



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:39 PM GMT

PDB ID : 4UXG  
Title : Crystal structure of the carboxy-terminal region of the bacteriophage T4 proximal long tail fibre protein gp34, R32 native crystal  
Authors : Granell, M.; Alvira, S.; Garcia-Doval, C.; Singh, A.K.; van Raaij, M.J.  
Deposited on : 2014-08-22  
Resolution : 3.00 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.

---

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20026982

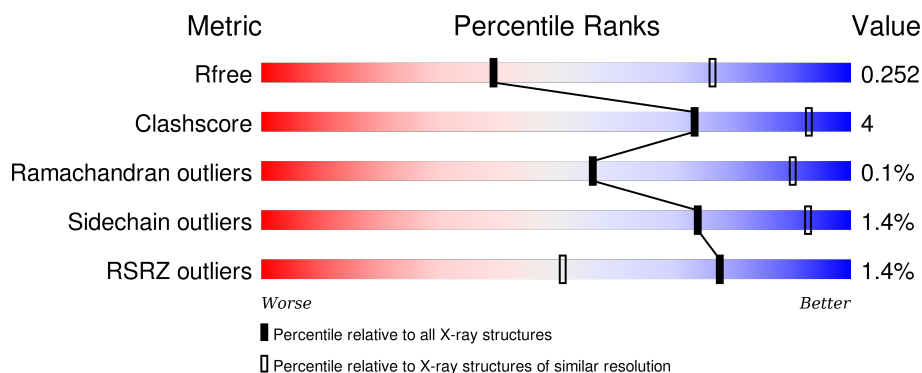
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	410	<div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	B	410	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	C	410	<div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	D	410	<div> <div>81%</div> <div>14%</div> <div>.</div> </div>
1	E	410	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	410	<div><div><div>%</div><div><div></div><div>86%</div><div>10%</div><div></div></div><div></div></div></div>
1	G	410	<div><div><div>3%</div><div><div></div><div>85%</div><div>11%</div><div></div></div><div></div></div></div>
1	H	410	<div><div><div>2%</div><div><div></div><div>89%</div><div>7%</div><div></div></div><div></div></div></div>
1	I	410	<div><div><div>%</div><div><div></div><div>85%</div><div>11%</div><div></div></div><div></div></div></div>
1	J	410	<div><div><div>3%</div><div><div></div><div>83%</div><div>13%</div><div></div></div><div></div></div></div>
1	K	410	<div><div><div>%</div><div><div></div><div>82%</div><div>13%</div><div></div></div><div></div></div></div>
1	L	410	<div><div><div>3%</div><div><div></div><div>82%</div><div>13%</div><div></div></div><div></div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 36241 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 LARGE TAIL FIBER PROTEIN P34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			
1	B	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			
1	C	398	Total	C	N	O	S	0	0	0
			3043	1898	536	604	5			
1	D	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			
1	E	398	Total	C	N	O	S	0	0	0
			3043	1898	536	604	5			
1	F	396	Total	C	N	O	S	0	0	0
			3027	1891	533	598	5			
1	G	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			
1	H	394	Total	C	N	O	S	0	0	0
			3013	1881	531	596	5			
1	I	394	Total	C	N	O	S	0	0	0
			3014	1883	531	595	5			
1	J	394	Total	C	N	O	S	0	0	0
			3014	1883	531	595	5			
1	K	391	Total	C	N	O	S	0	0	0
			2987	1864	527	591	5			
1	L	395	Total	C	N	O	S	0	0	0
			3020	1886	532	597	5			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	880	MET	-	EXPRESSION TAG	UNP P18771
A	881	GLY	-	EXPRESSION TAG	UNP P18771
A	882	SER	-	EXPRESSION TAG	UNP P18771
A	883	SER	-	EXPRESSION TAG	UNP P18771
A	884	HIS	-	EXPRESSION TAG	UNP P18771

