



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2025 – 02:10 PM JST

PDB ID : 8ZQ7 / pdb\_00008zq7  
Title : Crystal structure of prefusion RSV F protein  
Authors : Huang, Q.; Lang, Q.; Han, X.; 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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

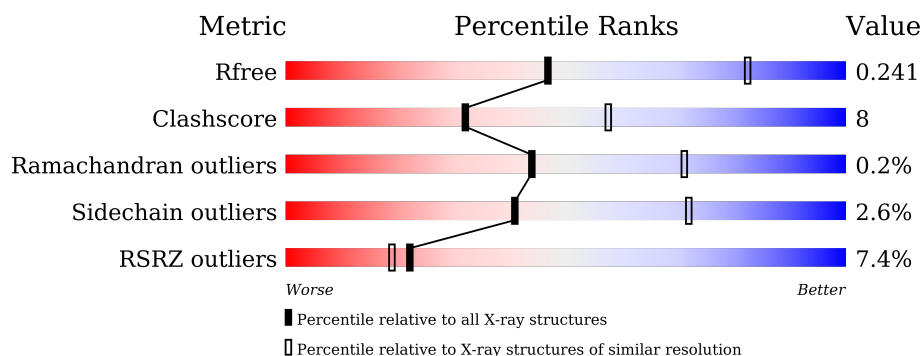
# 1 Overall quality at a glance

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>7%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	522	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	522	<div> <div>8%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	522	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>•</div> <div>13%</div> </div> </div>
1	E	522	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div></div> <div>14%</div> </div> </div>
1	F	522	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21095 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	466	Total	C	N	O	S	0	0	0
			3568	2252	591	704	21			
1	B	459	Total	C	N	O	S	0	0	0
			3531	2233	581	696	21			
1	C	460	Total	C	N	O	S	0	0	0
			3535	2235	582	697	21			
1	D	456	Total	C	N	O	S	0	0	0
			3517	2226	578	692	21			
1	E	451	Total	C	N	O	S	0	0	0
			3474	2193	573	687	21			
1	F	450	Total	C	N	O	S	0	0	0
			3470	2191	572	686	21			

There are 324 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	127	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	216	PRO	ASN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	TYR	-	expression tag	UNP P12568
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	100	GLY	-	linker	UNP P12568
B	101	GLY	-	linker	UNP P12568
B	102	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	216	PRO	ASN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	HIS	-	expression tag	UNP A0A346FJN8
B	547	HIS	-	expression tag	UNP A0A346FJN8
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	100	GLY	-	linker	UNP P12568
C	101	GLY	-	linker	UNP P12568
C	102	GLY	-	linker	UNP P12568
C	103	GLY	-	linker	UNP P12568
C	104	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	141	PRO	LEU	conflict	UNP P12568
C	152	VAL	ILE	conflict	UNP P12568
C	213	SER	ARG	conflict	UNP P12568
C	215	PRO	SER	conflict	UNP P12568
C	216	PRO	ASN	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	100	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	126	GLY	-	linker	UNP P12568
D	127	GLY	-	linker	UNP P12568
D	128	GLY	-	linker	UNP P12568
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	216	PRO	ASN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
E	25	CYS	-	expression tag	UNP P12568
E	67	PRO	ASN	conflict	UNP P12568
E	80	LYS	ASN	conflict	UNP P12568
E	100	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	216	PRO	ASN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	216	PRO	ASN	conflict	UNP P12568
F	279	PRO	GLN	conflict	UNP P12568

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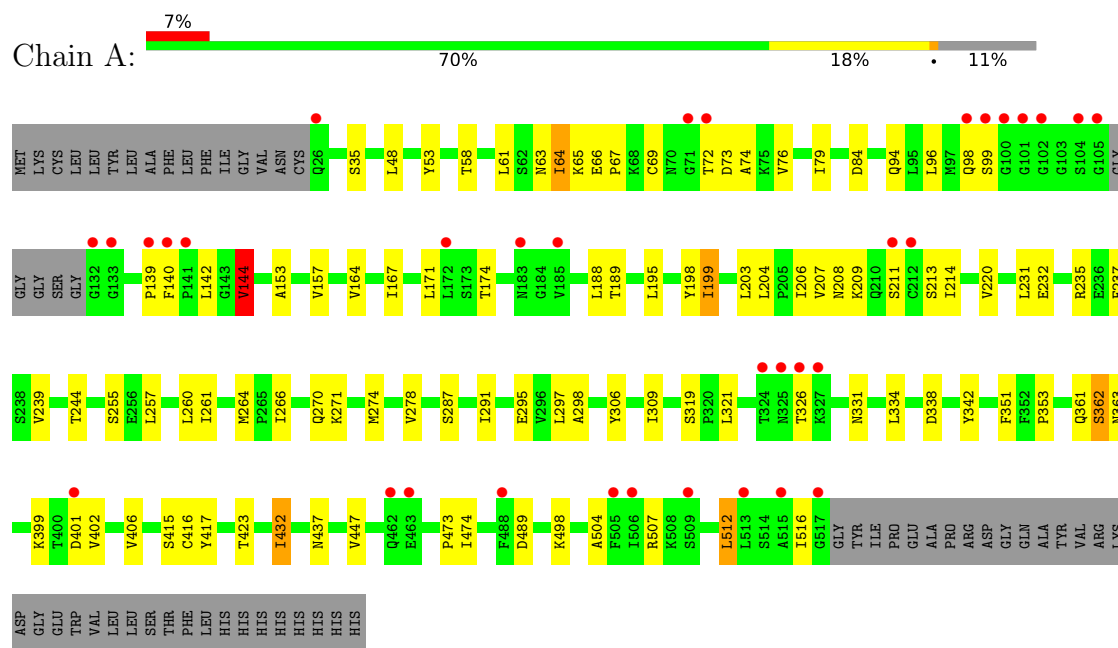
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Chain	Residue	Modelled	Actual	Comment	Reference
F	377	PRO	SER	conflict	UNP P12568
F	514	SER	-	linker	UNP P12568
F	515	ALA	-	linker	UNP P12568
F	516	ILE	-	linker	UNP P12568
F	517	GLY	-	linker	UNP P12568
F	545	HIS	-	expression tag	UNP A0A346FJN8
F	546	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

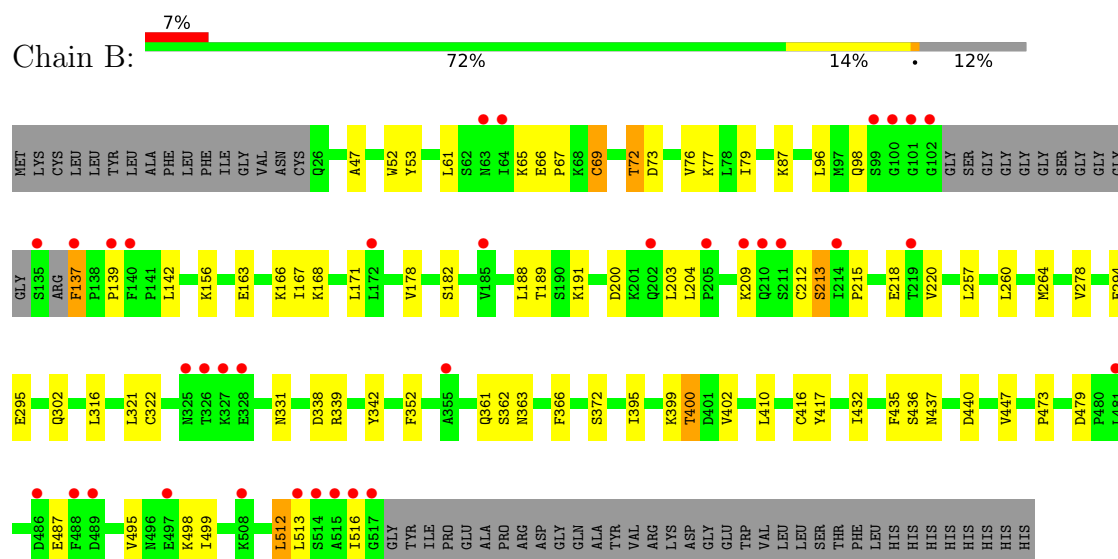
### 3 Residue-property plots [i](#)

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.

