



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:32 am GMT

PDB ID : 2DHR  
Title : Whole cytosolic region of ATP-dependent metalloprotease FtsH (G399L)  
Authors : Suno, R.; Niwa, H.; Tsuchiya, D.; Zhang, X.; Yoshida, M.; Morikawa, K.  
Deposited on : 2006-03-24  
Resolution : 3.90 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.

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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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28683  
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

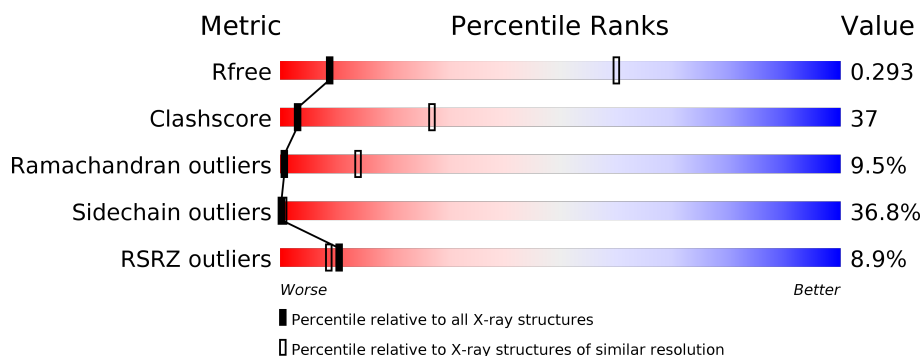
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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	1007 (4.20-3.60)
Clashscore	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)

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	499	<div> <div>8%</div> <div> <div>34%</div> <div>36%</div> <div>19%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	499	<div> <div>9%</div> <div> <div>29%</div> <div>38%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	499	<div> <div>10%</div> <div> <div>34%</div> <div>36%</div> <div>19%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	499	<div> <div>7%</div> <div> <div>30%</div> <div>36%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	499	<div> <div>8%</div> <div> <div>34%</div> <div>36%</div> <div>19%</div> <div>•</div> <div>8%</div> </div> </div>
1	F	499	<div> <div>8%</div> <div> <div>30%</div> <div>38%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21460 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 FtsH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3579	2245	659	662	13			
1	B	446	Total	C	N	O	S	0	0	0
			3511	2206	641	651	13			
1	C	458	Total	C	N	O	S	0	0	0
			3583	2247	659	664	13			
1	D	445	Total	C	N	O	S	0	0	0
			3503	2200	640	650	13			
1	E	458	Total	C	N	O	S	0	0	0
			3583	2247	659	664	13			
1	F	450	Total	C	N	O	S	0	0	0
			3539	2223	648	655	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
B	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
C	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
D	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
E	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
F	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

