



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2025 – 02:39 PM JST

PDB ID : 8ZQ6 / pdb\_00008zq6  
Title : preF6P of RSV glycoprotein  
Authors : Han, X.; Lang, Q.; Huang, Q.; Yan, J.  
Deposited on : 2024-06-01  
Resolution : 2.77 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](mailto: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

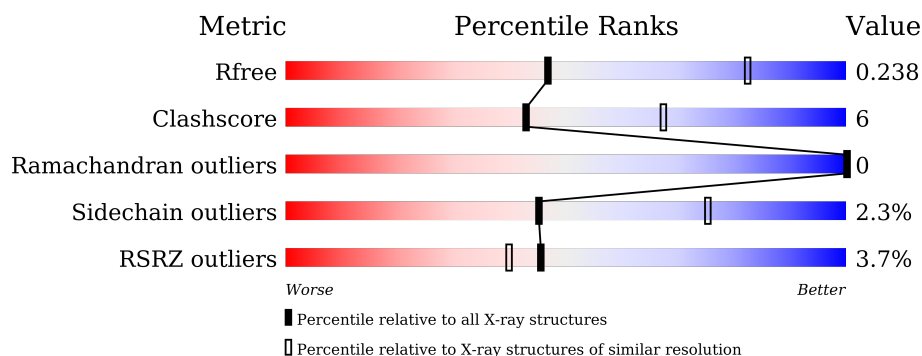
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

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  $\geq 3$ , 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> <div></div> <div>69%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	522	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	522	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div></div> <div>14%</div> </div> </div>
1	D	522	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div></div> <div>13%</div> </div> </div>
1	E	522	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div></div> <div>13%</div> </div> </div>
1	F	522	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>•</div> <div>13%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20971 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	451	Total	C	N	O	S	0	0	0
			3482	2201	573	687	21			
1	B	455	Total	C	N	O	S	0	0	0
			3500	2210	577	692	21			
1	C	451	Total	C	N	O	S	0	0	0
			3480	2201	572	686	21			
1	D	452	Total	C	N	O	S	0	0	0
			3489	2206	574	688	21			
1	E	454	Total	C	N	O	S	0	0	0
			3507	2220	576	690	21			
1	F	455	Total	C	N	O	S	0	0	0
			3513	2223	577	692	21			

There are 318 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP C3UPB8
A	11	LYS	-	expression tag	UNP C3UPB8
A	12	CYS	-	expression tag	UNP C3UPB8
A	13	LEU	-	expression tag	UNP C3UPB8
A	14	LEU	-	expression tag	UNP C3UPB8
A	15	TYR	-	expression tag	UNP C3UPB8
A	16	LEU	-	expression tag	UNP C3UPB8
A	17	ALA	-	expression tag	UNP C3UPB8
A	18	PHE	-	expression tag	UNP C3UPB8
A	19	LEU	-	expression tag	UNP C3UPB8
A	20	PHE	-	expression tag	UNP C3UPB8
A	21	ILE	-	expression tag	UNP C3UPB8
A	22	GLY	-	expression tag	UNP C3UPB8
A	23	VAL	-	expression tag	UNP C3UPB8
A	24	ASN	-	expression tag	UNP C3UPB8
A	25	CYS	-	expression tag	UNP C3UPB8
A	66	GLU	LYS	conflict	UNP C3UPB8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	PRO	ASN	conflict	UNP C3UPB8
A	76	VAL	ILE	conflict	UNP C3UPB8
A	121	GLY	-	linker	UNP C3UPB8
A	122	GLY	-	linker	UNP C3UPB8
A	123	GLY	-	linker	UNP C3UPB8
A	124	GLY	-	linker	UNP C3UPB8
A	125	SER	-	linker	UNP C3UPB8
A	126	GLY	-	linker	UNP C3UPB8
A	127	GLY	-	linker	UNP C3UPB8
A	128	GLY	-	linker	UNP C3UPB8
A	129	GLY	-	linker	UNP C3UPB8
A	130	SER	-	linker	UNP C3UPB8
A	131	GLY	-	linker	UNP C3UPB8
A	132	GLY	-	linker	UNP C3UPB8
A	133	GLY	-	linker	UNP C3UPB8
A	134	GLY	-	linker	UNP C3UPB8
A	135	SER	-	linker	UNP C3UPB8
A	136	ARG	-	linker	UNP C3UPB8
A	137	PHE	-	linker	UNP C3UPB8
A	138	PRO	-	linker	UNP C3UPB8
A	139	PRO	-	linker	UNP C3UPB8
A	215	PRO	SER	conflict	UNP C3UPB8
A	216	PRO	ASN	conflict	UNP C3UPB8
A	279	PRO	GLN	conflict	UNP C3UPB8
A	514	SER	-	linker	UNP C3UPB8
A	515	ALA	-	linker	UNP C3UPB8
A	516	ILE	-	linker	UNP C3UPB8
A	517	GLY	-	linker	UNP C3UPB8
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 C3UPB8
B	11	LYS	-	expression tag	UNP C3UPB8
B	12	CYS	-	expression tag	UNP C3UPB8
B	13	LEU	-	expression tag	UNP C3UPB8
B	14	LEU	-	expression tag	UNP C3UPB8
B	15	TYR	-	expression tag	UNP C3UPB8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	LEU	-	expression tag	UNP C3UPB8
B	17	ALA	-	expression tag	UNP C3UPB8
B	18	PHE	-	expression tag	UNP C3UPB8
B	19	LEU	-	expression tag	UNP C3UPB8
B	20	PHE	-	expression tag	UNP C3UPB8
B	21	ILE	-	expression tag	UNP C3UPB8
B	22	GLY	-	expression tag	UNP C3UPB8
B	23	VAL	-	expression tag	UNP C3UPB8
B	24	ASN	-	expression tag	UNP C3UPB8
B	25	CYS	-	expression tag	UNP C3UPB8
B	66	GLU	LYS	conflict	UNP C3UPB8
B	67	PRO	ASN	conflict	UNP C3UPB8
B	76	VAL	ILE	conflict	UNP C3UPB8
B	100	GLY	-	linker	UNP C3UPB8
B	101	GLY	-	linker	UNP C3UPB8
B	102	GLY	-	linker	UNP C3UPB8
B	124	GLY	-	linker	UNP C3UPB8
B	125	SER	-	linker	UNP C3UPB8
B	126	GLY	-	linker	UNP C3UPB8
B	127	GLY	-	linker	UNP C3UPB8
B	128	GLY	-	linker	UNP C3UPB8
B	129	GLY	-	linker	UNP C3UPB8
B	130	SER	-	linker	UNP C3UPB8
B	131	GLY	-	linker	UNP C3UPB8
B	132	GLY	-	linker	UNP C3UPB8
B	133	GLY	-	linker	UNP C3UPB8
B	134	GLY	-	linker	UNP C3UPB8
B	135	SER	-	linker	UNP C3UPB8
B	136	ARG	-	linker	UNP C3UPB8
B	137	PHE	-	linker	UNP C3UPB8
B	138	PRO	-	linker	UNP C3UPB8
B	139	PRO	-	linker	UNP C3UPB8
B	215	PRO	SER	conflict	UNP C3UPB8
B	216	PRO	ASN	conflict	UNP C3UPB8
B	279	PRO	GLN	conflict	UNP C3UPB8
B	514	SER	-	linker	UNP C3UPB8
B	515	ALA	-	linker	UNP C3UPB8
B	516	ILE	-	linker	UNP C3UPB8
B	517	GLY	-	linker	UNP C3UPB8
B	545	HIS	-	expression tag	UNP A0A346FJN8
B	546	HIS	-	expression tag	UNP A0A346FJN8
B	547	HIS	-	expression tag	UNP A0A346FJN8