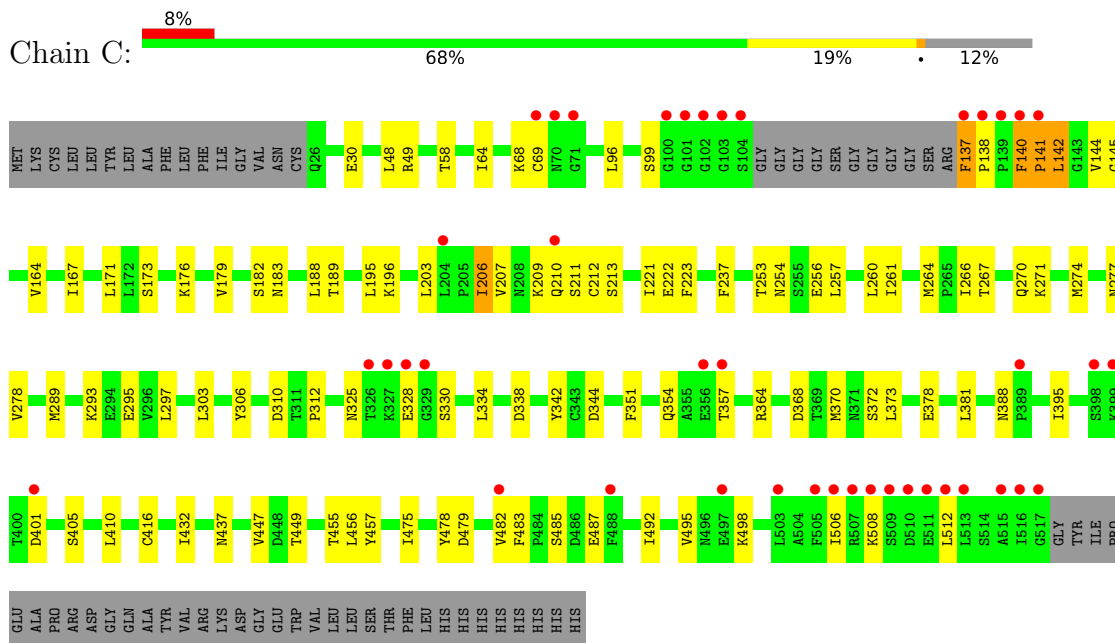
#### • Molecule 1: Fusion glycoprotein F0,Fibritin



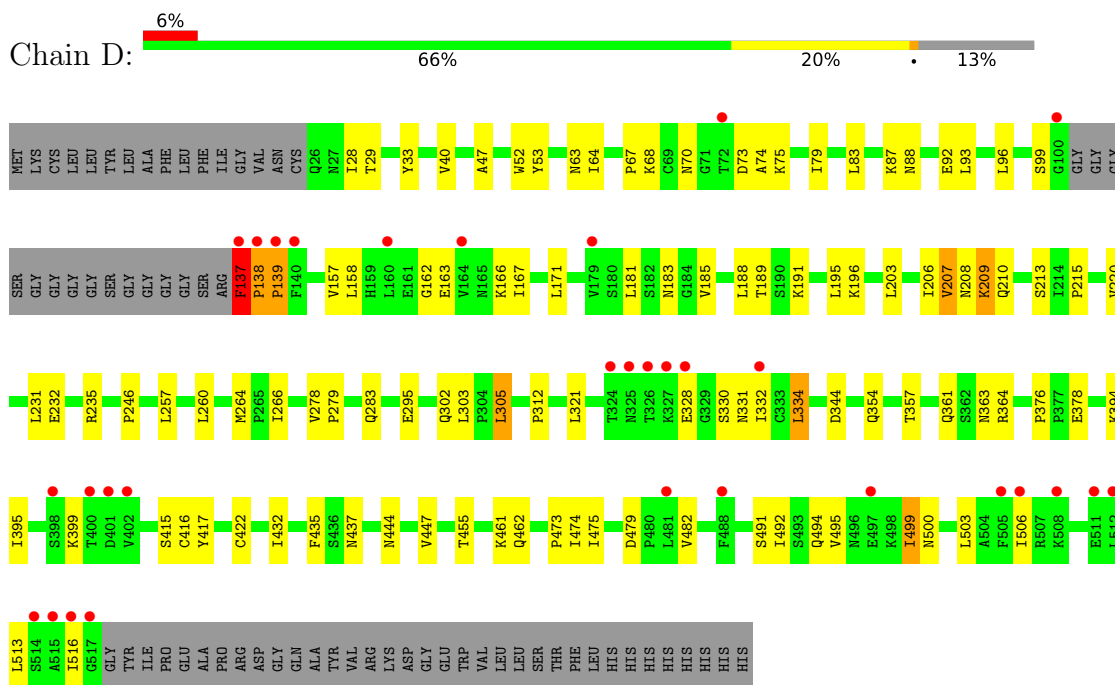
#### • Molecule 1: Fusion glycoprotein F0,Fibritin



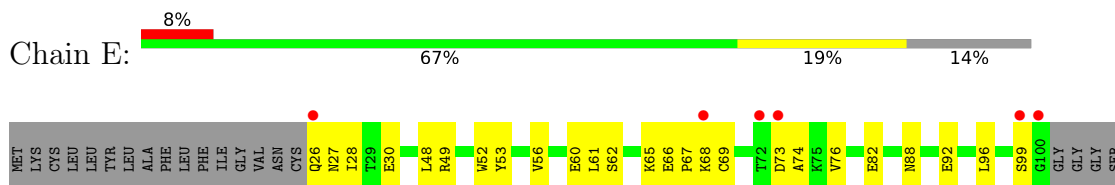
- Molecule 1: Fusion glycoprotein F0,Fibritin

