



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2025 – 07:37 pm BST

PDB ID : 9FSW / pdb\_00009fsw  
Title : ClpP from Staphylococcus epidermidis with glycerol in some of the catalytic sites.  
Authors : Alves Franca, B.; Rohde, H.; Betzel, C.  
Deposited on : 2024-06-22  
Resolution : 2.39 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

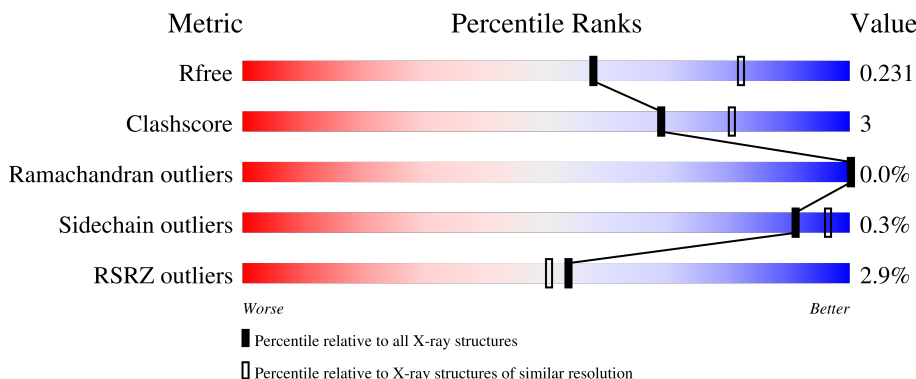
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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.






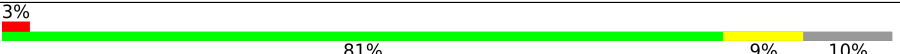
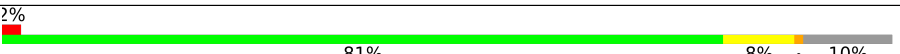
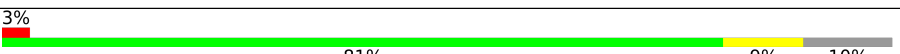
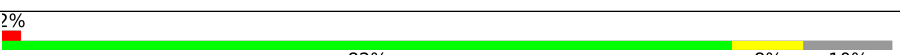
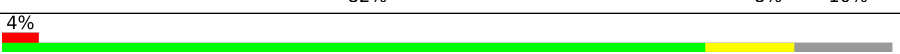

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 of 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	199	<div> <div>4%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
1	B	199	<div> <div>3%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	C	199	<div> <div>3%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
1	D	199	<div> <div>2%</div> <div>85%</div> <div>•</div> <div>10%</div> </div>
1	E	199	<div> <div>3%</div> <div>81%</div> <div>10%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	199	 4% 84% 7% 9%
1	G	199	 4% 86% 10%
1	H	199	 2% 84% 7% 10%
1	I	199	 3% 81% 9% 10%
1	J	199	 2% 81% 8% 10%
1	K	199	 3% 81% 9% 10%
1	L	199	 2% 82% 8% 10%
1	M	199	 4% 79% 10% 11%
1	N	199	 1% 85% 6% 10%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20061 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 proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1372	862	234	270	6			
1	B	184	Total	C	N	O	S	0	0	0
			1407	885	239	277	6			
1	C	181	Total	C	N	O	S	0	0	0
			1388	874	236	272	6			
1	D	179	Total	C	N	O	S	0	0	0
			1371	862	234	269	6			
1	E	181	Total	C	N	O	S	0	0	0
			1392	876	236	274	6			
1	F	182	Total	C	N	O	S	0	0	0
			1398	881	234	277	6			
1	G	179	Total	C	N	O	S	0	0	0
			1366	861	231	268	6			
1	H	180	Total	C	N	O	S	0	0	0
			1379	868	234	271	6			
1	I	179	Total	C	N	O	S	0	0	0
			1380	868	234	272	6			
1	J	179	Total	C	N	O	S	0	0	0
			1374	865	233	270	6			
1	K	179	Total	C	N	O	S	0	0	0
			1374	865	233	270	6			
1	L	179	Total	C	N	O	S	0	0	0
			1372	864	234	268	6			
1	M	178	Total	C	N	O	S	0	0	0
			1367	860	232	269	6			
1	N	180	Total	C	N	O	S	0	0	0
			1387	873	235	273	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	HIS	-	expression tag	UNP A0A0N1MQL5

