



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Nov 21, 2016 – 08:44 PM EST

PDB ID : 5KYH
EMDB ID: : EMD-8298
Title : Structure of Iho670 Flagellar-like Filament
Authors : Braun, T.; Vos, M.; Kalisman, N.; Sherman, N.E.; Rachel, R.; Wirth, R.;
Schroeder, G.F.; Egelman, E.H.
Deposited on : 2016-07-21
Resolution : 4.00 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

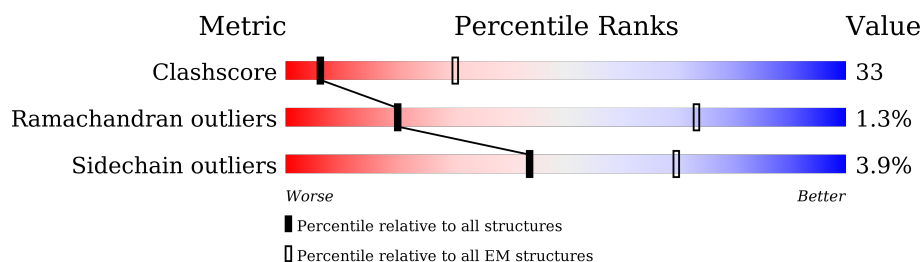
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	303	
1	B	303	
1	C	303	
1	D	303	
1	E	303	
1	F	303	
1	G	303	
1	H	303	
1	I	303	

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Mol	Chain	Length	Quality of chain
1	J	303	 50% 28% .. 20%
1	K	303	 50% 27% .. 20%
1	L	303	 50% 28% .. 20%
1	M	303	 50% 28% .. 20%
1	N	303	 50% 28% .. 20%
1	O	303	 52% 25% .. 20%
1	P	303	 52% 25% .. 20%
1	Q	303	 52% 25% .. 20%
1	R	303	 53% 24% .. 20%
1	S	303	 53% 25% .. 20%
1	T	303	 53% 25% .. 20%
1	U	303	 53% 24% .. 20%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 38892 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Iho670.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	B	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	C	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	D	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	E	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	F	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	G	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	H	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	I	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	J	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	K	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	L	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	M	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	N	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	O	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	P	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	Q	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		

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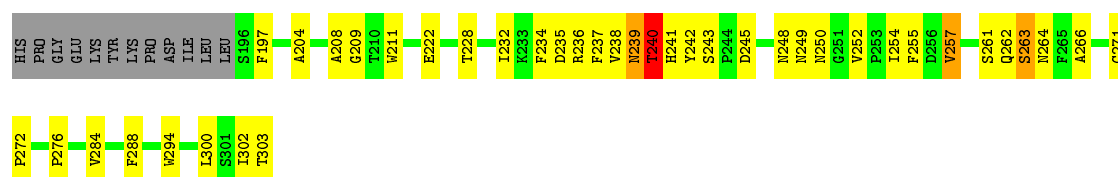
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	S	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	T	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		
1	U	242	Total	C	N	O	S	0	0
			1852	1193	301	353	5		