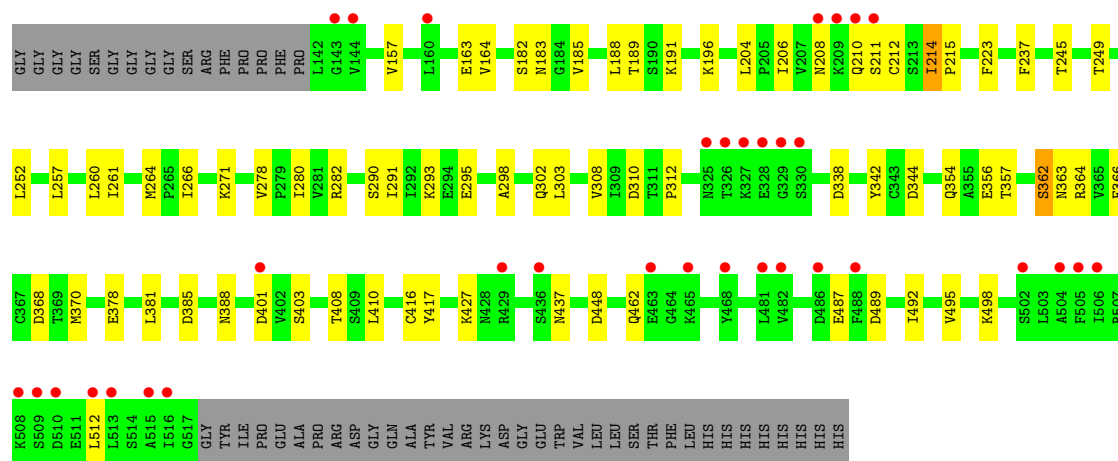


- Molecule 1: Fusion glycoprotein F0,Fibritin

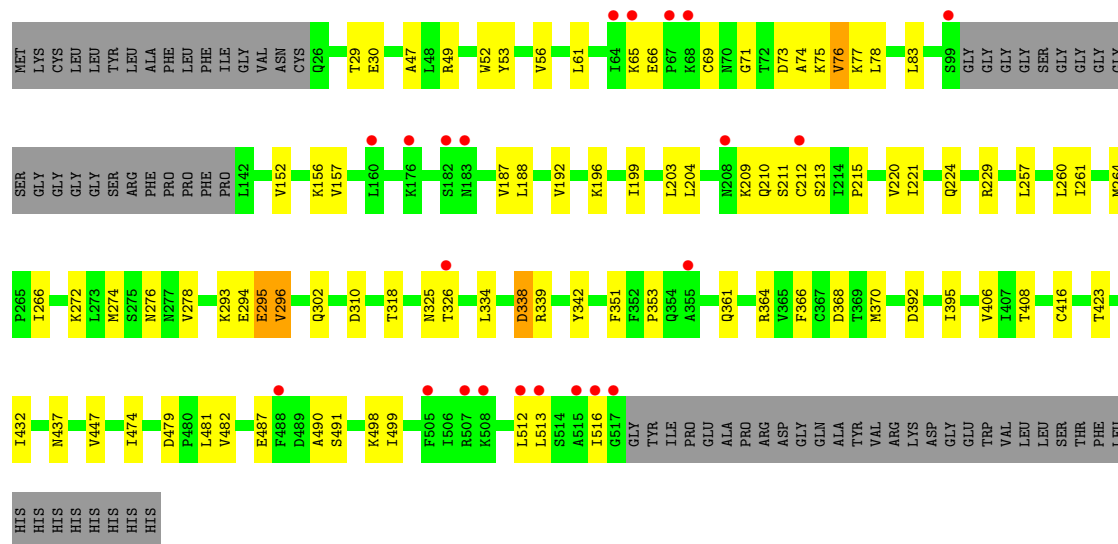


- Molecule 1: Fusion glycoprotein F0,Fibritin





• Molecule 1: Fusion glycoprotein F0,Fibritin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.42Å 168.70Å 190.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	126.35 – 2.77 126.35 – 2.77	Depositor EDS
% Data completeness (in resolution range)	76.7 (126.35-2.77) 76.7 (126.35-2.77)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.207 , 0.242 0.206 , 0.241	Depositor DCC
$R_{free}$ test set	127721 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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	0.30	1/3625 (0.0%)	0.55	3/4915 (0.1%)
1	B	0.25	0/3587	0.63	3/4865 (0.1%)
1	C	0.33	2/3592 (0.1%)	0.57	9/4873 (0.2%)
1	D	0.24	1/3574 (0.0%)	0.49	2/4850 (0.0%)
1	E	0.18	0/3526	0.43	0/4782
1	F	0.20	0/3522	0.46	0/4777
All	All	0.26	4/21426 (0.0%)	0.53	17/29062 (0.1%)

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	2
1	B	0	3
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	PRO	CA-C	-7.59	1.44	1.52
1	C	140	PHE	CA-C	-7.40	1.44	1.53
1	A	139	PRO	CA-C	-6.06	1.45	1.52
1	D	138	PRO	CA-C	-5.82	1.48	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	PHE	CA-C-N	21.84	142.88	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	PHE	C-N-CA	21.84	142.88	120.38
1	C	140	PHE	N-CA-C	-13.47	90.08	109.48
1	C	142	LEU	N-CA-C	-8.62	95.88	109.50
1	A	142	LEU	N-CA-C	7.26	120.12	110.53
1	C	138	PRO	N-CA-C	6.94	117.13	110.47
1	C	277	ASN	CA-C-N	6.61	124.40	120.24
1	C	277	ASN	C-N-CA	6.61	124.40	120.24
1	D	137	PHE	CA-C-N	-6.39	115.00	119.66
1	D	137	PHE	C-N-CA	-6.39	115.00	119.66
1	C	137	PHE	CA-C-N	-6.26	115.09	119.66
1	C	137	PHE	C-N-CA	-6.26	115.09	119.66
1	C	140	PHE	CA-C-N	-6.11	112.89	119.98
1	C	140	PHE	C-N-CA	-6.11	112.89	119.98
1	A	199	ILE	CA-CB-CG1	5.79	120.24	110.40
1	A	144	VAL	N-CA-C	5.39	115.72	108.17
1	B	137	PHE	C-N-CD	-5.12	104.02	125.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ASN	Peptide
1	A	211	SER	Peptide
1	B	137	PHE	Peptide
1	B	400	THR	Peptide
1	B	98	GLN	Peptide
1	C	325	ASN	Peptide
1	E	67	PRO	Peptide
1	F	211	SER	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	3568	0	3607	54	0
1	B	3531	0	3573	51	0
1	C	3535	0	3577	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3517	0	3563	72	0
1	E	3474	0	3524	69	0
1	F	3470	0	3521	48	0
All	All	21095	0	21365	337	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 8.

