



# wwPDB EM Model Validation Summary Report ⓘ

Mar 25, 2020 – 10:38 AM EDT

PDB ID : 6V6D  
EMDB ID : EMD-21071  
Title : Cryo-EM structure of human pannexin 1  
Authors : Deng, Z.; He, Z.; Yuan, P.  
Deposited on : 2019-12-05  
Resolution : 3.77 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.8



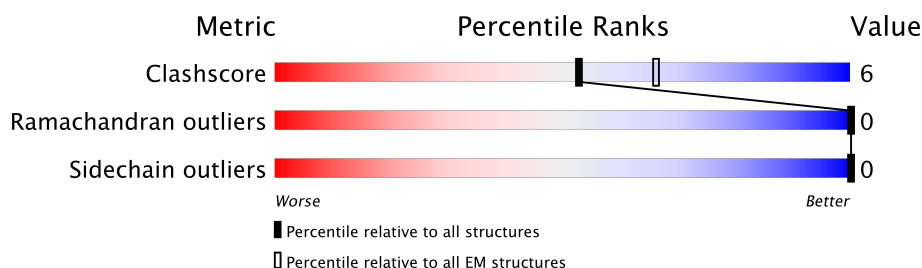
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.77 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	435	41% 7% 52%
1	B	435	41% 7% 52%
1	C	435	41% 7% 52%
1	D	435	41% 7% 52%
1	E	435	41% 7% 52%
1	F	435	41% 7% 52%
1	G	435	41% 7% 52%



## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11739 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Pannexin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	209	Total	C	N	O	S	0	0
			1677	1132	254	282	9		
1	B	209	Total	C	N	O	S	0	0
			1677	1132	254	282	9		
1	C	209	Total	C	N	O	S	0	0
			1677	1132	254	282	9		
1	D	209	Total	C	N	O	S	0	0
			1677	1132	254	282	9		
1	E	209	Total	C	N	O	S	0	0
			1677	1132	254	282	9		
1	F	209	Total	C	N	O	S	0	0
			1677	1132	254	282	9		
1	G	209	Total	C	N	O	S	0	0
			1677	1132	254	282	9		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	SER	-	expression tag	UNP Q96RD7
A	428	ASN	-	expression tag	UNP Q96RD7
A	429	SER	-	expression tag	UNP Q96RD7
A	430	LEU	-	expression tag	UNP Q96RD7
A	431	GLU	-	expression tag	UNP Q96RD7
A	432	VAL	-	expression tag	UNP Q96RD7
A	433	LEU	-	expression tag	UNP Q96RD7
A	434	PHE	-	expression tag	UNP Q96RD7
A	435	GLN	-	expression tag	UNP Q96RD7
B	427	SER	-	expression tag	UNP Q96RD7
B	428	ASN	-	expression tag	UNP Q96RD7
B	429	SER	-	expression tag	UNP Q96RD7
B	430	LEU	-	expression tag	UNP Q96RD7
B	431	GLU	-	expression tag	UNP Q96RD7
B	432	VAL	-	expression tag	UNP Q96RD7
B	433	LEU	-	expression tag	UNP Q96RD7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	434	PHE	-	expression tag	UNP Q96RD7
B	435	GLN	-	expression tag	UNP Q96RD7
C	427	SER	-	expression tag	UNP Q96RD7
C	428	ASN	-	expression tag	UNP Q96RD7
C	429	SER	-	expression tag	UNP Q96RD7
C	430	LEU	-	expression tag	UNP Q96RD7
C	431	GLU	-	expression tag	UNP Q96RD7
C	432	VAL	-	expression tag	UNP Q96RD7
C	433	LEU	-	expression tag	UNP Q96RD7
C	434	PHE	-	expression tag	UNP Q96RD7
C	435	GLN	-	expression tag	UNP Q96RD7
D	427	SER	-	expression tag	UNP Q96RD7
D	428	ASN	-	expression tag	UNP Q96RD7
D	429	SER	-	expression tag	UNP Q96RD7
D	430	LEU	-	expression tag	UNP Q96RD7
D	431	GLU	-	expression tag	UNP Q96RD7
D	432	VAL	-	expression tag	UNP Q96RD7
D	433	LEU	-	expression tag	UNP Q96RD7
D	434	PHE	-	expression tag	UNP Q96RD7
D	435	GLN	-	expression tag	UNP Q96RD7
E	427	SER	-	expression tag	UNP Q96RD7
E	428	ASN	-	expression tag	UNP Q96RD7
E	429	SER	-	expression tag	UNP Q96RD7
E	430	LEU	-	expression tag	UNP Q96RD7
E	431	GLU	-	expression tag	UNP Q96RD7
E	432	VAL	-	expression tag	UNP Q96RD7
E	433	LEU	-	expression tag	UNP Q96RD7
E	434	PHE	-	expression tag	UNP Q96RD7
E	435	GLN	-	expression tag	UNP Q96RD7
F	427	SER	-	expression tag	UNP Q96RD7
F	428	ASN	-	expression tag	UNP Q96RD7
F	429	SER	-	expression tag	UNP Q96RD7
F	430	LEU	-	expression tag	UNP Q96RD7
F	431	GLU	-	expression tag	UNP Q96RD7
F	432	VAL	-	expression tag	UNP Q96RD7
F	433	LEU	-	expression tag	UNP Q96RD7
F	434	PHE	-	expression tag	UNP Q96RD7
F	435	GLN	-	expression tag	UNP Q96RD7
G	427	SER	-	expression tag	UNP Q96RD7
G	428	ASN	-	expression tag	UNP Q96RD7
G	429	SER	-	expression tag	UNP Q96RD7
G	430	LEU	-	expression tag	UNP Q96RD7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	431	GLU	-	expression tag	UNP Q96RD7
G	432	VAL	-	expression tag	UNP Q96RD7
G	433	LEU	-	expression tag	UNP Q96RD7
G	434	PHE	-	expression tag	UNP Q96RD7
G	435	GLN	-	expression tag	UNP Q96RD7