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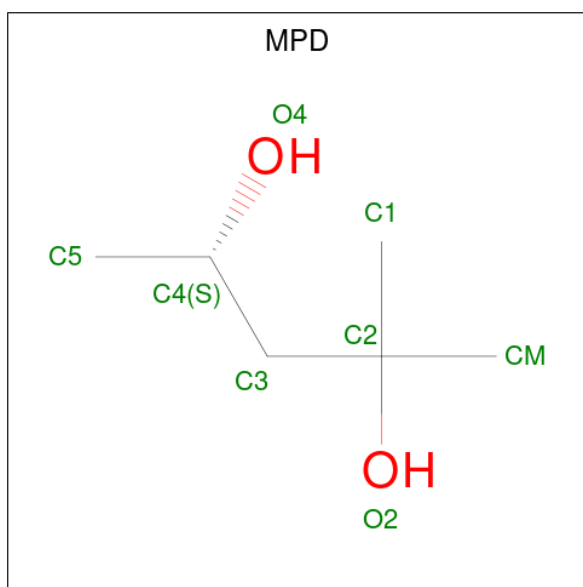
Chain	Residue	Modelled	Actual	Comment	Reference
A	195	HIS	-	expression tag	UNP A0A0N1MQL5
A	196	HIS	-	expression tag	UNP A0A0N1MQL5
A	197	HIS	-	expression tag	UNP A0A0N1MQL5
A	198	HIS	-	expression tag	UNP A0A0N1MQL5
A	199	HIS	-	expression tag	UNP A0A0N1MQL5
B	194	HIS	-	expression tag	UNP A0A0N1MQL5
B	195	HIS	-	expression tag	UNP A0A0N1MQL5
B	196	HIS	-	expression tag	UNP A0A0N1MQL5
B	197	HIS	-	expression tag	UNP A0A0N1MQL5
B	198	HIS	-	expression tag	UNP A0A0N1MQL5
B	199	HIS	-	expression tag	UNP A0A0N1MQL5
C	194	HIS	-	expression tag	UNP A0A0N1MQL5
C	195	HIS	-	expression tag	UNP A0A0N1MQL5
C	196	HIS	-	expression tag	UNP A0A0N1MQL5
C	197	HIS	-	expression tag	UNP A0A0N1MQL5
C	198	HIS	-	expression tag	UNP A0A0N1MQL5
C	199	HIS	-	expression tag	UNP A0A0N1MQL5
D	194	HIS	-	expression tag	UNP A0A0N1MQL5
D	195	HIS	-	expression tag	UNP A0A0N1MQL5
D	196	HIS	-	expression tag	UNP A0A0N1MQL5
D	197	HIS	-	expression tag	UNP A0A0N1MQL5
D	198	HIS	-	expression tag	UNP A0A0N1MQL5
D	199	HIS	-	expression tag	UNP A0A0N1MQL5
E	194	HIS	-	expression tag	UNP A0A0N1MQL5
E	195	HIS	-	expression tag	UNP A0A0N1MQL5
E	196	HIS	-	expression tag	UNP A0A0N1MQL5
E	197	HIS	-	expression tag	UNP A0A0N1MQL5
E	198	HIS	-	expression tag	UNP A0A0N1MQL5
E	199	HIS	-	expression tag	UNP A0A0N1MQL5
F	194	HIS	-	expression tag	UNP A0A0N1MQL5
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F	196	HIS	-	expression tag	UNP A0A0N1MQL5
F	197	HIS	-	expression tag	UNP A0A0N1MQL5
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F	199	HIS	-	expression tag	UNP A0A0N1MQL5
G	194	HIS	-	expression tag	UNP A0A0N1MQL5
G	195	HIS	-	expression tag	UNP A0A0N1MQL5
G	196	HIS	-	expression tag	UNP A0A0N1MQL5
G	197	HIS	-	expression tag	UNP A0A0N1MQL5
G	198	HIS	-	expression tag	UNP A0A0N1MQL5
G	199	HIS	-	expression tag	UNP A0A0N1MQL5
H	194	HIS	-	expression tag	UNP A0A0N1MQL5