All (337) 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:209:LYS:NZ	1:B:213:SER:OG	1.95	1.00
1:A:361:GLN:HE21	1:C:99:SER:HA	1.29	0.98
1:D:64:ILE:O	1:D:87:LYS:NZ	2.02	0.90
1:E:310:ASP:OD1	1:E:364:ARG:NH1	2.11	0.83
1:E:26:GLN:HG3	1:E:27:ASN:H	1.46	0.80
1:D:321:LEU:HD11	1:D:473:PRO:HB3	1.65	0.77
1:D:73:ASP:OD1	1:D:74:ALA:N	2.18	0.76
1:E:356:GLU:OE1	1:E:356:GLU:N	2.16	0.75
1:C:310:ASP:OD1	1:C:364:ARG:NH1	2.18	0.75
1:C:270:GLN:NE2	1:C:306:TYR:O	2.20	0.74
1:B:65:LYS:H	1:B:65:LYS:HD3	1.53	0.73
1:F:432:ILE:HD11	1:F:447:VAL:HG22	1.71	0.72
1:D:432:ILE:HD11	1:D:447:VAL:HG22	1.73	0.70
1:C:449:THR:HB	1:C:456:LEU:HD11	1.72	0.70
1:E:48:LEU:HB2	1:E:308:VAL:HB	1.75	0.69
1:C:432:ILE:HD11	1:C:447:VAL:HG22	1.74	0.68
1:A:73:ASP:OD1	1:A:74:ALA:N	2.28	0.67
1:C:479:ASP:HB3	1:C:482:VAL:HG22	1.78	0.66
1:B:209:LYS:HB3	1:B:212:CYS:H	1.61	0.66
1:D:167:ILE:HG23	1:D:189:THR:HG21	1.78	0.66
1:A:264:MET:HE2	1:A:266:ILE:HD13	1.77	0.65
1:A:512:LEU:HD21	1:C:512:LEU:HD21	1.79	0.65
1:E:378:GLU:O	1:E:381:LEU:HB2	1.97	0.64
1:F:487:GLU:HB3	1:F:490:ALA:HB2	1.80	0.64
1:D:264:MET:HE2	1:D:266:ILE:HD13	1.79	0.64
1:F:192:VAL:HB	1:F:229:ARG:HH12	1.62	0.64
1:A:512:LEU:HD13	1:F:512:LEU:HD21	1.81	0.63
1:C:141:PRO:O	1:C:373:LEU:HD21	1.97	0.63
1:E:252:LEU:O	1:E:282:ARG:NH2	2.25	0.63
1:C:260:LEU:HD23	1:C:303:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:HG22	1:B:188:LEU:HD23	1.81	0.63
1:D:171:LEU:HD11	1:D:189:THR:HG22	1.80	0.62
1:A:73:ASP:OD2	1:A:214:ILE:HD13	1.98	0.62
1:A:432:ILE:HD11	1:A:447:VAL:HG22	1.81	0.62
1:B:163:GLU:HA	1:B:166:LYS:HG3	1.81	0.62
1:A:167:ILE:HG23	1:A:189:THR:HG21	1.80	0.62
1:B:495:VAL:O	1:B:499:ILE:HG13	2.00	0.61
1:E:183:ASN:OD1	1:E:185:VAL:HG12	2.01	0.61
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.84	0.60
1:E:264:MET:HE2	1:E:266:ILE:HD13	1.84	0.60
1:D:395:ILE:HD13	1:D:492:ILE:HD12	1.84	0.60
1:F:73:ASP:OD1	1:F:74:ALA:N	2.35	0.59
1:F:264:MET:HE2	1:F:266:ILE:HD13	1.84	0.59
1:D:332:ILE:HG13	1:D:475:ILE:HD11	1.85	0.59
1:E:28:ILE:HG22	1:E:410:LEU:HD11	1.85	0.59
1:E:260:LEU:HD23	1:E:303:LEU:HD11	1.84	0.58
1:B:331:ASN:O	1:B:399:LYS:HG2	2.03	0.58
1:E:53:TYR:OH	1:E:188:LEU:HD23	2.03	0.58
1:A:261:ILE:HG12	1:A:274:MET:HE2	1.85	0.58
1:A:171:LEU:HD11	1:A:189:THR:HG22	1.85	0.58
1:C:30:GLU:HB2	1:C:410:LEU:HD21	1.86	0.58
1:A:270:GLN:HG2	1:A:309:ILE:HD12	1.86	0.57
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.85	0.57
1:C:487:GLU:OE2	1:C:498:LYS:HE2	2.03	0.57
1:E:206:ILE:HD12	1:E:215:PRO:HG3	1.86	0.57
1:E:163:GLU:OE2	1:E:182:SER:HB3	2.04	0.57
1:E:66:GLU:O	1:E:68:LYS:HG2	2.03	0.57
1:F:209:LYS:NZ	1:F:213:SER:H	2.01	0.57
1:F:220:VAL:O	1:F:224:GLN:HG3	2.04	0.57
1:C:145:GLY:HA3	1:C:370:MET:SD	2.45	0.57
1:D:137:PHE:HD1	1:D:138:PRO:HD3	1.70	0.57
1:C:164:VAL:HG21	1:C:293:LYS:HD2	1.86	0.56
1:A:321:LEU:HD11	1:A:473:PRO:HB3	1.86	0.56
1:C:328:GLU:C	1:C:330:SER:H	2.13	0.56
1:E:157:VAL:HG21	1:E:183:ASN:HB3	1.87	0.56
1:E:381:LEU:HD23	1:E:388:ASN:HD22	1.70	0.56
1:D:260:LEU:O	1:D:264:MET:HG3	2.06	0.56
1:E:26:GLN:HG2	1:E:363:ASN:ND2	2.21	0.56
1:F:209:LYS:HZ1	1:F:213:SER:H	1.53	0.56
1:B:167:ILE:HG23	1:B:189:THR:HG21	1.87	0.56
1:E:68:LYS:HB2	1:E:208:ASN:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:HD23	1:D:303:LEU:HD11	1.88	0.55
1:D:67:PRO:HB3	1:D:207:VAL:HG13	1.88	0.55
1:D:88:ASN:O	1:D:92:GLU:HG3	2.06	0.55
1:B:156:LYS:HE3	1:E:462:GLN:HG3	1.87	0.55
1:B:416:CYS:O	1:B:437:ASN:HA	2.07	0.55
1:F:56:VAL:HG23	1:F:187:VAL:HG21	1.88	0.55
1:D:503:LEU:HD23	1:D:506:ILE:HD12	1.89	0.55
1:C:312:PRO:HG2	1:C:344:ASP:OD2	2.06	0.54
1:F:53:TYR:OH	1:F:188:LEU:HD12	2.07	0.54
1:B:400:THR:O	1:B:402:VAL:HG23	2.08	0.54
1:F:310:ASP:OD1	1:F:364:ARG:NH1	2.40	0.54
1:A:291:ILE:HG12	1:A:298:ALA:HB3	1.90	0.54
1:C:167:ILE:HG12	1:C:179:VAL:HG21	1.89	0.54
1:D:139:PRO:HG3	1:D:354:GLN:HE21	1.72	0.54
1:E:73:ASP:HB3	1:E:76:VAL:HG23	1.90	0.54
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.90	0.53
1:C:49:ARG:NH1	1:C:368:ASP:OD1	2.40	0.53
1:B:513:LEU:HA	1:B:516:ILE:HG23	1.91	0.53
1:B:400:THR:HG23	1:D:394:LYS:NZ	2.23	0.53
1:A:206:ILE:HB	1:A:213:SER:HB2	1.91	0.53
1:A:231:LEU:O	1:A:235:ARG:HG3	2.09	0.53
1:D:513:LEU:HD21	1:E:512:LEU:HG	1.92	0.53
1:E:62:SER:HB2	1:E:196:LYS:HA	1.90	0.53
1:A:53:TYR:OH	1:A:188:LEU:HD12	2.08	0.52
1:D:513:LEU:HA	1:D:516:ILE:HG23	1.92	0.52
1:B:260:LEU:O	1:B:264:MET:HG3	2.08	0.52
1:D:334:LEU:HD21	1:D:474:ILE:HD11	1.92	0.52
1:A:406:VAL:HG13	1:C:144:VAL:HB	1.92	0.52
1:D:416:CYS:O	1:D:437:ASN:HA	2.10	0.52
1:F:338:ASP:HB2	1:F:342:TYR:OH	2.10	0.51
1:F:152:VAL:O	1:F:156:LYS:HG2	2.09	0.51
1:C:140:PHE:O	1:C:141:PRO:C	2.51	0.51
1:E:278:VAL:O	1:E:282:ARG:HG3	2.11	0.51
1:E:492:ILE:O	1:E:495:VAL:HG12	2.10	0.51
1:F:338:ASP:OD1	1:F:338:ASP:N	2.30	0.51
1:E:487:GLU:OE2	1:E:498:LYS:HD2	2.11	0.51
1:B:171:LEU:HD13	1:B:191:LYS:HB2	1.93	0.51
1:C:478:TYR:HE2	1:C:495:VAL:HG11	1.76	0.51
1:C:270:GLN:O	1:C:274:MET:HG3	2.12	0.50
1:E:49:ARG:HE	1:E:368:ASP:CG	2.20	0.50
1:E:65:LYS:HB2	1:E:68:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:489:ASP:OD1	1:E:489:ASP:C	2.54	0.50
1:A:58:THR:HA	1:A:297:LEU:O	2.12	0.50