i

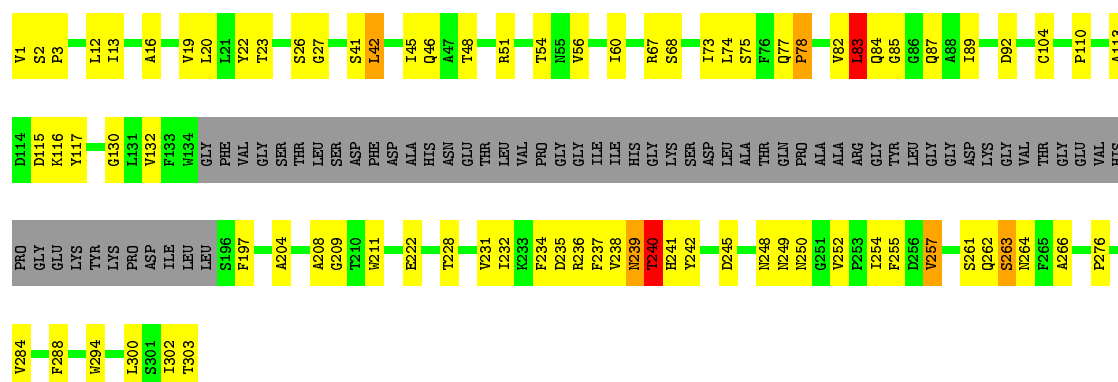
- Molecule 1: Iho670





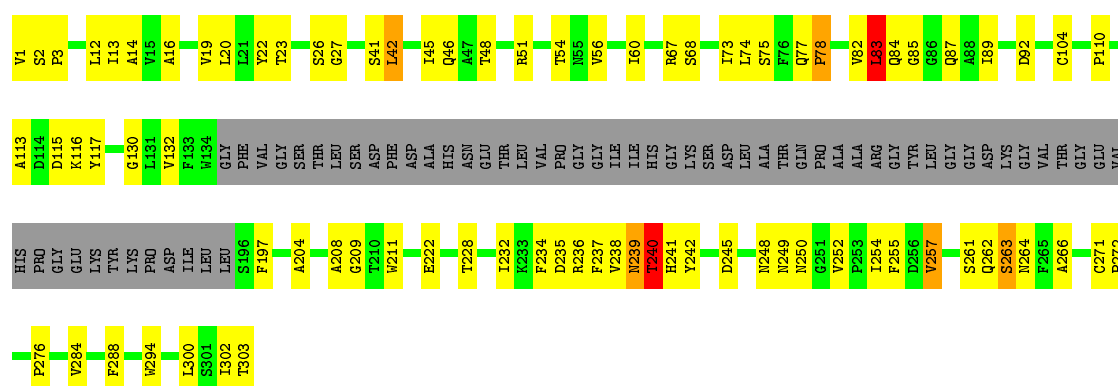
• Molecule 1: Iho670

Chain D: 53% 24% 20%



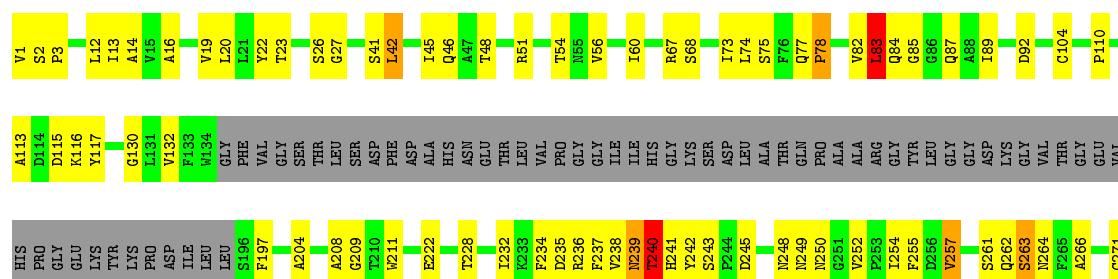
• Molecule 1: Iho670

Chain E: 52% 25% 20%

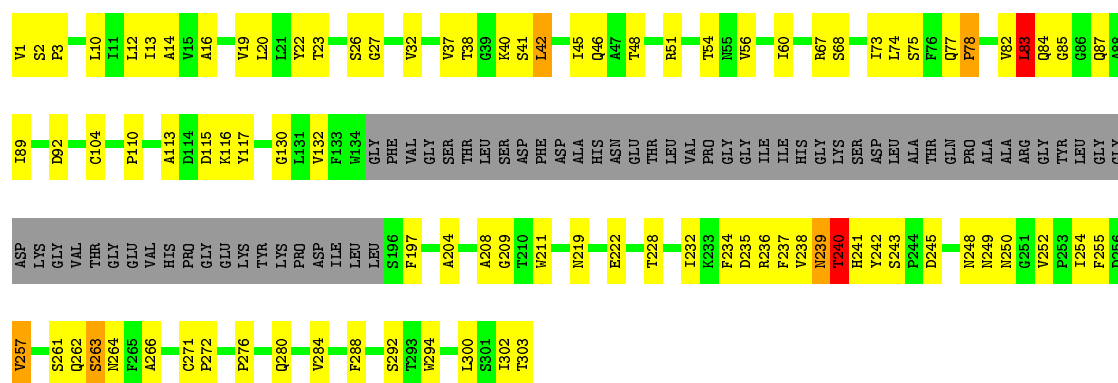