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	885	HIS	-	EXPRESSION TAG	UNP P18771
A	886	HIS	-	EXPRESSION TAG	UNP P18771
A	887	HIS	-	EXPRESSION TAG	UNP P18771
A	888	HIS	-	EXPRESSION TAG	UNP P18771
A	889	HIS	-	EXPRESSION TAG	UNP P18771
A	890	SER	-	EXPRESSION TAG	UNP P18771
A	891	GLN	-	EXPRESSION TAG	UNP P18771
A	892	ASP	-	EXPRESSION TAG	UNP P18771
A	893	PRO	-	EXPRESSION TAG	UNP P18771
B	880	MET	-	EXPRESSION TAG	UNP P18771
B	881	GLY	-	EXPRESSION TAG	UNP P18771
B	882	SER	-	EXPRESSION TAG	UNP P18771
B	883	SER	-	EXPRESSION TAG	UNP P18771
B	884	HIS	-	EXPRESSION TAG	UNP P18771
B	885	HIS	-	EXPRESSION TAG	UNP P18771
B	886	HIS	-	EXPRESSION TAG	UNP P18771
B	887	HIS	-	EXPRESSION TAG	UNP P18771
B	888	HIS	-	EXPRESSION TAG	UNP P18771
B	889	HIS	-	EXPRESSION TAG	UNP P18771
B	890	SER	-	EXPRESSION TAG	UNP P18771
B	891	GLN	-	EXPRESSION TAG	UNP P18771
B	892	ASP	-	EXPRESSION TAG	UNP P18771
B	893	PRO	-	EXPRESSION TAG	UNP P18771
C	880	MET	-	EXPRESSION TAG	UNP P18771
C	881	GLY	-	EXPRESSION TAG	UNP P18771
C	882	SER	-	EXPRESSION TAG	UNP P18771
C	883	SER	-	EXPRESSION TAG	UNP P18771
C	884	HIS	-	EXPRESSION TAG	UNP P18771
C	885	HIS	-	EXPRESSION TAG	UNP P18771
C	886	HIS	-	EXPRESSION TAG	UNP P18771
C	887	HIS	-	EXPRESSION TAG	UNP P18771
C	888	HIS	-	EXPRESSION TAG	UNP P18771
C	889	HIS	-	EXPRESSION TAG	UNP P18771
C	890	SER	-	EXPRESSION TAG	UNP P18771
C	891	GLN	-	EXPRESSION TAG	UNP P18771
C	892	ASP	-	EXPRESSION TAG	UNP P18771
C	893	PRO	-	EXPRESSION TAG	UNP P18771
D	880	MET	-	EXPRESSION TAG	UNP P18771
D	881	GLY	-	EXPRESSION TAG	UNP P18771
D	882	SER	-	EXPRESSION TAG	UNP P18771
D	883	SER	-	EXPRESSION TAG	UNP P18771
D	884	HIS	-	EXPRESSION TAG	UNP P18771

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	885	HIS	-	EXPRESSION TAG	UNP P18771
D	886	HIS	-	EXPRESSION TAG	UNP P18771
D	887	HIS	-	EXPRESSION TAG	UNP P18771
D	888	HIS	-	EXPRESSION TAG	UNP P18771
D	889	HIS	-	EXPRESSION TAG	UNP P18771
D	890	SER	-	EXPRESSION TAG	UNP P18771
D	891	GLN	-	EXPRESSION TAG	UNP P18771
D	892	ASP	-	EXPRESSION TAG	UNP P18771
D	893	PRO	-	EXPRESSION TAG	UNP P18771
E	880	MET	-	EXPRESSION TAG	UNP P18771
E	881	GLY	-	EXPRESSION TAG	UNP P18771
E	882	SER	-	EXPRESSION TAG	UNP P18771
E	883	SER	-	EXPRESSION TAG	UNP P18771
E	884	HIS	-	EXPRESSION TAG	UNP P18771
E	885	HIS	-	EXPRESSION TAG	UNP P18771
E	886	HIS	-	EXPRESSION TAG	UNP P18771
E	887	HIS	-	EXPRESSION TAG	UNP P18771
E	888	HIS	-	EXPRESSION TAG	UNP P18771
E	889	HIS	-	EXPRESSION TAG	UNP P18771
E	890	SER	-	EXPRESSION TAG	UNP P18771
E	891	GLN	-	EXPRESSION TAG	UNP P18771
E	892	ASP	-	EXPRESSION TAG	UNP P18771
E	893	PRO	-	EXPRESSION TAG	UNP P18771
F	880	MET	-	EXPRESSION TAG	UNP P18771
F	881	GLY	-	EXPRESSION TAG	UNP P18771
F	882	SER	-	EXPRESSION TAG	UNP P18771
F	883	SER	-	EXPRESSION TAG	UNP P18771
F	884	HIS	-	EXPRESSION TAG	UNP P18771
F	885	HIS	-	EXPRESSION TAG	UNP P18771
F	886	HIS	-	EXPRESSION TAG	UNP P18771
F	887	HIS	-	EXPRESSION TAG	UNP P18771
F	888	HIS	-	EXPRESSION TAG	UNP P18771
F	889	HIS	-	EXPRESSION TAG	UNP P18771
F	890	SER	-	EXPRESSION TAG	UNP P18771
F	891	GLN	-	EXPRESSION TAG	UNP P18771
F	892	ASP	-	EXPRESSION TAG	UNP P18771
F	893	PRO	-	EXPRESSION TAG	UNP P18771
G	880	MET	-	EXPRESSION TAG	UNP P18771
G	881	GLY	-	EXPRESSION TAG	UNP P18771
G	882	SER	-	EXPRESSION TAG	UNP P18771
G	883	SER	-	EXPRESSION TAG	UNP P18771
G	884	HIS	-	EXPRESSION TAG	UNP P18771

