



Full wwPDB EM Model Validation 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 Full wwPDB EM Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

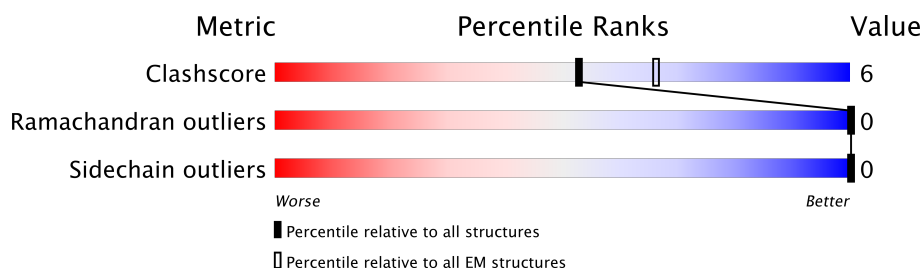
1 Overall quality at a glance

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 ≥ 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 1677	C 1132	N 254	O 282	S 9	0	0
1	B	209	Total 1677	C 1132	N 254	O 282	S 9	0	0
1	C	209	Total 1677	C 1132	N 254	O 282	S 9	0	0
1	D	209	Total 1677	C 1132	N 254	O 282	S 9	0	0
1	E	209	Total 1677	C 1132	N 254	O 282	S 9	0	0
1	F	209	Total 1677	C 1132	N 254	O 282	S 9	0	0
1	G	209	Total 1677	C 1132	N 254	O 282	S 9	0	0

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

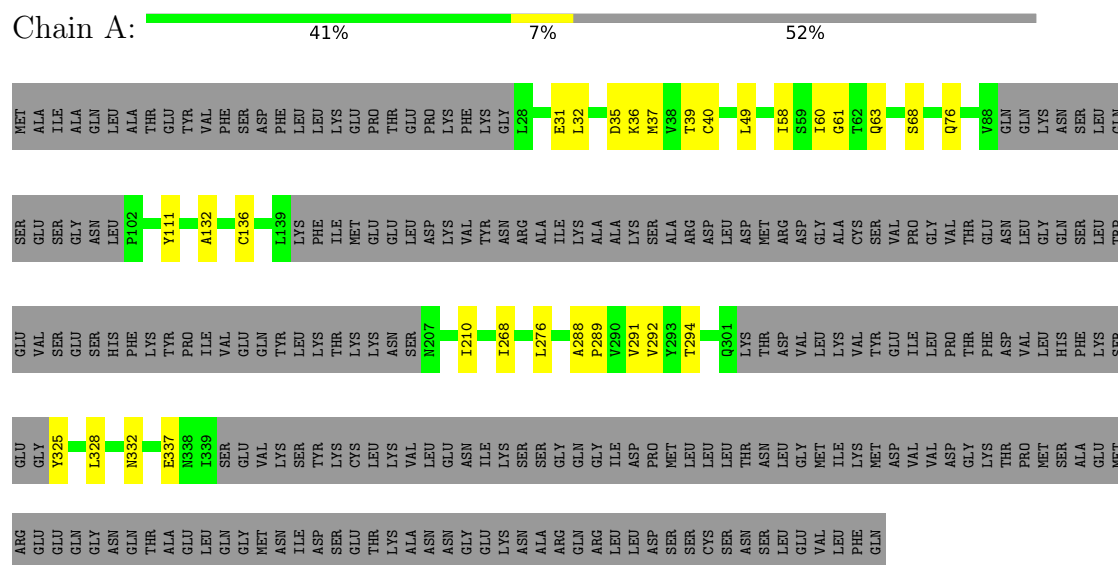
Continued from previous page...