• Molecule 1: Iho670

Chain F: 52% 25% 20%

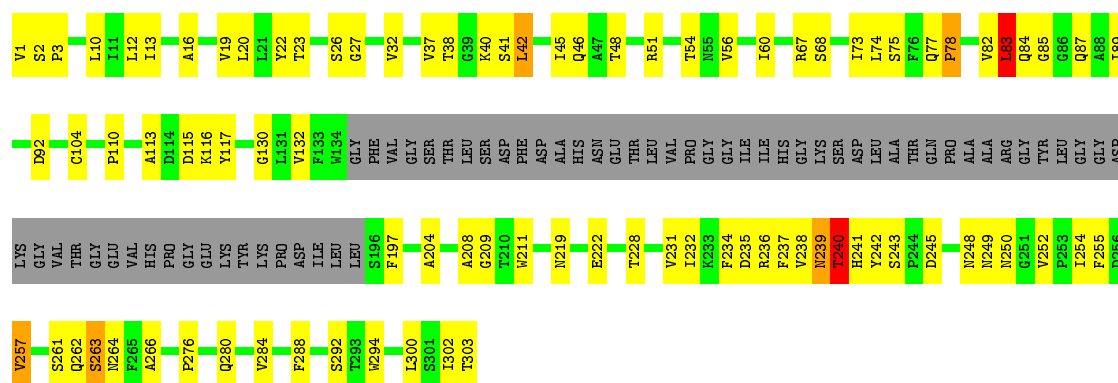


Chain J: 



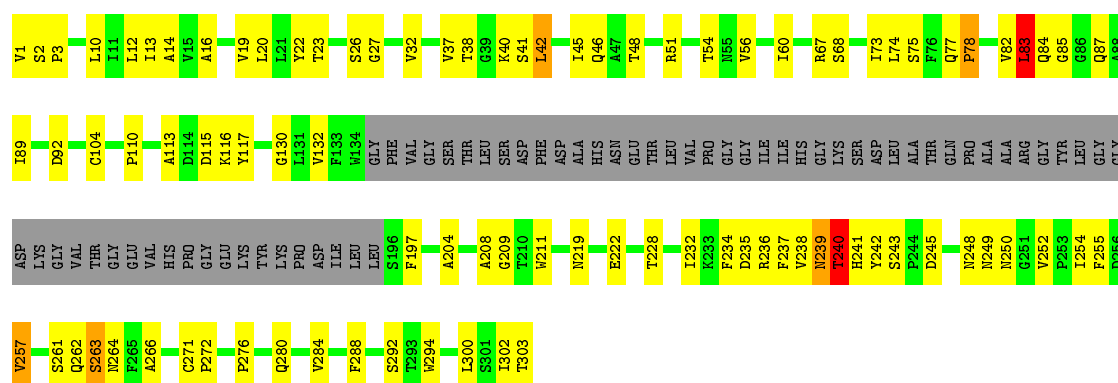
• Molecule 1: Iho670

Chain K: 



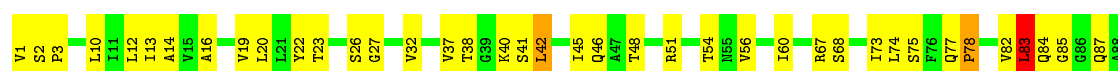
• Molecule 1: Iho670

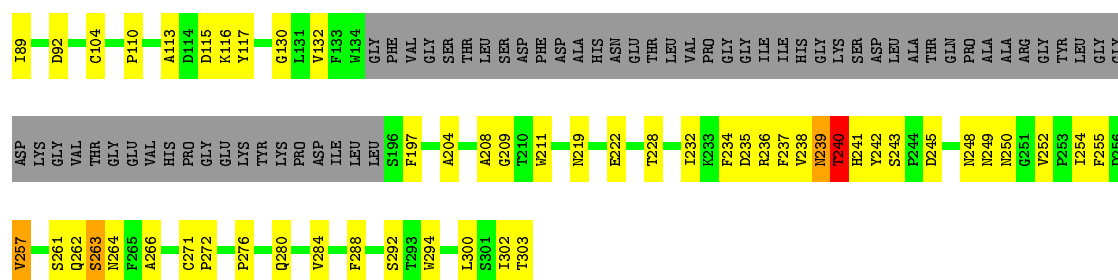
Chain L: 