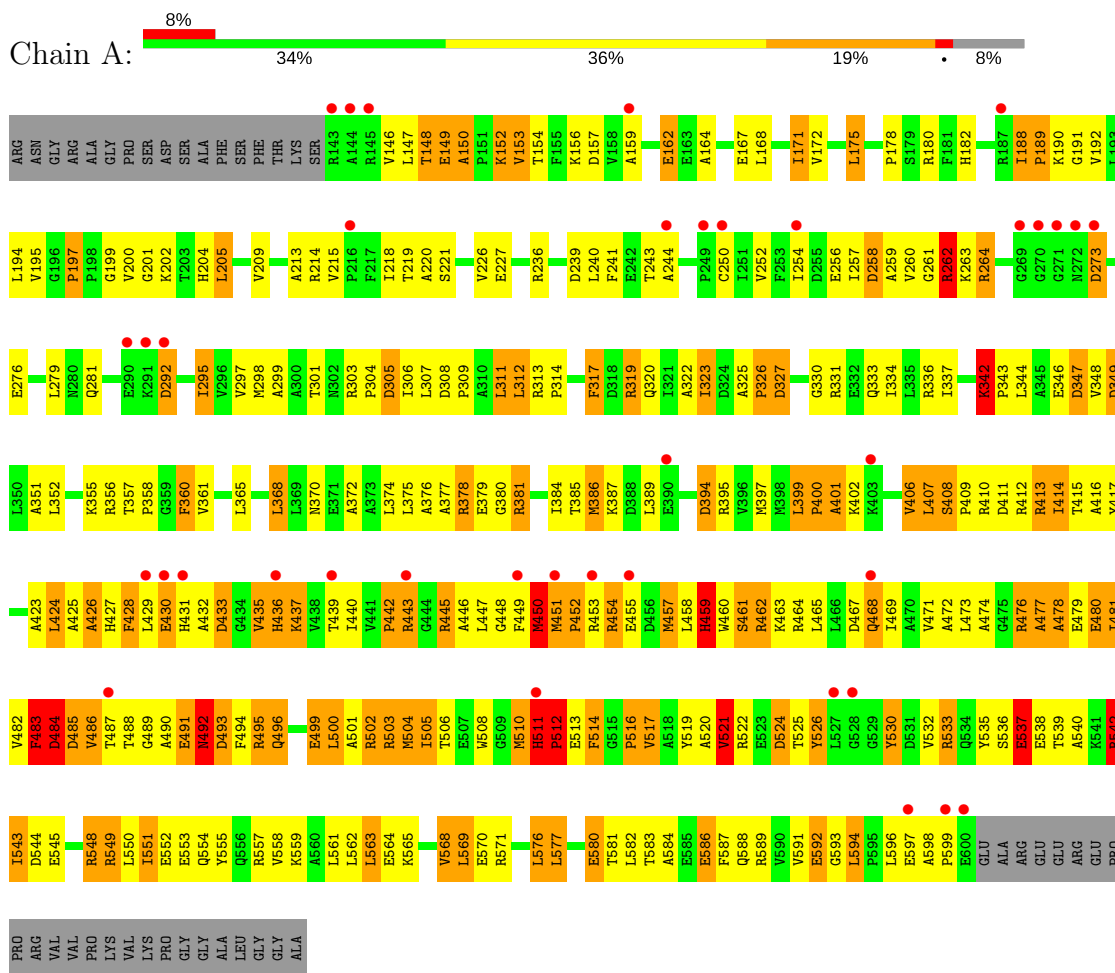


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

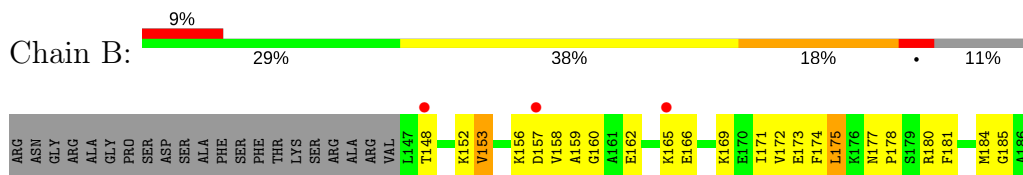
### 3 Residue-property plots

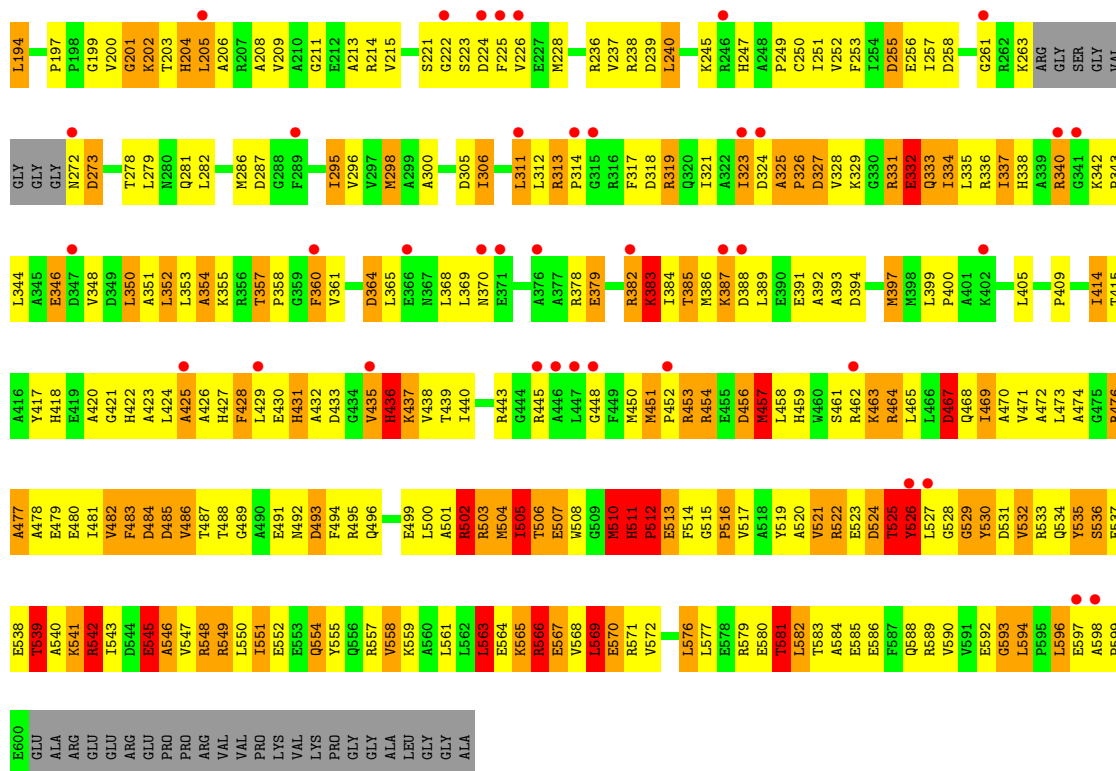
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: FtsH