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

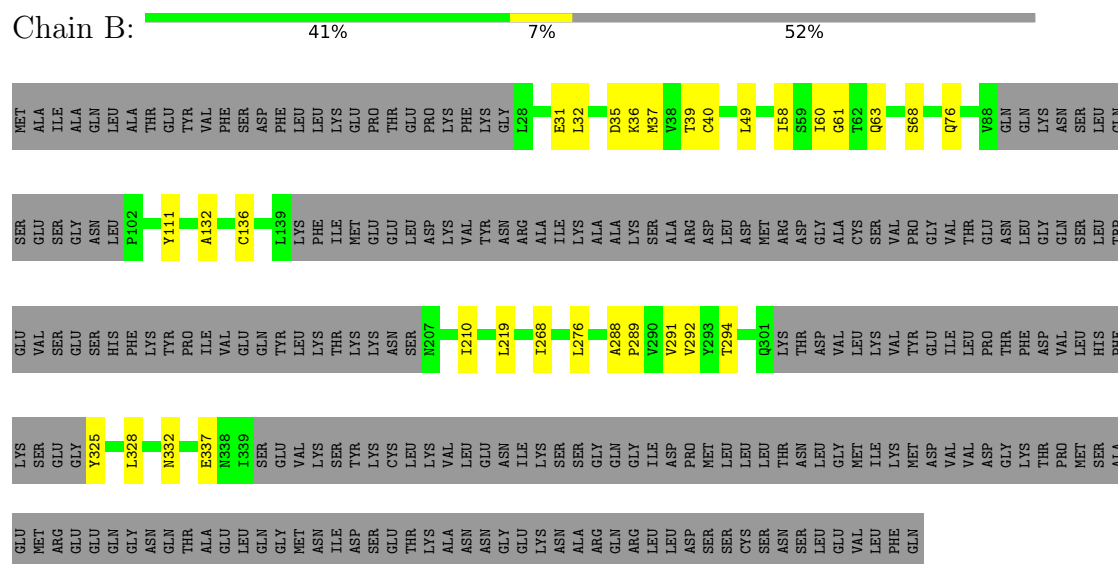
3 Residue-property plots

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

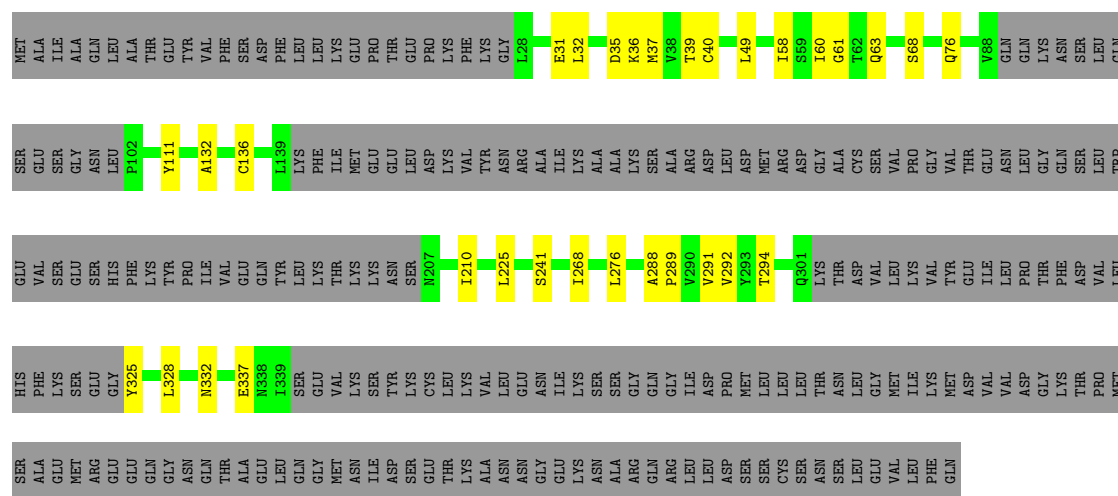


• Molecule 1: Pannexin-1



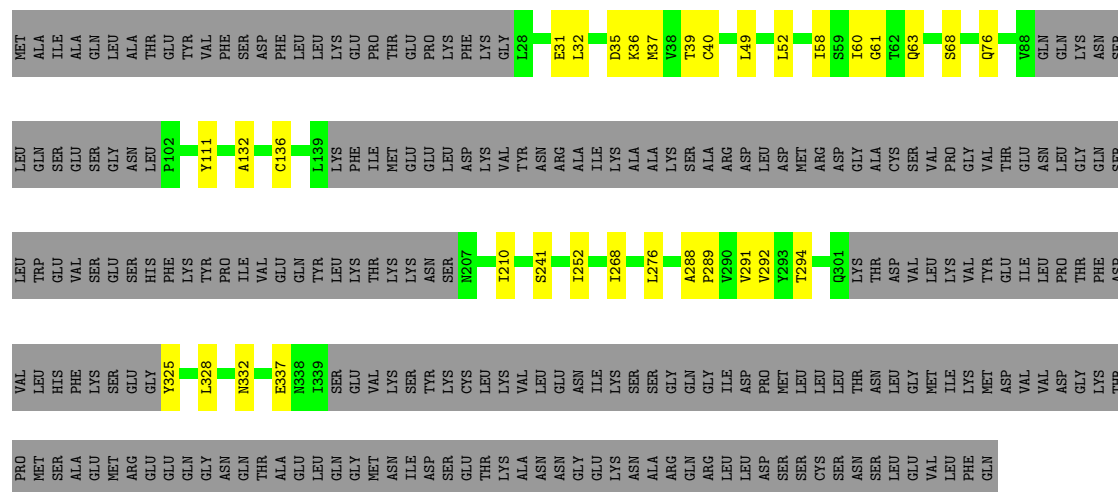
• Molecule 1: Pannexin-1

Chain C:  41% 7% 52%




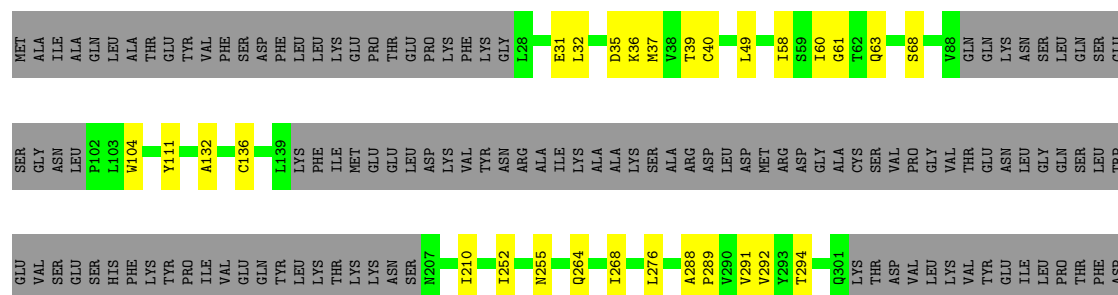
• Molecule 1: Pannexin-1

Chain D:  41% 7% 52%



• Molecule 1: Pannexin-1

Chain E:  41% 7% 52%



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
ILE
LYS
SER
SER
GLY
GLN
GLY
ILE
ASP
PRO
MET
SER
LEU
LEU
LEU
THR
LEU
GLY
MET
ILE
LYS
MET
ASP
VAL
ASP
GLY
LYS
THR

PRO
MET
SER
ALA
GLU
MET
ARG
GLU
GLY
GLN
ASN
GLN
THR
ALA
GLU
LEU
GLN
MET
GLY
MET
ASN
ILE
SER
ASP
PRO
TYR
LYS
SER
GLU
THR
LYS
ALA
ASN
GLY
GLU
LYS
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
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
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
TYR
ASN
ARG
ALA
ILE
LYS
ALA
LYS
SER
SER
ALA
GLN