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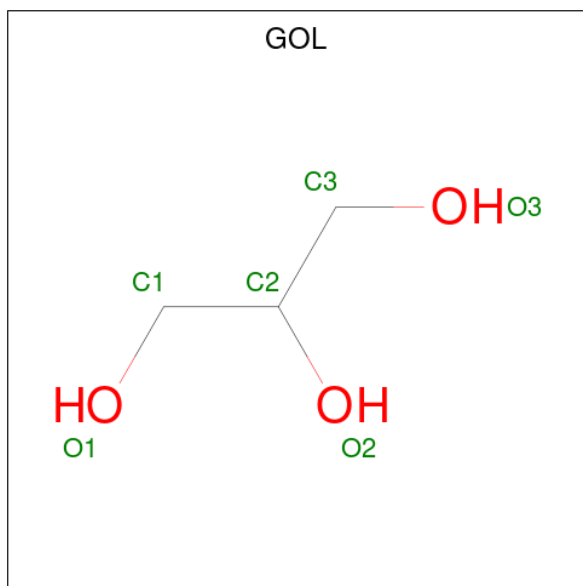
Chain	Residue	Modelled	Actual	Comment	Reference
H	195	HIS	-	expression tag	UNP A0A0N1MQL5
H	196	HIS	-	expression tag	UNP A0A0N1MQL5
H	197	HIS	-	expression tag	UNP A0A0N1MQL5
H	198	HIS	-	expression tag	UNP A0A0N1MQL5
H	199	HIS	-	expression tag	UNP A0A0N1MQL5
I	194	HIS	-	expression tag	UNP A0A0N1MQL5
I	195	HIS	-	expression tag	UNP A0A0N1MQL5
I	196	HIS	-	expression tag	UNP A0A0N1MQL5
I	197	HIS	-	expression tag	UNP A0A0N1MQL5
I	198	HIS	-	expression tag	UNP A0A0N1MQL5
I	199	HIS	-	expression tag	UNP A0A0N1MQL5
J	194	HIS	-	expression tag	UNP A0A0N1MQL5
J	195	HIS	-	expression tag	UNP A0A0N1MQL5
J	196	HIS	-	expression tag	UNP A0A0N1MQL5
J	197	HIS	-	expression tag	UNP A0A0N1MQL5
J	198	HIS	-	expression tag	UNP A0A0N1MQL5
J	199	HIS	-	expression tag	UNP A0A0N1MQL5
K	194	HIS	-	expression tag	UNP A0A0N1MQL5
K	195	HIS	-	expression tag	UNP A0A0N1MQL5
K	196	HIS	-	expression tag	UNP A0A0N1MQL5
K	197	HIS	-	expression tag	UNP A0A0N1MQL5
K	198	HIS	-	expression tag	UNP A0A0N1MQL5
K	199	HIS	-	expression tag	UNP A0A0N1MQL5
L	194	HIS	-	expression tag	UNP A0A0N1MQL5
L	195	HIS	-	expression tag	UNP A0A0N1MQL5
L	196	HIS	-	expression tag	UNP A0A0N1MQL5
L	197	HIS	-	expression tag	UNP A0A0N1MQL5
L	198	HIS	-	expression tag	UNP A0A0N1MQL5
L	199	HIS	-	expression tag	UNP A0A0N1MQL5
M	194	HIS	-	expression tag	UNP A0A0N1MQL5
M	195	HIS	-	expression tag	UNP A0A0N1MQL5
M	196	HIS	-	expression tag	UNP A0A0N1MQL5
M	197	HIS	-	expression tag	UNP A0A0N1MQL5
M	198	HIS	-	expression tag	UNP A0A0N1MQL5
M	199	HIS	-	expression tag	UNP A0A0N1MQL5
N	194	HIS	-	expression tag	UNP A0A0N1MQL5
N	195	HIS	-	expression tag	UNP A0A0N1MQL5
N	196	HIS	-	expression tag	UNP A0A0N1MQL5
N	197	HIS	-	expression tag	UNP A0A0N1MQL5
N	198	HIS	-	expression tag	UNP A0A0N1MQL5
N	199	HIS	-	expression tag	UNP A0A0N1MQL5

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	C 6	O 2	0	0
2	B	1	Total 8	C 6	O 2	0	0
2	C	1	Total 8	C 6	O 2	0	0
2	D	1	Total 8	C 6	O 2	0	0
2	E	1	Total 8	C 6	O 2	0	0
2	F	1	Total 8	C 6	O 2	0	0
2	G	1	Total 8	C 6	O 2	0	0
2	H	1	Total 8	C 6	O 2	0	0
2	I	1	Total 8	C 6	O 2	0	0
2	J	1	Total 8	C 6	O 2	0	0
2	K	1	Total 8	C 6	O 2	0	0
2	L	1	Total 8	C 6	O 2	0	0
2	M	1	Total 8	C 6	O 2	0	0
2	N	1	Total 8	C 6	O 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		

