



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 11:25 pm GMT

PDB ID : 2WST
Title : Head domain of porcine adenovirus type 4 NADC-1 isolate fibre
Authors : Guardado-Calvo, P.; Munoz, E.M.; Llamas-Saiz, A.L.; Fox, G.C.; Glasgow, J.N.; van Raaij, M.J.
Deposited on : 2009-09-09
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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>.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

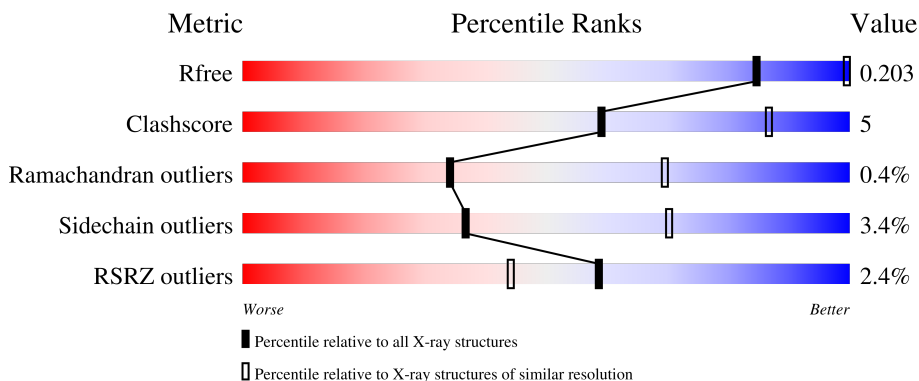
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



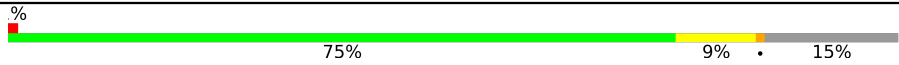
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 ≥ 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	208	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
1	B	208	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
1	C	208	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
1	D	208	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
1	E	208	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	208	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment representing 75%, a yellow segment representing 9%, and a grey segment representing 15%. A small red square is at the beginning of the bar, and a small black dot is at the end of the grey segment. The percentage values are labeled below the bar.</p>

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 7984 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 PUTATIVE FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	176	1330	839	219	267	5	0	0	0
1	B	176	1330	839	219	267	5	0	0	0
1	C	176	1330	839	219	267	5	0	0	0
1	D	176	1330	839	219	267	5	0	0	0
1	E	176	1330	839	219	267	5	0	0	0
1	F	176	1330	839	219	267	5	0	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	MET	-	expression tag	UNP Q83467
A	85	GLY	-	expression tag	UNP Q83467
A	86	SER	-	expression tag	UNP Q83467
A	87	SER	-	expression tag	UNP Q83467
A	88	HIS	-	expression tag	UNP Q83467
A	89	HIS	-	expression tag	UNP Q83467
A	90	HIS	-	expression tag	UNP Q83467
A	91	HIS	-	expression tag	UNP Q83467
A	92	HIS	-	expression tag	UNP Q83467
A	93	HIS	-	expression tag	UNP Q83467
A	94	SER	-	expression tag	UNP Q83467
A	95	SER	-	expression tag	UNP Q83467
A	96	GLY	-	expression tag	UNP Q83467
A	97	LEU	-	expression tag	UNP Q83467
A	98	VAL	-	expression tag	UNP Q83467
A	99	PRO	-	expression tag	UNP Q83467
A	100	ARG	-	expression tag	UNP Q83467