A288
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

SER
GLU
HIS
PHE
LYS
TYR
PRO
ILE
VAL
GLU
GLN
TYR
LEU
LYS
LYS
SER
ASN
SER
T207
I210
I252
Q264
I268
L275
L276
A288
P289
V290
V291
V292
T293
Q301
LYS
THR
ASP
VAL
LEU
LYS
VAL
TYR
GLU
ILE
LEU
PRO
PHE
ASP
VAL
HIS

PHE
LYS
GLU
GLY
Y325
L328
N332
E337
N338
I339
SER
GLU
SER
VAL
LYS
LYS
SER
TYR
LYS
CYS
LEU
LYS
VAL
LEU
LYS
VAL
LEU
GLY
THR
ILE
MET
ASN
ILE
ASP
SER
SER
GLU
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

ALA
GLU
MET
ARG
GLU
GLY
GLN
GLY
ASN
GLN
THR
ALA
GLU
LEU
GLN
SER
ASN
ILE
ASP
SER
SER
GLU
THR
THR
LYS
ALA
ASN
ASN
GLY
GLU
LYS
ALA
ASN
ALA
ARG
GLN
ARG
LEU
LEU
ASP
SER
CYS
SER
ASN
SER
LEU
GLU
VAL
PHE
GLN

● Molecule 1: Pannexin-1

Chain G: 41% 7% 52%

MET
ALA
ILE
ALA
GLN
LEU
ALA
THR
GLU
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
V68
GLN
GLN
LYS
ASN
SER
SER
GLU
SER
THR
GLN

SER
GLY
ASN
LEU
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
Q301
LYS
THR
ASP
VAL
LEU
LYS
VAL
TYR
GLU
ILE
LEU
PRO
PHE
ASP
VAL
HIS
LYS