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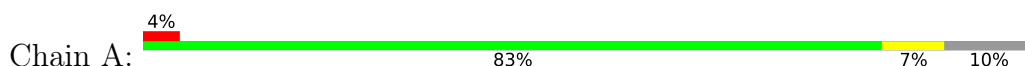
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	36	Total 36	O 36	0	0
4	C	36	Total 36	O 36	0	0
4	D	40	Total 40	O 40	0	0
4	E	48	Total 48	O 48	0	0
4	F	44	Total 44	O 44	0	0
4	G	49	Total 49	O 49	0	0
4	H	44	Total 44	O 44	0	0
4	I	44	Total 44	O 44	0	0
4	J	44	Total 44	O 44	0	0
4	K	34	Total 34	O 34	0	0
4	L	24	Total 24	O 24	0	0
4	M	34	Total 34	O 34	0	0
4	N	36	Total 36	O 36	0	0

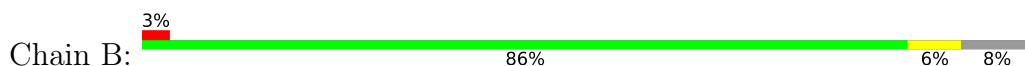
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

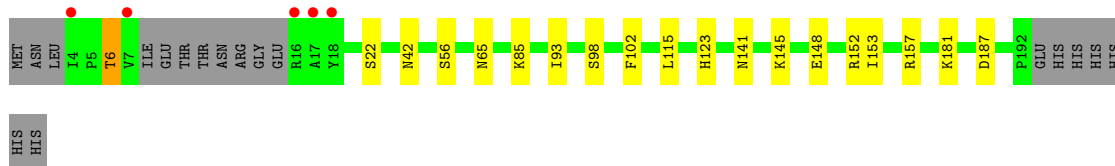
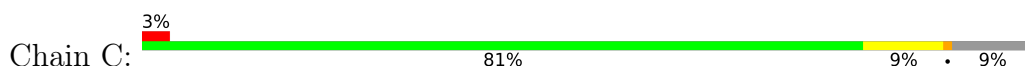
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



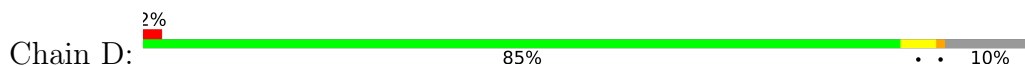
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



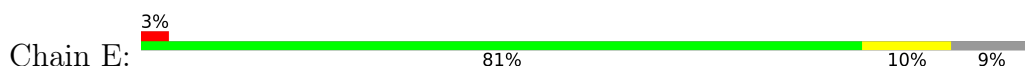
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



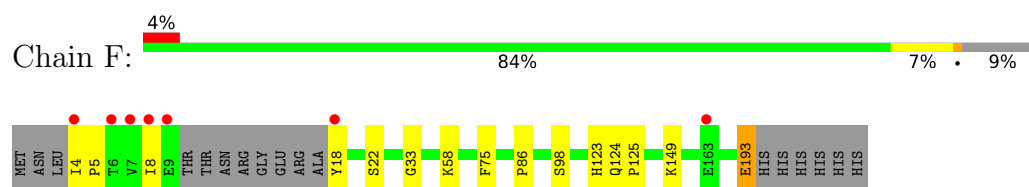
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



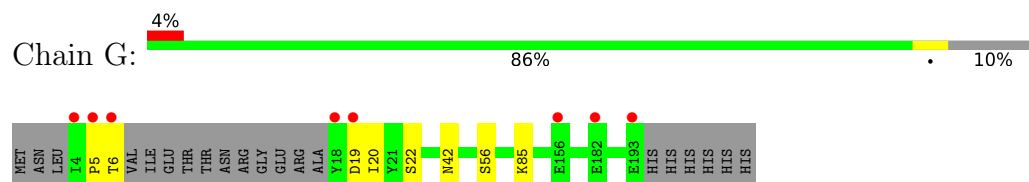
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