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLY	-	expression tag	UNP Q83467
A	102	SER	-	expression tag	UNP Q83467
A	103	HIS	-	expression tag	UNP Q83467
A	104	MET	-	expression tag	UNP Q83467
A	105	ALA	-	expression tag	UNP Q83467
A	106	SER	-	expression tag	UNP Q83467
A	107	MET	-	expression tag	UNP Q83467
A	108	THR	-	expression tag	UNP Q83467
A	109	GLY	-	expression tag	UNP Q83467
A	110	GLY	-	expression tag	UNP Q83467
A	111	GLN	-	expression tag	UNP Q83467
A	112	GLN	-	expression tag	UNP Q83467
A	113	GLY	-	expression tag	UNP Q83467
A	114	ARG	-	expression tag	UNP Q83467
A	115	ILE	-	expression tag	UNP Q83467
B	84	MET	-	expression tag	UNP Q83467
B	85	GLY	-	expression tag	UNP Q83467
B	86	SER	-	expression tag	UNP Q83467
B	87	SER	-	expression tag	UNP Q83467
B	88	HIS	-	expression tag	UNP Q83467
B	89	HIS	-	expression tag	UNP Q83467
B	90	HIS	-	expression tag	UNP Q83467
B	91	HIS	-	expression tag	UNP Q83467
B	92	HIS	-	expression tag	UNP Q83467
B	93	HIS	-	expression tag	UNP Q83467
B	94	SER	-	expression tag	UNP Q83467
B	95	SER	-	expression tag	UNP Q83467
B	96	GLY	-	expression tag	UNP Q83467
B	97	LEU	-	expression tag	UNP Q83467
B	98	VAL	-	expression tag	UNP Q83467
B	99	PRO	-	expression tag	UNP Q83467
B	100	ARG	-	expression tag	UNP Q83467
B	101	GLY	-	expression tag	UNP Q83467
B	102	SER	-	expression tag	UNP Q83467
B	103	HIS	-	expression tag	UNP Q83467
B	104	MET	-	expression tag	UNP Q83467
B	105	ALA	-	expression tag	UNP Q83467
B	106	SER	-	expression tag	UNP Q83467
B	107	MET	-	expression tag	UNP Q83467
B	108	THR	-	expression tag	UNP Q83467
B	109	GLY	-	expression tag	UNP Q83467
B	110	GLY	-	expression tag	UNP Q83467

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	111	GLN	-	expression tag	UNP Q83467
B	112	GLN	-	expression tag	UNP Q83467
B	113	GLY	-	expression tag	UNP Q83467
B	114	ARG	-	expression tag	UNP Q83467
B	115	ILE	-	expression tag	UNP Q83467
C	84	MET	-	expression tag	UNP Q83467
C	85	GLY	-	expression tag	UNP Q83467
C	86	SER	-	expression tag	UNP Q83467
C	87	SER	-	expression tag	UNP Q83467
C	88	HIS	-	expression tag	UNP Q83467
C	89	HIS	-	expression tag	UNP Q83467
C	90	HIS	-	expression tag	UNP Q83467
C	91	HIS	-	expression tag	UNP Q83467
C	92	HIS	-	expression tag	UNP Q83467
C	93	HIS	-	expression tag	UNP Q83467
C	94	SER	-	expression tag	UNP Q83467
C	95	SER	-	expression tag	UNP Q83467
C	96	GLY	-	expression tag	UNP Q83467
C	97	LEU	-	expression tag	UNP Q83467
C	98	VAL	-	expression tag	UNP Q83467
C	99	PRO	-	expression tag	UNP Q83467
C	100	ARG	-	expression tag	UNP Q83467
C	101	GLY	-	expression tag	UNP Q83467
C	102	SER	-	expression tag	UNP Q83467
C	103	HIS	-	expression tag	UNP Q83467
C	104	MET	-	expression tag	UNP Q83467
C	105	ALA	-	expression tag	UNP Q83467
C	106	SER	-	expression tag	UNP Q83467
C	107	MET	-	expression tag	UNP Q83467
C	108	THR	-	expression tag	UNP Q83467
C	109	GLY	-	expression tag	UNP Q83467
C	110	GLY	-	expression tag	UNP Q83467
C	111	GLN	-	expression tag	UNP Q83467
C	112	GLN	-	expression tag	UNP Q83467
C	113	GLY	-	expression tag	UNP Q83467
C	114	ARG	-	expression tag	UNP Q83467
C	115	ILE	-	expression tag	UNP Q83467
D	84	MET	-	expression tag	UNP Q83467
D	85	GLY	-	expression tag	UNP Q83467
D	86	SER	-	expression tag	UNP Q83467
D	87	SER	-	expression tag	UNP Q83467
D	88	HIS	-	expression tag	UNP Q83467