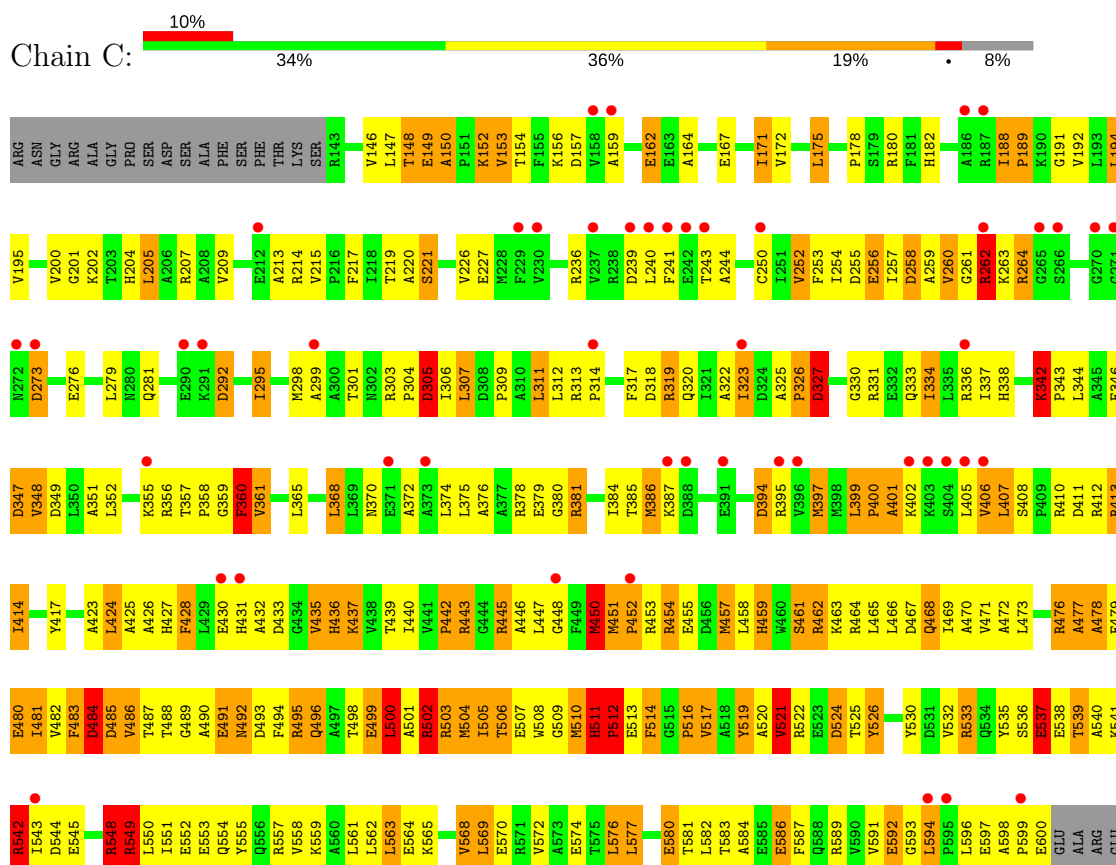


#### • Molecule 1: FtsH



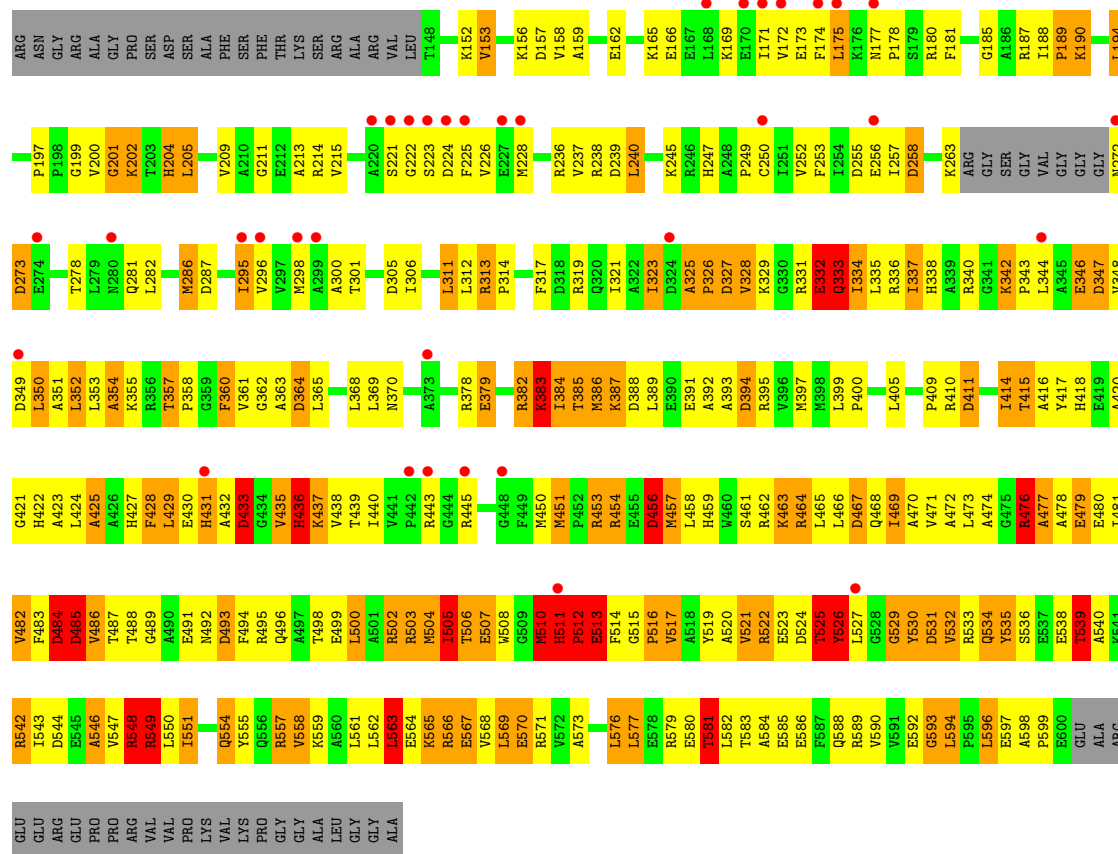


### • Molecule 1: FtsH

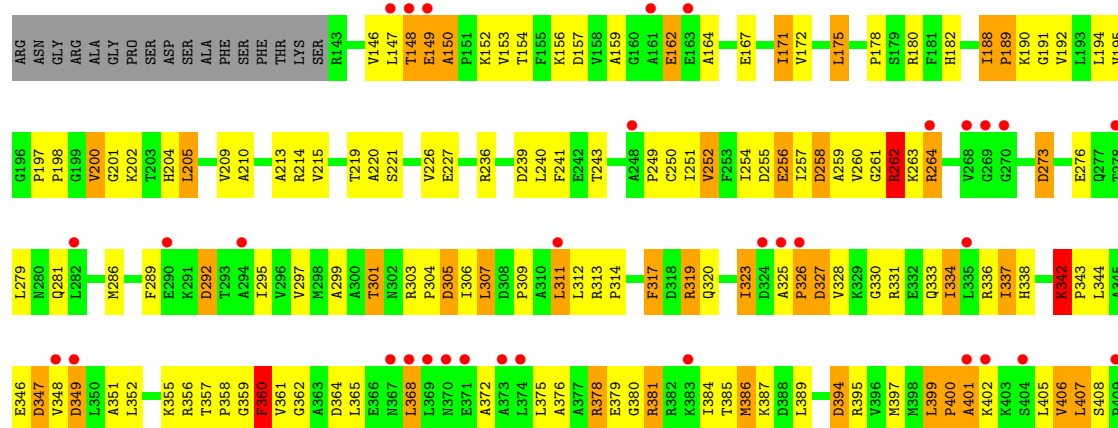