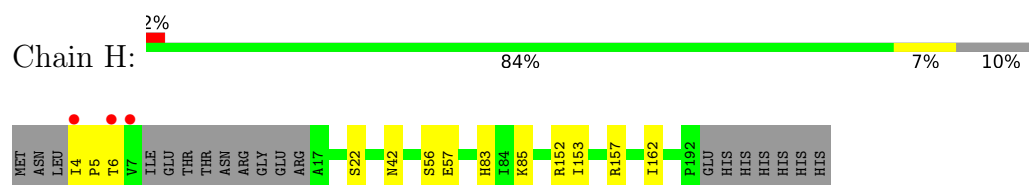
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



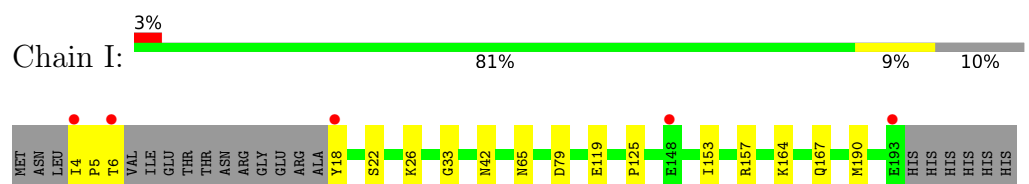
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



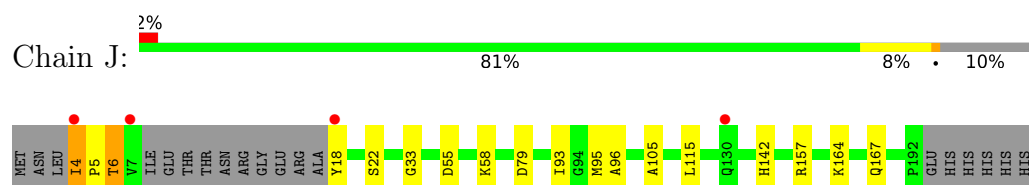
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



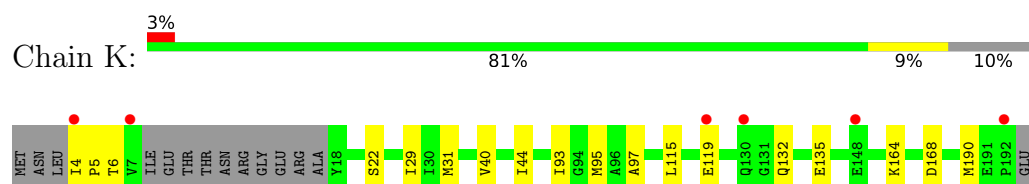
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



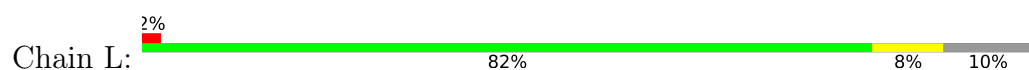
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

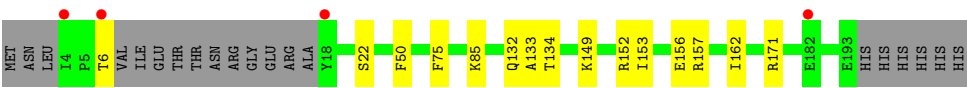


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

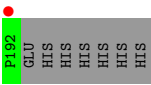
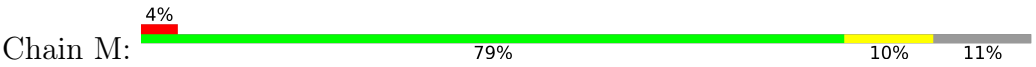