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	885	HIS	-	EXPRESSION TAG	UNP P18771
G	886	HIS	-	EXPRESSION TAG	UNP P18771
G	887	HIS	-	EXPRESSION TAG	UNP P18771
G	888	HIS	-	EXPRESSION TAG	UNP P18771
G	889	HIS	-	EXPRESSION TAG	UNP P18771
G	890	SER	-	EXPRESSION TAG	UNP P18771
G	891	GLN	-	EXPRESSION TAG	UNP P18771
G	892	ASP	-	EXPRESSION TAG	UNP P18771
G	893	PRO	-	EXPRESSION TAG	UNP P18771
H	880	MET	-	EXPRESSION TAG	UNP P18771
H	881	GLY	-	EXPRESSION TAG	UNP P18771
H	882	SER	-	EXPRESSION TAG	UNP P18771
H	883	SER	-	EXPRESSION TAG	UNP P18771
H	884	HIS	-	EXPRESSION TAG	UNP P18771
H	885	HIS	-	EXPRESSION TAG	UNP P18771
H	886	HIS	-	EXPRESSION TAG	UNP P18771
H	887	HIS	-	EXPRESSION TAG	UNP P18771
H	888	HIS	-	EXPRESSION TAG	UNP P18771
H	889	HIS	-	EXPRESSION TAG	UNP P18771
H	890	SER	-	EXPRESSION TAG	UNP P18771
H	891	GLN	-	EXPRESSION TAG	UNP P18771
H	892	ASP	-	EXPRESSION TAG	UNP P18771
H	893	PRO	-	EXPRESSION TAG	UNP P18771
I	880	MET	-	EXPRESSION TAG	UNP P18771
I	881	GLY	-	EXPRESSION TAG	UNP P18771
I	882	SER	-	EXPRESSION TAG	UNP P18771
I	883	SER	-	EXPRESSION TAG	UNP P18771
I	884	HIS	-	EXPRESSION TAG	UNP P18771
I	885	HIS	-	EXPRESSION TAG	UNP P18771
I	886	HIS	-	EXPRESSION TAG	UNP P18771
I	887	HIS	-	EXPRESSION TAG	UNP P18771
I	888	HIS	-	EXPRESSION TAG	UNP P18771
I	889	HIS	-	EXPRESSION TAG	UNP P18771
I	890	SER	-	EXPRESSION TAG	UNP P18771
I	891	GLN	-	EXPRESSION TAG	UNP P18771
I	892	ASP	-	EXPRESSION TAG	UNP P18771
I	893	PRO	-	EXPRESSION TAG	UNP P18771
J	880	MET	-	EXPRESSION TAG	UNP P18771
J	881	GLY	-	EXPRESSION TAG	UNP P18771
J	882	SER	-	EXPRESSION TAG	UNP P18771
J	883	SER	-	EXPRESSION TAG	UNP P18771
J	884	HIS	-	EXPRESSION TAG	UNP P18771

