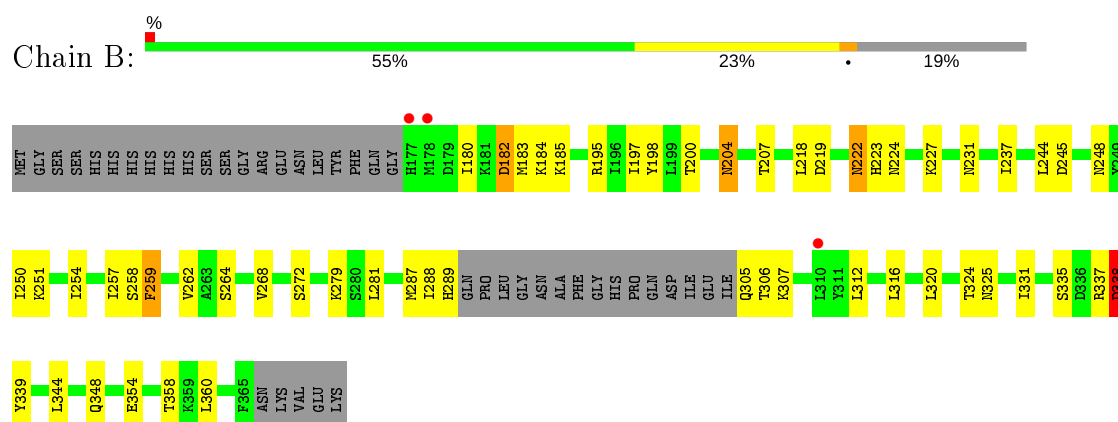
### 3 Residue-property plots

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.

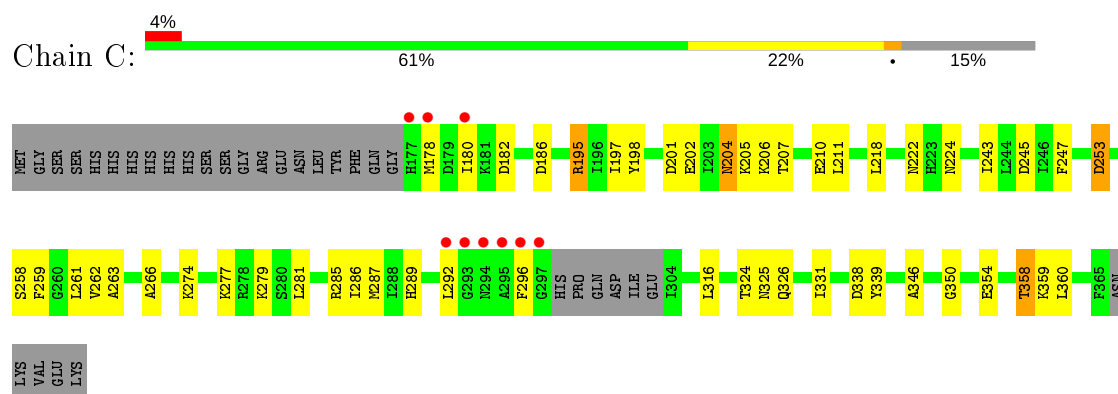
- Molecule 1: ATP-dependent CLP protease, putative



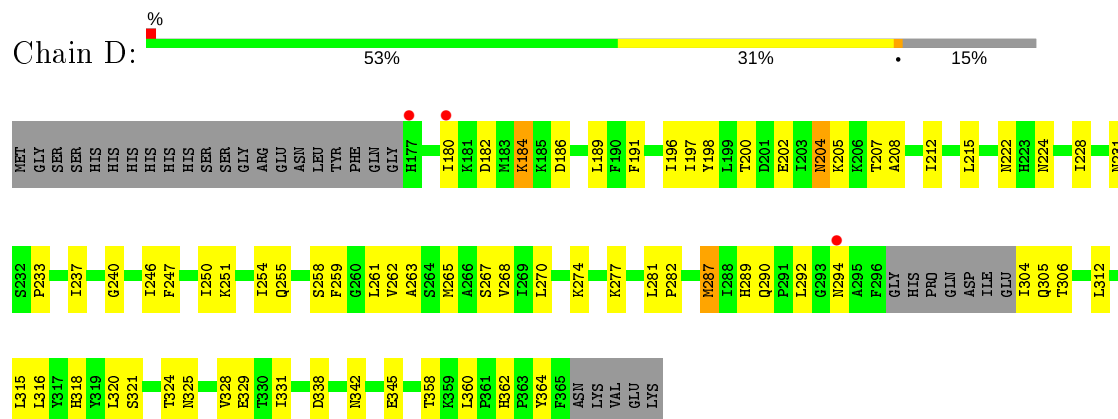
- Molecule 1: ATP-dependent CLP protease, putative