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	89	HIS	-	expression tag	UNP Q83467
D	90	HIS	-	expression tag	UNP Q83467
D	91	HIS	-	expression tag	UNP Q83467
D	92	HIS	-	expression tag	UNP Q83467
D	93	HIS	-	expression tag	UNP Q83467
D	94	SER	-	expression tag	UNP Q83467
D	95	SER	-	expression tag	UNP Q83467
D	96	GLY	-	expression tag	UNP Q83467
D	97	LEU	-	expression tag	UNP Q83467
D	98	VAL	-	expression tag	UNP Q83467
D	99	PRO	-	expression tag	UNP Q83467
D	100	ARG	-	expression tag	UNP Q83467
D	101	GLY	-	expression tag	UNP Q83467
D	102	SER	-	expression tag	UNP Q83467
D	103	HIS	-	expression tag	UNP Q83467
D	104	MET	-	expression tag	UNP Q83467
D	105	ALA	-	expression tag	UNP Q83467
D	106	SER	-	expression tag	UNP Q83467
D	107	MET	-	expression tag	UNP Q83467
D	108	THR	-	expression tag	UNP Q83467
D	109	GLY	-	expression tag	UNP Q83467
D	110	GLY	-	expression tag	UNP Q83467
D	111	GLN	-	expression tag	UNP Q83467
D	112	GLN	-	expression tag	UNP Q83467
D	113	GLY	-	expression tag	UNP Q83467
D	114	ARG	-	expression tag	UNP Q83467
D	115	ILE	-	expression tag	UNP Q83467
E	84	MET	-	expression tag	UNP Q83467
E	85	GLY	-	expression tag	UNP Q83467
E	86	SER	-	expression tag	UNP Q83467
E	87	SER	-	expression tag	UNP Q83467
E	88	HIS	-	expression tag	UNP Q83467
E	89	HIS	-	expression tag	UNP Q83467
E	90	HIS	-	expression tag	UNP Q83467
E	91	HIS	-	expression tag	UNP Q83467
E	92	HIS	-	expression tag	UNP Q83467
E	93	HIS	-	expression tag	UNP Q83467
E	94	SER	-	expression tag	UNP Q83467
E	95	SER	-	expression tag	UNP Q83467
E	96	GLY	-	expression tag	UNP Q83467
E	97	LEU	-	expression tag	UNP Q83467
E	98	VAL	-	expression tag	UNP Q83467