*Continued on next page...*

*Continued from previous page...*

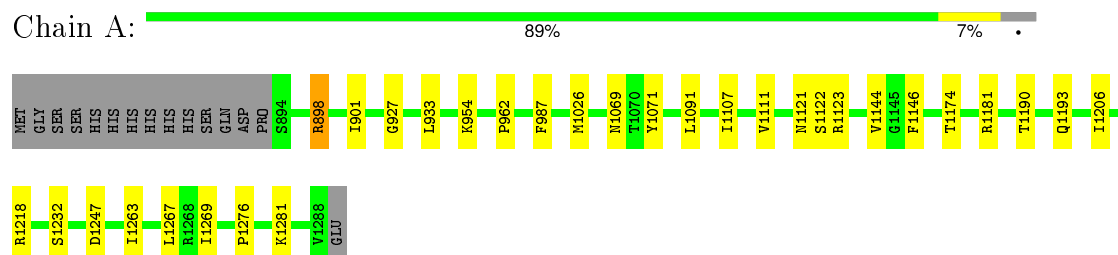
Chain	Residue	Modelled	Actual	Comment	Reference
J	885	HIS	-	EXPRESSION TAG	UNP P18771
J	886	HIS	-	EXPRESSION TAG	UNP P18771
J	887	HIS	-	EXPRESSION TAG	UNP P18771
J	888	HIS	-	EXPRESSION TAG	UNP P18771
J	889	HIS	-	EXPRESSION TAG	UNP P18771
J	890	SER	-	EXPRESSION TAG	UNP P18771
J	891	GLN	-	EXPRESSION TAG	UNP P18771
J	892	ASP	-	EXPRESSION TAG	UNP P18771
J	893	PRO	-	EXPRESSION TAG	UNP P18771
K	880	MET	-	EXPRESSION TAG	UNP P18771
K	881	GLY	-	EXPRESSION TAG	UNP P18771
K	882	SER	-	EXPRESSION TAG	UNP P18771
K	883	SER	-	EXPRESSION TAG	UNP P18771
K	884	HIS	-	EXPRESSION TAG	UNP P18771
K	885	HIS	-	EXPRESSION TAG	UNP P18771
K	886	HIS	-	EXPRESSION TAG	UNP P18771
K	887	HIS	-	EXPRESSION TAG	UNP P18771
K	888	HIS	-	EXPRESSION TAG	UNP P18771
K	889	HIS	-	EXPRESSION TAG	UNP P18771
K	890	SER	-	EXPRESSION TAG	UNP P18771
K	891	GLN	-	EXPRESSION TAG	UNP P18771
K	892	ASP	-	EXPRESSION TAG	UNP P18771
K	893	PRO	-	EXPRESSION TAG	UNP P18771
L	880	MET	-	EXPRESSION TAG	UNP P18771
L	881	GLY	-	EXPRESSION TAG	UNP P18771
L	882	SER	-	EXPRESSION TAG	UNP P18771
L	883	SER	-	EXPRESSION TAG	UNP P18771
L	884	HIS	-	EXPRESSION TAG	UNP P18771
L	885	HIS	-	EXPRESSION TAG	UNP P18771
L	886	HIS	-	EXPRESSION TAG	UNP P18771
L	887	HIS	-	EXPRESSION TAG	UNP P18771
L	888	HIS	-	EXPRESSION TAG	UNP P18771
L	889	HIS	-	EXPRESSION TAG	UNP P18771
L	890	SER	-	EXPRESSION TAG	UNP P18771
L	891	GLN	-	EXPRESSION TAG	UNP P18771
L	892	ASP	-	EXPRESSION TAG	UNP P18771
L	893	PRO	-	EXPRESSION TAG	UNP P18771



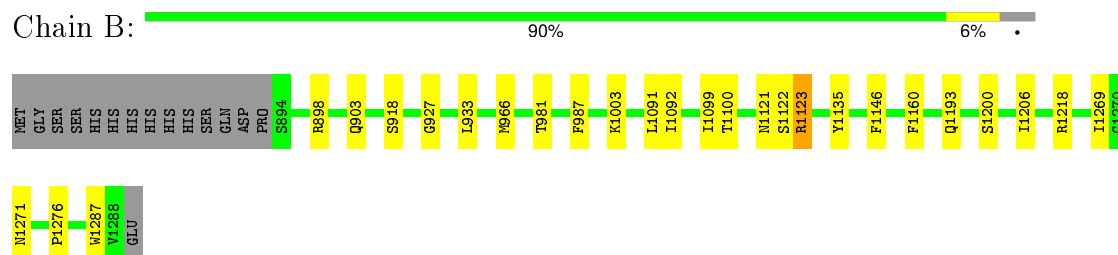
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

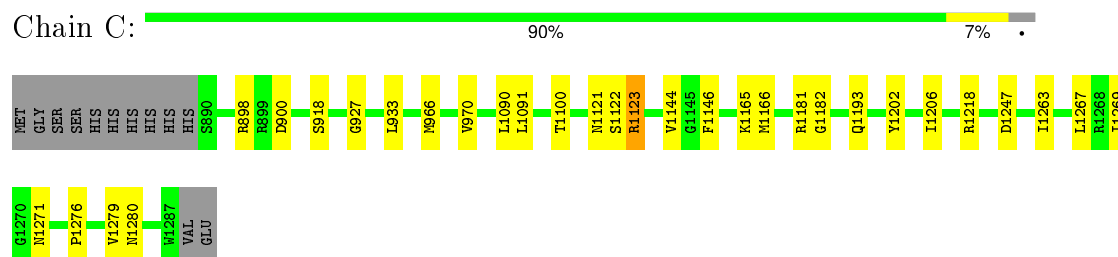
#### • Molecule 1: LARGE TAIL FIBER PROTEIN P34



