



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 8, 2025 – 02:33 PM JST

PDB ID : 8ZPY / pdb_00008zpy
Title : Crystal structure of prefusion F of RSV
Authors : Huang, Q.; Lang, Q.; Han, X.; Yan, J.
Deposited on : 2024-05-31
Resolution : 2.92 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

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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.47

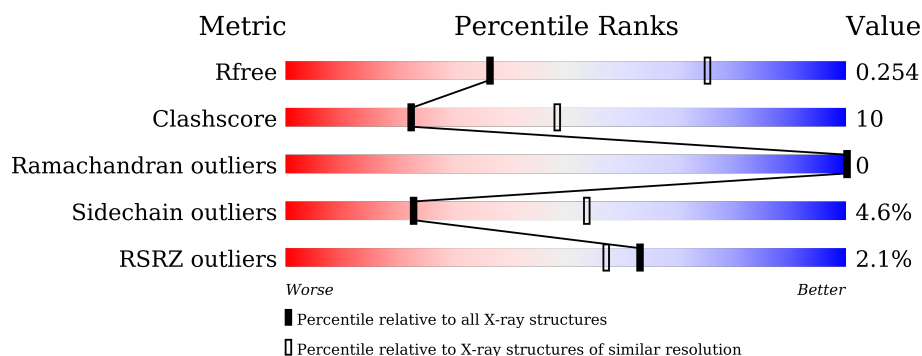
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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	522	<div> <div>2%</div> <div>64%</div> <div>21%</div> <div>•</div> <div>12%</div> </div>
1	B	522	<div> <div>2%</div> <div>62%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
1	C	522	<div> <div>%</div> <div>62%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
1	D	522	<div> <div>2%</div> <div>63%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
1	E	522	<div> <div>2%</div> <div>63%</div> <div>22%</div> <div>•</div> <div>14%</div> </div>
1	F	522	<div> <div>2%</div> <div>64%</div> <div>21%</div> <div>•</div> <div>14%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20848 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 Fusion glycoprotein F0,Fibritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3510	2215	580	694	21			
1	B	449	Total	C	N	O	S	0	0	0
			3472	2193	572	686	21			
1	C	448	Total	C	N	O	S	0	0	0
			3466	2190	571	684	21			
1	D	450	Total	C	N	O	S	0	0	0
			3472	2192	573	686	21			
1	E	449	Total	C	N	O	S	0	0	0
			3465	2187	572	685	21			
1	F	449	Total	C	N	O	S	0	0	0
			3463	2187	571	684	21			