*Continued on next page...*

*Continued from previous page...*

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 C3UPB8
C	11	LYS	-	expression tag	UNP C3UPB8
C	12	CYS	-	expression tag	UNP C3UPB8
C	13	LEU	-	expression tag	UNP C3UPB8
C	14	LEU	-	expression tag	UNP C3UPB8
C	15	TYR	-	expression tag	UNP C3UPB8
C	16	LEU	-	expression tag	UNP C3UPB8
C	17	ALA	-	expression tag	UNP C3UPB8
C	18	PHE	-	expression tag	UNP C3UPB8
C	19	LEU	-	expression tag	UNP C3UPB8
C	20	PHE	-	expression tag	UNP C3UPB8
C	21	ILE	-	expression tag	UNP C3UPB8
C	22	GLY	-	expression tag	UNP C3UPB8
C	23	VAL	-	expression tag	UNP C3UPB8
C	24	ASN	-	expression tag	UNP C3UPB8
C	25	CYS	-	expression tag	UNP C3UPB8
C	66	GLU	LYS	conflict	UNP C3UPB8
C	67	PRO	ASN	conflict	UNP C3UPB8
C	76	VAL	ILE	conflict	UNP C3UPB8
C	121	GLY	-	linker	UNP C3UPB8
C	122	GLY	-	linker	UNP C3UPB8
C	123	GLY	-	linker	UNP C3UPB8
C	124	GLY	-	linker	UNP C3UPB8
C	125	SER	-	linker	UNP C3UPB8
C	126	GLY	-	linker	UNP C3UPB8
C	127	GLY	-	linker	UNP C3UPB8
C	128	GLY	-	linker	UNP C3UPB8
C	129	GLY	-	linker	UNP C3UPB8
C	130	SER	-	linker	UNP C3UPB8
C	131	GLY	-	linker	UNP C3UPB8
C	132	GLY	-	linker	UNP C3UPB8
C	133	GLY	-	linker	UNP C3UPB8
C	134	GLY	-	linker	UNP C3UPB8
C	135	SER	-	linker	UNP C3UPB8
C	136	ARG	-	linker	UNP C3UPB8
C	137	PHE	-	linker	UNP C3UPB8
C	138	PRO	-	linker	UNP C3UPB8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	139	PRO	-	linker	UNP C3UPB8
C	215	PRO	SER	conflict	UNP C3UPB8
C	216	PRO	ASN	conflict	UNP C3UPB8
C	279	PRO	GLN	conflict	UNP C3UPB8
C	514	SER	-	linker	UNP C3UPB8
C	515	ALA	-	linker	UNP C3UPB8
C	516	ILE	-	linker	UNP C3UPB8
C	517	GLY	-	linker	UNP C3UPB8
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 C3UPB8
D	11	LYS	-	expression tag	UNP C3UPB8
D	12	CYS	-	expression tag	UNP C3UPB8
D	13	LEU	-	expression tag	UNP C3UPB8
D	14	LEU	-	expression tag	UNP C3UPB8
D	15	TYR	-	expression tag	UNP C3UPB8
D	16	LEU	-	expression tag	UNP C3UPB8
D	17	ALA	-	expression tag	UNP C3UPB8
D	18	PHE	-	expression tag	UNP C3UPB8
D	19	LEU	-	expression tag	UNP C3UPB8
D	20	PHE	-	expression tag	UNP C3UPB8
D	21	ILE	-	expression tag	UNP C3UPB8
D	22	GLY	-	expression tag	UNP C3UPB8
D	23	VAL	-	expression tag	UNP C3UPB8
D	24	ASN	-	expression tag	UNP C3UPB8
D	25	CYS	-	expression tag	UNP C3UPB8
D	66	GLU	LYS	conflict	UNP C3UPB8
D	67	PRO	ASN	conflict	UNP C3UPB8
D	76	VAL	ILE	conflict	UNP C3UPB8
D	121	GLY	-	linker	UNP C3UPB8
D	122	GLY	-	linker	UNP C3UPB8
D	123	GLY	-	linker	UNP C3UPB8
D	124	GLY	-	linker	UNP C3UPB8
D	125	SER	-	linker	UNP C3UPB8
D	126	GLY	-	linker	UNP C3UPB8
D	127	GLY	-	linker	UNP C3UPB8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	128	GLY	-	linker	UNP C3UPB8
D	129	GLY	-	linker	UNP C3UPB8
D	130	SER	-	linker	UNP C3UPB8
D	131	GLY	-	linker	UNP C3UPB8
D	132	GLY	-	linker	UNP C3UPB8
D	133	GLY	-	linker	UNP C3UPB8
D	134	GLY	-	linker	UNP C3UPB8
D	135	SER	-	linker	UNP C3UPB8
D	136	ARG	-	linker	UNP C3UPB8
D	137	PHE	-	linker	UNP C3UPB8
D	138	PRO	-	linker	UNP C3UPB8
D	139	PRO	-	linker	UNP C3UPB8
D	215	PRO	SER	conflict	UNP C3UPB8
D	216	PRO	ASN	conflict	UNP C3UPB8
D	279	PRO	GLN	conflict	UNP C3UPB8
D	514	SER	-	linker	UNP C3UPB8
D	515	ALA	-	linker	UNP C3UPB8
D	516	ILE	-	linker	UNP C3UPB8
D	517	GLY	-	linker	UNP C3UPB8
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 C3UPB8
E	11	LYS	-	expression tag	UNP C3UPB8
E	12	CYS	-	expression tag	UNP C3UPB8
E	13	LEU	-	expression tag	UNP C3UPB8
E	14	LEU	-	expression tag	UNP C3UPB8
E	15	TYR	-	expression tag	UNP C3UPB8
E	16	LEU	-	expression tag	UNP C3UPB8
E	17	ALA	-	expression tag	UNP C3UPB8
E	18	PHE	-	expression tag	UNP C3UPB8
E	19	LEU	-	expression tag	UNP C3UPB8
E	20	PHE	-	expression tag	UNP C3UPB8
E	21	ILE	-	expression tag	UNP C3UPB8
E	22	GLY	-	expression tag	UNP C3UPB8
E	23	VAL	-	expression tag	UNP C3UPB8
E	24	ASN	-	expression tag	UNP C3UPB8