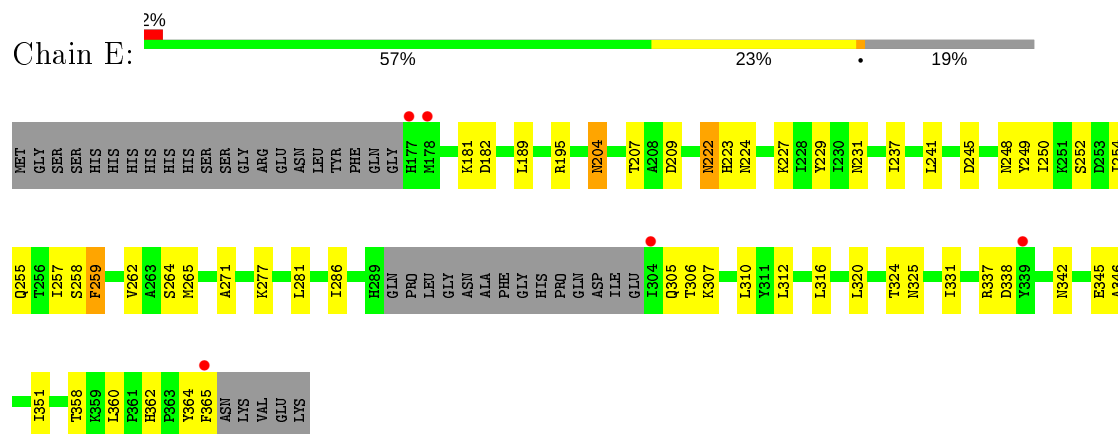
- Molecule 1: ATP-dependent CLP protease, putative



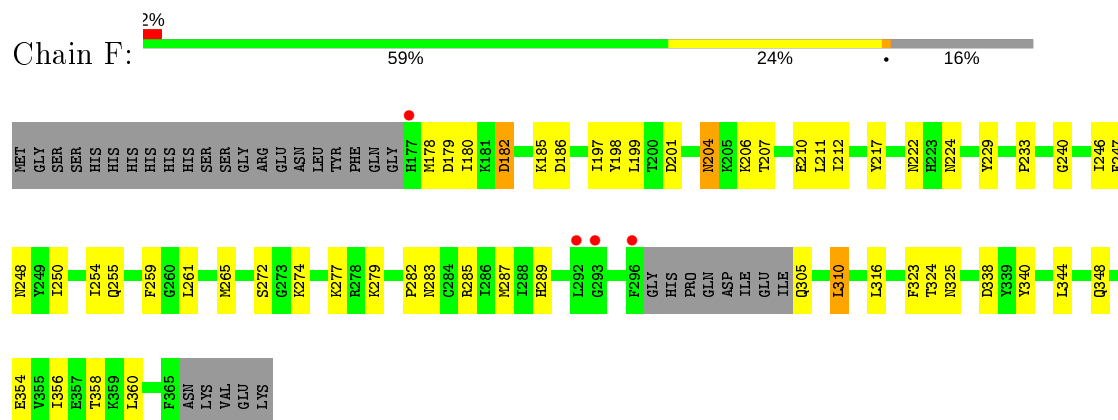
- Molecule 1: ATP-dependent CLP protease, putative



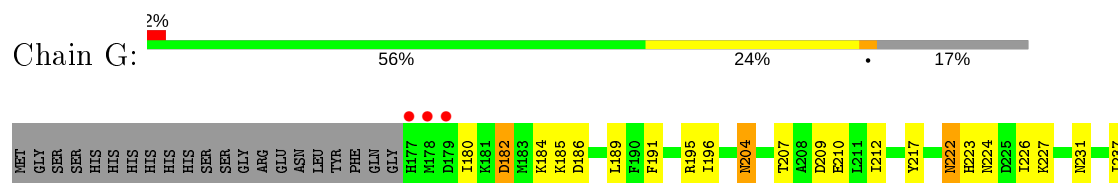
- Molecule 1: ATP-dependent CLP protease, putative

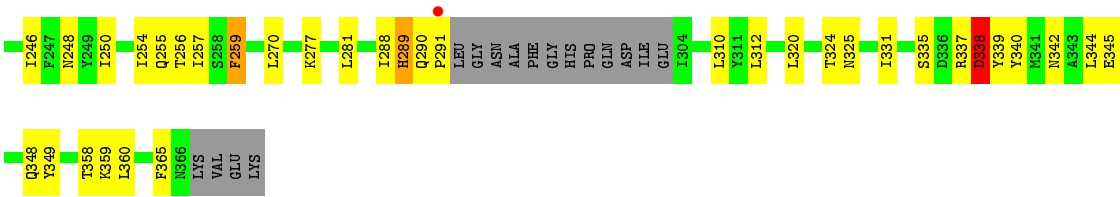


- Molecule 1: ATP-dependent CLP protease, putative



- Molecule 1: ATP-dependent CLP protease, putative





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.30Å 196.46Å 139.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.45 47.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.45) 96.3 (47.85-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.238 0.210 , 0.238	Depositor DCC
$R_{free}$ test set	3911 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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](#)