There are 318 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP P12568
A	11	LYS	-	expression tag	UNP P12568
A	12	CYS	-	expression tag	UNP P12568
A	13	LEU	-	expression tag	UNP P12568
A	14	LEU	-	expression tag	UNP P12568
A	15	TYR	-	expression tag	UNP P12568
A	16	LEU	-	expression tag	UNP P12568
A	17	ALA	-	expression tag	UNP P12568
A	18	PHE	-	expression tag	UNP P12568
A	19	LEU	-	expression tag	UNP P12568
A	20	PHE	-	expression tag	UNP P12568
A	21	ILE	-	expression tag	UNP P12568
A	22	GLY	-	expression tag	UNP P12568
A	23	VAL	-	expression tag	UNP P12568
A	24	ASN	-	expression tag	UNP P12568
A	25	CYS	-	expression tag	UNP P12568
A	67	PRO	ASN	conflict	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
A	80	LYS	ASN	conflict	UNP P12568
A	100	GLY	-	linker	UNP P12568
A	101	GLY	-	linker	UNP P12568
A	102	GLY	-	linker	UNP P12568
A	103	GLY	-	linker	UNP P12568
A	104	SER	-	linker	UNP P12568
A	105	GLY	-	linker	UNP P12568
A	106	GLY	-	linker	UNP P12568
A	128	GLY	-	linker	UNP P12568
A	129	GLY	-	linker	UNP P12568
A	130	SER	-	linker	UNP P12568
A	131	GLY	-	linker	UNP P12568
A	132	GLY	-	linker	UNP P12568
A	133	GLY	-	linker	UNP P12568
A	134	GLY	-	linker	UNP P12568
A	135	SER	-	linker	UNP P12568
A	138	PRO	LEU	conflict	UNP P12568
A	139	PRO	GLY	conflict	UNP P12568
A	141	PRO	LEU	conflict	UNP P12568
A	152	VAL	ILE	conflict	UNP P12568
A	213	SER	ARG	conflict	UNP P12568
A	215	PRO	SER	conflict	UNP P12568
A	279	PRO	GLN	conflict	UNP P12568
A	377	PRO	SER	conflict	UNP P12568
A	514	SER	-	linker	UNP P12568
A	515	ALA	-	linker	UNP P12568
A	516	ILE	-	linker	UNP P12568
A	517	GLY	-	linker	UNP P12568
A	545	HIS	-	expression tag	UNP A0A346FJN8
A	546	HIS	-	expression tag	UNP A0A346FJN8
A	547	HIS	-	expression tag	UNP A0A346FJN8
A	548	HIS	-	expression tag	UNP A0A346FJN8
A	549	HIS	-	expression tag	UNP A0A346FJN8
A	550	HIS	-	expression tag	UNP A0A346FJN8
A	551	HIS	-	expression tag	UNP A0A346FJN8
A	552	HIS	-	expression tag	UNP A0A346FJN8
B	10	MET	-	initiating methionine	UNP P12568
B	11	LYS	-	expression tag	UNP P12568
B	12	CYS	-	expression tag	UNP P12568
B	13	LEU	-	expression tag	UNP P12568
B	14	LEU	-	expression tag	UNP P12568
B	15	TYR	-	expression tag	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	LEU	-	expression tag	UNP P12568
B	17	ALA	-	expression tag	UNP P12568
B	18	PHE	-	expression tag	UNP P12568
B	19	LEU	-	expression tag	UNP P12568
B	20	PHE	-	expression tag	UNP P12568
B	21	ILE	-	expression tag	UNP P12568
B	22	GLY	-	expression tag	UNP P12568
B	23	VAL	-	expression tag	UNP P12568
B	24	ASN	-	expression tag	UNP P12568
B	25	CYS	-	expression tag	UNP P12568
B	67	PRO	ASN	conflict	UNP P12568
B	80	LYS	ASN	conflict	UNP P12568
B	121	GLY	-	linker	UNP P12568
B	122	GLY	-	linker	UNP P12568
B	123	GLY	-	linker	UNP P12568
B	124	GLY	-	linker	UNP P12568
B	125	SER	-	linker	UNP P12568
B	126	GLY	-	linker	UNP P12568
B	127	GLY	-	linker	UNP P12568
B	128	GLY	-	linker	UNP P12568
B	129	GLY	-	linker	UNP P12568
B	130	SER	-	linker	UNP P12568
B	131	GLY	-	linker	UNP P12568
B	132	GLY	-	linker	UNP P12568
B	133	GLY	-	linker	UNP P12568
B	134	GLY	-	linker	UNP P12568
B	135	SER	-	linker	UNP P12568
B	138	PRO	LEU	conflict	UNP P12568
B	139	PRO	GLY	conflict	UNP P12568
B	141	PRO	LEU	conflict	UNP P12568
B	152	VAL	ILE	conflict	UNP P12568
B	213	SER	ARG	conflict	UNP P12568
B	215	PRO	SER	conflict	UNP P12568
B	279	PRO	GLN	conflict	UNP P12568
B	377	PRO	SER	conflict	UNP P12568
B	514	SER	-	linker	UNP P12568
B	515	ALA	-	linker	UNP P12568
B	516	ILE	-	linker	UNP P12568
B	517	GLY	-	linker	UNP P12568
B	545	HIS	-	expression tag	UNP A0A346FJN8
B	546	HIS	-	expression tag	UNP A0A346FJN8
B	547	HIS	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	548	HIS	-	expression tag	UNP A0A346FJN8
B	549	HIS	-	expression tag	UNP A0A346FJN8
B	550	HIS	-	expression tag	UNP A0A346FJN8
B	551	HIS	-	expression tag	UNP A0A346FJN8
B	552	HIS	-	expression tag	UNP A0A346FJN8
C	10	MET	-	initiating methionine	UNP P12568
C	11	LYS	-	expression tag	UNP P12568
C	12	CYS	-	expression tag	UNP P12568
C	13	LEU	-	expression tag	UNP P12568
C	14	LEU	-	expression tag	UNP P12568
C	15	TYR	-	expression tag	UNP P12568
C	16	LEU	-	expression tag	UNP P12568
C	17	ALA	-	expression tag	UNP P12568
C	18	PHE	-	expression tag	UNP P12568
C	19	LEU	-	expression tag	UNP P12568
C	20	PHE	-	expression tag	UNP P12568
C	21	ILE	-	expression tag	UNP P12568
C	22	GLY	-	expression tag	UNP P12568
C	23	VAL	-	expression tag	UNP P12568
C	24	ASN	-	expression tag	UNP P12568
C	25	CYS	-	expression tag	UNP P12568
C	67	PRO	ASN	conflict	UNP P12568
C	80	LYS	ASN	conflict	UNP P12568
C	121	GLY	-	linker	UNP P12568
C	122	GLY	-	linker	UNP P12568
C	123	GLY	-	linker	UNP P12568
C	124	GLY	-	linker	UNP P12568
C	125	SER	-	linker	UNP P12568
C	126	GLY	-	linker	UNP P12568
C	127	GLY	-	linker	UNP P12568
C	128	GLY	-	linker	UNP P12568
C	129	GLY	-	linker	UNP P12568
C	130	SER	-	linker	UNP P12568
C	131	GLY	-	linker	UNP P12568