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	25	CYS	-	expression tag	UNP C3UPB8
E	66	GLU	LYS	conflict	UNP C3UPB8
E	67	PRO	ASN	conflict	UNP C3UPB8
E	76	VAL	ILE	conflict	UNP C3UPB8
E	121	GLY	-	linker	UNP C3UPB8
E	122	GLY	-	linker	UNP C3UPB8
E	123	GLY	-	linker	UNP C3UPB8
E	124	GLY	-	linker	UNP C3UPB8
E	125	SER	-	linker	UNP C3UPB8
E	126	GLY	-	linker	UNP C3UPB8
E	127	GLY	-	linker	UNP C3UPB8
E	128	GLY	-	linker	UNP C3UPB8
E	129	GLY	-	linker	UNP C3UPB8
E	130	SER	-	linker	UNP C3UPB8
E	131	GLY	-	linker	UNP C3UPB8
E	132	GLY	-	linker	UNP C3UPB8
E	133	GLY	-	linker	UNP C3UPB8
E	134	GLY	-	linker	UNP C3UPB8
E	135	SER	-	linker	UNP C3UPB8
E	136	ARG	-	linker	UNP C3UPB8
E	137	PHE	-	linker	UNP C3UPB8
E	138	PRO	-	linker	UNP C3UPB8
E	139	PRO	-	linker	UNP C3UPB8
E	215	PRO	SER	conflict	UNP C3UPB8
E	216	PRO	ASN	conflict	UNP C3UPB8
E	279	PRO	GLN	conflict	UNP C3UPB8
E	514	SER	-	linker	UNP C3UPB8
E	515	ALA	-	linker	UNP C3UPB8
E	516	ILE	-	linker	UNP C3UPB8
E	517	GLY	-	linker	UNP C3UPB8
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 C3UPB8
F	11	LYS	-	expression tag	UNP C3UPB8
F	12	CYS	-	expression tag	UNP C3UPB8
F	13	LEU	-	expression tag	UNP C3UPB8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	14	LEU	-	expression tag	UNP C3UPB8
F	15	TYR	-	expression tag	UNP C3UPB8
F	16	LEU	-	expression tag	UNP C3UPB8
F	17	ALA	-	expression tag	UNP C3UPB8
F	18	PHE	-	expression tag	UNP C3UPB8
F	19	LEU	-	expression tag	UNP C3UPB8
F	20	PHE	-	expression tag	UNP C3UPB8
F	21	ILE	-	expression tag	UNP C3UPB8
F	22	GLY	-	expression tag	UNP C3UPB8
F	23	VAL	-	expression tag	UNP C3UPB8
F	24	ASN	-	expression tag	UNP C3UPB8
F	25	CYS	-	expression tag	UNP C3UPB8
F	66	GLU	LYS	conflict	UNP C3UPB8
F	67	PRO	ASN	conflict	UNP C3UPB8
F	76	VAL	ILE	conflict	UNP C3UPB8
F	121	GLY	-	linker	UNP C3UPB8
F	122	GLY	-	linker	UNP C3UPB8
F	123	GLY	-	linker	UNP C3UPB8
F	124	GLY	-	linker	UNP C3UPB8
F	125	SER	-	linker	UNP C3UPB8
F	126	GLY	-	linker	UNP C3UPB8
F	127	GLY	-	linker	UNP C3UPB8
F	128	GLY	-	linker	UNP C3UPB8
F	129	GLY	-	linker	UNP C3UPB8
F	130	SER	-	linker	UNP C3UPB8
F	131	GLY	-	linker	UNP C3UPB8
F	132	GLY	-	linker	UNP C3UPB8
F	133	GLY	-	linker	UNP C3UPB8
F	134	GLY	-	linker	UNP C3UPB8
F	135	SER	-	linker	UNP C3UPB8
F	136	ARG	-	linker	UNP C3UPB8
F	137	PHE	-	linker	UNP C3UPB8
F	138	PRO	-	linker	UNP C3UPB8
F	139	PRO	-	linker	UNP C3UPB8
F	215	PRO	SER	conflict	UNP C3UPB8
F	216	PRO	ASN	conflict	UNP C3UPB8
F	279	PRO	GLN	conflict	UNP C3UPB8
F	514	SER	-	linker	UNP C3UPB8
F	515	ALA	-	linker	UNP C3UPB8
F	516	ILE	-	linker	UNP C3UPB8
F	517	GLY	-	linker	UNP C3UPB8
F	545	HIS	-	expression tag	UNP A0A346FJN8