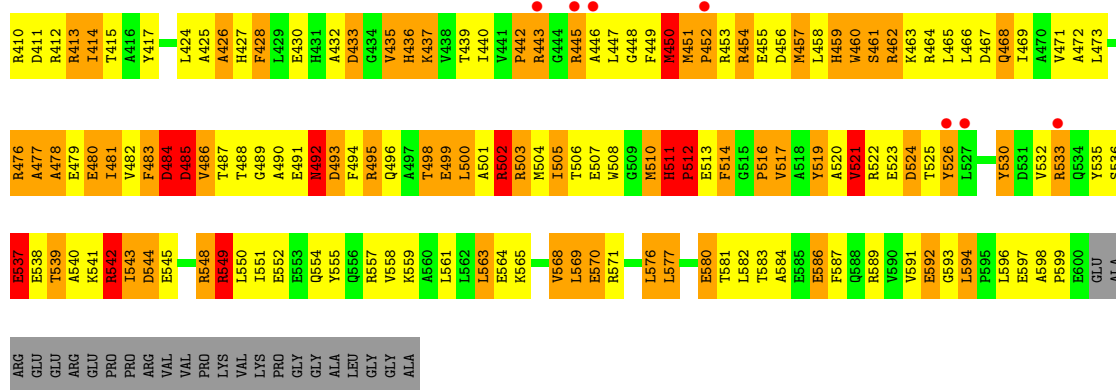
GLU ARG  
GLU GLY  
PRO PRO  
PRO ARG  
VAL VAL  
VAL VAL  
PRO LYS  
PRO LYS  
GLY GLY  
GLY ALA  
LEU LEU  
GLY GLY  
ALA