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

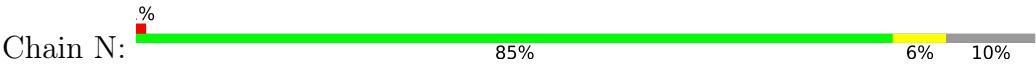




● Molecule 1: ATP-dependent Clp protease proteolytic subunit



● Molecule 1: ATP-dependent Clp protease proteolytic subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.61Å 123.99Å 126.69Å 90.00° 91.18° 90.00°	Depositor
Resolution (Å)	63.33 – 2.39 63.33 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.33-2.39) 99.9 (63.33-2.39)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.199 , 0.233 0.199 , 0.231	Depositor DCC
$R_{free}$ test set	5708 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.005 for -h,-l,-k 0.017 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20061	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.18	0/1389	0.37	0/1877
1	B	0.18	0/1425	0.39	0/1925
1	C	0.19	0/1406	0.39	0/1899
1	D	0.19	0/1388	0.38	0/1874
1	E	0.20	0/1410	0.40	0/1904
1	F	0.20	0/1416	0.40	0/1913
1	G	0.21	0/1384	0.38	0/1870
1	H	0.19	0/1397	0.40	0/1888
1	I	0.21	0/1398	0.41	0/1887
1	J	0.19	0/1392	0.43	0/1881
1	K	0.19	0/1392	0.41	0/1881
1	L	0.18	0/1390	0.40	0/1877
1	M	0.18	0/1385	0.39	0/1871
1	N	0.20	0/1405	0.39	0/1897
All	All	0.19	0/19577	0.40	0/26444

There are no bond length outliers.

There are no bond angle outliers.

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	1372	0	1371	10	0
1	B	1407	0	1404	9	0
1	C	1388	0	1394	15	0
1	D	1371	0	1380	8	0
1	E	1392	0	1398	16	0
1	F	1398	0	1399	14	0
1	G	1366	0	1365	5	0
1	H	1379	0	1381	11	0
1	I	1380	0	1384	16	0
1	J	1374	0	1376	14	0
1	K	1374	0	1376	14	0
1	L	1372	0	1376	13	0
1	M	1367	0	1367	14	0
1	N	1387	0	1393	9	0
2	A	8	0	14	2	0
2	B	8	0	14	3	0
2	C	8	0	14	3	0
2	D	8	0	14	0	0
2	E	8	0	14	0	0
2	F	8	0	14	0	0
2	G	8	0	14	0	0
2	H	8	0	14	0	0
2	I	8	0	14	0	0
2	J	8	0	14	0	0
2	K	8	0	14	0	0
2	L	8	0	14	0	0
2	M	8	0	14	1	0
2	N	8	0	14	1	0
3	B	12	0	16	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
3	I	6	0	8	1	0
3	N	12	0	16	2	0
4	A	49	0	0	1	0
4	B	36	0	0	0	0
4	C	36	0	0	0	0
4	D	40	0	0	0	0
4	E	48	0	0	1	0
4	F	44	0	0	0	0
4	G	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	44	0	0	0	0
4	I	44	0	0	1	0
4	J	44	0	0	0	0
4	K	34	0	0	1	0
4	L	24	0	0	0	0
4	M	34	0	0	0	0
4	N	36	0	0	0	0
All	All	20061	0	19640	133	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 3.

The worst 5 of 133 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:H:42:ASN:HD21	1:I:33:GLY:HA3	1.46	0.80
1:N:152:ARG:HA	1:N:162:ILE:HD11	1.63	0.79
1:L:152:ARG:HA	1:L:162:ILE:HD11	1.69	0.74
1:J:93:ILE:HG22	1:J:115:LEU:HD22	1.71	0.72
1:K:93:ILE:HG22	1:K:115:LEU:HD22	1.71	0.72

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	176/199 (88%)	172 (98%)	4 (2%)	0	100	100
1	B	180/199 (90%)	176 (98%)	4 (2%)	0	100	100
1	C	177/199 (89%)	174 (98%)	3 (2%)	0	100	100
1	D	175/199 (88%)	172 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	177/199 (89%)	174 (98%)	3 (2%)	0	100	100
1	F	178/199 (89%)	175 (98%)	3 (2%)	0	100	100
1	G	175/199 (88%)	171 (98%)	3 (2%)	1 (1%)	22	33
1	H	176/199 (88%)	173 (98%)	3 (2%)	0	100	100
1	I	175/199 (88%)	171 (98%)	4 (2%)	0	100	100
1	J	175/199 (88%)	172 (98%)	3 (2%)	0	100	100
1	K	175/199 (88%)	171 (98%)	4 (2%)	0	100	100
1	L	175/199 (88%)	172 (98%)	3 (2%)	0	100	100
1	M	174/199 (87%)	171 (98%)	3 (2%)	0	100	100
1	N	176/199 (88%)	173 (98%)	3 (2%)	0	100	100
All	All	2464/2786 (88%)	2417 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	5	PRO