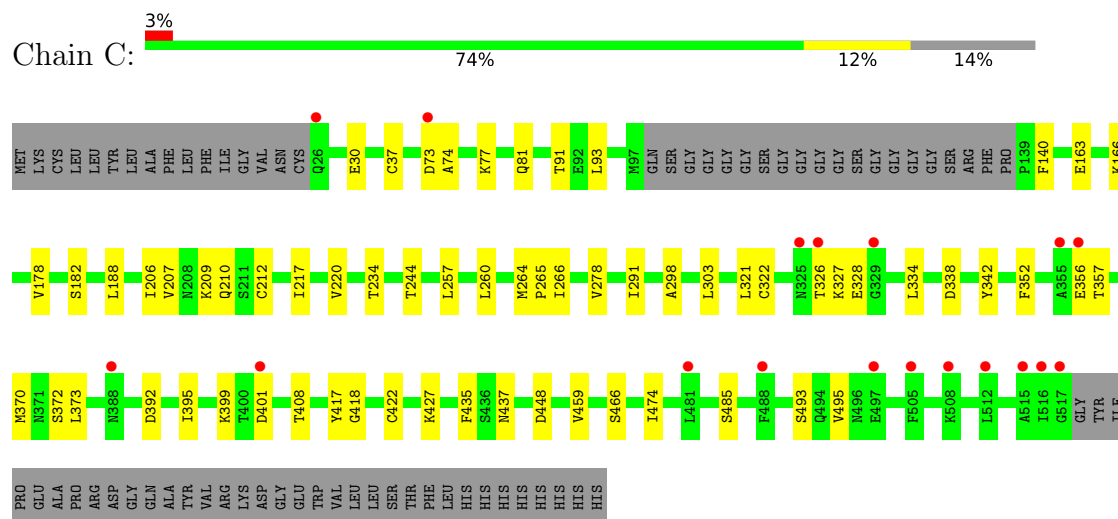
*Continued on next page...*

*Continued from previous page...*

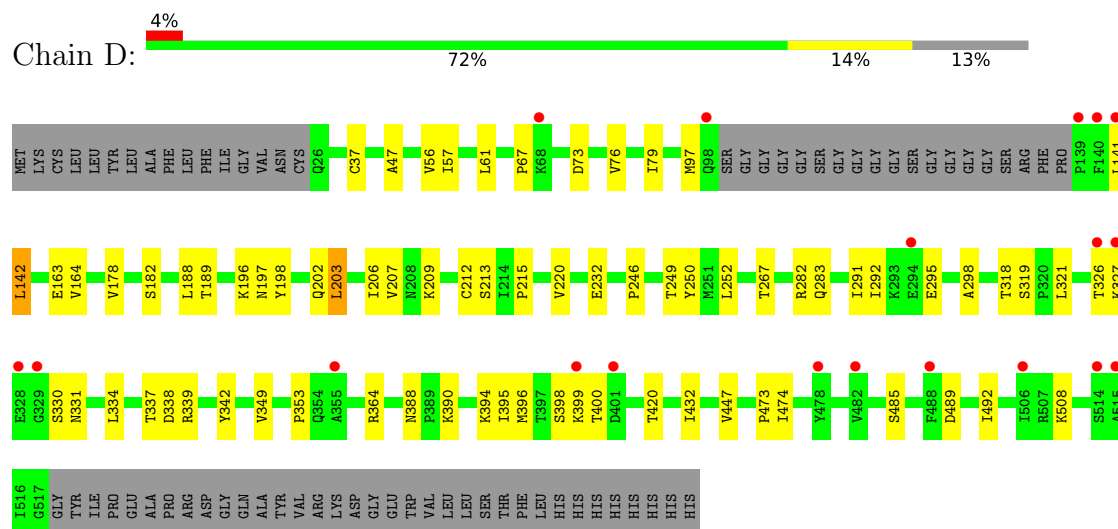
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	HIS	-	expression tag	UNP A0A346FJN8
F	547	HIS	-	expression tag	UNP A0A346FJN8
F	548	HIS	-	expression tag	UNP A0A346FJN8
F	549	HIS	-	expression tag	UNP A0A346FJN8
F	550	HIS	-	expression tag	UNP A0A346FJN8
F	551	HIS	-	expression tag	UNP A0A346FJN8
F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



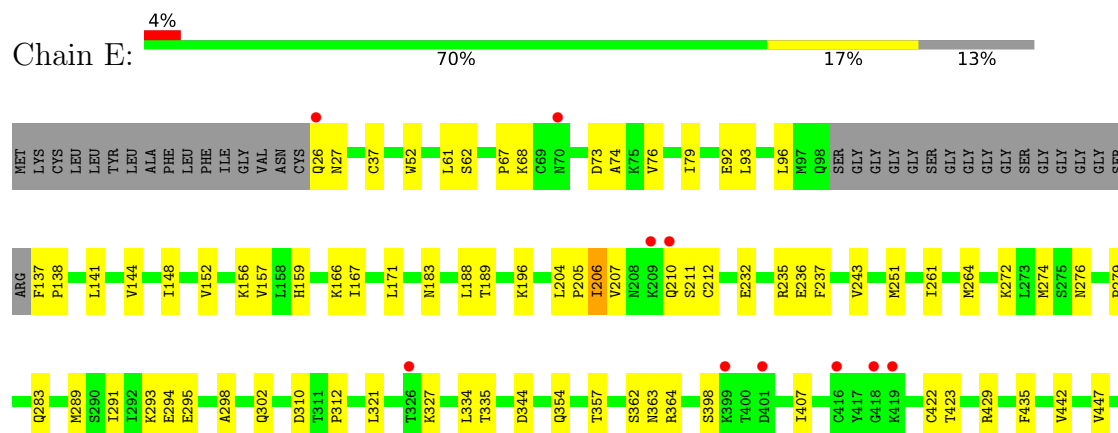
- Molecule 1: Fusion glycoprotein F0,Fibrin



- 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, $\alpha$ , $\beta$ , $\gamma$	159.16Å 170.08Å 190.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.94 – 2.77 26.94 – 2.77	Depositor EDS
% Data completeness (in resolution range)	86.6 (26.94-2.77) 86.8 (26.94-2.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.198 , 0.237 0.198 , 0.238	Depositor DCC
$R_{free}$ test set	1997 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	20971	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 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	0.14	0/3534	0.34	0/4792
1	B	0.13	0/3552	0.33	0/4815
1	C	0.12	0/3533	0.33	0/4791
1	D	0.15	0/3542	0.35	0/4803
1	E	0.12	0/3562	0.35	0/4832
1	F	0.13	0/3568	0.33	0/4840
All	All	0.13	0/21291	0.34	0/28873

There are no bond length outliers.

There are no bond angle outliers.

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	3482	0	3534	53	0
1	B	3500	0	3548	48	0
1	C	3480	0	3534	38	0
1	D	3489	0	3542	40	0
1	E	3507	0	3557	53	0
1	F	3513	0	3562	39	0
All	All	20971	0	21277	259	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 6.