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	99	PRO	-	expression tag	UNP Q83467
E	100	ARG	-	expression tag	UNP Q83467
E	101	GLY	-	expression tag	UNP Q83467
E	102	SER	-	expression tag	UNP Q83467
E	103	HIS	-	expression tag	UNP Q83467
E	104	MET	-	expression tag	UNP Q83467
E	105	ALA	-	expression tag	UNP Q83467
E	106	SER	-	expression tag	UNP Q83467
E	107	MET	-	expression tag	UNP Q83467
E	108	THR	-	expression tag	UNP Q83467
E	109	GLY	-	expression tag	UNP Q83467
E	110	GLY	-	expression tag	UNP Q83467
E	111	GLN	-	expression tag	UNP Q83467
E	112	GLN	-	expression tag	UNP Q83467
E	113	GLY	-	expression tag	UNP Q83467
E	114	ARG	-	expression tag	UNP Q83467
E	115	ILE	-	expression tag	UNP Q83467
F	84	MET	-	expression tag	UNP Q83467
F	85	GLY	-	expression tag	UNP Q83467
F	86	SER	-	expression tag	UNP Q83467
F	87	SER	-	expression tag	UNP Q83467
F	88	HIS	-	expression tag	UNP Q83467
F	89	HIS	-	expression tag	UNP Q83467
F	90	HIS	-	expression tag	UNP Q83467
F	91	HIS	-	expression tag	UNP Q83467
F	92	HIS	-	expression tag	UNP Q83467
F	93	HIS	-	expression tag	UNP Q83467
F	94	SER	-	expression tag	UNP Q83467
F	95	SER	-	expression tag	UNP Q83467
F	96	GLY	-	expression tag	UNP Q83467
F	97	LEU	-	expression tag	UNP Q83467
F	98	VAL	-	expression tag	UNP Q83467
F	99	PRO	-	expression tag	UNP Q83467
F	100	ARG	-	expression tag	UNP Q83467
F	101	GLY	-	expression tag	UNP Q83467
F	102	SER	-	expression tag	UNP Q83467
F	103	HIS	-	expression tag	UNP Q83467
F	104	MET	-	expression tag	UNP Q83467
F	105	ALA	-	expression tag	UNP Q83467
F	106	SER	-	expression tag	UNP Q83467
F	107	MET	-	expression tag	UNP Q83467
F	108	THR	-	expression tag	UNP Q83467

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	109	GLY	-	expression tag	UNP Q83467
F	110	GLY	-	expression tag	UNP Q83467
F	111	GLN	-	expression tag	UNP Q83467
F	112	GLN	-	expression tag	UNP Q83467
F	113	GLY	-	expression tag	UNP Q83467
F	114	ARG	-	expression tag	UNP Q83467
F	115	ILE	-	expression tag	UNP Q83467

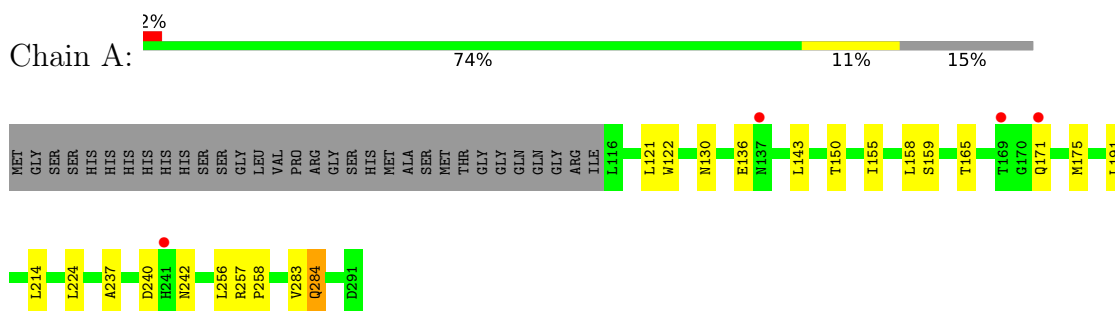
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	C	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0
2	F	1	Total O 1 1	0	0

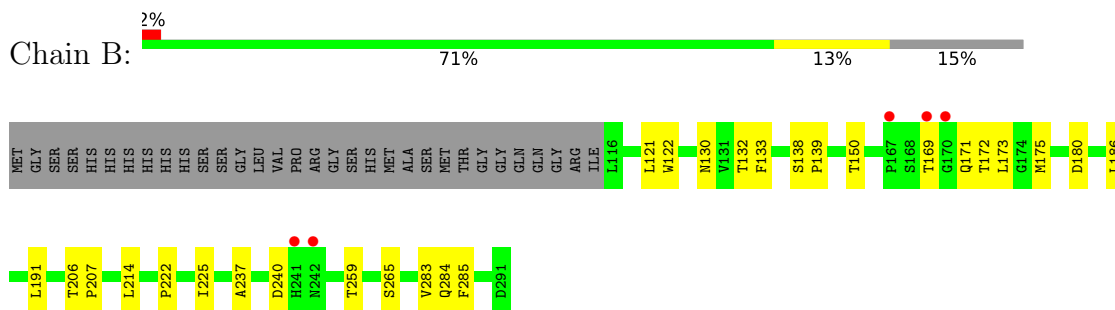
3 Residue-property plots [i](#)

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.