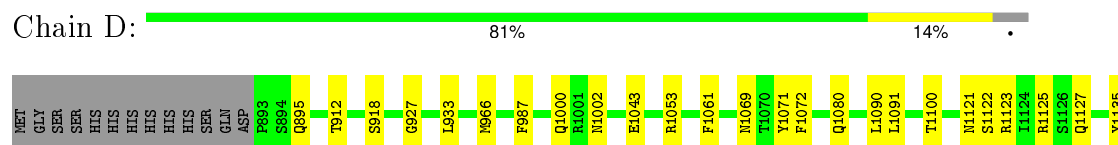
#### • Molecule 1: LARGE TAIL FIBER PROTEIN P34



#### • Molecule 1: LARGE TAIL FIBER PROTEIN P34

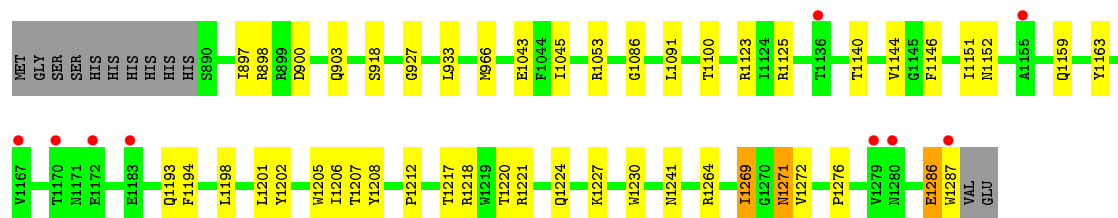
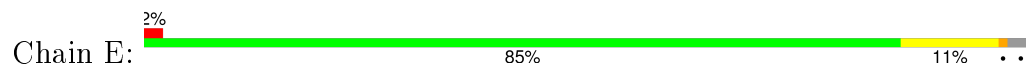


#### • Molecule 1: LARGE TAIL FIBER PROTEIN P34

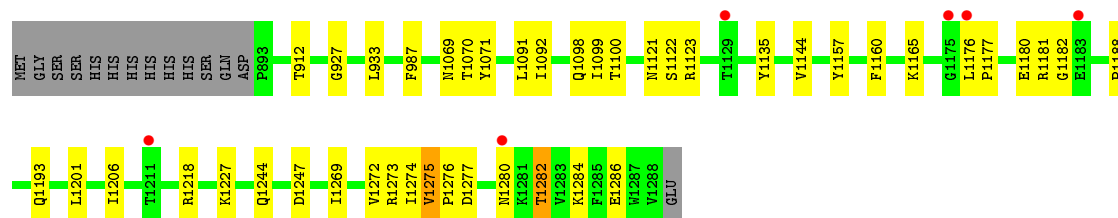
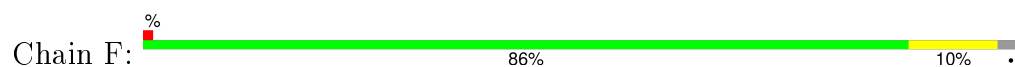




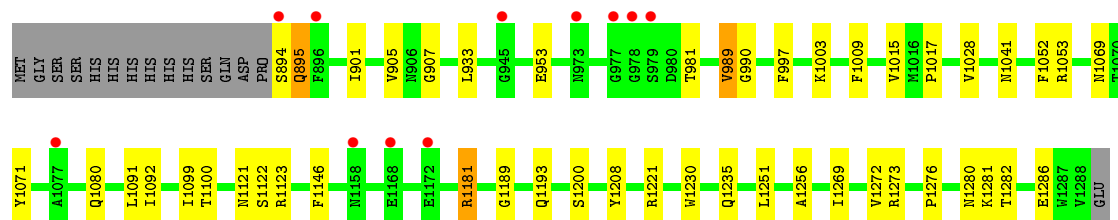
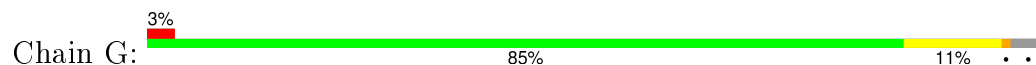
• Molecule 1: LARGE TAIL FIBER PROTEIN P34