C	132	GLY	-	linker	UNP P12568
C	133	GLY	-	linker	UNP P12568
C	134	GLY	-	linker	UNP P12568
C	135	SER	-	linker	UNP P12568
C	138	PRO	LEU	conflict	UNP P12568
C	139	PRO	GLY	conflict	UNP P12568
C	141	PRO	LEU	conflict	UNP P12568
C	152	VAL	ILE	conflict	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
C	213	SER	ARG	conflict	UNP P12568
C	215	PRO	SER	conflict	UNP P12568
C	279	PRO	GLN	conflict	UNP P12568
C	377	PRO	SER	conflict	UNP P12568
C	514	SER	-	linker	UNP P12568
C	515	ALA	-	linker	UNP P12568
C	516	ILE	-	linker	UNP P12568
C	517	GLY	-	linker	UNP P12568
C	545	HIS	-	expression tag	UNP A0A346FJN8
C	546	HIS	-	expression tag	UNP A0A346FJN8
C	547	HIS	-	expression tag	UNP A0A346FJN8
C	548	HIS	-	expression tag	UNP A0A346FJN8
C	549	HIS	-	expression tag	UNP A0A346FJN8
C	550	HIS	-	expression tag	UNP A0A346FJN8
C	551	HIS	-	expression tag	UNP A0A346FJN8
C	552	HIS	-	expression tag	UNP A0A346FJN8
D	10	MET	-	initiating methionine	UNP P12568
D	11	LYS	-	expression tag	UNP P12568
D	12	CYS	-	expression tag	UNP P12568
D	13	LEU	-	expression tag	UNP P12568
D	14	LEU	-	expression tag	UNP P12568
D	15	TYR	-	expression tag	UNP P12568
D	16	LEU	-	expression tag	UNP P12568
D	17	ALA	-	expression tag	UNP P12568
D	18	PHE	-	expression tag	UNP P12568
D	19	LEU	-	expression tag	UNP P12568
D	20	PHE	-	expression tag	UNP P12568
D	21	ILE	-	expression tag	UNP P12568
D	22	GLY	-	expression tag	UNP P12568
D	23	VAL	-	expression tag	UNP P12568
D	24	ASN	-	expression tag	UNP P12568
D	25	CYS	-	expression tag	UNP P12568
D	67	PRO	ASN	conflict	UNP P12568
D	80	LYS	ASN	conflict	UNP P12568
D	121	GLY	-	linker	UNP P12568
D	122	GLY	-	linker	UNP P12568
D	123	GLY	-	linker	UNP P12568
D	124	GLY	-	linker	UNP P12568
D	125	SER	-	linker	UNP P12568
D	126	GLY	-	linker	UNP P12568
D	127	GLY	-	linker	UNP P12568
D	128	GLY	-	linker	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
D	129	GLY	-	linker	UNP P12568
D	130	SER	-	linker	UNP P12568
D	131	GLY	-	linker	UNP P12568
D	132	GLY	-	linker	UNP P12568
D	133	GLY	-	linker	UNP P12568
D	134	GLY	-	linker	UNP P12568
D	135	SER	-	linker	UNP P12568
D	138	PRO	LEU	conflict	UNP P12568
D	139	PRO	GLY	conflict	UNP P12568
D	141	PRO	LEU	conflict	UNP P12568
D	152	VAL	ILE	conflict	UNP P12568
D	213	SER	ARG	conflict	UNP P12568
D	215	PRO	SER	conflict	UNP P12568
D	279	PRO	GLN	conflict	UNP P12568
D	377	PRO	SER	conflict	UNP P12568
D	514	SER	-	linker	UNP P12568
D	515	ALA	-	linker	UNP P12568
D	516	ILE	-	linker	UNP P12568
D	517	GLY	-	linker	UNP P12568
D	545	HIS	-	expression tag	UNP A0A346FJN8
D	546	HIS	-	expression tag	UNP A0A346FJN8
D	547	HIS	-	expression tag	UNP A0A346FJN8
D	548	HIS	-	expression tag	UNP A0A346FJN8
D	549	HIS	-	expression tag	UNP A0A346FJN8
D	550	HIS	-	expression tag	UNP A0A346FJN8
D	551	HIS	-	expression tag	UNP A0A346FJN8
D	552	HIS	-	expression tag	UNP A0A346FJN8
E	10	MET	-	initiating methionine	UNP P12568
E	11	LYS	-	expression tag	UNP P12568
E	12	CYS	-	expression tag	UNP P12568
E	13	LEU	-	expression tag	UNP P12568
E	14	LEU	-	expression tag	UNP P12568
E	15	TYR	-	expression tag	UNP P12568
E	16	LEU	-	expression tag	UNP P12568
E	17	ALA	-	expression tag	UNP P12568
E	18	PHE	-	expression tag	UNP P12568
E	19	LEU	-	expression tag	UNP P12568
E	20	PHE	-	expression tag	UNP P12568
E	21	ILE	-	expression tag	UNP P12568
E	22	GLY	-	expression tag	UNP P12568
E	23	VAL	-	expression tag	UNP P12568
E	24	ASN	-	expression tag	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
E	25	CYS	-	expression tag	UNP P12568
E	67	PRO	ASN	conflict	UNP P12568
E	80	LYS	ASN	conflict	UNP P12568
E	121	GLY	-	linker	UNP P12568
E	122	GLY	-	linker	UNP P12568
E	123	GLY	-	linker	UNP P12568
E	124	GLY	-	linker	UNP P12568
E	125	SER	-	linker	UNP P12568
E	126	GLY	-	linker	UNP P12568
E	127	GLY	-	linker	UNP P12568
E	128	GLY	-	linker	UNP P12568
E	129	GLY	-	linker	UNP P12568
E	130	SER	-	linker	UNP P12568
E	131	GLY	-	linker	UNP P12568
E	132	GLY	-	linker	UNP P12568
E	133	GLY	-	linker	UNP P12568
E	134	GLY	-	linker	UNP P12568
E	135	SER	-	linker	UNP P12568
E	138	PRO	LEU	conflict	UNP P12568
E	139	PRO	GLY	conflict	UNP P12568
E	141	PRO	LEU	conflict	UNP P12568
E	152	VAL	ILE	conflict	UNP P12568
E	213	SER	ARG	conflict	UNP P12568
E	215	PRO	SER	conflict	UNP P12568
E	279	PRO	GLN	conflict	UNP P12568
E	377	PRO	SER	conflict	UNP P12568
E	514	SER	-	linker	UNP P12568
E	515	ALA	-	linker	UNP P12568
E	516	ILE	-	linker	UNP P12568
E	517	GLY	-	linker	UNP P12568
E	545	HIS	-	expression tag	UNP A0A346FJN8
E	546	HIS	-	expression tag	UNP A0A346FJN8
E	547	HIS	-	expression tag	UNP A0A346FJN8
E	548	HIS	-	expression tag	UNP A0A346FJN8
E	549	HIS	-	expression tag	UNP A0A346FJN8
E	550	HIS	-	expression tag	UNP A0A346FJN8
E	551	HIS	-	expression tag	UNP A0A346FJN8
E	552	HIS	-	expression tag	UNP A0A346FJN8
F	10	MET	-	initiating methionine	UNP P12568
F	11	LYS	-	expression tag	UNP P12568
F	12	CYS	-	expression tag	UNP P12568
F	13	LEU	-	expression tag	UNP P12568