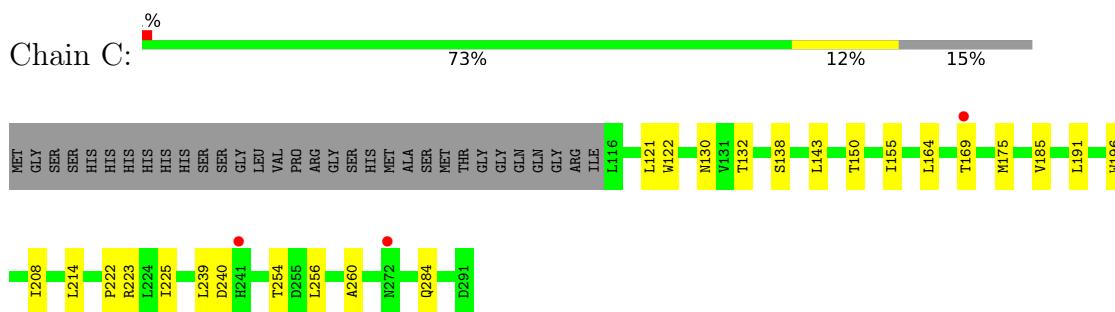
- Molecule 1: PUTATIVE FIBER PROTEIN



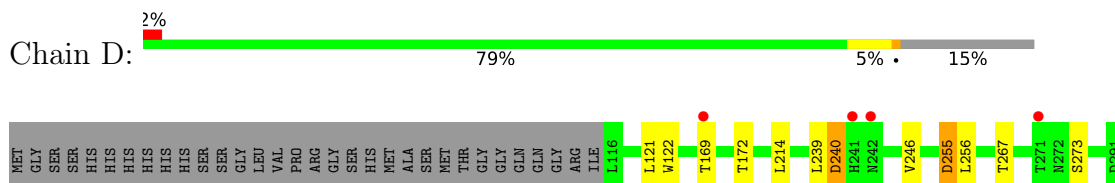
- Molecule 1: PUTATIVE FIBER PROTEIN



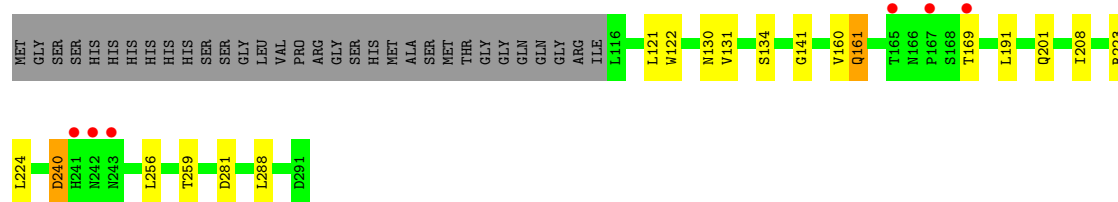
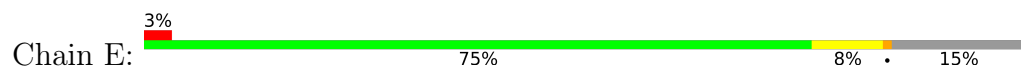
- Molecule 1: PUTATIVE FIBER PROTEIN