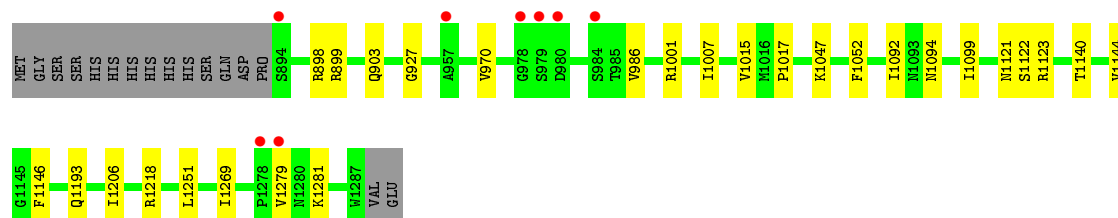
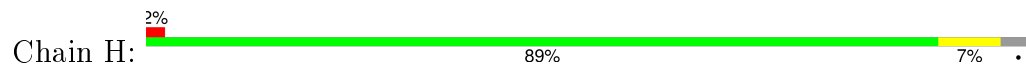
• Molecule 1: LARGE TAIL FIBER PROTEIN P34



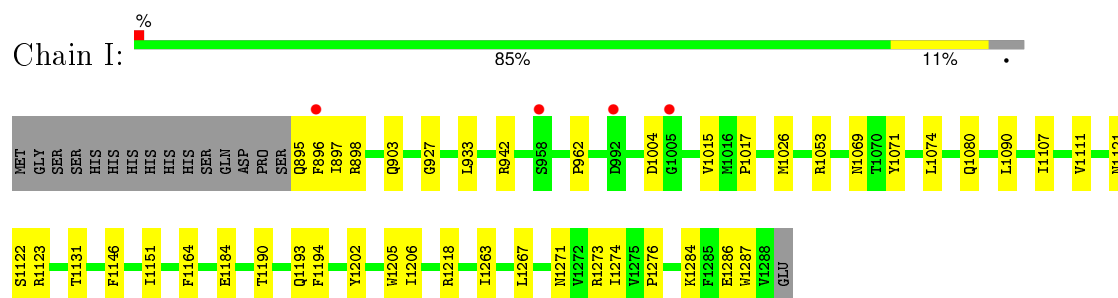
• Molecule 1: LARGE TAIL FIBER PROTEIN P34



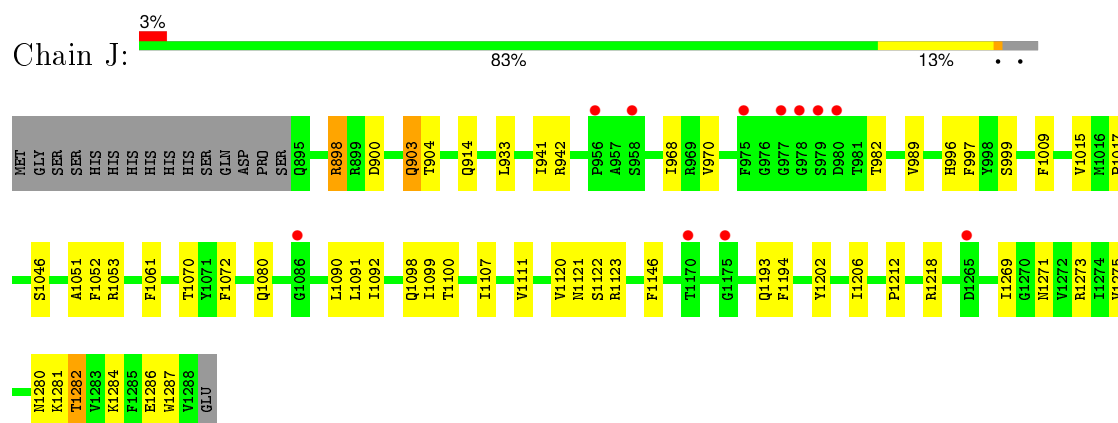
• Molecule 1: LARGE TAIL FIBER PROTEIN P34