All (259) 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:B:270:GLN:HG2	1:B:309:ILE:HD12	1.58	0.84
1:E:293:LYS:HG3	1:E:294:GLU:HG3	1.64	0.80
1:D:67:PRO:HB3	1:D:207:VAL:HB	1.65	0.79
1:F:49:ARG:NH1	1:F:368:ASP:OD1	2.19	0.75
1:B:206:ILE:HD12	1:B:215:PRO:HB3	1.67	0.74
1:B:92:GLU:OE1	1:B:238:SER:OG	2.06	0.71
1:D:388:ASN:OD1	1:D:390:LYS:N	2.23	0.71
1:C:73:ASP:OD2	1:C:74:ALA:N	2.24	0.70
1:C:418:GLY:H	1:C:437:ASN:HD21	1.40	0.69
1:A:512:LEU:HD22	1:B:512:LEU:HD21	1.73	0.69
1:F:310:ASP:OD1	1:F:364:ARG:NH1	2.26	0.68
1:D:318:THR:OG1	1:D:339:ARG:NH1	2.25	0.68
1:C:264:MET:HB2	1:C:266:ILE:HG12	1.76	0.68
1:D:395:ILE:HD13	1:D:492:ILE:HD13	1.77	0.65
1:A:97:MET:HE3	1:A:292:ILE:H	1.60	0.65
1:A:432:ILE:HD11	1:A:447:VAL:HG22	1.79	0.65
1:B:209:LYS:HB2	1:B:211:SER:H	1.61	0.65
1:B:270:GLN:NE2	1:B:306:TYR:O	2.29	0.64
1:D:394:LYS:NZ	1:D:489:ASP:OD1	2.26	0.64
1:E:171:LEU:HD11	1:E:189:THR:HG22	1.77	0.64
1:A:334:LEU:HB2	1:A:475:ILE:HD13	1.81	0.63
1:B:99:SER:HB2	1:B:152:VAL:HG22	1.80	0.63
1:B:65:LYS:HE3	1:B:66:GLU:H	1.64	0.63
1:B:67:PRO:HB3	1:B:207:VAL:HG22	1.79	0.62
1:E:264:MET:HE1	1:E:274:MET:HE1	1.82	0.62
1:E:272:LYS:O	1:E:276:ASN:ND2	2.30	0.62
1:C:209:LYS:HD3	1:C:210:GLN:H	1.64	0.62
1:B:338:ASP:OD2	1:B:338:ASP:N	2.31	0.61
1:C:291:ILE:HG22	1:C:298:ALA:HB3	1.81	0.61
1:A:422:CYS:HB2	1:A:435:PHE:HB2	1.82	0.61
1:A:206:ILE:HD12	1:A:215:PRO:HB3	1.84	0.60
1:F:331:ASN:ND2	1:F:401:ASP:OD2	2.33	0.60
1:B:208:ASN:HB3	1:B:209:LYS:HD3	1.82	0.60
1:E:144:VAL:HG21	1:E:152:VAL:HG21	1.84	0.59
1:F:210:GLN:H	1:F:210:GLN:CD	2.11	0.58
1:A:169:SER:HA	1:A:172:LEU:HG	1.86	0.58
1:A:429:ARG:HH12	1:C:265:PRO:HG2	1.67	0.58
1:E:167:ILE:HG23	1:E:189:THR:HG21	1.86	0.58
1:F:73:ASP:HB2	1:F:76:VAL:HG12	1.86	0.58
1:A:486:ASP:OD1	1:B:498:LYS:NZ	2.37	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:SER:OG	1:A:363:ASN:N	2.38	0.57
1:B:472:GLU:HG2	1:B:477:PHE:HE2	1.69	0.57
1:F:63:ASN:HB3	1:F:295:GLU:HG2	1.85	0.57
1:D:97:MET:HE3	1:D:291:ILE:HG13	1.87	0.57
1:B:167:ILE:HG22	1:B:179:VAL:HG21	1.84	0.57
1:A:163:GLU:OE2	1:A:182:SER:HB3	2.04	0.57
1:E:37:CYS:HB2	1:E:321:LEU:HD13	1.86	0.57
1:A:487:GLU:HB3	1:A:490:ALA:HB2	1.87	0.56
1:C:163:GLU:OE2	1:C:182:SER:N	2.38	0.56
1:E:68:LYS:HE2	1:E:68:LYS:HA	1.86	0.56
1:B:140:PHE:HE2	1:B:338:ASP:HA	1.71	0.56
1:E:422:CYS:HB2	1:E:435:PHE:HB2	1.87	0.56
1:E:497:GLU:O	1:E:501:GLN:HG3	2.05	0.56
1:B:97:MET:HE3	1:B:292:ILE:H	1.71	0.55
1:E:148:ILE:HD13	1:E:243:VAL:HG11	1.87	0.55
1:E:362:SER:OG	1:E:363:ASN:N	2.39	0.55
1:D:400:THR:HG21	1:E:489:ASP:OD2	2.06	0.55
1:C:392:ASP:OD2	1:C:493:SER:HB2	2.06	0.55
1:E:423:THR:HB	1:E:451:SER:HB3	1.89	0.55
1:F:73:ASP:OD2	1:F:214:ILE:HD11	2.07	0.55
1:D:337:THR:HG21	1:D:396:MET:HB3	1.88	0.55
1:B:338:ASP:HB2	1:B:342:TYR:OH	2.07	0.54
1:E:210:GLN:HG2	1:E:211:SER:H	1.72	0.54
1:C:370:MET:HE1	1:E:457:TYR:CE2	2.43	0.53
1:F:75:LYS:HB3	1:F:215:PRO:HD2	1.89	0.53
1:A:257:LEU:HD23	1:A:278:VAL:HG13	1.90	0.53
1:D:338:ASP:HB2	1:D:342:TYR:OH	2.08	0.53
1:E:138:PRO:HD3	1:E:159:HIS:CE1	2.44	0.53
1:F:432:ILE:HD11	1:F:447:VAL:HG22	1.91	0.53
1:D:73:ASP:HB3	1:D:76:VAL:HG23	1.90	0.53
1:F:48:LEU:HB2	1:F:308:VAL:HB	1.90	0.53
1:A:60:GLU:HG2	1:A:196:LYS:HD2	1.89	0.53
1:A:163:GLU:OE2	1:A:166:LYS:HE3	2.09	0.53
1:E:291:ILE:HG22	1:E:298:ALA:HB3	1.91	0.52
1:A:61:LEU:O	1:A:196:LYS:HB2	2.09	0.52
1:A:291:ILE:HG22	1:A:298:ALA:HB3	1.91	0.52
1:B:276:ASN:O	1:F:99:SER:HB2	2.10	0.52
1:E:354:GLN:O	1:E:357:THR:HG22	2.10	0.52
1:D:79:ILE:HD12	1:D:203:LEU:HD11	1.91	0.52
1:F:56:VAL:HB	1:F:189:THR:HG22	1.91	0.52
1:E:206:ILE:HG13	1:E:207:VAL:HG23	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:H	1:A:65:LYS:HD2	1.75	0.51
1:B:73:ASP:HB3	1:B:76:VAL:HG23	1.91	0.51
1:E:73:ASP:OD1	1:E:74:ALA:N	2.43	0.51
1:E:291:ILE:HD11	1:E:293:LYS:HD2	1.92	0.51
1:B:49:ARG:NE	1:B:368:ASP:OD1	2.42	0.51
1:C:427:LYS:HG3	1:C:448:ASP:OD2	2.10	0.51
1:A:429:ARG:NH1	1:C:265:PRO:HG2	2.25	0.51
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.93	0.51
1:A:61:LEU:O	1:A:295:GLU:HB3	2.10	0.51
1:A:338:ASP:HB2	1:A:342:TYR:OH	2.11	0.51
1:D:321:LEU:HD11	1:D:473:PRO:HB3	1.93	0.51
1:D:432:ILE:HD11	1:D:447:VAL:HG22	1.92	0.51
1:C:260:LEU:HD23	1:C:303:LEU:HD11	1.92	0.51
1:C:338:ASP:HB2	1:C:342:TYR:OH	2.10	0.51
1:D:61:LEU:HD11	1:D:292:ILE:HD11	1.93	0.50
1:F:157:VAL:HG21	1:F:183:ASN:CG	2.35	0.50
1:A:479:ASP:HB3	1:A:482:VAL:HG22	1.94	0.50
1:F:97:MET:HE1	1:F:289:MET:HG3	1.93	0.49
1:E:251:MET:HE1	1:E:289:MET:HE2	1.94	0.49
1:F:79:ILE:HG12	1:F:220:VAL:HG22	1.92	0.49
1:D:326:THR:HB	1:D:330:SER:OG	2.13	0.49
1:C:37:CYS:HB2	1:C:321:LEU:HD13	1.95	0.49
1:D:56:VAL:HB	1:D:189:THR:HG22	1.94	0.49
1:A:69:CYS:HB3	1:A:209:LYS:O	2.13	0.49
1:F:72:THR:O	1:F:72:THR:OG1	2.28	0.48
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.95	0.48
1:A:513:LEU:HA	1:A:516:ILE:HG12	1.93	0.48
1:B:147:ALA:HA	1:B:370:MET:HE1	1.94	0.48
1:D:47:ALA:HB2	1:D:364:ARG:HD2	1.96	0.48
1:D:249:THR:OG1	1:E:235:ARG:HD3	2.13	0.48
1:F:163:GLU:OE2	1:F:182:SER:HB3	2.12	0.48
1:A:53:TYR:OH	1:A:188:LEU:HB2	2.14	0.48
1:B:163:GLU:OE2	1:B:182:SER:HB3	2.14	0.48
1:C:257:LEU:HD23	1:C:278:VAL:HG13	1.94	0.48
1:E:310:ASP:OD1	1:E:364:ARG:NH1	2.45	0.48
1:C:178:VAL:HG22	1:C:188:LEU:HD23	1.96	0.48
1:C:352:PHE:CE1	1:C:372:SER:HB3	2.48	0.48
1:E:312:PRO:HG2	1:E:344:ASP:OD2	2.13	0.48
1:C:334:LEU:HD11	1:C:474:ILE:HD11	1.96	0.48
1:E:157:VAL:HG21	1:E:183:ASN:CG	2.38	0.48
1:E:491:SER:H	1:E:494:GLN:HB2	1.79	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:THR:HG22	1:B:396:MET:HG2	1.96	0.47
1:B:357:THR:HG21	1:B:371:ASN:HB2	1.97	0.47
1:D:178:VAL:HG22	1:D:188:LEU:HD12	1.97	0.47
1:A:321:LEU:HD11	1:A:473:PRO:HB3	1.97	0.47
1:B:26:GLN:HB3	1:B:363:ASN:ND2	2.30	0.47
1:C:356:GLU:HG3	1:C:357:THR:N	2.29	0.47