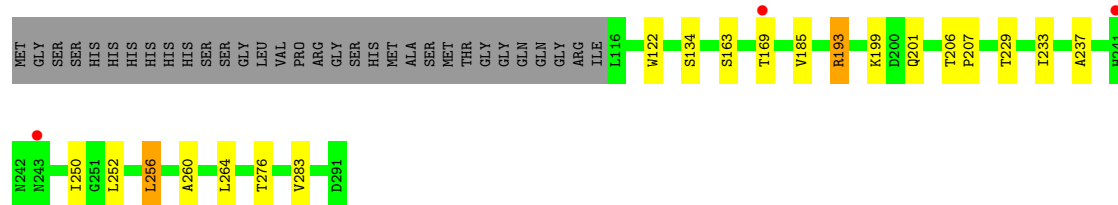
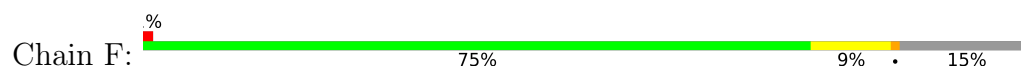
- Molecule 1: PUTATIVE FIBER PROTEIN



- Molecule 1: PUTATIVE FIBER PROTEIN



- Molecule 1: PUTATIVE FIBER PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.73Å 145.44Å 147.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.21 – 3.20 28.93 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.4 (29.21-3.20) 93.7 (28.93-3.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.18Å)	Xtrriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.173 , 0.201 0.178 , 0.203	Depositor DCC
R_{free} test set	2026 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtrriage
Anisotropy	0.270	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7984	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/1360	0.66	0/1861
1	B	0.45	0/1360	0.65	0/1861
1	C	0.45	0/1360	0.65	0/1861
1	D	0.44	0/1360	0.62	0/1861
1	E	0.45	0/1360	0.64	0/1861
1	F	0.48	0/1360	0.68	0/1861
All	All	0.45	0/8160	0.65	0/11166

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	ASN	Peptide

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	1330	0	1295	20	0
1	B	1330	0	1295	25	0
1	C	1330	0	1295	14	0
1	D	1330	0	1295	6	0
1	E	1330	0	1295	11	0
1	F	1330	0	1295	10	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
All	All	7984	0	7770	74	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 5.