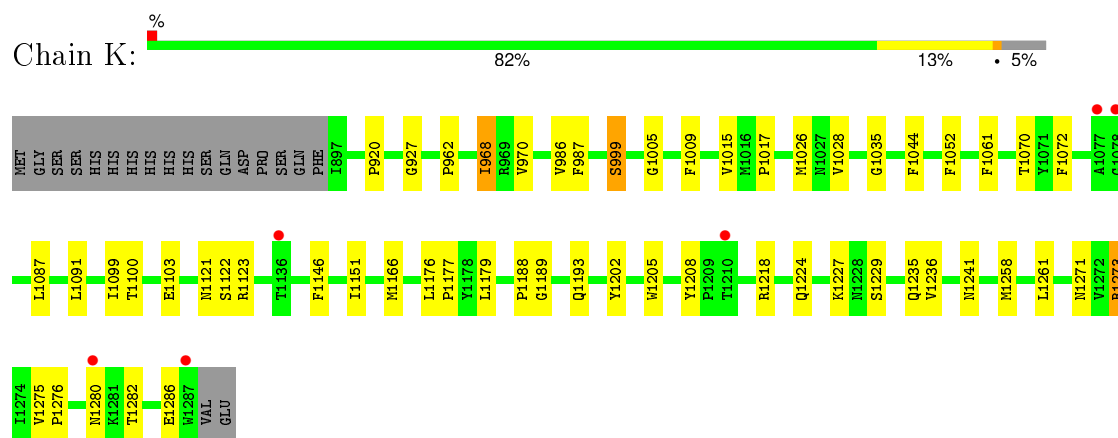
- Molecule 1: LARGE TAIL FIBER PROTEIN P34



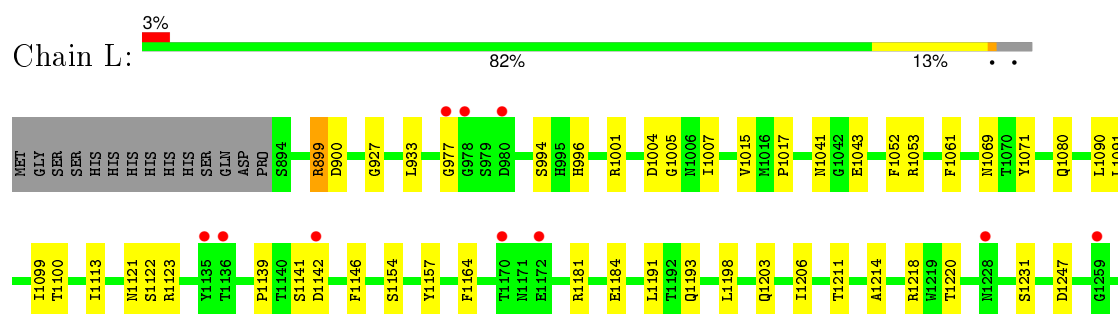
- Molecule 1: LARGE TAIL FIBER PROTEIN P34

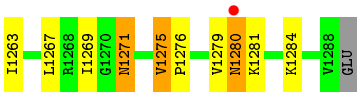


- Molecule 1: LARGE TAIL FIBER PROTEIN P34



- Molecule 1: LARGE TAIL FIBER PROTEIN P34





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.49Å 228.49Å 1069.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.99 – 3.00 29.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.99-3.00) 99.9 (29.99-3.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.226 , 0.249 0.232 , 0.252	Depositor DCC
$R_{free}$ test set	3005 reflections (1.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	1.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	11 of 214065 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	36241	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 13.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	0/3085	0.52	0/4197
1	B	0.32	0/3085	0.51	0/4197
1	C	0.32	0/3109	0.51	0/4230
1	D	0.29	0/3086	0.52	1/4198 (0.0%)
1	E	0.30	0/3109	0.52	0/4230
1	F	0.29	0/3093	0.49	0/4208
1	G	0.25	0/3085	0.49	0/4197
1	H	0.25	0/3078	0.48	0/4187
1	I	0.26	0/3079	0.47	0/4189
1	J	0.26	0/3079	0.48	0/4189
1	K	0.25	0/3051	0.49	0/4151
1	L	0.26	0/3085	0.48	0/4197
All	All	0.28	0/37024	0.50	1/50370 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1267	LEU	CA-CB-CG	6.75	130.81	115.30

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	3020	0	2921	19	0
1	B	3020	0	2921	19	0
1	C	3043	0	2936	22	0
1	D	3020	0	2920	42	0
1	E	3043	0	2936	38	0
1	F	3027	0	2929	29	0
1	G	3020	0	2921	29	0
1	H	3013	0	2912	20	0
1	I	3014	0	2916	29	0
1	J	3014	0	2916	38	0
1	K	2987	0	2890	43	0
1	L	3020	0	2921	40	0
All	All	36241	0	35039	290	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 4.