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Chain	Residue	Modelled	Actual	Comment	Reference
F	14	LEU	-	expression tag	UNP P12568
F	15	TYR	-	expression tag	UNP P12568
F	16	LEU	-	expression tag	UNP P12568
F	17	ALA	-	expression tag	UNP P12568
F	18	PHE	-	expression tag	UNP P12568
F	19	LEU	-	expression tag	UNP P12568
F	20	PHE	-	expression tag	UNP P12568
F	21	ILE	-	expression tag	UNP P12568
F	22	GLY	-	expression tag	UNP P12568
F	23	VAL	-	expression tag	UNP P12568
F	24	ASN	-	expression tag	UNP P12568
F	25	CYS	-	expression tag	UNP P12568
F	67	PRO	ASN	conflict	UNP P12568
F	80	LYS	ASN	conflict	UNP P12568
F	121	GLY	-	linker	UNP P12568
F	122	GLY	-	linker	UNP P12568
F	123	GLY	-	linker	UNP P12568
F	124	GLY	-	linker	UNP P12568
F	125	SER	-	linker	UNP P12568
F	126	GLY	-	linker	UNP P12568
F	127	GLY	-	linker	UNP P12568
F	128	GLY	-	linker	UNP P12568
F	129	GLY	-	linker	UNP P12568
F	130	SER	-	linker	UNP P12568
F	131	GLY	-	linker	UNP P12568
F	132	GLY	-	linker	UNP P12568
F	133	GLY	-	linker	UNP P12568
F	134	GLY	-	linker	UNP P12568
F	135	SER	-	linker	UNP P12568
F	138	PRO	LEU	conflict	UNP P12568
F	139	PRO	GLY	conflict	UNP P12568
F	141	PRO	LEU	conflict	UNP P12568
F	152	VAL	ILE	conflict	UNP P12568
F	213	SER	ARG	conflict	UNP P12568
F	215	PRO	SER	conflict	UNP P12568
F	279	PRO	GLN	conflict	UNP P12568
F	377	PRO	SER	conflict	UNP P12568
F	514	SER	-	linker	UNP P12568
F	515	ALA	-	linker	UNP P12568
F	516	ILE	-	linker	UNP P12568
F	517	GLY	-	linker	UNP P12568
F	545	HIS	-	expression tag	UNP A0A346FJN8