All (74) 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:150:THR:CG2	1:B:150:THR:HG21	1.45	1.43
1:A:150:THR:HG23	1:B:150:THR:CG2	1.82	1.10
1:A:150:THR:CG2	1:B:150:THR:CG2	2.34	1.05
1:A:150:THR:HG23	1:B:150:THR:HG21	0.92	0.90
1:A:150:THR:HG21	1:C:150:THR:HB	1.64	0.77
1:C:169:THR:O	1:C:169:THR:HG22	1.90	0.70
1:B:150:THR:HG23	1:C:150:THR:OG1	1.92	0.69
1:A:150:THR:HG22	1:B:150:THR:HG21	1.67	0.66
1:C:223:ARG:NH1	1:C:260:ALA:O	2.29	0.64
1:C:223:ARG:HG2	1:C:256:LEU:HD11	1.79	0.63
1:C:130:ASN:O	1:C:191:LEU:HD12	2.02	0.59
1:C:121:LEU:HD22	1:C:208:ILE:HD13	1.84	0.58
1:E:224:LEU:HD13	1:E:256:LEU:HB2	1.85	0.58
1:B:132:THR:HG22	1:B:139:PRO:HA	1.85	0.57
1:E:224:LEU:CD1	1:E:256:LEU:HB2	2.34	0.57
1:B:132:THR:HG22	1:B:139:PRO:CA	2.35	0.57
1:B:130:ASN:O	1:B:191:LEU:HD12	2.04	0.56
1:E:121:LEU:HD22	1:E:208:ILE:HD13	1.86	0.56
1:B:237:ALA:HB2	1:B:283:VAL:HG21	1.88	0.55
1:A:257:ARG:HB3	1:A:258:PRO:HD2	1.89	0.55
1:F:169:THR:HG23	1:F:169:THR:O	2.06	0.54
1:D:239:LEU:HD21	1:D:246:VAL:HG21	1.88	0.53
1:A:143:LEU:HD11	1:A:158:LEU:HD11	1.91	0.53
1:B:121:LEU:HD13	1:B:214:LEU:HD13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PHE:HE1	1:B:175:MET:HE2	1.73	0.52
1:A:143:LEU:HD13	1:A:175:MET:CE	2.41	0.51
1:F:237:ALA:HB2	1:F:283:VAL:HG21	1.92	0.50
1:E:130:ASN:O	1:E:191:LEU:HD12	2.11	0.49
1:C:185:VAL:HG13	1:C:196:TRP:CD1	2.47	0.49
1:B:132:THR:HG22	1:B:139:PRO:N	2.28	0.49
1:A:155:ILE:HD11	1:C:155:ILE:CD1	2.43	0.49
1:B:186:LEU:HD13	1:B:259:THR:HG23	1.95	0.49
1:A:136:GLU:OE1	1:A:165:THR:HG23	2.13	0.48
1:E:240:ASP:N	1:E:240:ASP:OD1	2.46	0.48
1:B:133:PHE:CE1	1:B:175:MET:HE2	2.48	0.48
1:A:155:ILE:HD11	1:C:155:ILE:HD13	1.94	0.48
1:B:180:ASP:HB3	1:B:186:LEU:HD21	1.96	0.48
1:A:121:LEU:HG	1:A:214:LEU:HD13	1.96	0.47
1:A:150:THR:HG21	1:B:150:THR:CG2	2.36	0.47
1:E:223:ARG:HG2	1:E:256:LEU:HD13	1.96	0.47
1:D:240:ASP:N	1:D:240:ASP:OD1	2.48	0.47
1:B:138:SER:HB2	1:B:139:PRO:HD2	1.98	0.46
1:F:163:SER:HA	1:F:276:THR:O	2.15	0.46
1:B:240:ASP:OD2	1:B:240:ASP:N	2.49	0.46
1:E:169:THR:O	1:E:169:THR:HG23	2.16	0.45
1:A:284:GLN:HE22	1:B:285:PHE:HA	1.81	0.45
1:F:252:LEU:HD23	1:F:264:LEU:HD12	1.97	0.45
1:D:239:LEU:HG	1:D:246:VAL:HG23	1.98	0.45
1:C:164:LEU:HD22	1:C:164:LEU:N	2.31	0.45
1:F:185:VAL:HG23	1:F:193:ARG:HB3	1.99	0.45
1:F:206:THR:OG1	1:F:207:PRO:HD3	2.17	0.45
1:C:223:ARG:HG2	1:C:256:LEU:CD1	2.46	0.44
1:E:160:VAL:HG12	1:E:161:GLN:N	2.32	0.44
1:D:121:LEU:HG	1:D:214:LEU:HD13	1.99	0.44
1:E:131:VAL:HG12	1:E:141:GLY:C	2.39	0.43
1:A:224:LEU:HG	1:A:256:LEU:HD11	2.00	0.43
1:B:133:PHE:HE1	1:B:175:MET:CE	2.31	0.43
1:A:130:ASN:O	1:A:191:LEU:HD12	2.19	0.43
1:A:143:LEU:HD13	1:A:175:MET:HE3	2.00	0.43
1:D:255:ASP:O	1:D:256:LEU:HD12	2.19	0.43
1:E:281:ASP:HA	1:F:229:THR:HG22	2.00	0.43
1:B:222:PRO:HB2	1:B:225:ILE:HD12	2.00	0.43
1:A:237:ALA:HB2	1:A:283:VAL:HG21	2.02	0.42
1:D:169:THR:O	1:D:169:THR:HG22	2.20	0.42
1:C:143:LEU:HD13	1:C:175:MET:CE	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:LYS:HE3	1:F:201:GLN:O	2.20	0.41
1:A:143:LEU:HD13	1:A:175:MET:HE1	2.02	0.41
1:F:233:ILE:HB	1:F:250:ILE:HB	2.02	0.41
1:E:259:THR:HG22	1:E:259:THR:O	2.20	0.41
1:F:256:LEU:HD12	1:F:260:ALA:HB3	2.03	0.41
1:B:169:THR:O	1:B:169:THR:HG22	2.21	0.41
1:B:186:LEU:CD1	1:B:259:THR:HG23	2.50	0.41
1:B:206:THR:OG1	1:B:207:PRO:HD3	2.20	0.41
1:C:225:ILE:O	1:C:254:THR:HG22	2.21	0.41