• Molecule 1: FtsH

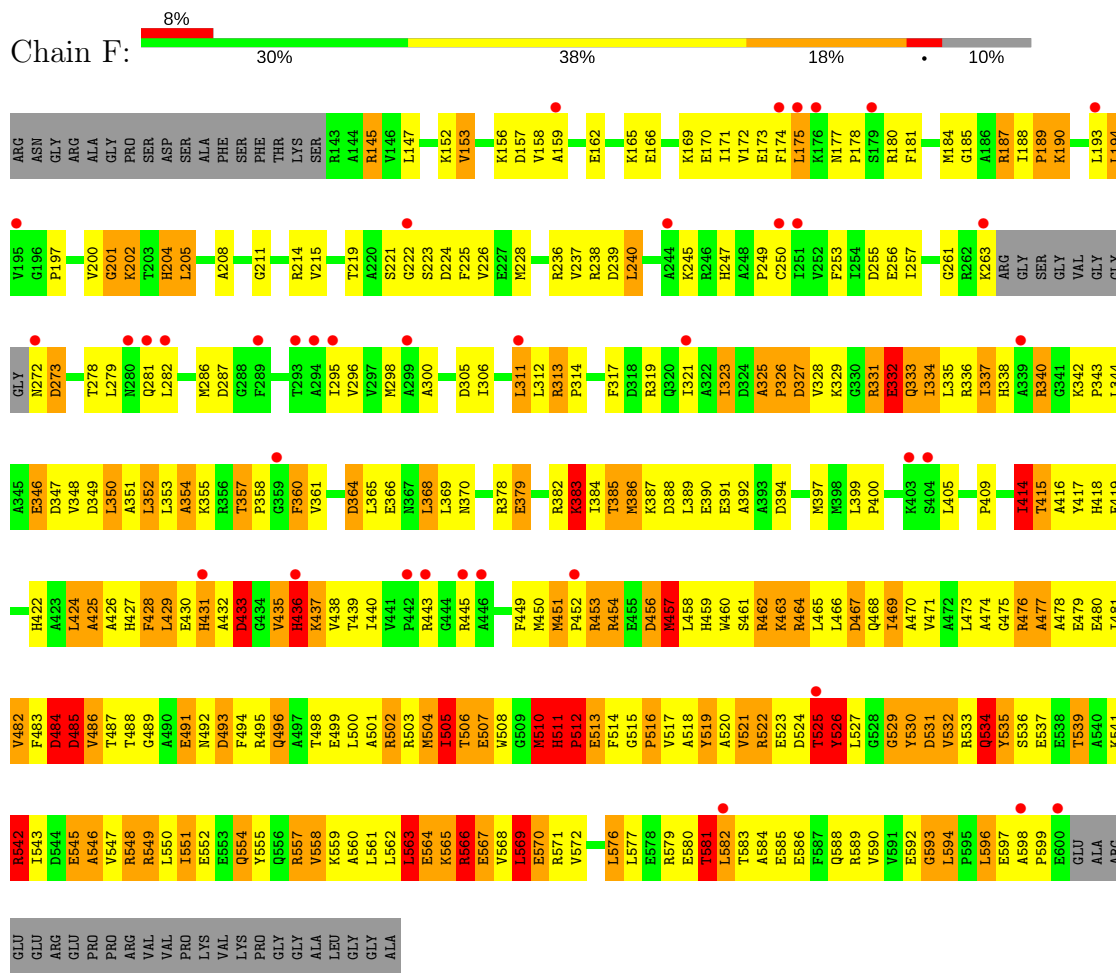


• Molecule 1: FtsH





### • Molecule 1: FtsH





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.15Å 146.15Å 349.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.90 73.08 – 3.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.90) 97.4 (73.08-3.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.79 (at 3.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.299 , 0.342 0.292 , 0.293	Depositor DCC
$R_{free}$ test set	1960 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , -17.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.27$ , $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.247 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	21460	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: ADP

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	0.78	4/3637 (0.1%)	0.96	14/4908 (0.3%)
1	B	0.77	4/3568 (0.1%)	0.98	18/4815 (0.4%)
1	C	0.78	4/3641 (0.1%)	0.97	19/4913 (0.4%)
1	D	0.79	2/3560 (0.1%)	0.99	22/4804 (0.5%)
1	E	0.74	2/3641 (0.1%)	0.95	20/4913 (0.4%)
1	F	0.77	4/3596 (0.1%)	0.97	18/4853 (0.4%)
All	All	0.77	20/21643 (0.1%)	0.97	111/29206 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	3
1	D	0	4
1	E	0	2
1	F	0	6
All	All	0	22

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	549	ARG	NE-CZ	7.12	1.42	1.33
1	C	553	GLU	CD-OE1	6.86	1.33	1.25
1	D	549	ARG	NE-CZ	6.80	1.41	1.33
1	C	537	GLU	CD-OE1	6.61	1.32	1.25
1	E	537	GLU	CD-OE1	6.42	1.32	1.25