1:D:37:CYS:SG	1:D:319:SER:HB3	2.55	0.47
1:D:232:GLU:HG3	1:D:250:TYR:CZ	2.48	0.47
1:D:334:LEU:HD21	1:D:474:ILE:HD11	1.95	0.47
1:E:67:PRO:HB3	1:E:207:VAL:CG1	2.44	0.47
1:F:280:ILE:HG21	1:F:366:PHE:CG	2.50	0.47
1:A:410:LEU:HD22	1:A:464:GLY:HA3	1.95	0.47
1:C:93:LEU:HG	1:C:234:THR:HG23	1.97	0.47
1:A:64:ILE:HG21	1:A:199:ILE:HG21	1.96	0.46
1:B:37:CYS:SG	1:B:319:SER:HB3	2.55	0.46
1:E:61:LEU:O	1:E:295:GLU:HB3	2.15	0.46
1:A:162:GLY:O	1:A:166:LYS:HG3	2.15	0.46
1:B:240:ASN:HB3	1:B:243:VAL:O	2.16	0.46
1:A:221:ILE:HD12	1:B:217:ILE:HD11	1.97	0.46
1:C:326:THR:HG22	1:C:328:GLU:HG3	1.98	0.46
1:E:232:GLU:O	1:E:236:GLU:HG3	2.16	0.46
1:E:472:GLU:HG2	1:E:477:PHE:CE1	2.51	0.46
1:D:246:PRO:HB3	1:D:283:GLN:HA	1.97	0.46
1:E:67:PRO:HB3	1:E:207:VAL:HG11	1.98	0.46
1:E:73:ASP:O	1:E:76:VAL:HG22	2.16	0.46
1:B:327:LYS:HB3	1:B:330:SER:HB3	1.97	0.46
1:F:209:LYS:HE3	1:F:211:SER:O	2.16	0.46
1:E:196:LYS:HE2	1:E:196:LYS:HB3	1.68	0.46
1:C:370:MET:HE3	1:C:370:MET:O	2.15	0.45
1:E:52:TRP:CE3	1:E:302:GLN:HG2	2.51	0.45
1:D:508:LYS:HE3	1:D:508:LYS:HA	1.98	0.45
1:F:26:GLN:HA	1:F:363:ASN:OD1	2.16	0.45
1:F:293:LYS:HG2	1:F:294:GLU:OE2	2.16	0.45
1:C:77:LYS:HG2	1:C:81:GLN:HE21	1.81	0.45
1:E:62:SER:HB2	1:E:196:LYS:HA	1.97	0.45
1:C:338:ASP:OD1	1:C:338:ASP:N	2.37	0.45
1:C:422:CYS:HB2	1:C:435:PHE:HB2	1.99	0.45
1:F:49:ARG:HH11	1:F:368:ASP:CG	2.24	0.45
1:A:165:ASN:ND2	1:A:294:GLU:OE1	2.49	0.44
1:F:49:ARG:HD3	1:F:368:ASP:OD2	2.17	0.44
1:F:168:LYS:NZ	1:F:294:GLU:O	2.32	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLU:OE2	1:D:182:SER:N	2.51	0.44
1:A:293:LYS:O	1:A:296:VAL:HG12	2.17	0.44
1:A:357:THR:HG21	1:A:371:ASN:HB2	1.99	0.44
1:D:142:LEU:HD11	1:D:353:PRO:HG3	1.99	0.44
1:B:61:LEU:O	1:B:295:GLU:HB3	2.18	0.44
1:D:291:ILE:HG23	1:D:298:ALA:HB3	2.00	0.44
1:E:92:GLU:O	1:E:96:LEU:HG	2.18	0.44
1:E:138:PRO:HD2	1:E:141:LEU:HD12	1.99	0.44
1:B:444:ASN:ND2	1:B:462:GLN:O	2.51	0.44
1:E:26:GLN:HB3	1:E:27:ASN:H	1.56	0.44
1:C:217:ILE:HD12	1:C:217:ILE:HA	1.90	0.44
1:F:37:CYS:SG	1:F:319:SER:HB3	2.58	0.44
1:E:442:VAL:HG21	1:E:447:VAL:HG21	2.00	0.44
1:C:418:GLY:H	1:C:437:ASN:ND2	2.14	0.43
1:D:79:ILE:HG12	1:D:220:VAL:HG22	1.99	0.43
1:E:327:LYS:HA	1:E:327:LYS:HD3	1.74	0.43
1:B:487:GLU:HB3	1:B:490:ALA:HB2	2.00	0.43
1:B:67:PRO:HB3	1:B:207:VAL:CG2	2.46	0.43
1:D:331:ASN:O	1:D:399:LYS:HG2	2.18	0.43
1:E:334:LEU:HD21	1:E:474:ILE:HD11	2.00	0.43
1:B:265:PRO:HB3	1:E:429:ARG:NH2	2.34	0.43
1:D:196:LYS:HE3	1:D:295:GLU:OE2	2.18	0.43
1:B:291:ILE:HG12	1:B:298:ALA:HB3	1.99	0.43
1:C:326:THR:C	1:C:327:LYS:HG2	2.43	0.43
1:E:93:LEU:HD23	1:E:237:PHE:HD2	1.82	0.43
1:A:240:ASN:HB3	1:A:243:VAL:O	2.18	0.43
1:A:399:LYS:HB3	1:A:399:LYS:HE2	1.72	0.43
1:B:221:ILE:HD12	1:F:217:ILE:HD11	2.01	0.43
1:E:261:ILE:HD13	1:E:274:MET:HB3	2.00	0.43
1:E:507:ARG:HD2	1:E:507:ARG:HA	1.91	0.43
1:B:432:ILE:HD11	1:B:447:VAL:HG22	2.01	0.43
1:A:60:GLU:HG2	1:A:196:LYS:HB3	2.01	0.42
1:A:445:LYS:NZ	1:A:465:LYS:HA	2.34	0.42
1:E:398:SER:HA	1:E:485:SER:O	2.20	0.42
1:F:338:ASP:OD1	1:F:338:ASP:N	2.49	0.42
1:F:30:GLU:OE1	1:F:408:THR:OG1	2.31	0.42
1:A:426:ASN:OD1	1:A:427:LYS:N	2.53	0.42
1:B:140:PHE:CE2	1:B:338:ASP:HA	2.50	0.42
1:D:203:LEU:O	1:D:207:VAL:HG22	2.19	0.42
1:F:261:ILE:HD13	1:F:274:MET:HB3	2.01	0.42
1:A:176:LYS:HD3	1:A:263:ASP:OD2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:LYS:HB3	1:C:399:LYS:HE3	1.70	0.42
1:D:141:LEU:HD12	1:D:142:LEU:H	1.85	0.42
1:E:204:LEU:N	1:E:205:PRO:HD2	2.34	0.42
1:F:507:ARG:HD3	1:F:507:ARG:HA	1.80	0.42
1:D:206:ILE:HD12	1:D:215:PRO:HB3	2.02	0.42
1:F:321:LEU:HD11	1:F:473:PRO:HB3	1.99	0.42
1:F:53:TYR:CE2	1:F:188:LEU:HD12	2.55	0.42
1:B:280:ILE:HG21	1:B:366:PHE:CG	2.55	0.41
1:B:427:LYS:HG3	1:B:448:ASP:OD2	2.20	0.41
1:E:79:ILE:HD13	1:E:79:ILE:HA	1.90	0.41
1:A:96:LEU:HD11	1:A:238:SER:HA	2.02	0.41
1:C:30:GLU:OE2	1:C:408:THR:OG1	2.31	0.41
1:C:166:LYS:HB2	1:C:166:LYS:HE2	1.68	0.41
1:C:395:ILE:HD11	1:C:495:VAL:HG21	2.01	0.41
1:A:56:VAL:HB	1:A:189:THR:HG22	2.02	0.41
1:A:63:ASN:O	1:A:65:LYS:HE3	2.20	0.41
1:D:327:LYS:HE3	1:D:327:LYS:HA	2.02	0.41
1:A:96:LEU:HD13	1:A:237:PHE:HB3	2.01	0.41
1:A:318:THR:O	1:A:339:ARG:NH2	2.54	0.41
1:F:75:LYS:HD3	1:F:215:PRO:O	2.20	0.41
1:A:217:ILE:HD11	1:F:221:ILE:HD12	2.02	0.41
1:B:48:LEU:O	1:B:306:TYR:HA	2.19	0.41
1:D:198:TYR:CD1	1:D:202:GLN:HG3	2.55	0.41
1:D:342:TYR:HD2	1:D:349:VAL:HG11	1.85	0.41
1:E:279:PRO:O	1:E:283:GLN:HG3	2.20	0.41
1:F:368:ASP:OD1	1:F:370:MET:HB3	2.21	0.41
1:A:58:THR:HA	1:A:297:LEU:O	2.20	0.41
1:C:322:CYS:HB2	1:C:417:TYR:CE1	2.55	0.41
1:D:209:LYS:CE	1:D:213:SER:HB3	2.50	0.41
1:F:370:MET:HE3	1:F:370:MET:HB2	1.87	0.41
1:F:410:LEU:HD22	1:F:464:GLY:HA3	2.02	0.41
1:A:167:ILE:HG12	1:A:189:THR:HG21	2.03	0.41
1:A:505:PHE:CD1	1:A:505:PHE:C	2.99	0.41
1:B:56:VAL:HG23	1:B:187:VAL:HG11	2.02	0.41
1:B:246:PRO:HB3	1:B:283:GLN:HA	2.02	0.41
1:C:140:PHE:HB3	1:C:373:LEU:HD11	2.01	0.41
1:C:427:LYS:N	1:C:448:ASP:OD2	2.50	0.41
1:B:415:SER:HB3	1:B:417:TYR:CE2	2.56	0.41
1:D:57:ILE:CD1	1:D:252:LEU:HD13	2.51	0.41
1:E:137:PHE:HZ	1:E:156:LYS:HD3	1.85	0.41
1:A:209:LYS:HE2	1:A:213:SER:OG	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:VAL:N	1:A:279:PRO:HD2	2.36	0.41
1:B:503:LEU:HD23	1:B:503:LEU:HA	1.87	0.41
1:C:260:LEU:O	1:C:264:MET:HG2	2.21	0.41
1:C:73:ASP:OD2	1:C:73:ASP:C	2.64	0.40
1:C:401:ASP:OD2	1:C:417:TYR:HB3	2.21	0.40
1:D:249:THR:HG22	1:D:282:ARG:NH2	2.36	0.40
1:E:407:ILE:HD11	1:E:457:TYR:HB3	2.03	0.40
1:A:484:PRO:HD3	1:A:499:ILE:HG13	2.04	0.40
1:B:375:LEU:HD13	1:B:379:VAL:HG21	2.04	0.40
1:B:499:ILE:O	1:B:503:LEU:HB2	2.22	0.40
1:A:266:ILE:HG13	1:A:271:LYS:HG3	2.03	0.40
1:D:398:SER:HA	1:D:485:SER:O	2.22	0.40
1:F:210:GLN:CD	1:F:210:GLN:N	2.78	0.40
1:F:352:PHE:CE1	1:F:372:SER:HB3	2.56	0.40