1:B:171:LEU:HD11	1:B:189:THR:HG22	1.94	0.50
1:C:395:ILE:HD13	1:C:492:ILE:HD13	1.94	0.50
1:A:362:SER:OG	1:A:363:ASN:N	2.40	0.50
1:E:354:GLN:HB2	1:E:357:THR:HG23	1.93	0.50
1:E:210:GLN:O	1:E:212:CYS:HA	2.11	0.50
1:A:338:ASP:HB2	1:A:342:TYR:OH	2.11	0.49
1:F:257:LEU:HD23	1:F:278:VAL:HG13	1.94	0.49
1:F:351:PHE:CE2	1:F:353:PRO:HB3	2.47	0.49
1:A:270:GLN:NE2	1:A:306:TYR:O	2.43	0.49
1:C:209:LYS:C	1:C:211:SER:H	2.20	0.49
1:E:362:SER:OG	1:E:363:ASN:N	2.39	0.49
1:F:192:VAL:HB	1:F:229:ARG:NH1	2.27	0.49
1:D:444:ASN:ND2	1:D:462:GLN:O	2.45	0.49
1:A:99:SER:HB2	1:F:361:GLN:OE1	2.13	0.49
1:A:195:LEU:O	1:A:198:TYR:N	2.46	0.49
1:A:144:VAL:HG13	1:F:406:VAL:HG22	1.95	0.49
1:D:513:LEU:HD11	1:E:512:LEU:HD12	1.95	0.49
1:B:72:THR:O	1:B:72:THR:OG1	2.31	0.49
1:D:47:ALA:HB2	1:D:364:ARG:HD2	1.93	0.49
1:A:361:GLN:NE2	1:C:99:SER:HA	2.12	0.49
1:B:512:LEU:CD2	1:E:512:LEU:HD21	2.43	0.49
1:C:266:ILE:HG13	1:C:271:LYS:HG3	1.93	0.49
1:A:73:ASP:HB3	1:A:76:VAL:HG23	1.94	0.49
1:A:203:LEU:O	1:A:207:VAL:HG22	2.12	0.49
1:B:512:LEU:HD22	1:E:512:LEU:HD21	1.94	0.49
1:C:176:LYS:HG3	1:C:188:LEU:HD11	1.94	0.49
1:F:487:GLU:OE2	1:F:498:LYS:NZ	2.43	0.48
1:B:352:PHE:CE1	1:B:372:SER:HB3	2.48	0.48
1:E:60:GLU:OE1	1:E:191:LYS:NZ	2.35	0.48
1:F:75:LYS:HB3	1:F:215:PRO:HG2	1.93	0.48
1:F:513:LEU:O	1:F:516:ILE:HG12	2.14	0.48
1:C:267:THR:HG23	1:C:270:GLN:H	1.77	0.48
1:D:28:ILE:HD11	1:D:363:ASN:HB3	1.94	0.48
1:D:79:ILE:HG13	1:D:215:PRO:HG3	1.96	0.48
1:B:432:ILE:HD11	1:B:447:VAL:HG22	1.94	0.48
1:E:312:PRO:HG2	1:E:344:ASP:OD2	2.12	0.48
1:F:61:LEU:O	1:F:196:LYS:HB2	2.13	0.48
1:B:73:ASP:O	1:B:77:LYS:HG3	2.13	0.48
1:F:199:ILE:O	1:F:204:LEU:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:CYS:O	1:A:437:ASN:HA	2.14	0.48
1:D:232:GLU:CD	1:D:235:ARG:HH11	2.22	0.48
1:E:56:VAL:HB	1:E:189:THR:HG22	1.96	0.48
1:B:218:GLU:OE2	1:D:75:LYS:HE3	2.14	0.48
1:B:400:THR:O	1:B:400:THR:HG22	2.14	0.48
1:C:222:GLU:HG3	1:F:78:LEU:HD21	1.95	0.48
1:B:53:TYR:OH	1:B:188:LEU:HG	2.13	0.48
1:D:331:ASN:O	1:D:399:LYS:HG2	2.14	0.48
1:B:47:ALA:O	1:B:366:PHE:HA	2.14	0.48
1:D:210:GLN:CD	1:D:210:GLN:H	2.22	0.48
1:A:94:GLN:O	1:A:98:GLN:NE2	2.47	0.47
1:C:261:ILE:HG12	1:C:274:MET:HE2	1.96	0.47
1:B:479:ASP:C	1:B:479:ASP:OD1	2.57	0.47
1:A:257:LEU:HD23	1:A:278:VAL:HG13	1.95	0.47
1:B:487:GLU:OE2	1:B:498:LYS:HE2	2.14	0.47
1:D:330:SER:O	1:D:330:SER:OG	2.27	0.47
1:E:261:ILE:HA	1:E:264:MET:HG3	1.96	0.47
1:A:331:ASN:O	1:A:399:LYS:HG2	2.15	0.47
1:B:79:ILE:HG13	1:B:220:VAL:HG22	1.96	0.47
1:F:260:LEU:O	1:F:264:MET:HG3	2.14	0.47
1:D:93:LEU:HD23	1:D:96:LEU:HD12	1.96	0.47
1:E:30:GLU:OE2	1:E:408:THR:OG1	2.30	0.47
1:A:415:SER:HB3	1:A:417:TYR:CE2	2.49	0.47
1:B:79:ILE:HD12	1:B:215:PRO:HG2	1.95	0.47
1:E:416:CYS:O	1:E:437:ASN:HA	2.15	0.47
1:B:200:ASP:HA	1:B:204:LEU:HD12	1.97	0.47
1:D:499:ILE:HG13	1:D:500:ASN:N	2.28	0.47
1:E:73:ASP:OD1	1:E:74:ALA:N	2.48	0.46
1:C:354:GLN:HB2	1:C:357:THR:HG23	1.97	0.46
1:E:381:LEU:HB3	1:E:388:ASN:ND2	2.30	0.46
1:F:52:TRP:CE3	1:F:302:GLN:HG2	2.49	0.46
1:C:416:CYS:O	1:C:437:ASN:HA	2.15	0.46
1:E:280:ILE:HG21	1:E:366:PHE:CG	2.50	0.46
1:E:401:ASP:OD1	1:E:417:TYR:HB3	2.15	0.46
1:A:61:LEU:O	1:A:295:GLU:HB3	2.15	0.46
1:A:79:ILE:HG12	1:A:220:VAL:HG22	1.96	0.46
1:D:479:ASP:HB3	1:D:482:VAL:HG22	1.98	0.46
1:E:61:LEU:O	1:E:295:GLU:HB3	2.15	0.46
1:B:362:SER:OG	1:B:363:ASN:N	2.45	0.46
1:C:261:ILE:HA	1:C:264:MET:HG3	1.97	0.46
1:B:435:PHE:HD2	1:B:440:ASP:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ILE:HD12	1:D:215:PRO:HB3	1.98	0.46
1:D:361:GLN:O	1:D:364:ARG:HB3	2.15	0.46
1:E:82:GLU:HB3	1:E:223:PHE:CE2	2.51	0.46
1:C:378:GLU:O	1:C:381:LEU:HB2	2.16	0.46
1:D:75:LYS:HD2	1:D:215:PRO:O	2.16	0.45
1:E:157:VAL:HG21	1:E:183:ASN:ND2	2.31	0.45
1:E:157:VAL:O	1:E:163:GLU:HG3	2.15	0.45
1:D:376:PRO:HB2	1:D:378:GLU:OE1	2.16	0.45
1:E:26:GLN:HG3	1:E:27:ASN:N	2.22	0.45
1:A:401:ASP:OD1	1:A:417:TYR:HB3	2.17	0.45
1:C:182:SER:OG	1:C:183:ASN:N	2.49	0.45
1:E:96:LEU:CD2	1:E:237:PHE:HB3	2.46	0.45
1:D:209:LYS:NZ	1:D:213:SER:OG	2.48	0.45
1:E:338:ASP:OD1	1:E:338:ASP:N	2.41	0.45
1:D:455:THR:HG23	1:E:370:MET:HA	1.99	0.45
1:F:49:ARG:HE	1:F:368:ASP:CG	2.25	0.45
1:D:246:PRO:HB3	1:D:283:GLN:HA	1.98	0.45
1:F:272:LYS:HE3	1:F:276:ASN:HD21	1.81	0.45
1:A:504:ALA:O	1:A:507:ARG:HB3	2.17	0.45
1:D:181:LEU:HD23	1:D:185:VAL:HG13	1.98	0.45
1:D:495:VAL:O	1:D:499:ILE:HG23	2.16	0.45
1:C:209:LYS:O	1:C:210:GLN:HB3	2.17	0.45
1:D:68:LYS:O	1:D:70:ASN:ND2	2.50	0.45
1:A:195:LEU:HB3	1:A:199:ILE:CD1	2.47	0.45
1:B:52:TRP:CE3	1:B:302:GLN:HG2	2.51	0.45
1:C:221:ILE:HD11	1:F:221:ILE:HD11	1.98	0.44
1:D:183:ASN:OD1	1:D:183:ASN:C	2.59	0.44
1:D:257:LEU:HD23	1:D:278:VAL:HG13	1.99	0.44
1:C:257:LEU:HD23	1:C:278:VAL:HG13	1.99	0.44
1:F:209:LYS:HZ1	1:F:213:SER:N	2.14	0.44
1:F:479:ASP:OD1	1:F:481:LEU:HD12	2.17	0.44
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.92	0.44
1:C:381:LEU:HB3	1:C:388:ASN:ND2	2.32	0.44
1:D:157:VAL:HG21	1:D:183:ASN:ND2	2.32	0.44
1:D:162:GLY:O	1:D:166:LYS:HG3	2.17	0.44
1:E:68:LYS:HD2	1:E:208:ASN:ND2	2.32	0.44
1:B:513:LEU:HD23	1:B:516:ILE:HG21	1.99	0.44
1:F:325:ASN:HA	1:F:326:THR:HA	1.66	0.44
