



wwPDB EM Validation Summary Report ⓘ

May 31, 2026 – 12:24 AM JST

PDB ID : 9VIN / pdb_00009vin
EMDB ID : EMD-65094
Title : Ternary complex of TNFR1-DD, TRADD-DD and RIPK1-DD
Authors : Liu, J.; Han, Y.; Zhao, J.; Gao, J.; Yuan, J.
Deposited on : 2025-06-18
Resolution : 3.41 Å(reported)
Based on initial models : 6ac0, 6AC5, 1ICH

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

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

A user guide is available at

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

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

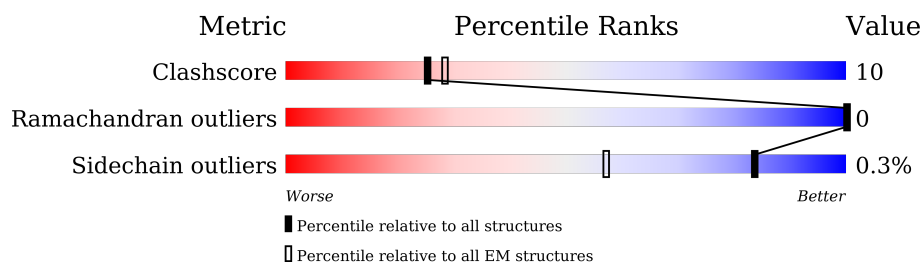
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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.



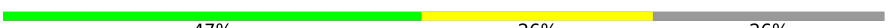
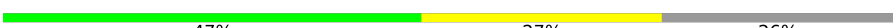
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 of 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	E	118	73% 18% 9%
1	F	118	69% 21% 9%
1	N	118	66% 24% 9%
1	V	118	64% 27% 9%
1	W	118	69% 21% 9%
2	i	116	71% 16% 14%
2	j	116	70% 16% 14%
2	k	116	67% 19% 14%
2	l	116	76% 10% 14%

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Mol	Chain	Length	Quality of chain
2	m	116	
2	n	116	
2	o	116	
2	p	116	
2	q	116	
2	r	116	
2	s	116	
2	t	116	
2	u	116	
3	A	118	
3	B	118	
3	C	118	
3	D	118	
3	G	118	
3	a	118	
3	b	118	
3	c	118	
3	d	118	
3	e	118	
3	f	118	
3	g	118	
3	h	118	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24273 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 Tumor necrosis factor receptor type 1-associated DEATH domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			867	544	162	160	1		
1	F	107	Total	C	N	O	S	0	0
			867	544	162	160	1		
1	N	107	Total	C	N	O	S	0	0
			867	544	162	160	1		
1	V	107	Total	C	N	O	S	0	0
			867	544	162	160	1		
1	W	107	Total	C	N	O	S	0	0
			867	544	162	160	1		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	195	GLY	-	expression tag	UNP Q15628
E	196	PRO	-	expression tag	UNP Q15628
E	197	GLY	-	expression tag	UNP Q15628
E	198	SER	-	expression tag	UNP Q15628
F	195	GLY	-	expression tag	UNP Q15628
F	196	PRO	-	expression tag	UNP Q15628
F	197	GLY	-	expression tag	UNP Q15628
F	198	SER	-	expression tag	UNP Q15628
N	195	GLY	-	expression tag	UNP Q15628
N	196	PRO	-	expression tag	UNP Q15628
N	197	GLY	-	expression tag	UNP Q15628
N	198	SER	-	expression tag	UNP Q15628
V	195	GLY	-	expression tag	UNP Q15628
V	196	PRO	-	expression tag	UNP Q15628
V	197	GLY	-	expression tag	UNP Q15628
V	198	SER	-	expression tag	UNP Q15628
W	195	GLY	-	expression tag	UNP Q15628
W	196	PRO	-	expression tag	UNP Q15628
W	197	GLY	-	expression tag	UNP Q15628

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Chain	Residue	Modelled	Actual	Comment	Reference
W	198	SER	-	expression tag	UNP Q15628

- Molecule 2 is a protein called Receptor-interacting serine/threonine-protein kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	i	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	j	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	k	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	l	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	m	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	n	100	Total	C	N	O	S	1	0
			818	515	146	153	4		
2	o	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	p	100	Total	C	N	O	S	1	0
			818	515	146	152	5		
2	q	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	r	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	s	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	t	100	Total	C	N	O	S	0	0
			815	513	146	152	4		
2	u	100	Total	C	N	O	S	1	0
			818	515	146	152	5		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	556	GLY	-	expression tag	UNP Q13546
i	557	PRO	-	expression tag	UNP Q13546
i	558	GLY	-	expression tag	UNP Q13546
j	556	GLY	-	expression tag	UNP Q13546
j	557	PRO	-	expression tag	UNP Q13546
j	558	GLY	-	expression tag	UNP Q13546
k	556	GLY	-	expression tag	UNP Q13546