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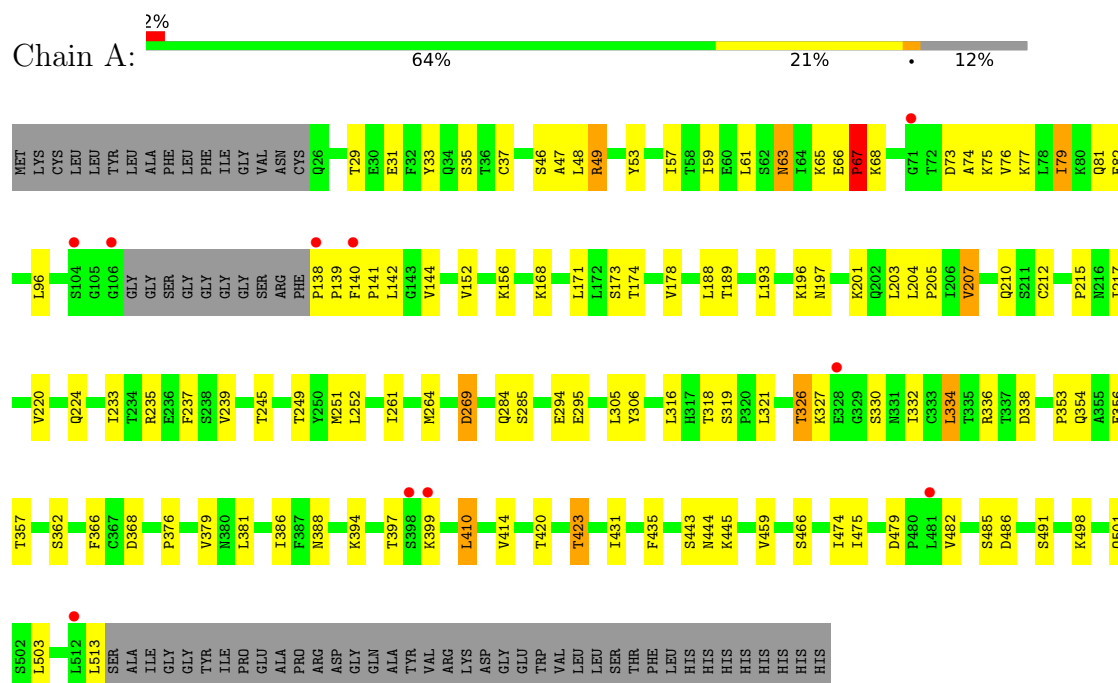
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Chain	Residue	Modelled	Actual	Comment	Reference
F	546	HIS	-	expression tag	UNP A0A346FJN8
F	547	HIS	-	expression tag	UNP A0A346FJN8
F	548	HIS	-	expression tag	UNP A0A346FJN8
F	549	HIS	-	expression tag	UNP A0A346FJN8
F	550	HIS	-	expression tag	UNP A0A346FJN8
F	551	HIS	-	expression tag	UNP A0A346FJN8
F	552	HIS	-	expression tag	UNP A0A346FJN8