SER
GLU
HIS
PHE
LYS
TYR
PRO
ILE
VAL
GLU
GLN
TYR
LEU
LYS
LYS
SER
ASN
SER
T207
I210
I252
Q264
I268
L275
L276
A288
P289
V290
V291
V292
T293
Q301
LYS
THR
ASP
VAL
LEU
LYS
VAL
TYR
GLU
ILE
LEU
PRO
PHE
ASP
VAL
HIS
LYS

SER
GLU
Y325
L328
N332
E337
N338
I339
SER
GLU
VAL
SER
TYR
LYS
CYS
LEU
LYS
LYS
SER
THR
ASN
GLY
L28
E31
L32
D35
K36
M37
V38
T39
C40
L49
I58
S59
I60
G61
T62
Q63
V68
GLN
GLN
LYS
ASN
SER
SER
GLU
SER
THR
GLN

MET
ARG
GLU
GLY
GLN
ASN
GLN
THR
ALA
GLU
GLN
SER
ASP
SER
GLU
THR
LEU
LYS
VAL
ALA
ASN
GLY
LYS
ASN
ARG
GLN
ARG
LEU
LEU
ASP
SER
SER
CYS
SER
SER
ASN
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.

All (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
1:A:111:TYR:OH	1:B:58:ILE:HG21	1.81	0.81
1:B:111:TYR:OH	1:C:58:ILE:HG21	1.81	0.80
1:E:36:LYS:O	1:E:39:THR:HG22	1.82	0.80
1:F:36:LYS:O	1:F:39:THR:HG22	1.82	0.80
1:G:36:LYS:O	1:G:39:THR:HG22	1.82	0.79
1:D:36:LYS:O	1:D:39:THR:HG22	1.82	0.79
1:A:36:LYS:O	1:A:39:THR:HG22	1.82	0.79
1:C:36:LYS:O	1:C:39:THR:HG22	1.82	0.78
1:B:36:LYS:O	1:B:39:THR:HG22	1.82	0.78
1:E:111:TYR:OH	1:F:58:ILE:CG2	2.42	0.68
1:F:111:TYR:OH	1:G:58:ILE:CG2	2.43	0.65
1:G:49:LEU:HD22	1:G:276:LEU:HD22	1.83	0.60
1:F:49:LEU:HD22	1:F:276:LEU:HD22	1.84	0.60
1:E:49:LEU:HD22	1:E:276:LEU:HD22	1.84	0.60
1:A:210:ILE:HG21	1:A:325:TYR:HB3	1.84	0.60
1:B:210:ILE:HG21	1:B:325:TYR:HB3	1.84	0.59
1:C:49:LEU:HD22	1:C:276:LEU:HD22	1.84	0.59
1:E:111:TYR:CE2	1:F:58:ILE:HG12	2.37	0.59
1:G:210:ILE:HG21	1:G:325:TYR:HB3	1.84	0.59
1:B:49:LEU:HD22	1:B:276:LEU:HD22	1.84	0.59
1:A:49:LEU:HD22	1:A:276:LEU:HD22	1.84	0.59
1:C:210:ILE:HG21	1:C:325:TYR:HB3	1.84	0.59
1:D:210:ILE:HG21	1:D:325:TYR:HB3	1.84	0.59
1:A:60:ILE:HG22	1:A:61:GLY:N	2.18	0.59
1:D:49:LEU:HD22	1:D:276:LEU:HD22	1.84	0.59
1:D:60:ILE:HG22	1:D:61:GLY:N	2.18	0.59
1:E:210:ILE:HG21	1:E:325:TYR:HB3	1.84	0.59
1:F:210:ILE:HG21	1:F:325:TYR:HB3	1.84	0.59
1:E:60:ILE:HG22	1:E:61:GLY:N	2.18	0.59
1:F:111:TYR:CE2	1:G:58:ILE:HG12	2.38	0.59
1:C:60:ILE:HG22	1:C:61:GLY:N	2.18	0.58
1:D:111:TYR:OH	1:E:58:ILE:CG2	2.49	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:ILE:HG22	1:F:61:GLY:N	2.18	0.58
1:B:60:ILE:HG22	1:B:61:GLY:N	2.18	0.58
1:C:111:TYR:OH	1:D:58:ILE:CG2	2.50	0.58
1:G:60:ILE:HG22	1:G:61:GLY:N	2.18	0.57
1:A:111:TYR:OH	1:B:58:ILE:CG2	2.52	0.57
1:A:58:ILE:CG2	1:G:111:TYR:OH	2.51	0.56