• Molecule 1: Iho670

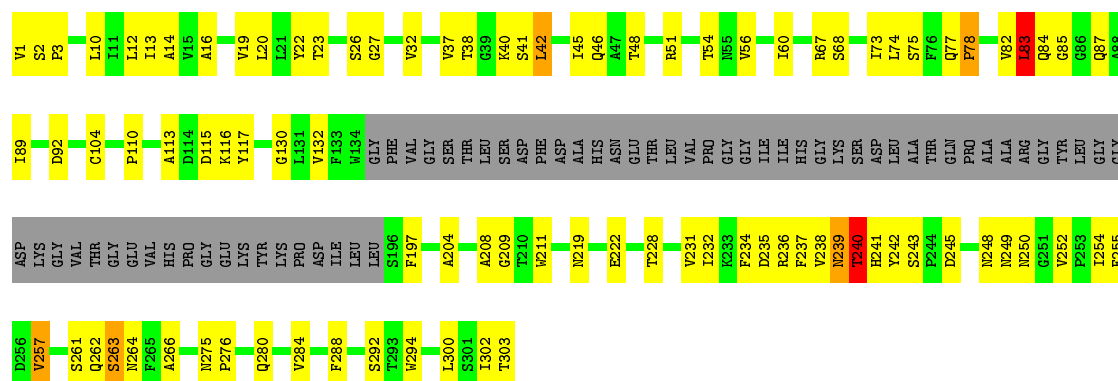
Chain M: 