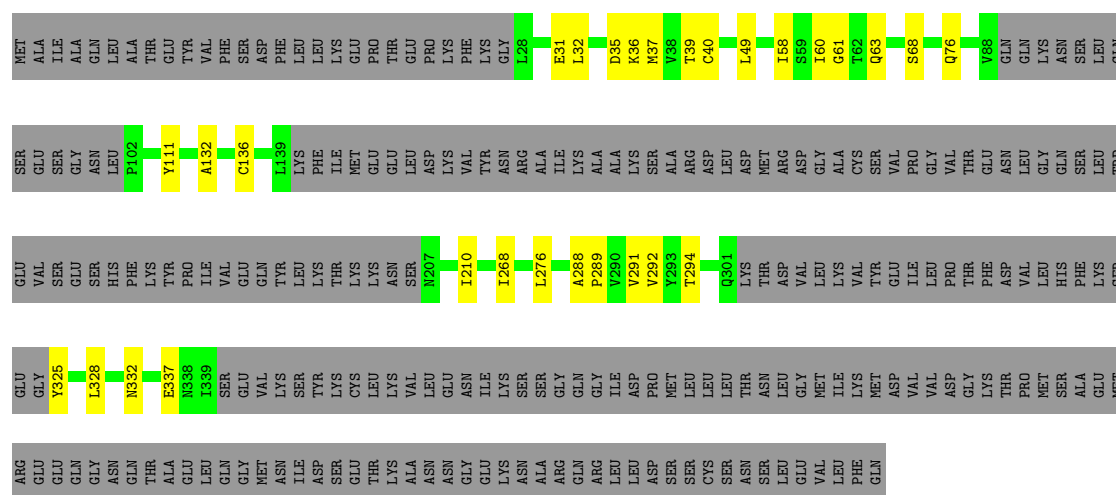


### 3 Residue-property plots

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

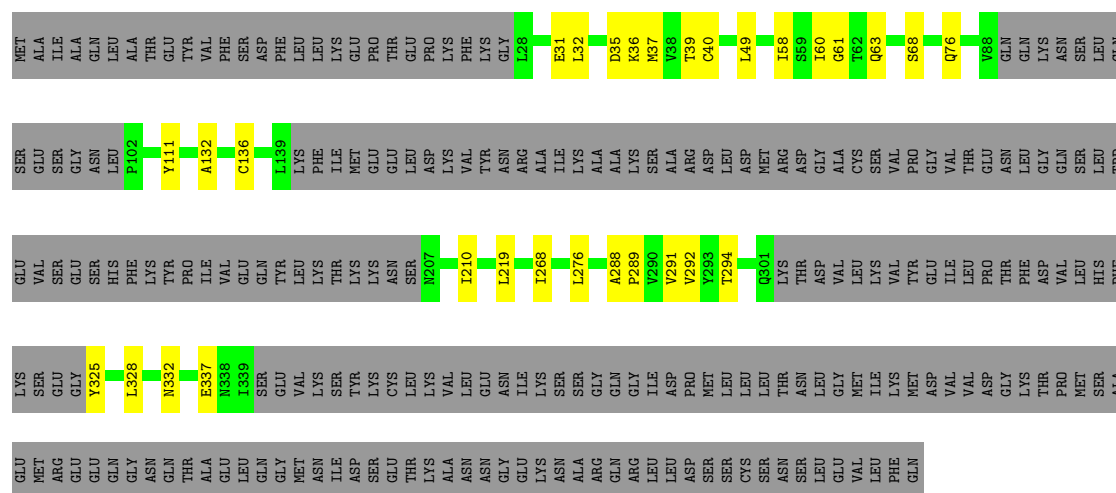
#### • Molecule 1: Pannexin-1

Chain A: 