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	174/208 (84%)	163 (94%)	10 (6%)	1 (1%)	25	64
1	B	174/208 (84%)	158 (91%)	16 (9%)	0	100	100
1	C	174/208 (84%)	160 (92%)	13 (8%)	1 (1%)	25	64
1	D	174/208 (84%)	164 (94%)	9 (5%)	1 (1%)	25	64
1	E	174/208 (84%)	161 (92%)	12 (7%)	1 (1%)	25	64
1	F	174/208 (84%)	159 (91%)	15 (9%)	0	100	100
All	All	1044/1248 (84%)	965 (92%)	75 (7%)	4 (0%)	34	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	240	ASP
1	E	240	ASP
1	A	240	ASP
1	C	240	ASP

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	150/175 (86%)	146 (97%)	4 (3%)	44	75
1	B	150/175 (86%)	144 (96%)	6 (4%)	31	66
1	C	150/175 (86%)	143 (95%)	7 (5%)	26	62
1	D	150/175 (86%)	145 (97%)	5 (3%)	38	71
1	E	150/175 (86%)	145 (97%)	5 (3%)	38	71
1	F	150/175 (86%)	146 (97%)	4 (3%)	44	75
All	All	900/1050 (86%)	869 (97%)	31 (3%)	37	70

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	TRP
1	A	159	SER
1	A	171	GLN
1	A	284	GLN
1	B	122	TRP
1	B	171	GLN
1	B	172	THR
1	B	173	LEU
1	B	265	SER
1	B	284	GLN
1	C	122	TRP
1	C	132	THR
1	C	138	SER
1	C	214	LEU
1	C	222	PRO
1	C	239	LEU
1	C	284	GLN
1	D	122	TRP
1	D	172	THR
1	D	255	ASP
1	D	267	THR
1	D	273	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	122	TRP
1	E	134	SER
1	E	161	GLN
1	E	201	GLN
1	E	288	LEU
1	F	122	TRP
1	F	134	SER
1	F	193	ARG
1	F	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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

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, 95th 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 ²)	Q<0.9
1	A	176/208 (84%)	-0.49	4 (2%) 60 47	37, 57, 103, 119	0
1	B	176/208 (84%)	-0.39	5 (2%) 53 37	40, 67, 121, 142	0
1	C	176/208 (84%)	-0.56	3 (1%) 70 57	37, 56, 107, 123	0
1	D	176/208 (84%)	-0.43	4 (2%) 60 47	40, 67, 125, 144	0
1	E	176/208 (84%)	-0.45	6 (3%) 45 29	40, 60, 121, 141	0
1	F	176/208 (84%)	-0.62	3 (1%) 70 57	36, 53, 99, 112	0
All	All	1056/1248 (84%)	-0.49	25 (2%) 59 44	36, 59, 112, 144	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	THR	4.5
1	D	169	THR	3.8
1	E	242	ASN	3.4
1	C	169	THR	3.4
1	E	167	PRO	3.0
1	B	167	PRO	2.8
1	A	241	HIS	2.8
1	B	241	HIS	2.8
1	E	241	HIS	2.6
1	E	169	THR	2.6
1	F	169	THR	2.5
1	A	137	ASN	2.4
1	B	170	GLY	2.4
1	C	241	HIS	2.4
1	F	241	HIS	2.4
1	C	272	ASN	2.2
1	E	165	THR	2.2
1	D	271	THR	2.1
1	F	243	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	241	HIS	2.1
1	E	243	ASN	2.1
1	A	169	THR	2.0
1	A	171	GLN	2.0
1	B	242	ASN	2.0
1	D	242	ASN	2.0

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 monosaccharides 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.