1:D:137:PHE:CD1	1:D:138:PRO:HD3	2.51	0.44
1:E:356:GLU:H	1:E:356:GLU:CD	2.18	0.44
1:A:63:ASN:HB2	1:A:295:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:THR:OG1	1:C:256:GLU:HG3	2.17	0.44
1:A:334:LEU:HD11	1:A:474:ILE:HD11	1.99	0.43
1:C:338:ASP:OD1	1:C:338:ASP:N	2.37	0.43
1:D:422:CYS:HB2	1:D:435:PHE:HB2	2.00	0.43
1:E:385:ASP:OD1	1:E:388:ASN:N	2.50	0.43
1:D:196:LYS:NZ	1:D:295:GLU:OE1	2.48	0.43
1:D:415:SER:HB3	1:D:417:TYR:CE2	2.53	0.43
1:B:87:LYS:HD2	1:B:87:LYS:HA	1.69	0.43
1:E:214:ILE:HA	1:E:215:PRO:HD3	1.82	0.43
1:A:266:ILE:HG13	1:A:271:LYS:HG3	2.00	0.43
1:C:58:THR:HA	1:C:297:LEU:O	2.19	0.43
1:C:203:LEU:HD21	1:C:223:PHE:CD2	2.54	0.43
1:D:208:ASN:O	1:D:209:LYS:HG3	2.18	0.43
1:A:351:PHE:CE2	1:A:353:PRO:HB3	2.54	0.43
1:B:73:ASP:HB3	1:B:76:VAL:HG23	2.00	0.43
1:D:79:ILE:HG12	1:D:220:VAL:HG22	2.00	0.43
1:D:279:PRO:O	1:D:283:GLN:HG3	2.19	0.43
1:C:351:PHE:O	1:C:372:SER:HA	2.19	0.42
1:D:461:LYS:HA	1:D:461:LYS:HD2	1.82	0.42
1:E:257:LEU:HD23	1:E:278:VAL:HG13	2.01	0.42
1:A:232:GLU:OE2	1:A:235:ARG:NH1	2.52	0.42
1:C:338:ASP:HB2	1:C:342:TYR:OH	2.19	0.42
1:A:79:ILE:HD12	1:A:203:LEU:HD11	2.02	0.42
1:A:195:LEU:HB3	1:A:199:ILE:HD12	2.01	0.42
1:B:96:LEU:HD23	1:B:96:LEU:HA	1.88	0.42
1:C:48:LEU:O	1:C:306:TYR:HA	2.19	0.42
1:E:338:ASP:HB2	1:E:342:TYR:OH	2.20	0.42
1:F:47:ALA:O	1:F:366:PHE:HA	2.19	0.42
1:A:489:ASP:OD1	1:A:489:ASP:C	2.61	0.42
1:B:61:LEU:O	1:B:295:GLU:HB3	2.20	0.42
1:E:249:THR:HA	1:E:282:ARG:NH2	2.35	0.42
1:F:261:ILE:HG12	1:F:274:MET:HE2	2.00	0.42
1:B:69:CYS:HB2	1:B:212:CYS:HB3	1.89	0.42
1:D:33:TYR:HE2	1:D:40:VAL:HG23	1.83	0.42
1:C:96:LEU:HD13	1:C:237:PHE:HB3	2.00	0.42
1:D:171:LEU:HD13	1:D:191:LYS:HB2	2.02	0.42
1:F:61:LEU:O	1:F:295:GLU:HB3	2.19	0.42
1:F:293:LYS:O	1:F:296:VAL:HG12	2.19	0.42
1:F:334:LEU:HD21	1:F:474:ILE:HD11	2.02	0.42
1:B:338:ASP:HB2	1:B:342:TYR:OH	2.19	0.42
1:D:53:TYR:HB2	1:D:305:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:O	1:A:157:VAL:HG23	2.20	0.42
1:C:237:PHE:CE2	1:C:289:MET:HB2	2.54	0.42
1:E:291:ILE:HD12	1:E:293:LYS:HG2	2.01	0.42
1:C:69:CYS:HB3	1:C:207:VAL:O	2.20	0.42
1:A:48:LEU:O	1:A:306:TYR:HA	2.19	0.41
1:B:168:LYS:NZ	1:B:294:GLU:O	2.51	0.41
1:C:483:PHE:HD2	1:C:485:SER:HB3	1.85	0.41
1:D:231:LEU:O	1:D:235:ARG:HG3	2.20	0.41
1:E:164:VAL:HG21	1:E:293:LYS:HD3	2.02	0.41
1:B:513:LEU:O	1:B:516:ILE:HG12	2.20	0.41
1:D:163:GLU:HA	1:D:166:LYS:HD2	2.03	0.41
1:C:508:LYS:O	1:C:512:LEU:HB3	2.20	0.41
1:E:88:ASN:O	1:E:92:GLU:HG3	2.20	0.41
1:F:71:GLY:HA3	1:F:76:VAL:HG11	2.02	0.41
1:A:63:ASN:O	1:A:64:ILE:O	2.39	0.41
1:C:68:LYS:HA	1:C:68:LYS:HD3	1.90	0.41
1:C:171:LEU:HD11	1:C:189:THR:HG22	2.02	0.41
1:E:52:TRP:CE3	1:E:302:GLN:HG2	2.56	0.41
1:A:244:THR:OG1	1:A:287:SER:HB3	2.21	0.41
1:B:322:CYS:HB2	1:B:417:TYR:CZ	2.55	0.41
1:B:316:LEU:HD23	1:B:339:ARG:HA	2.02	0.41
1:C:206:ILE:HG23	1:C:213:SER:O	2.20	0.41
1:C:405:SER:HB3	1:C:457:TYR:CE2	2.55	0.41
1:E:266:ILE:HG13	1:E:271:LYS:HG3	2.02	0.41
1:F:30:GLU:OE2	1:F:408:THR:OG1	2.28	0.41
1:A:512:LEU:O	1:A:516:ILE:HG23	2.21	0.41
1:B:79:ILE:HD12	1:B:215:PRO:CG	2.51	0.41
1:D:196:LYS:HZ3	1:D:295:GLU:CD	2.29	0.41
1:E:290:SER:HB3	1:E:298:ALA:O	2.21	0.41
1:A:96:LEU:HD13	1:A:237:PHE:HB3	2.01	0.41
1:C:167:ILE:HG23	1:C:189:THR:HG21	2.02	0.41
1:D:158:LEU:HD23	1:D:158:LEU:HA	1.80	0.41
1:E:68:LYS:HZ2	1:E:204:LEU:HD11	1.85	0.41
1:E:427:LYS:HB3	1:E:448:ASP:OD2	2.20	0.41
1:A:260:LEU:O	1:A:264:MET:HG3	2.21	0.41
1:C:267:THR:HG22	1:C:270:GLN:OE1	2.21	0.41
1:F:318:THR:HG23	1:F:339:ARG:HB3	2.03	0.41
1:F:392:ASP:OD2	1:F:491:SER:OG	2.32	0.41
1:B:361:GLN:NE2	1:D:99:SER:O	2.54	0.41
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.92	0.41
1:C:196:LYS:HD2	1:C:295:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:LEU:HD23	1:D:195:LEU:HA	1.87	0.41
1:D:513:LEU:O	1:D:516:ILE:HG12	2.21	0.41
1:F:83:LEU:HD23	1:F:83:LEU:HA	1.85	0.41
1:C:334:LEU:HB3	1:C:475:ILE:HD13	2.04	0.40
1:D:491:SER:OG	1:D:494:GLN:HG3	2.21	0.40
1:B:395:ILE:HD11	1:B:495:VAL:HG21	2.03	0.40
1:E:26:GLN:HG2	1:E:363:ASN:HD22	1.84	0.40
1:F:65:LYS:HG3	1:F:66:GLU:N	2.35	0.40
1:D:52:TRP:CE3	1:D:302:GLN:HG2	2.56	0.40
1:E:69:CYS:HB2	1:E:211:SER:HB3	2.03	0.40
1:A:164:VAL:HG22	1:A:291:ILE:HD12	2.02	0.40
1:C:506:ILE:HD13	1:C:506:ILE:HA	1.88	0.40
1:D:312:PRO:HG2	1:D:344:ASP:OD2	2.21	0.40
1:B:257:LEU:HD23	1:B:278:VAL:HG13	2.03	0.40
1:C:455:THR:HG23	1:F:370:MET:HA	2.04	0.40
1:D:63:ASN:HB2	1:D:295:GLU:OE2	2.22	0.40
1:D:83:LEU:HD23	1:D:83:LEU:HA	1.89	0.40
1:D:183:ASN:OD1	1:D:185:VAL:HG12	2.22	0.40
1:F:416:CYS:O	1:F:437:ASN:HA	2.22	0.40
1:F:482:VAL:O	1:F:499:ILE:HG12	2.21	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	462/522 (88%)	435 (94%)	26 (6%)	1 (0%)	44 71
1	B	454/522 (87%)	433 (95%)	20 (4%)	1 (0%)	44 71
1	C	456/522 (87%)	426 (93%)	29 (6%)	1 (0%)	44 71
1	D	452/522 (87%)	432 (96%)	18 (4%)	2 (0%)	30 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	447/522 (86%)	424 (95%)	23 (5%)	0	100	100
1	F	446/522 (85%)	424 (95%)	22 (5%)	0	100	100
All	All	2717/3132 (87%)	2574 (95%)	138 (5%)	5 (0%)	44	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	B	139	PRO
1	C	64	ILE
1	D	328	GLU
1	D	139	PRO