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	447/522 (86%)	434 (97%)	13 (3%)	0	100	100
1	B	451/522 (86%)	426 (94%)	25 (6%)	0	100	100
1	C	447/522 (86%)	434 (97%)	13 (3%)	0	100	100
1	D	448/522 (86%)	434 (97%)	14 (3%)	0	100	100
1	E	450/522 (86%)	440 (98%)	10 (2%)	0	100	100
1	F	451/522 (86%)	437 (97%)	14 (3%)	0	100	100
All	All	2694/3132 (86%)	2605 (97%)	89 (3%)	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	411/463 (89%)	402 (98%)	9 (2%)	47	76
1	B	412/463 (89%)	398 (97%)	14 (3%)	32	63
1	C	411/463 (89%)	402 (98%)	9 (2%)	47	76
1	D	412/463 (89%)	405 (98%)	7 (2%)	56	81
1	E	414/463 (89%)	409 (99%)	5 (1%)	67	87
1	F	415/463 (90%)	402 (97%)	13 (3%)	35	66
All	All	2475/2778 (89%)	2418 (98%)	57 (2%)	45	75

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	LEU
1	A	212	CYS
1	A	213	SER
1	A	238	SER
1	A	254	ASN
1	A	402	VAL
1	A	410	LEU
1	A	423	THR
1	A	432	ILE
1	B	69	CYS
1	B	99	SER
1	B	141	LEU
1	B	253	THR
1	B	319	SER
1	B	324	THR
1	B	338	ASP
1	B	381	LEU
1	B	384	VAL
1	B	420	THR
1	B	425	SER
1	B	432	ILE
1	B	503	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	509	SER
1	C	91	THR
1	C	206	ILE
1	C	207	VAL
1	C	212	CYS
1	C	220	VAL
1	C	244	THR
1	C	459	VAL
1	C	466	SER
1	C	485	SER
1	D	142	LEU
1	D	164	VAL
1	D	197	ASN
1	D	203	LEU
1	D	212	CYS
1	D	267	THR
1	D	420	THR
1	E	166	LYS
1	E	188	LEU
1	E	206	ILE
1	E	212	CYS
1	E	335	THR
1	F	35	SER
1	F	141	LEU
1	F	152	VAL
1	F	212	CYS
1	F	213	SER
1	F	214	ILE
1	F	249	THR
1	F	267	THR
1	F	295	GLU
1	F	296	VAL
1	F	410	LEU
1	F	423	THR
1	F	427	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	388	ASN
1	A	460	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	183	ASN
1	B	283	GLN
1	C	26	GLN
1	C	81	GLN
1	C	202	GLN
1	C	345	ASN
1	C	437	ASN
1	C	454	ASN
1	D	27	ASN
1	D	283	GLN
1	D	460	ASN
1	E	26	GLN
1	E	165	ASN
1	E	361	GLN
1	E	460	ASN
1	E	462	GLN
1	F	202	GLN
1	F	276	ASN
1	F	283	GLN
1	F	354	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 ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