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	0.29	0/1472	0.53	0/1985
1	B	0.29	0/1411	0.54	0/1904
1	C	0.29	0/1476	0.52	0/1992
1	D	0.28	0/1459	0.50	0/1971
1	E	0.28	0/1415	0.52	0/1910
1	F	0.29	0/1459	0.53	0/1970
1	G	0.30	0/1422	0.56	1/1922 (0.1%)
All	All	0.29	0/10114	0.53	1/13654 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	G	291	PRO	N-CA-CB	5.75	110.20	103.30

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	1447	0	1452	37	0
1	B	1387	0	1386	49	0
1	C	1450	0	1447	50	0
1	D	1434	0	1426	56	0
1	E	1391	0	1386	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1434	0	1430	53	0
1	G	1398	0	1376	57	1
2	A	55	0	0	4	0
2	B	41	0	0	6	0
2	C	33	0	0	3	0
2	D	23	0	0	8	0
2	E	27	0	0	3	0
2	F	35	0	0	7	0
2	G	34	0	0	4	0
All	All	10189	0	9903	330	1

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 17.

The worst 5 of 330 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:C:358:THR:HG22	1:C:360:LEU:H	1.20	1.02
1:D:240:GLY:HA3	1:D:265:MET:HG2	1.41	1.02
1:G:212:ILE:HB	2:G:402:HOH:O	1.59	1.01
1:G:358:THR:HG22	1:G:360:LEU:H	1.31	0.94
1:C:222:ASN:HD22	1:C:224:ASN:H	1.14	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:LEU:CD1	1:G:310:LEU:CD1[3_555]	2.01	0.19

## 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	178/215 (83%)	171 (96%)	7 (4%)	0	100	100
1	B	170/215 (79%)	163 (96%)	6 (4%)	1 (1%)	25	29
1	C	179/215 (83%)	170 (95%)	8 (4%)	1 (1%)	25	29
1	D	178/215 (83%)	163 (92%)	14 (8%)	1 (1%)	25	29
1	E	171/215 (80%)	165 (96%)	6 (4%)	0	100	100
1	F	177/215 (82%)	165 (93%)	10 (6%)	2 (1%)	14	14
1	G	174/215 (81%)	164 (94%)	7 (4%)	3 (2%)	9	7
All	All	1227/1505 (82%)	1161 (95%)	58 (5%)	8 (1%)	22	25

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	305	GLN
1	G	290	GLN
1	B	338	ASP
1	G	338	ASP
1	F	178	MET

### 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	157/195 (80%)	154 (98%)	3 (2%)	57	69
1	B	151/195 (77%)	145 (96%)	6 (4%)	31	41
1	C	157/195 (80%)	151 (96%)	6 (4%)	33	43
1	D	154/195 (79%)	149 (97%)	5 (3%)	39	50
1	E	151/195 (77%)	146 (97%)	5 (3%)	38	49
1	F	155/195 (80%)	151 (97%)	4 (3%)	46	58
1	G	149/195 (76%)	143 (96%)	6 (4%)	31	41
All	All	1074/1365 (79%)	1039 (97%)	35 (3%)	38	49

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	182	ASP
1	D	287	MET
1	G	259	PHE
1	D	184	LYS
1	D	204	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	289	HIS
1	D	248	ASN
1	G	204	ASN
1	D	204	ASN
1	D	222	ASN

### 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](#)

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	182/215 (84%)	-0.12	7 (3%) 40 37	34, 44, 69, 93	0
1	B	174/215 (80%)	-0.15	3 (1%) 70 67	32, 45, 70, 92	0
1	C	183/215 (85%)	-0.02	9 (4%) 29 27	41, 53, 74, 89	0
1	D	182/215 (84%)	0.06	3 (1%) 72 69	45, 57, 73, 88	0
1	E	175/215 (81%)	0.00	5 (2%) 51 47	38, 50, 76, 93	0
1	F	181/215 (84%)	-0.19	4 (2%) 62 58	34, 47, 72, 89	0
1	G	178/215 (82%)	-0.09	4 (2%) 62 58	32, 43, 72, 97	0
All	All	1255/1505 (83%)	-0.07	35 (2%) 53 49	32, 50, 74, 97	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	177	HIS	4.9
1	A	177	HIS	4.5
1	C	295	ALA	4.5
1	B	178	MET	4.1
1	E	177	HIS	3.7

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.