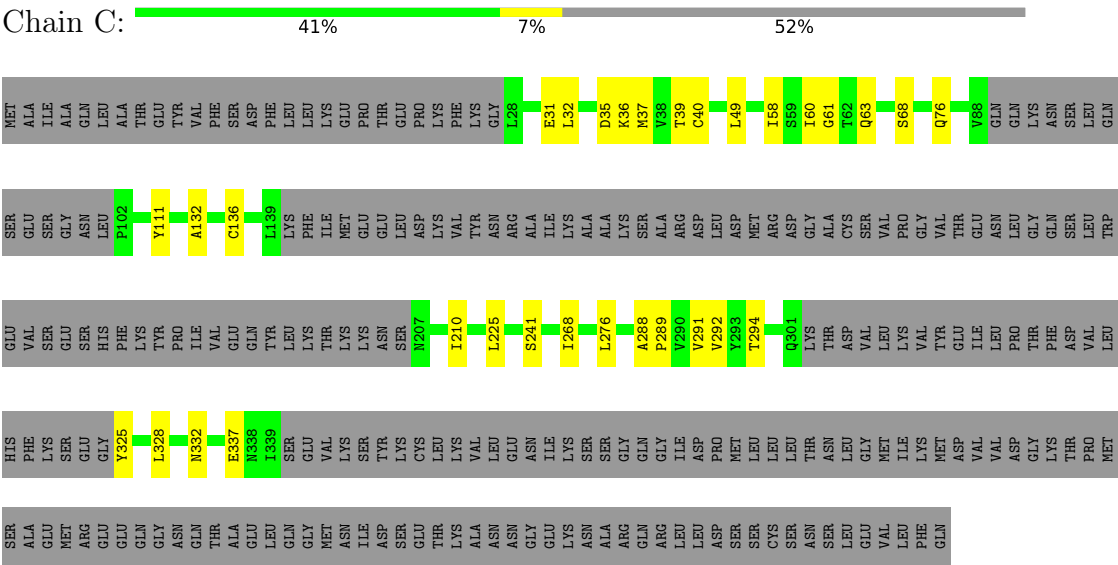
#### • Molecule 1: Pannexin-1

Chain B: 