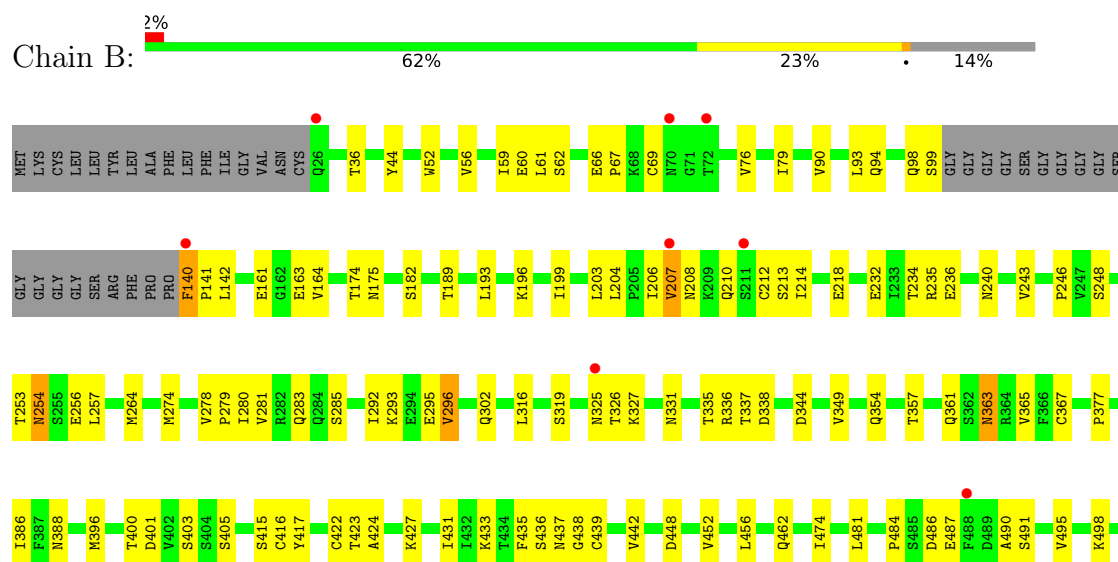
3 Residue-property plots [i](#)