### 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	418/463 (90%)	398 (95%)	20 (5%)	21	50
1	B	416/463 (90%)	407 (98%)	9 (2%)	47	76
1	C	416/463 (90%)	410 (99%)	6 (1%)	62	85
1	D	415/463 (90%)	405 (98%)	10 (2%)	44	74
1	E	410/463 (89%)	405 (99%)	5 (1%)	67	87
1	F	410/463 (89%)	396 (97%)	14 (3%)	32	63
All	All	2485/2778 (90%)	2421 (97%)	64 (3%)	41	72

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	65	LYS
1	A	69	CYS
1	A	72	THR
1	A	84	ASP

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Mol	Chain	Res	Type
1	A	140	PHE
1	A	144	VAL
1	A	174	THR
1	A	204	LEU
1	A	209	LYS
1	A	239	VAL
1	A	255	SER
1	A	319	SER
1	A	326	THR
1	A	362	SER
1	A	402	VAL
1	A	423	THR
1	A	432	ILE
1	A	498	LYS
1	A	512	LEU
1	B	69	CYS
1	B	72	THR
1	B	142	LEU
1	B	182	SER
1	B	203	LEU
1	B	213	SER
1	B	410	LEU
1	B	436	SER
1	B	512	LEU
1	C	137	PHE
1	C	173	SER
1	C	206	ILE
1	C	212	CYS
1	C	254	ASN
1	C	401	ASP
1	D	29	THR
1	D	137	PHE
1	D	188	LEU
1	D	203	LEU
1	D	207	VAL
1	D	209	LYS
1	D	305	LEU
1	D	334	LEU
1	D	357	THR
1	D	499	ILE
1	E	99	SER
1	E	214	ILE

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Mol	Chain	Res	Type
1	E	245	THR
1	E	362	SER
1	E	403	SER
1	F	29	THR
1	F	69	CYS
1	F	76	VAL
1	F	77	LYS
1	F	157	VAL
1	F	203	LEU
1	F	210	GLN
1	F	212	CYS
1	F	294	GLU
1	F	295	GLU
1	F	296	VAL
1	F	338	ASP
1	F	395	ILE
1	F	423	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	283	GLN
1	A	354	GLN
1	A	361	GLN
1	A	371	ASN
1	B	27	ASN
1	B	165	ASN
1	B	227	ASN
1	B	361	GLN
1	B	380	ASN
1	C	317	HIS
1	C	361	GLN
1	D	70	ASN
1	D	165	ASN
1	D	371	ASN
1	E	70	ASN
1	E	208	ASN
1	E	225	GLN
1	E	276	ASN
1	E	317	HIS
1	E	361	GLN

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Mol	Chain	Res	Type
1	F	70	ASN
1	F	224	GLN
1	F	240	ASN
1	F	268	ASN
1	F	276	ASN
1	F	325	ASN
1	F	501	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 ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