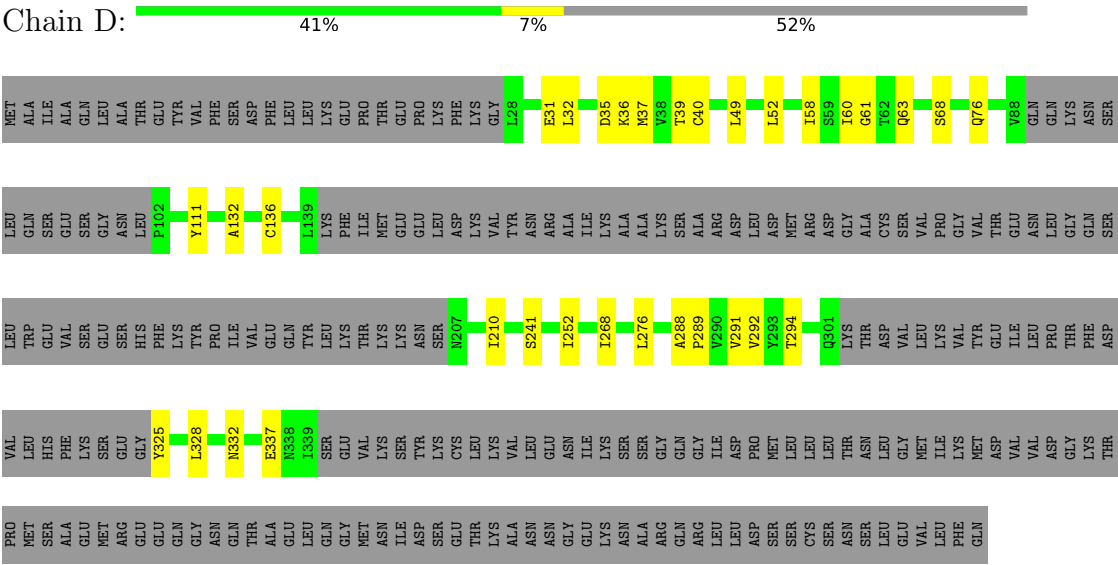


#### • Molecule 1: Pannexin-1

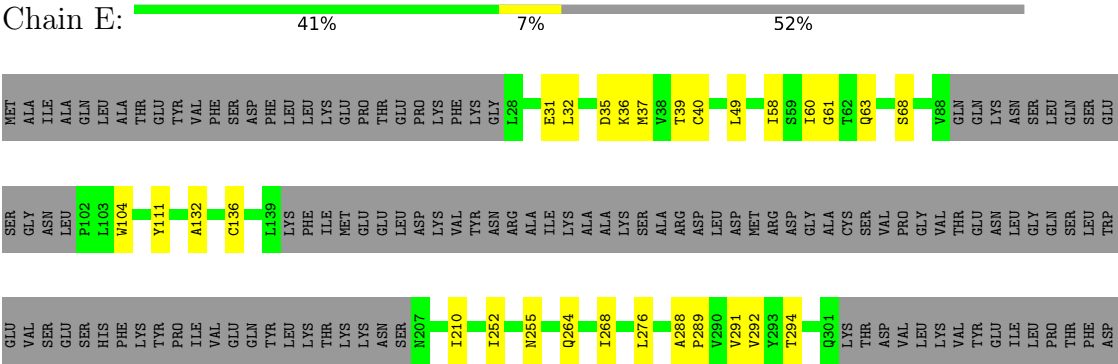




● Molecule 1: Pannexin-1



● Molecule 1: Pannexin-1





VAL  
LEU  
PHE  
LYS  
SER  
GLU  
GLY  
Y325  
L328  
N332  
E337  
N338  
I339  
SER  
GLU  
VAL  
LYS  
LYS  
SER  
TYR  
LYS  
CYS  
LEU  
LYS  
VAL  
LEU  
GLU  
ASN  
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ASP  
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LEU  
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ASP  
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ASP  
GLY  
LYS  
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ARG  
GLU  
GLU  
GLN  
GLY  
ASN  
GLN  
THR  
ALA  
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LEU  
LEU  
GLN  
MET  
GLY  
MET  
ASN  
ILE  
SER  
ASP  
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ALA  
ASN  
GLY  
GLU  
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ASN  
ALA  
D35  
K36  
M37  
V38  
T39  
C40  
L49  
I58  
S59  
I60  
G61  
T62  
Q63  
V68  
GLN  
GLN  
LYS  
ASN  
SER  
SER  
GLN  
SER  
GLU  
SER  
THR  
GLN

● Molecule 1: Pannexin-1

Chain F: 41% 7% 52%

MET  
ALA  
ILE  
ALA  
GLN  
LEU  
ALA  
THR  
GLU  
THR  
TYR  
VAL  
PHE  
SER  
ASP  
PHE  
LEU  
LEU  
LYS  
GLU  
PRO  
THR  
ASN  
GLU  
VAL  
GLU  
PRO  
TYR  
LYS  
PHE  
LYS  
GLY  
L28  
E31  
L32  
D35  
K36  
M37  
V38  
T39  
C40  
L49  
I58  
S59  
I60  
G61  
T62  
Q63  
V68  
GLN  
GLN  
LYS  
ASN  
SER  
SER  
GLN  
SER  
GLU  
SER  
THR  
GLN

ASN  
LEU  
P102  
I103  
W104  
Y111  
A132  
C136  
L139  
LYS  
PHE  
ILE  
MET  
GLU  
GLU  
LEU  
LEU  
ASP  
LYS  
VAL  
VAL  
ASN  
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ALA  
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LYS  
ALA  
LYS  
SER  
SER  
ALA  
GLN  
A288  
K36  
P289  
V290  
V291  
V292  
T293  
Q301  
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LEU  
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GLN  
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VAL

SER  
GLU  
HIS  
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TYR  
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TYR  
LEU  
LYS  
LYS  
SER  
ASN  
SER  
T207  
I210  
I252  
Q264  
I268  
L275  
L276  
A288  
P289  
V290  
V291  
V292  
T293  
Q301  
LYS  
THR  
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PHE  
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GLY  
Y325  
L328  
N332  
E337  
N338  
I339  
SER  
GLU  
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VAL  
LYS  
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SER  
GLY  
GLN  
A288  
K36  
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V290  
V291  
V292  
T293  
Q301  
LYS  
THR  
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THR  
ALA  
GLU  
LEU  
GLN  
MET  
ASN  
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ASP  
SER  
GLU  
THR  
LYS  
ALA  
ASN  
ASN  
GLY  
GLU  
LYS  
ALA  
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ALA  
ARG  
GLN  
ARG  
LEU  
LEU  
ASP  
SER  
CYS  
SER  
ASN  
SER  
LEU  
GLU  
VAL  
LEU  
PHE  
GLN