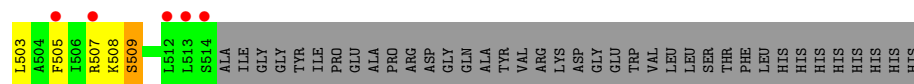
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Fusion glycoprotein F0,Fibritin

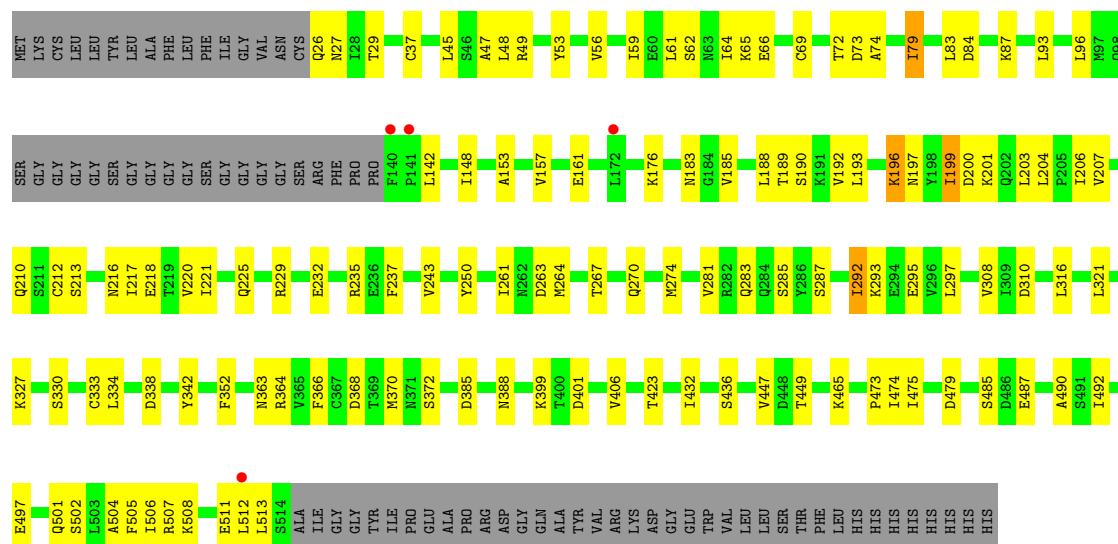


• Molecule 1: Fusion glycoprotein F0,Fibritin

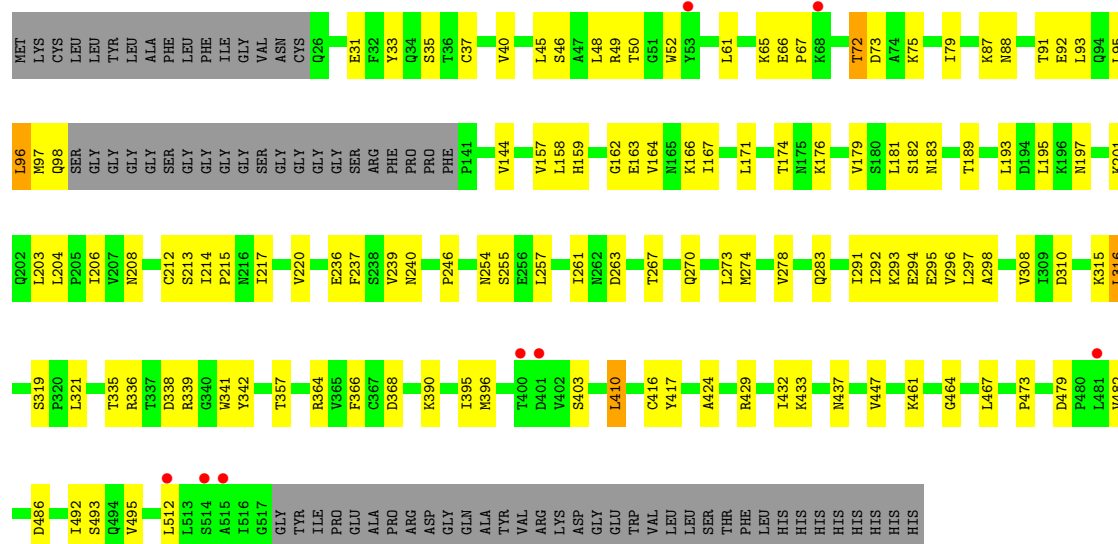




• Molecule 1: Fusion glycoprotein F0,Fibrin

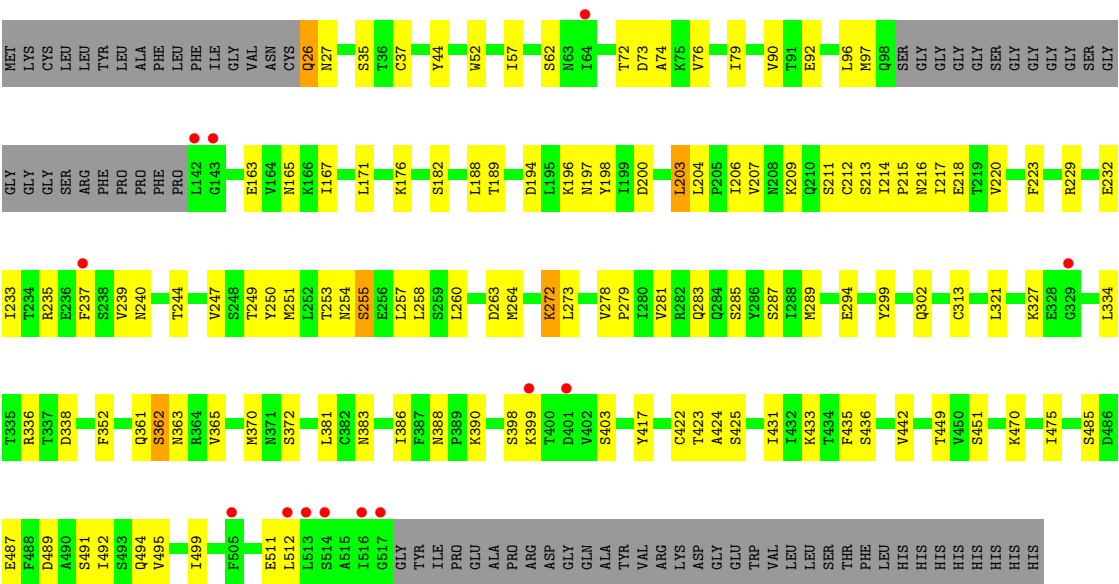


• Molecule 1: Fusion glycoprotein F0,Fibrin

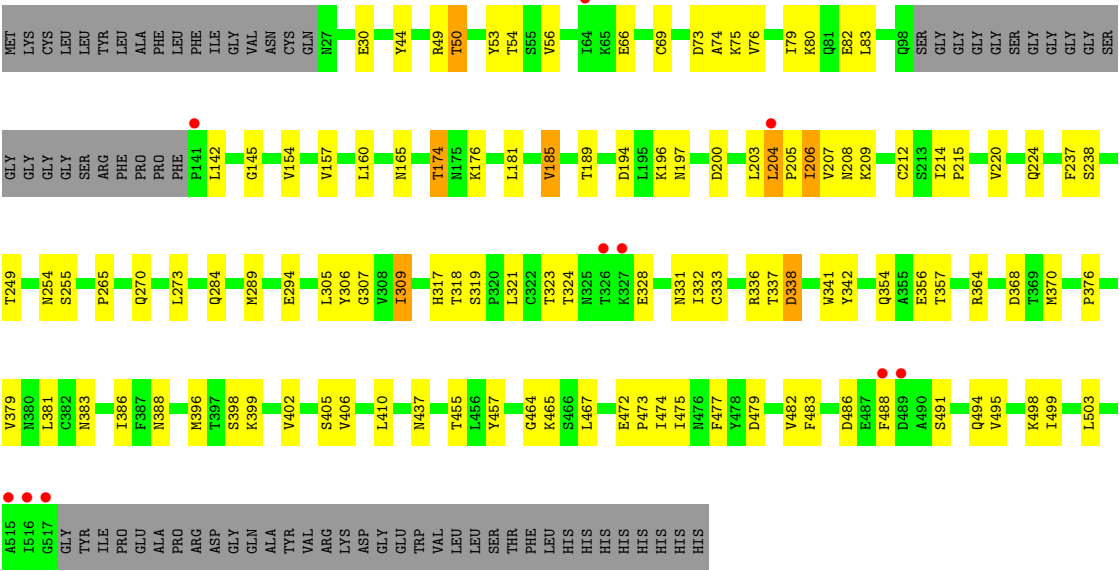


• Molecule 1: Fusion glycoprotein F0,Fibrin





● Molecule 1: Fusion glycoprotein F0,Fibrin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	159.33Å 168.67Å 189.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	126.01 – 2.92 126.01 – 2.92	Depositor EDS
% Data completeness (in resolution range)	67.2 (126.01-2.92) 67.3 (126.01-2.92)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.197 , 0.255 0.197 , 0.254	Depositor DCC
R_{free} test set	2005 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20848	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/3565	0.42	1/4834 (0.0%)
1	B	0.18	0/3525	0.44	2/4781 (0.0%)
1	C	0.19	0/3519	0.44	0/4773
1	D	0.16	0/3524	0.39	0/4779
1	E	0.17	0/3516	0.40	0/4768
1	F	0.17	0/3515	0.42	1/4767 (0.0%)
All	All	0.18	0/21164	0.42	4/28702 (0.0%)

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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ILE	CG1-CB-CG2	-6.66	90.72	110.70
1	A	67	PRO	N-CA-CB	-5.73	97.23	103.25
1	B	214	ILE	CB-CA-C	5.18	116.08	111.00
1	F	265	PRO	CA-N-CD	-5.03	104.95	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	PHE	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	3510	0	3550	76	0
1	B	3472	0	3517	73	0
1	C	3466	0	3512	81	0
1	D	3472	0	3523	74	0
1	E	3465	0	3517	80	0
1	F	3463	0	3515	70	0
All	All	20848	0	21134	437	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 10.

The worst 5 of 437 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:F:324:THR:HG21	1:F:437:ASN:HB3	1.53	0.90
1:C:216:ASN:OD1	1:C:218:GLU:N	2.08	0.85