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Chain	Residue	Modelled	Actual	Comment	Reference
k	557	PRO	-	expression tag	UNP Q13546
k	558	GLY	-	expression tag	UNP Q13546
l	556	GLY	-	expression tag	UNP Q13546
l	557	PRO	-	expression tag	UNP Q13546
l	558	GLY	-	expression tag	UNP Q13546
m	556	GLY	-	expression tag	UNP Q13546
m	557	PRO	-	expression tag	UNP Q13546
m	558	GLY	-	expression tag	UNP Q13546
n	556	GLY	-	expression tag	UNP Q13546
n	557	PRO	-	expression tag	UNP Q13546
n	558	GLY	-	expression tag	UNP Q13546
o	556	GLY	-	expression tag	UNP Q13546
o	557	PRO	-	expression tag	UNP Q13546
o	558	GLY	-	expression tag	UNP Q13546
p	556	GLY	-	expression tag	UNP Q13546
p	557	PRO	-	expression tag	UNP Q13546
p	558	GLY	-	expression tag	UNP Q13546
q	556	GLY	-	expression tag	UNP Q13546
q	557	PRO	-	expression tag	UNP Q13546
q	558	GLY	-	expression tag	UNP Q13546
r	556	GLY	-	expression tag	UNP Q13546
r	557	PRO	-	expression tag	UNP Q13546
r	558	GLY	-	expression tag	UNP Q13546
s	556	GLY	-	expression tag	UNP Q13546
s	557	PRO	-	expression tag	UNP Q13546
s	558	GLY	-	expression tag	UNP Q13546
t	556	GLY	-	expression tag	UNP Q13546
t	557	PRO	-	expression tag	UNP Q13546
t	558	GLY	-	expression tag	UNP Q13546
u	556	GLY	-	expression tag	UNP Q13546
u	557	PRO	-	expression tag	UNP Q13546
u	558	GLY	-	expression tag	UNP Q13546

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 1A, membrane form.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	87	Total	C	N	O	S	0	0
			718	448	135	131	4		
3	B	87	Total	C	N	O	S	0	0
			718	448	135	131	4		
3	C	87	Total	C	N	O	S	0	0
			718	448	135	131	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	87	Total 718	C 448	N 135	O 131	S 4	0	0
3	G	87	Total 718	C 448	N 135	O 131	S 4	0	0
3	a	87	Total 718	C 448	N 135	O 131	S 4	0	0
3	b	87	Total 718	C 448	N 135	O 131	S 4	0	0
3	c	87	Total 718	C 448	N 135	O 131	S 4	0	0
3	d	87	Total 718	C 448	N 135	O 131	S 4	0	0
3	e	87	Total 718	C 448	N 135	O 131	S 4	0	0
3	f	87	Total 718	C 448	N 135	O 131	S 4	0	0
3	g	87	Total 718	C 448	N 135	O 131	S 4	0	0
3	h	87	Total 718	C 448	N 135	O 131	S 4	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	338	GLY	-	expression tag	UNP P19438
A	339	PRO	-	expression tag	UNP P19438
A	340	GLY	-	expression tag	UNP P19438
A	341	SER	-	expression tag	UNP P19438
B	338	GLY	-	expression tag	UNP P19438
B	339	PRO	-	expression tag	UNP P19438
B	340	GLY	-	expression tag	UNP P19438
B	341	SER	-	expression tag	UNP P19438
C	338	GLY	-	expression tag	UNP P19438
C	339	PRO	-	expression tag	UNP P19438
C	340	GLY	-	expression tag	UNP P19438
C	341	SER	-	expression tag	UNP P19438
D	338	GLY	-	expression tag	UNP P19438
D	339	PRO	-	expression tag	UNP P19438
D	340	GLY	-	expression tag	UNP P19438
D	341	SER	-	expression tag	UNP P19438
G	338	GLY	-	expression tag	UNP P19438
G	339	PRO	-	expression tag	UNP P19438
G	340	GLY	-	expression tag	UNP P19438