### 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	146/166 (88%)	146 (100%)	0	100	100
1	B	149/166 (90%)	149 (100%)	0	100	100
1	C	148/166 (89%)	147 (99%)	1 (1%)	81	91
1	D	147/166 (89%)	146 (99%)	1 (1%)	81	91
1	E	149/166 (90%)	149 (100%)	0	100	100
1	F	150/166 (90%)	149 (99%)	1 (1%)	81	91
1	G	145/166 (87%)	145 (100%)	0	100	100
1	H	147/166 (89%)	146 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	148/166 (89%)	148 (100%)	0	100	100
1	J	147/166 (89%)	145 (99%)	2 (1%)	62	79
1	K	147/166 (89%)	147 (100%)	0	100	100
1	L	146/166 (88%)	146 (100%)	0	100	100
1	M	146/166 (88%)	146 (100%)	0	100	100
1	N	149/166 (90%)	149 (100%)	0	100	100
All	All	2064/2324 (89%)	2058 (100%)	6 (0%)	91	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	6	THR
1	J	4	ILE
1	J	6	THR
1	D	6	THR
1	C	6	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	82	GLN
1	J	167	GLN
1	L	151	ASN
1	J	39	ASN
1	K	65	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	F	201	-	5,5,5	0.35	0	5,5,5	0.49	0
3	GOL	N	203	-	5,5,5	0.30	0	5,5,5	0.53	0
2	MPD	E	202	-	7,7,7	0.38	0	9,10,10	0.42	0
2	MPD	N	202	-	7,7,7	0.43	0	9,10,10	0.38	0
3	GOL	H	201	-	5,5,5	0.30	0	5,5,5	0.36	0
3	GOL	E	201	-	5,5,5	0.32	0	5,5,5	0.34	0
2	MPD	H	202	-	7,7,7	0.37	0	9,10,10	0.65	0
2	MPD	C	201	-	7,7,7	0.44	0	9,10,10	0.79	0
3	GOL	N	201	-	5,5,5	0.33	0	5,5,5	0.30	0
2	MPD	M	201	-	7,7,7	0.39	0	9,10,10	0.58	0
2	MPD	A	201	-	7,7,7	0.41	0	9,10,10	0.53	0
3	GOL	B	201	-	5,5,5	0.35	0	5,5,5	0.43	0
2	MPD	I	202	-	7,7,7	0.48	0	9,10,10	0.62	0
3	GOL	B	202	-	5,5,5	0.29	0	5,5,5	0.40	0
2	MPD	G	202	-	7,7,7	0.40	0	9,10,10	0.42	0
2	MPD	K	201	-	7,7,7	0.43	0	9,10,10	0.40	0
3	GOL	G	201	-	5,5,5	0.31	0	5,5,5	0.38	0
3	GOL	D	201	-	5,5,5	0.34	0	5,5,5	0.45	0
2	MPD	L	201	-	7,7,7	0.35	0	9,10,10	0.41	0
2	MPD	D	202	-	7,7,7	0.39	0	9,10,10	0.50	0
2	MPD	F	202	-	7,7,7	0.38	0	9,10,10	0.39	0
2	MPD	B	203	-	7,7,7	0.41	0	9,10,10	0.46	0
2	MPD	J	201	-	7,7,7	0.36	0	9,10,10	0.50	0
3	GOL	I	201	-	5,5,5	0.32	0	5,5,5	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	F	201	-	-	3/4/4/4	-
3	GOL	N	203	-	-	2/4/4/4	-
2	MPD	E	202	-	-	0/5/5/5	-
2	MPD	N	202	-	-	0/5/5/5	-
3	GOL	H	201	-	-	2/4/4/4	-
3	GOL	E	201	-	-	4/4/4/4	-
2	MPD	H	202	-	-	2/5/5/5	-
2	MPD	C	201	-	-	0/5/5/5	-
3	GOL	N	201	-	-	0/4/4/4	-
2	MPD	M	201	-	-	2/5/5/5	-
2	MPD	A	201	-	-	0/5/5/5	-
3	GOL	B	201	-	-	2/4/4/4	-
2	MPD	I	202	-	-	4/5/5/5	-
3	GOL	B	202	-	-	0/4/4/4	-
2	MPD	G	202	-	-	0/5/5/5	-
2	MPD	K	201	-	-	2/5/5/5	-
3	GOL	G	201	-	-	0/4/4/4	-
3	GOL	D	201	-	-	2/4/4/4	-
2	MPD	L	201	-	-	0/5/5/5	-
2	MPD	D	202	-	-	0/5/5/5	-
2	MPD	F	202	-	-	0/5/5/5	-
2	MPD	B	203	-	-	2/5/5/5	-
2	MPD	J	201	-	-	2/5/5/5	-
3	GOL	I	201	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	202	MPD	C1-C2-C3-C4
2	I	202	MPD	C2-C3-C4-O4
2	J	201	MPD	C2-C3-C4-O4
2	J	201	MPD	C2-C3-C4-C5
2	K	201	MPD	C1-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	203	GOL	2	0
2	N	202	MPD	1	0
2	C	201	MPD	3	0
2	M	201	MPD	1	0
2	A	201	MPD	2	0
2	B	203	MPD	3	0
3	I	201	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	180/199 (90%)	0.09	7 (3%) 44 41	37, 45, 63, 73	0
1	B	184/199 (92%)	0.02	5 (2%) 56 53	37, 45, 64, 90	0
1	C	181/199 (90%)	0.15	5 (2%) 55 51	38, 46, 62, 90	0
1	D	179/199 (89%)	0.04	4 (2%) 62 59	33, 44, 62, 78	0
1	E	181/199 (90%)	-0.08	5 (2%) 55 51	35, 43, 60, 73	0
1	F	182/199 (91%)	0.08	7 (3%) 44 42	36, 43, 62, 101	0
1	G	179/199 (89%)	0.06	8 (4%) 39 36	37, 46, 62, 89	0
1	H	180/199 (90%)	-0.01	3 (1%) 69 65	35, 45, 63, 69	0
1	I	179/199 (89%)	0.14	5 (2%) 55 51	38, 44, 61, 87	0
1	J	179/199 (89%)	0.07	4 (2%) 62 59	36, 46, 62, 81	0
1	K	179/199 (89%)	0.10	6 (3%) 48 45	39, 48, 64, 72	0
1	L	179/199 (89%)	0.26	4 (2%) 62 59	41, 50, 65, 83	0
1	M	178/199 (89%)	0.12	7 (3%) 44 41	38, 47, 64, 86	0
1	N	180/199 (90%)	-0.00	2 (1%) 77 75	36, 44, 59, 73	0
All	All	2520/2786 (90%)	0.07	72 (2%) 54 50	33, 46, 63, 101	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	4	ILE	6.3
1	A	4	ILE	5.6
1	L	4	ILE	5.6
1	B	4	ILE	5.5
1	I	4	ILE	5.5