The worst 5 of 290 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:A:1190:THR:HG1	1:B:1200:SER:HG	1.16	0.86
1:G:989:VAL:HG12	1:G:990:GLY:H	1.46	0.79
1:E:1207:THR:HG22	1:E:1217:THR:H	1.50	0.76
1:F:1275:VAL:HG13	1:F:1284:LYS:HB2	1.66	0.76
1:J:904:THR:O	1:L:899:ARG:NH2	2.21	0.73

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	393/410 (96%)	379 (96%)	14 (4%)	0	100 100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	393/410 (96%)	379 (96%)	14 (4%)	0	100	100
1	C	396/410 (97%)	379 (96%)	17 (4%)	0	100	100
1	D	393/410 (96%)	379 (96%)	14 (4%)	0	100	100
1	E	396/410 (97%)	382 (96%)	14 (4%)	0	100	100
1	F	394/410 (96%)	379 (96%)	15 (4%)	0	100	100
1	G	393/410 (96%)	377 (96%)	13 (3%)	3 (1%)	24	66
1	H	392/410 (96%)	378 (96%)	14 (4%)	0	100	100
1	I	392/410 (96%)	376 (96%)	16 (4%)	0	100	100
1	J	392/410 (96%)	377 (96%)	14 (4%)	1 (0%)	46	84
1	K	389/410 (95%)	375 (96%)	14 (4%)	0	100	100
1	L	393/410 (96%)	376 (96%)	14 (4%)	3 (1%)	24	66
All	All	4716/4920 (96%)	4536 (96%)	173 (4%)	7 (0%)	56	90

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1279	VAL
1	J	1281	LYS
1	L	1280	ASN
1	G	1281	LYS
1	L	977	GLY

### 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	329/343 (96%)	324 (98%)	5 (2%)	72	92
1	B	329/343 (96%)	326 (99%)	3 (1%)	84	95
1	C	332/343 (97%)	330 (99%)	2 (1%)	90	97
1	D	329/343 (96%)	325 (99%)	4 (1%)	78	94
1	E	332/343 (97%)	328 (99%)	4 (1%)	78	94

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	330/343 (96%)	326 (99%)	4 (1%)	78	94
1	G	329/343 (96%)	325 (99%)	4 (1%)	78	94
1	H	328/343 (96%)	326 (99%)	2 (1%)	90	97
1	I	328/343 (96%)	325 (99%)	3 (1%)	84	95
1	J	328/343 (96%)	318 (97%)	10 (3%)	48	83
1	K	325/343 (95%)	318 (98%)	7 (2%)	60	88
1	L	329/343 (96%)	322 (98%)	7 (2%)	61	89
All	All	3948/4116 (96%)	3893 (99%)	55 (1%)	74	93

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	1123	ARG
1	I	1131	THR
1	L	1004	ASP
1	G	1181	ARG
1	H	1279	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	1255	ASN
1	L	1203	GLN
1	L	1012	ASN
1	J	914	GLN
1	L	1193	GLN

### 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 [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	395/410 (96%)	-0.57	0	100 100	4, 19, 62, 121	0
1	B	395/410 (96%)	-0.53	0	100 100	5, 21, 56, 130	0
1	C	398/410 (97%)	-0.55	0	100 100	4, 19, 62, 124	0
1	D	395/410 (96%)	-0.21	2 (0%)	91 76	5, 42, 92, 135	0
1	E	398/410 (97%)	-0.12	9 (2%)	64 33	5, 42, 94, 129	0
1	F	396/410 (96%)	-0.20	6 (1%)	76 49	4, 43, 93, 125	0
1	G	395/410 (96%)	0.09	11 (2%)	56 27	36, 69, 103, 125	0
1	H	394/410 (96%)	-0.00	8 (2%)	68 39	31, 64, 100, 137	0
1	I	394/410 (96%)	-0.06	4 (1%)	84 60	26, 65, 100, 134	0
1	J	394/410 (96%)	0.02	11 (2%)	56 27	28, 62, 99, 134	0
1	K	391/410 (95%)	0.06	6 (1%)	76 49	27, 64, 105, 143	0
1	L	395/410 (96%)	0.06	11 (2%)	56 27	28, 64, 104, 152	0
All	All	4740/4920 (96%)	-0.17	68 (1%)	78 51	4, 52, 97, 152	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1183	GLU	4.3
1	J	978	GLY	4.3
1	G	979	SER	4.0
1	E	1279	VAL	3.8
1	D	1184	GLU	3.6

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.