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	549	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	C	493	ASP	CB-CG-OD2	8.24	125.72	118.30
1	E	493	ASP	CB-CG-OD2	7.17	124.75	118.30
1	F	549	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	C	548	ARG	NE-CZ-NH1	6.88	123.74	120.30

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	ALA	Peptide
1	A	511	HIS	Peptide
1	A	512	PRO	Peptide
1	B	457	MET	Peptide
1	B	505	ILE	Peptide

## 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	3579	0	3624	251	0
1	B	3511	0	3556	321	0
1	C	3583	0	3628	252	0
1	D	3503	0	3545	314	0
1	E	3583	0	3628	240	0
1	F	3539	0	3585	318	0
2	A	27	0	12	2	0
2	B	27	0	12	6	0
2	C	27	0	12	1	0
2	D	27	0	12	7	0
2	E	27	0	12	1	0
2	F	27	0	12	4	0
All	All	21460	0	21638	1596	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 37.

The worst 5 of 1596 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:D:502:ARG:CD	1:D:533:ARG:HH22	1.54	1.20
1:E:510:MET:O	1:E:512:PRO:HD2	1.41	1.17
1:F:502:ARG:CD	1:F:533:ARG:HH22	1.56	1.17
1:C:428:PHE:CD1	1:C:432:ALA:HB1	1.81	1.15
1:E:428:PHE:CD1	1:E:432:ALA:HB1	1.81	1.15

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	456/499 (91%)	311 (68%)	102 (22%)	43 (9%)	1	14
1	B	442/499 (89%)	320 (72%)	79 (18%)	43 (10%)	1	13
1	C	456/499 (91%)	319 (70%)	100 (22%)	37 (8%)	1	17
1	D	441/499 (88%)	314 (71%)	80 (18%)	47 (11%)	0	10
1	E	456/499 (91%)	320 (70%)	98 (22%)	38 (8%)	1	16
1	F	446/499 (89%)	315 (71%)	83 (19%)	48 (11%)	0	10
All	All	2697/2994 (90%)	1899 (70%)	542 (20%)	256 (10%)	1	14