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	F	201	6/6	0.65	0.26	56,59,62,66	0
3	GOL	H	201	6/6	0.68	0.17	60,67,67,73	0
3	GOL	B	202	6/6	0.71	0.21	55,66,68,73	0
3	GOL	N	201	6/6	0.73	0.19	64,67,72,75	0
3	GOL	E	201	6/6	0.74	0.22	47,59,60,64	0
3	GOL	G	201	6/6	0.74	0.15	65,66,70,72	0
3	GOL	N	203	6/6	0.77	0.19	49,52,64,64	0
3	GOL	B	201	6/6	0.78	0.20	51,57,61,62	0
2	MPD	B	203	8/8	0.78	0.18	52,54,55,55	0
2	MPD	M	201	8/8	0.80	0.19	45,55,59,63	0
3	GOL	I	201	6/6	0.80	0.20	47,57,59,61	0
2	MPD	H	202	8/8	0.82	0.19	46,53,60,61	0
3	GOL	D	201	6/6	0.83	0.18	49,53,62,63	0
2	MPD	K	201	8/8	0.83	0.17	47,53,57,64	0
2	MPD	A	201	8/8	0.84	0.18	41,51,54,56	0
2	MPD	C	201	8/8	0.85	0.19	48,52,56,66	0
2	MPD	I	202	8/8	0.88	0.15	42,53,54,55	0
2	MPD	L	201	8/8	0.89	0.14	43,51,55,60	0
2	MPD	N	202	8/8	0.89	0.15	38,45,50,60	0
2	MPD	E	202	8/8	0.90	0.14	42,45,49,52	0
2	MPD	J	201	8/8	0.90	0.14	51,53,56,63	0
2	MPD	F	202	8/8	0.90	0.13	45,48,55,57	0
2	MPD	D	202	8/8	0.90	0.12	41,51,53,58	0
2	MPD	G	202	8/8	0.93	0.10	47,53,54,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.