1:B:111:TYR:OH	1:C:58:ILE:CG2	2.54	0.53
1:D:111:TYR:CE2	1:E:58:ILE:HG12	2.43	0.52
1:A:58:ILE:HG12	1:G:111:TYR:CE2	2.45	0.52
1:C:111:TYR:CE2	1:D:58:ILE:HG12	2.44	0.52
1:A:111:TYR:CE2	1:B:58:ILE:HG12	2.45	0.51
1:E:252:ILE:HG22	1:F:264:GLN:HB2	1.94	0.50
1:B:111:TYR:CE2	1:C:58:ILE:HG12	2.47	0.49
1:F:32:LEU:HD23	1:F:337:GLU:OE2	2.12	0.49
1:E:32:LEU:HD23	1:E:337:GLU:OE2	2.12	0.49
1:D:32:LEU:HD23	1:D:337:GLU:OE2	2.12	0.49
1:B:32:LEU:HD23	1:B:337:GLU:OE2	2.12	0.49
1:G:32:LEU:HD23	1:G:337:GLU:OE2	2.12	0.49
1:F:252:ILE:HG22	1:G:264:GLN:HB2	1.95	0.49
1:C:32:LEU:HD23	1:C:337:GLU:OE2	2.12	0.48
1:A:32:LEU:HD23	1:A:337:GLU:OE2	2.12	0.48
1:A:76:GLN:NE2	1:B:68:SER:O	2.48	0.47
1:D:252:ILE:HG22	1:E:264:GLN:HB2	1.97	0.46
1:C:132:ALA:O	1:C:136:CYS:HB3	2.16	0.46
1:B:132:ALA:O	1:B:136:CYS:HB3	2.16	0.46
1:D:132:ALA:O	1:D:136:CYS:HB3	2.16	0.46
1:B:37:MET:SD	1:B:37:MET:C	2.95	0.46
1:B:76:GLN:NE2	1:C:68:SER:O	2.48	0.46
1:G:132:ALA:O	1:G:136:CYS:HB3	2.16	0.46
1:B:289:PRO:HA	1:B:292:VAL:HG12	1.99	0.45
1:C:289:PRO:HA	1:C:292:VAL:HG12	1.99	0.45
1:D:289:PRO:HA	1:D:292:VAL:HG12	1.99	0.45
1:E:37:MET:SD	1:E:37:MET:C	2.95	0.45
1:A:37:MET:SD	1:A:37:MET:C	2.95	0.45
1:E:132:ALA:O	1:E:136:CYS:HB3	2.16	0.45
1:A:289:PRO:HA	1:A:292:VAL:HG12	1.99	0.45
1:F:132:ALA:O	1:F:136:CYS:HB3	2.16	0.45
1:F:37:MET:SD	1:F:37:MET:C	2.95	0.45
1:G:37:MET:C	1:G:37:MET:SD	2.95	0.45
1:B:328:LEU:HD23	1:B:332:ASN:HD21	1.82	0.45
1:D:37:MET:C	1:D:37:MET:SD	2.95	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ALA:O	1:A:136:CYS:HB3	2.16	0.45
1:C:328:LEU:HD23	1:C:332:ASN:HD21	1.82	0.45
1:D:328:LEU:HD23	1:D:332:ASN:HD21	1.82	0.45
1:C:37:MET:C	1:C:37:MET:SD	2.95	0.45
1:E:289:PRO:HA	1:E:292:VAL:HG12	1.99	0.45
1:E:35:ASP:OD1	1:E:294:THR:HG21	2.17	0.45
1:G:289:PRO:HA	1:G:292:VAL:HG12	1.99	0.44
1:F:35:ASP:OD1	1:F:294:THR:HG21	2.18	0.44
1:D:35:ASP:OD1	1:D:294:THR:HG21	2.18	0.44
1:G:35:ASP:OD1	1:G:294:THR:HG21	2.17	0.44
1:E:60:ILE:CG2	1:E:61:GLY:N	2.81	0.44
1:F:60:ILE:CG2	1:F:61:GLY:N	2.81	0.44
1:B:60:ILE:CG2	1:B:61:GLY:N	2.81	0.44
1:F:328:LEU:HD23	1:F:332:ASN:HD21	1.82	0.44
1:F:289:PRO:HA	1:F:292:VAL:HG12	1.99	0.44
1:A:328:LEU:HD23	1:A:332:ASN:HD21	1.82	0.44
1:E:328:LEU:HD23	1:E:332:ASN:HD21	1.82	0.44
1:G:328:LEU:HD23	1:G:332:ASN:HD21	1.82	0.44
1:A:68:SER:O	1:G:76:GLN:NE2	2.51	0.43
1:A:36:LYS:O	1:A:39:THR:CG2	2.62	0.43