5 of 256 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ALA
1	A	401	ALA
1	A	442	PRO
1	A	457	MET
1	A	477	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/397 (92%)	234 (64%)	131 (36%)	0	1
1	B	361/397 (91%)	228 (63%)	133 (37%)	0	0
1	C	366/397 (92%)	232 (63%)	134 (37%)	0	1
1	D	360/397 (91%)	226 (63%)	134 (37%)	0	0
1	E	366/397 (92%)	230 (63%)	136 (37%)	0	0
1	F	363/397 (91%)	228 (63%)	135 (37%)	0	0
All	All	2181/2382 (92%)	1378 (63%)	803 (37%)	0	0

5 of 803 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	506	THR
1	D	368	LEU
1	F	436	HIS
1	C	532	VAL
1	D	205	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	338	HIS
1	C	554	GLN
1	F	338	HIS
1	C	370	ASN
1	C	468	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
2	ADP	A	1001	-	25,29,29	1.13	2 (8%)	24,45,45	1.98	2 (8%)
2	ADP	B	2001	-	25,29,29	1.14	2 (8%)	24,45,45	2.14	2 (8%)
2	ADP	C	3001	-	25,29,29	1.08	2 (8%)	24,45,45	2.14	2 (8%)
2	ADP	D	4001	-	25,29,29	1.13	2 (8%)	24,45,45	2.08	2 (8%)
2	ADP	E	5001	-	25,29,29	1.12	2 (8%)	24,45,45	2.10	1 (4%)
2	ADP	F	6001	-	25,29,29	1.12	2 (8%)	24,45,45	2.06	1 (4%)

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
2	ADP	A	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	B	2001	-	-	0/12/32/32	0/3/3/3
2	ADP	C	3001	-	-	0/12/32/32	0/3/3/3
2	ADP	D	4001	-	-	0/12/32/32	0/3/3/3
2	ADP	E	5001	-	-	0/12/32/32	0/3/3/3
2	ADP	F	6001	-	-	0/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4001	ADP	C2-N1	2.16	1.38	1.33
2	C	3001	ADP	C2-N1	2.40	1.38	1.33
2	E	5001	ADP	C2-N1	2.46	1.38	1.33
2	A	1001	ADP	C2-N1	2.49	1.38	1.33
2	F	6001	ADP	C2-N1	2.52	1.38	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	ADP	N3-C2-N1	-10.04	120.11	128.86
2	C	3001	ADP	N3-C2-N1	-9.68	120.43	128.86
2	F	6001	ADP	N3-C2-N1	-9.62	120.48	128.86
2	E	5001	ADP	N3-C2-N1	-9.54	120.55	128.86
2	D	4001	ADP	N3-C2-N1	-9.47	120.61	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ADP	2	0
2	B	2001	ADP	6	0
2	C	3001	ADP	1	0
2	D	4001	ADP	7	0
2	E	5001	ADP	1	0
2	F	6001	ADP	4	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 [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	458/499 (91%)	0.54	38 (8%) 12 10	2, 19, 55, 80	0
1	B	446/499 (89%)	0.58	43 (9%) 9 8	2, 19, 50, 97	0
1	C	458/499 (91%)	0.68	48 (10%) 7 6	2, 20, 57, 84	0
1	D	445/499 (89%)	0.53	35 (7%) 13 11	2, 18, 50, 97	0
1	E	458/499 (91%)	0.59	40 (8%) 11 9	2, 21, 55, 82	0
1	F	450/499 (90%)	0.62	38 (8%) 12 10	2, 19, 51, 94	0
All	All	2715/2994 (90%)	0.59	242 (8%) 10 9	2, 19, 54, 97	0

The worst 5 of 242 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	271	GLY	7.6
1	A	144	ALA	7.4
1	C	403	LYS	6.9
1	F	272	ASN	6.5
1	E	269	GLY	5.7

### 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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	A	1001	27/27	0.88	0.26	-0.39	14,15,17,18	0
2	ADP	C	3001	27/27	0.86	0.27	-0.64	18,18,19,19	0
2	ADP	D	4001	27/27	0.92	0.25	-0.85	2,2,8,8	0
2	ADP	E	5001	27/27	0.85	0.27	-1.01	14,17,18,18	0
2	ADP	F	6001	27/27	0.88	0.22	-1.04	11,15,15,18	0
2	ADP	B	2001	27/27	0.85	0.21	-1.08	5,9,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.