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, 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	451/522 (86%)	-0.24	8 (1%) 67 62	16, 40, 83, 122	0
1	B	455/522 (87%)	-0.04	19 (4%) 41 36	19, 44, 96, 126	0
1	C	451/522 (86%)	-0.22	18 (3%) 43 37	17, 39, 91, 140	0
1	D	452/522 (86%)	-0.11	19 (4%) 41 36	17, 43, 91, 154	0
1	E	454/522 (86%)	-0.02	20 (4%) 39 34	18, 42, 94, 131	0
1	F	455/522 (87%)	-0.10	16 (3%) 47 42	18, 44, 90, 142	0
All	All	2718/3132 (86%)	-0.12	100 (3%) 45 40	16, 42, 92, 154	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	140	PHE	5.5
1	F	515	ALA	5.0
1	B	517	GLY	4.7
1	B	141	LEU	4.6
1	F	144	VAL	4.5
1	C	488	PHE	4.5
1	C	515	ALA	4.4
1	D	401	ASP	4.4
1	B	26	GLN	4.3
1	E	401	ASP	4.2
1	A	211	SER	4.1
1	E	482	VAL	4.1
1	D	139	PRO	4.1
1	E	515	ALA	4.1
1	C	517	GLY	4.0
1	D	326	THR	4.0
1	E	517	GLY	3.9
1	B	516	ILE	3.9
1	F	338	ASP	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	326	THR	3.6
1	F	99	SER	3.5
1	C	516	ILE	3.4
1	B	488	PHE	3.4
1	C	329	GLY	3.4
1	F	326	THR	3.4
1	F	516	ILE	3.3
1	D	488	PHE	3.3
1	E	399	LYS	3.3
1	D	68	LYS	3.1
1	B	515	ALA	3.1
1	A	488	PHE	3.1
1	E	506	ILE	3.1
1	D	329	GLY	3.1
1	F	328	GLU	3.0
1	E	504	ALA	3.0
1	B	486	ASP	3.0
1	E	418	GLY	3.0
1	E	419	LYS	2.9
1	F	512	LEU	2.9
1	F	401	ASP	2.8
1	F	142	LEU	2.8
1	B	99	SER	2.7
1	C	388	ASN	2.7
1	E	209	LYS	2.7
1	E	481	LEU	2.7
1	C	356	GLU	2.7
1	B	355	ALA	2.6
1	F	514	SER	2.6
1	C	73	ASP	2.6
1	C	481	LEU	2.6
1	C	355	ALA	2.6
1	A	98	GLN	2.5
1	F	488	PHE	2.5
1	A	172	LEU	2.5
1	E	416	CYS	2.5
1	F	212	CYS	2.5
1	C	505	PHE	2.5
1	C	497	GLU	2.5
1	E	488	PHE	2.5
1	D	141	LEU	2.4
1	E	513	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	327	LYS	2.4
1	B	487	GLU	2.4
1	A	265	PRO	2.4
1	D	98	GLN	2.4
1	D	355	ALA	2.4
1	E	210	GLN	2.4
1	D	515	ALA	2.4
1	B	72	THR	2.3
1	D	328	GLU	2.3
1	F	325	ASN	2.3
1	B	100	GLY	2.3
1	F	70	ASN	2.3
1	C	512	LEU	2.3
1	D	506	ILE	2.3
1	D	327	LYS	2.2
1	C	326	THR	2.2
1	A	355	ALA	2.2
1	E	514	SER	2.2
1	B	497	GLU	2.2
1	E	70	ASN	2.2
1	B	489	ASP	2.2
1	B	206	ILE	2.2
1	C	26	GLN	2.2
1	D	399	LYS	2.2
1	C	325	ASN	2.1
1	A	212	CYS	2.1
1	D	478	TYR	2.1
1	E	26	GLN	2.1
1	A	506	ILE	2.1
1	B	101	GLY	2.1
1	C	508	LYS	2.1
1	D	514	SER	2.1
1	D	482	VAL	2.1
1	B	208	ASN	2.1
1	B	212	CYS	2.0
1	D	294	GLU	2.0
1	B	183	ASN	2.0
1	C	401	ASP	2.0
1	E	505	PHE	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 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.