1:C:35:ASP:OD1	1:C:294:THR:HG21	2.18	0.43
1:E:104:TRP:HZ3	1:F:275:LEU:HD12	1.83	0.43
1:C:39:THR:HG23	1:C:40:CYS:N	2.34	0.43
1:D:60:ILE:CG2	1:D:61:GLY:N	2.81	0.43
1:A:35:ASP:OD1	1:A:294:THR:HG21	2.18	0.43
1:C:60:ILE:CG2	1:C:61:GLY:N	2.80	0.43
1:F:104:TRP:HZ3	1:G:275:LEU:HD12	1.83	0.43
1:A:60:ILE:CG2	1:A:61:GLY:N	2.81	0.43
1:B:39:THR:HG23	1:B:40:CYS:N	2.34	0.43
1:E:288:ALA:HA	1:E:291:VAL:HG12	2.01	0.43
1:E:36:LYS:O	1:E:39:THR:CG2	2.62	0.43
1:D:39:THR:HG23	1:D:40:CYS:N	2.33	0.43
1:A:39:THR:HG23	1:A:40:CYS:N	2.34	0.42
1:F:288:ALA:HA	1:F:291:VAL:HG12	2.01	0.42
1:B:35:ASP:OD1	1:B:294:THR:HG21	2.18	0.42
1:D:288:ALA:HA	1:D:291:VAL:HG12	2.01	0.42
1:A:63:GLN:O	1:A:268:ILE:HG12	2.19	0.42
1:G:60:ILE:CG2	1:G:61:GLY:N	2.81	0.42
1:C:31:GLU:HA	1:C:31:GLU:OE1	2.20	0.42
1:E:255:ASN:N	1:E:255:ASN:OD1	2.53	0.42
1:E:39:THR:HG23	1:E:40:CYS:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:GLU:OE1	1:F:31:GLU:HA	2.20	0.42
1:F:39:THR:HG23	1:F:40:CYS:N	2.34	0.42
1:B:288:ALA:HA	1:B:291:VAL:HG12	2.01	0.42
1:E:31:GLU:OE1	1:E:31:GLU:HA	2.20	0.42
1:D:31:GLU:HA	1:D:31:GLU:OE1	2.20	0.42
1:D:76:GLN:NE2	1:E:68:SER:O	2.53	0.42
1:G:39:THR:HG23	1:G:40:CYS:N	2.34	0.42
1:G:31:GLU:HA	1:G:31:GLU:OE1	2.20	0.42
1:D:241:SER:OG	1:D:241:SER:O	2.35	0.41
1:A:288:ALA:HA	1:A:291:VAL:HG12	2.01	0.41
1:E:63:GLN:O	1:E:268:ILE:HG12	2.21	0.41
1:A:31:GLU:OE1	1:A:31:GLU:HA	2.20	0.41
1:B:31:GLU:HA	1:B:31:GLU:OE1	2.20	0.41
1:B:36:LYS:O	1:B:39:THR:CG2	2.62	0.41
1:G:288:ALA:HA	1:G:291:VAL:HG12	2.01	0.41
1:C:288:ALA:HA	1:C:291:VAL:HG12	2.01	0.41
1:D:63:GLN:O	1:D:268:ILE:HG12	2.21	0.41
1:B:63:GLN:O	1:B:268:ILE:HG12	2.21	0.41
1:C:63:GLN:O	1:C:268:ILE:HG12	2.20	0.41
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.94	0.41
1:G:63:GLN:O	1:G:268:ILE:HG12	2.20	0.41
1:C:76:GLN:NE2	1:D:68:SER:O	2.53	0.40
1:C:225:LEU:HA	1:C:225:LEU:HD23	1.93	0.40
1:C:241:SER:OG	1:C:241:SER:O	2.35	0.40
1:C:111:TYR:OH	1:D:52:LEU:O	2.32	0.40
1:F:63:GLN:O	1:F:268:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 ⓘ

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. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	332	ASN

Continued on next page...

Continued from previous page...

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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.