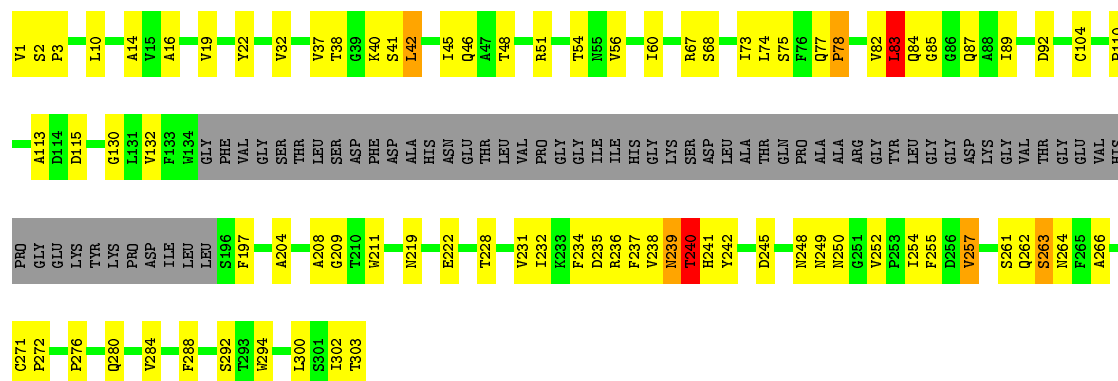
• Molecule 1: Iho670

Chain N: 50% 28% 20%



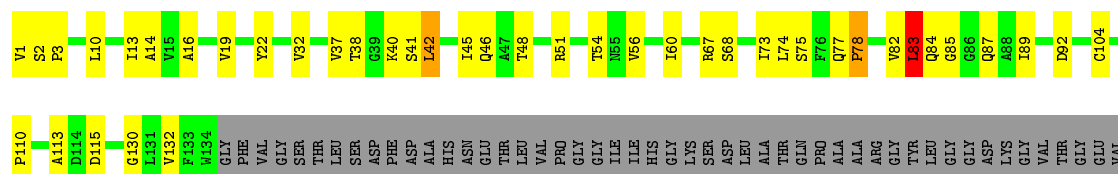
• Molecule 1: Iho670

Chain O: 52% 25% 20%



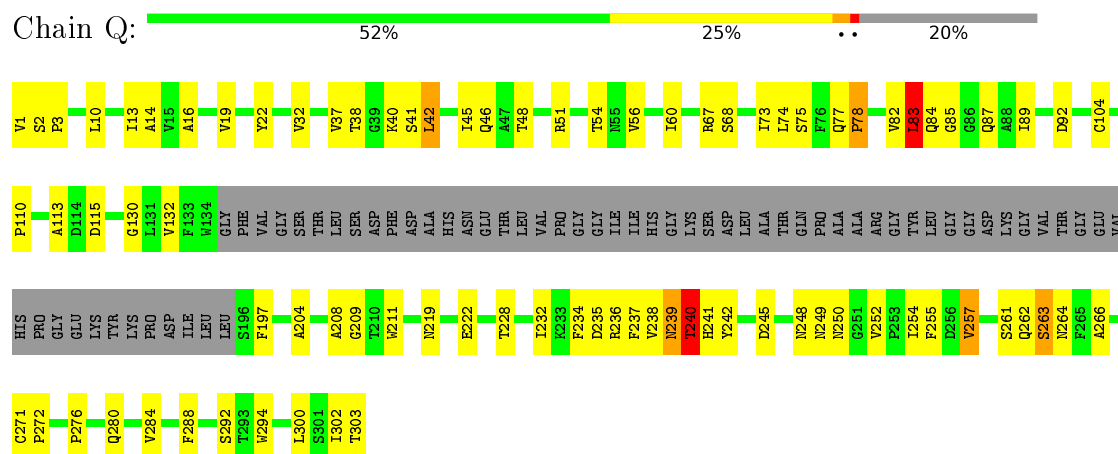
• Molecule 1: Iho670

Chain P: 52% 25% 20%

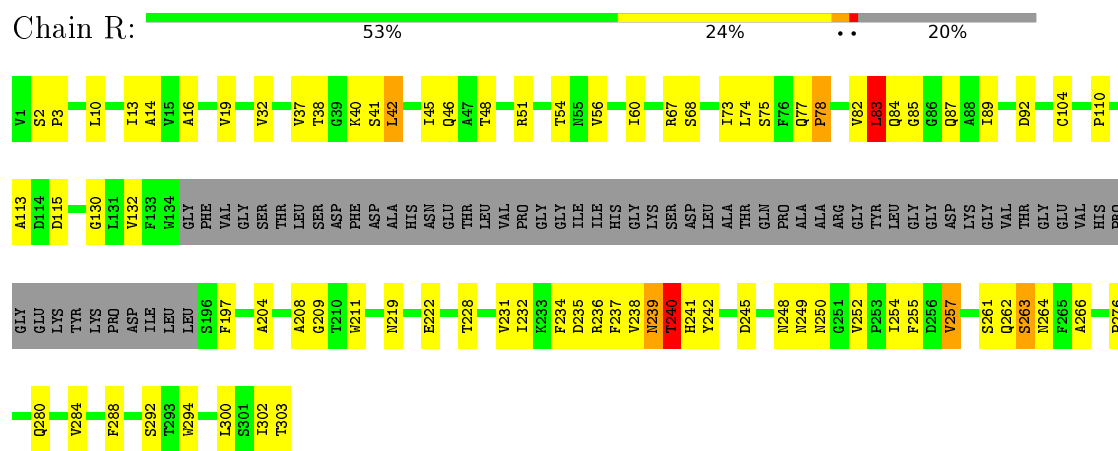




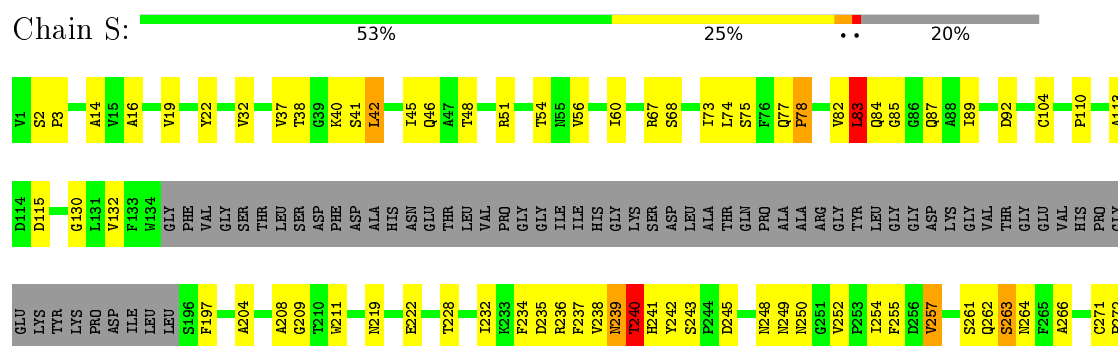
• Molecule 1: Iho670



• Molecule 1: Iho670



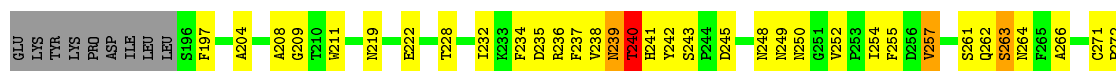
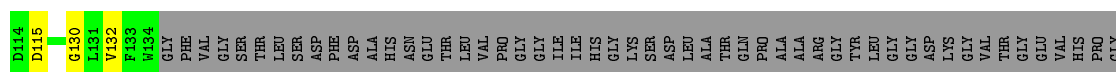
• Molecule 1: Iho670