● Molecule 1: Pannexin-1

Chain G: 41% 7% 52%

MET  
ALA  
ILE  
ALA  
GLN  
LEU  
ALA  
THR  
GLU  
THR  
TYR  
VAL  
PHE  
SER  
ASP  
PHE  
LEU  
LEU  
LYS  
GLU  
PRO  
THR  
ASN  
GLY  
L28  
E31  
L32  
D35  
K36  
M37  
V38  
T39  
C40  
L49  
I58  
S59  
I60  
G61  
T62  
Q63  
Q76  
V68  
GLN  
GLN  
LYS  
ASN  
SER  
LEU  
GLN  
SER  
GLU

SER  
GLY  
ASN  
P102  
Y111  
A132  
C136  
L139  
LYS  
PHE  
ILE  
MET  
GLU  
GLU  
LEU  
LYS  
LYS  
SER  
ASN  
SER  
T207  
I210  
I252  
Q264  
I268  
L275  
L276  
A288  
P289  
V290  
V291  
V292  
T293  
T294  
Q301  
LYS  
THR  
ASP  
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TYR  
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T207  
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L276  
A288  
P289  
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SER  
GLY  
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Y325  
L328  
N332  
E337  
N338  
I339  
SER  
GLU  
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ASN  
GLY  
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A288  
K36  
P289  
V290  
V291  
V292  
T293  
T294  
Q301  
LYS  
THR  
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ASP  
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MET  
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GLY  
MET  
ASN  
ILE  
SER  
ASP  
SER  
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THR  
LYS  
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ALA  
ASN  
ASN  
GLY  
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ASN  
ALA  
ARG  
GLN  
ARG  
ILE  
LEU  
LEU  
ASP  
SER  
SER  
CYS  
SER  
SER  
SER  
LEU  
GLY  
VAL  
PHE  
GLN



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	15796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	62	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/1720	0.51	0/2346
1	B	0.33	0/1720	0.51	0/2346
1	C	0.33	0/1720	0.51	0/2346
1	D	0.33	0/1720	0.51	0/2346
1	E	0.33	0/1720	0.51	0/2346
1	F	0.33	0/1720	0.51	0/2346
1	G	0.33	0/1720	0.51	0/2346
All	All	0.33	0/12040	0.51	0/16422

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1677	0	1732	24	0
1	B	1677	0	1732	25	0
1	C	1677	0	1732	26	0
1	D	1677	0	1732	26	0
1	E	1677	0	1732	27	0
1	F	1677	0	1732	25	0
1	G	1677	0	1732	24	0
All	All	11739	0	12124	145	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.

The worst 5 of 145 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:E:111:TYR:OH	1:F:58:ILE:HG21	1.72	0.89
1:F:111:TYR:OH	1:G:58:ILE:HG21	1.72	0.88
1:C:111:TYR:OH	1:D:58:ILE:HG21	1.77	0.84
1:A:58:ILE:HG21	1:G:111:TYR:OH	1.77	0.83
1:D:111:TYR:OH	1:E:58:ILE:HG21	1.78	0.83

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 PDB entries followed by that with respect to all EM entries.

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	201/435 (46%)	197 (98%)	4 (2%)	0	100	100
1	B	201/435 (46%)	197 (98%)	4 (2%)	0	100	100
1	C	201/435 (46%)	197 (98%)	4 (2%)	0	100	100
1	D	201/435 (46%)	197 (98%)	4 (2%)	0	100	100
1	E	201/435 (46%)	197 (98%)	4 (2%)	0	100	100
1	F	201/435 (46%)	197 (98%)	4 (2%)	0	100	100
1	G	201/435 (46%)	197 (98%)	4 (2%)	0	100	100
All	All	1407/3045 (46%)	1379 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	189/390 (48%)	189 (100%)	0	100	100
1	B	189/390 (48%)	189 (100%)	0	100	100
1	C	189/390 (48%)	189 (100%)	0	100	100
1	D	189/390 (48%)	189 (100%)	0	100	100
1	E	189/390 (48%)	189 (100%)	0	100	100
1	F	189/390 (48%)	189 (100%)	0	100	100
1	G	189/390 (48%)	189 (100%)	0	100	100
All	All	1323/2730 (48%)	1323 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	106	HIS
1	D	332	ASN
1	F	332	ASN
1	C	332	ASN
1	F	106	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.