1:F:66:GLU:OE2	1:F:66:GLU:N	2.10	0.84
1:A:381:LEU:HB3	1:A:388:ASN:HD22	1.44	0.83
1:D:176:LYS:NZ	1:D:263:ASP:OD2	2.10	0.81

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	453/522 (87%)	420 (93%)	33 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	445/522 (85%)	427 (96%)	18 (4%)	0	100	100
1	C	444/522 (85%)	426 (96%)	18 (4%)	0	100	100
1	D	446/522 (85%)	436 (98%)	10 (2%)	0	100	100
1	E	445/522 (85%)	423 (95%)	22 (5%)	0	100	100
1	F	445/522 (85%)	418 (94%)	27 (6%)	0	100	100
All	All	2678/3132 (86%)	2550 (95%)	128 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	413/463 (89%)	390 (94%)	23 (6%)	17	46
1	B	411/463 (89%)	391 (95%)	20 (5%)	21	51
1	C	410/463 (89%)	393 (96%)	17 (4%)	26	58
1	D	410/463 (89%)	394 (96%)	16 (4%)	27	60
1	E	409/463 (88%)	390 (95%)	19 (5%)	23	54
1	F	409/463 (88%)	391 (96%)	18 (4%)	24	55
All	All	2462/2778 (89%)	2349 (95%)	113 (5%)	23	54

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	423	THR
1	F	402	VAL
1	D	390	LYS
1	F	338	ASP
1	F	174	THR

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

Mol	Chain	Res	Type
1	C	462	GLN
1	D	262	ASN
1	E	501	GLN
1	D	208	ASN
1	D	277	ASN

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 oligosaccharides 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, 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	457/522 (87%)	0.03	10 (2%) 62 56	16, 39, 79, 113	0
1	B	449/522 (86%)	-0.12	13 (2%) 54 48	16, 35, 80, 118	0
1	C	448/522 (85%)	-0.07	4 (0%) 81 76	15, 41, 76, 103	0
1	D	450/522 (86%)	-0.13	8 (1%) 67 62	17, 37, 77, 122	0
1	E	449/522 (86%)	0.12	13 (2%) 54 48	18, 41, 83, 122	0
1	F	449/522 (86%)	0.06	10 (2%) 62 56	19, 40, 84, 120	0
All	All	2702/3132 (86%)	-0.02	58 (2%) 63 57	15, 39, 80, 122	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	PHE	5.5
1	E	142	LEU	4.5
1	E	516	ILE	4.4
1	A	104	SER	4.2
1	C	141	PRO	4.0

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 oligosaccharides 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.