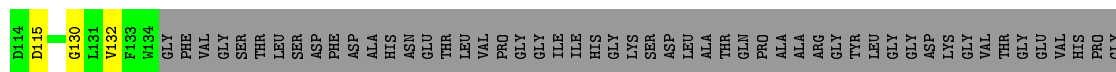
• Molecule 1: Iho670

Chain T: 53% 25% 20%



• Molecule 1: Iho670

Chain U: 53% 24% 20%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	146696	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	B	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	C	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	D	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	E	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	F	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	G	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	H	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	I	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	J	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	K	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	L	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	M	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	N	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	O	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	P	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	Q	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	R	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	S	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	T	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
1	U	0.68	1/1897 (0.1%)	0.82	2/2603 (0.1%)
All	All	0.68	21/39837 (0.1%)	0.82	42/54663 (0.1%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	222	GLU	CG-CD	7.70	1.63	1.51
1	S	222	GLU	CG-CD	7.69	1.63	1.51
1	H	222	GLU	CG-CD	7.68	1.63	1.51
1	U	222	GLU	CG-CD	7.68	1.63	1.51
1	L	222	GLU	CG-CD	7.67	1.63	1.51

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	N	92	ASP	CB-CG-OD1	5.83	123.55	118.30
1	T	92	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	92	ASP	CB-CG-OD1	5.80	123.52	118.30
1	K	92	ASP	CB-CG-OD1	5.79	123.52	118.30
1	J	92	ASP	CB-CG-OD1	5.77	123.49	118.30

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	1852	0	1820	141	0
1	B	1852	0	1820	137	0
1	C	1852	0	1820	139	0
1	D	1852	0	1820	139	0
1	E	1852	0	1820	140	0
1	F	1852	0	1820	146	0
1	G	1852	0	1820	137	0
1	H	1852	0	1820	194	0
1	I	1852	0	1820	197	0
1	J	1852	0	1820	194	0
1	K	1852	0	1820	191	0
1	L	1852	0	1820	195	0
1	M	1852	0	1820	192	0
1	N	1852	0	1820	194	0
1	O	1852	0	1820	143	0
1	P	1852	0	1820	147	0
1	Q	1852	0	1820	139	0
1	R	1852	0	1820	138	0
1	S	1852	0	1820	139	0
1	T	1852	0	1820	135	0
1	U	1852	0	1820	137	0
All	All	38892	0	38220	2572	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 33.

The worst 5 of 2572 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:K:117:TYR:CZ	1:R:302:ILE:CD1	2.00	1.45
1:D:27:GLY:CA	1:K:294:TRP:HZ3	1.29	1.44
1:C:117:TYR:CZ	1:J:302:ILE:HD11	1.53	1.44
1:L:117:TYR:CZ	1:S:302:ILE:HD11	1.53	1.44
1:M:117:TYR:CZ	1:T:302:ILE:HD11	1.52	1.44

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 PDB entries followed by that with respect to all EM entries.

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	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	B	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	C	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	D	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	E	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	F	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	G	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	H	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	I	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	J	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	K	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	L	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	M	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60
1	N	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	O	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15 60
1	P	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15 60
1	Q	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15 60
1	R	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15 60
1	S	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15 60
1	T	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15 60
1	U	238/303 (78%)	229 (96%)	6 (2%)	3 (1%)	15 60
All	All	4998/6363 (78%)	4809 (96%)	126 (2%)	63 (1%)	20 60

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	A	240	THR
1	B	83	LEU
1	B	240	THR
1	C	83	LEU

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 PDB entries followed by that with respect to all EM entries.

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	205/251 (82%)	197 (96%)	8 (4%)	39 74
1	B	205/251 (82%)	197 (96%)	8 (4%)	39 74
1	C	205/251 (82%)	197 (96%)	8 (4%)	39 74
1	D	205/251 (82%)	197 (96%)	8 (4%)	39 74
1	E	205/251 (82%)	197 (96%)	8 (4%)	39 74
1	F	205/251 (82%)	197 (96%)	8 (4%)	39 74
1	G	205/251 (82%)	197 (96%)	8 (4%)	39 74
1	H	205/251 (82%)	197 (96%)	8 (4%)	39 74
1	I	205/251 (82%)	197 (96%)	8 (4%)	39 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	K	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	L	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	M	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	N	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	O	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	P	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	Q	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	R	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	S	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	T	205/251 (82%)	197 (96%)	8 (4%)	39	74
1	U	205/251 (82%)	197 (96%)	8 (4%)	39	74
All	All	4305/5271 (82%)	4137 (96%)	168 (4%)	43	74

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	104	CYS
1	L	240	THR
1	T	104	CYS
1	J	240	THR
1	K	239	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	77	GLN
1	M	219	ASN
1	T	219	ASN
1	K	219	ASN
1	L	219	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.