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	466/522 (89%)	0.41	34 (7%)	22	19	38, 56, 98, 122	0
1	B	459/522 (87%)	0.37	35 (7%)	21	18	34, 54, 100, 127	0
1	C	460/522 (88%)	0.45	41 (8%)	17	14	38, 58, 102, 130	0
1	D	456/522 (87%)	0.41	31 (6%)	25	21	37, 58, 100, 131	0
1	E	451/522 (86%)	0.49	40 (8%)	17	14	36, 59, 97, 132	0
1	F	450/522 (86%)	0.36	22 (4%)	36	31	37, 57, 97, 138	0
All	All	2742/3132 (87%)	0.42	203 (7%)	22	19	34, 57, 100, 138	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	PHE	6.4
1	C	517	GLY	6.2
1	E	329	GLY	6.0
1	A	488	PHE	6.0
1	F	516	ILE	5.9
1	C	139	PRO	5.9
1	B	101	GLY	5.7
1	A	517	GLY	5.5
1	A	132	GLY	5.2
1	F	517	GLY	5.2
1	E	100	GLY	5.1
1	B	488	PHE	5.0
1	A	105	GLY	5.0
1	B	516	ILE	5.0
1	B	326	THR	5.0
1	C	104	SER	4.9
1	C	488	PHE	4.8
1	B	140	PHE	4.8
1	A	140	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	488	PHE	4.6
1	B	135	SER	4.5
1	B	517	GLY	4.5
1	D	517	GLY	4.5
1	C	137	PHE	4.4
1	C	515	ALA	4.2
1	F	355	ALA	4.2
1	C	100	GLY	4.2
1	E	210	GLN	4.1
1	D	137	PHE	4.1
1	B	211	SER	4.1
1	D	516	ILE	4.0
1	A	102	GLY	4.0
1	B	513	LEU	4.0
1	F	508	LYS	3.9
1	D	100	GLY	3.9
1	D	140	PHE	3.9
1	C	516	ILE	3.9
1	D	515	ALA	3.9
1	E	509	SER	3.8
1	B	63	ASN	3.8
1	E	327	LYS	3.7
1	C	482	VAL	3.7
1	E	513	LEU	3.7
1	A	211	SER	3.6
1	C	508	LYS	3.5
1	D	326	THR	3.5
1	C	398	SER	3.4
1	B	210	GLN	3.4
1	E	26	GLN	3.4
1	E	505	PHE	3.3
1	F	488	PHE	3.3
1	E	330	SER	3.3
1	C	505	PHE	3.3
1	E	143	GLY	3.3
1	E	488	PHE	3.3
1	C	399	LYS	3.2
1	F	326	THR	3.2
1	E	512	LEU	3.2
1	F	513	LEU	3.2
1	B	137	PHE	3.2
1	D	324	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	400	THR	3.1
1	A	104	SER	3.1
1	E	515	ALA	3.1
1	F	505	PHE	3.1
1	E	326	THR	3.1
1	C	507	ARG	3.1
1	D	508	LYS	3.1
1	E	72	THR	3.0
1	F	67	PRO	3.0
1	B	481	LEU	3.0
1	B	185	VAL	3.0
1	E	482	VAL	3.0
1	D	401	ASP	3.0
1	A	183	ASN	3.0
1	C	513	LEU	3.0
1	F	512	LEU	3.0
1	F	212	CYS	3.0
1	D	512	LEU	2.9
1	A	172	LEU	2.9
1	B	209	LYS	2.9
1	A	462	GLN	2.9
1	B	325	ASN	2.9
1	F	208	ASN	2.9
1	C	101	GLY	2.9
1	B	172	LEU	2.9
1	B	489	ASP	2.8
1	B	64	ILE	2.8
1	D	328	GLU	2.8
1	B	328	GLU	2.8
1	A	139	PRO	2.8
1	D	506	ILE	2.8
1	E	328	GLU	2.8
1	D	138	PRO	2.8
1	C	512	LEU	2.8
1	A	133	GLY	2.8
1	B	515	ALA	2.7
1	C	210	GLN	2.7
1	F	182	SER	2.7
1	E	468	TYR	2.7
1	A	506	ILE	2.7
1	A	101	GLY	2.7
1	D	164	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	209	LYS	2.7
1	B	486	ASP	2.7
1	E	144	VAL	2.7
1	A	513	LEU	2.7
1	E	99	SER	2.7
1	C	102	GLY	2.7
1	C	510	ASP	2.6
1	E	325	ASN	2.6
1	B	497	GLU	2.6
1	E	508	LYS	2.6
1	A	141	PRO	2.6
1	C	329	GLY	2.6
1	A	99	SER	2.6
1	E	463	GLU	2.6
1	D	325	ASN	2.6
1	C	103	GLY	2.6
1	C	356	GLU	2.6
1	E	401	ASP	2.6
1	B	327	LYS	2.5
1	F	65	LYS	2.5
1	F	515	ALA	2.5
1	E	68	LYS	2.5
1	C	328	GLU	2.5
1	B	202	GLN	2.5
1	A	326	THR	2.5
1	D	481	LEU	2.5
1	C	141	PRO	2.5
1	E	504	ALA	2.5
1	A	327	LYS	2.5
1	D	327	LYS	2.5
1	A	71	GLY	2.5
1	A	72	THR	2.5
1	B	508	LYS	2.5
1	C	327	LYS	2.5
1	C	401	ASP	2.5
1	E	486	ASP	2.5
1	E	160	LEU	2.4
1	D	505	PHE	2.4
1	B	355	ALA	2.4
1	C	326	THR	2.4
1	E	516	ILE	2.4
1	E	481	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	139	PRO	2.4
1	A	509	SER	2.4
1	B	99	SER	2.4
1	A	463	GLU	2.3
1	A	26	GLN	2.3
1	D	398	SER	2.3
1	A	100	GLY	2.3
1	D	160	LEU	2.3
1	F	160	LEU	2.3
1	B	100	GLY	2.3
1	A	324	THR	2.3
1	A	401	ASP	2.3
1	A	98	GLN	2.3
1	B	214	ILE	2.3
1	C	506	ILE	2.3
1	E	436	SER	2.3
1	F	183	ASN	2.2
1	C	389	PRO	2.2
1	C	69	CYS	2.2
1	D	179	VAL	2.2
1	B	102	GLY	2.2
1	F	99	SER	2.2
1	A	325	ASN	2.2
1	E	429	ARG	2.2
1	C	70	ASN	2.2
1	E	510	ASP	2.2
1	C	204	LEU	2.2
1	A	505	PHE	2.1
1	E	465	LYS	2.1
1	E	506	ILE	2.1
1	A	515	ALA	2.1
1	B	205	PRO	2.1
1	D	139	PRO	2.1
1	E	211	SER	2.1
1	D	402	VAL	2.1
1	E	502	SER	2.1
1	F	176	LYS	2.1
1	F	64	ILE	2.1
1	C	503	LEU	2.1
1	F	507	ARG	2.1
1	C	497	GLU	2.1
1	D	511	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	357	THR	2.1
1	B	514	SER	2.1
1	C	509	SER	2.1
1	C	138	PRO	2.0
1	A	212	CYS	2.0
1	F	68	LYS	2.0
1	D	72	THR	2.0
1	D	514	SER	2.0
1	E	208	ASN	2.0
1	C	71	GLY	2.0
1	C	511	GLU	2.0
1	D	497	GLU	2.0
1	B	219	THR	2.0
1	D	332	ILE	2.0
1	A	185	VAL	2.0
1	E	73	ASP	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.