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Chain	Residue	Modelled	Actual	Comment	Reference
G	341	SER	-	expression tag	UNP P19438
a	338	GLY	-	expression tag	UNP P19438
a	339	PRO	-	expression tag	UNP P19438
a	340	GLY	-	expression tag	UNP P19438
a	341	SER	-	expression tag	UNP P19438
b	338	GLY	-	expression tag	UNP P19438
b	339	PRO	-	expression tag	UNP P19438
b	340	GLY	-	expression tag	UNP P19438
b	341	SER	-	expression tag	UNP P19438
c	338	GLY	-	expression tag	UNP P19438
c	339	PRO	-	expression tag	UNP P19438
c	340	GLY	-	expression tag	UNP P19438
c	341	SER	-	expression tag	UNP P19438
d	338	GLY	-	expression tag	UNP P19438
d	339	PRO	-	expression tag	UNP P19438
d	340	GLY	-	expression tag	UNP P19438
d	341	SER	-	expression tag	UNP P19438
e	338	GLY	-	expression tag	UNP P19438
e	339	PRO	-	expression tag	UNP P19438
e	340	GLY	-	expression tag	UNP P19438
e	341	SER	-	expression tag	UNP P19438
f	338	GLY	-	expression tag	UNP P19438
f	339	PRO	-	expression tag	UNP P19438
f	340	GLY	-	expression tag	UNP P19438
f	341	SER	-	expression tag	UNP P19438
g	338	GLY	-	expression tag	UNP P19438
g	339	PRO	-	expression tag	UNP P19438
g	340	GLY	-	expression tag	UNP P19438
g	341	SER	-	expression tag	UNP P19438
h	338	GLY	-	expression tag	UNP P19438
h	339	PRO	-	expression tag	UNP P19438
h	340	GLY	-	expression tag	UNP P19438
h	341	SER	-	expression tag	UNP P19438

3 Residue-property plots

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. 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: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain E: 



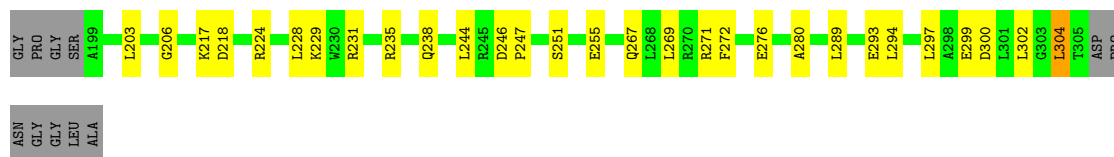
- Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain F: 



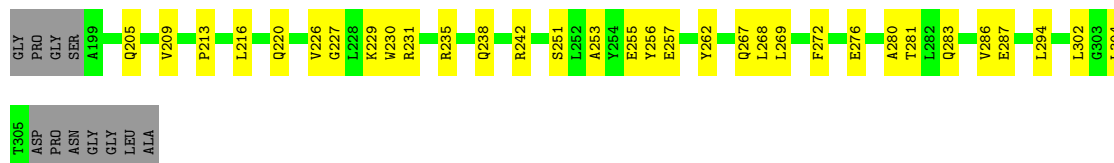
- Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain N: 



- Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain V: 



- Molecule 1: Tumor necrosis factor receptor type 1-associated DEATH domain protein

Chain W: 



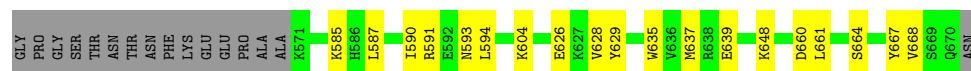
- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1

Chain i: 



- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1

Chain j: 



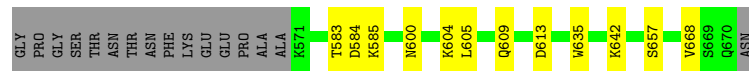
- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1

Chain k: 



- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1

Chain l: 



- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1

Chain m: 



- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1

Chain n: 



- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1

Chain o: 





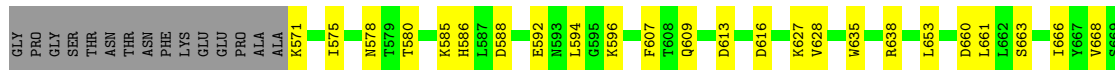
- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1



- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1



- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1



- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1



- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1



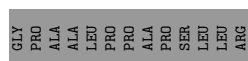
- Molecule 2: Receptor-interacting serine/threonine-protein kinase 1





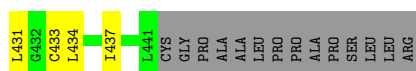
- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

Chain A: 53% 20% 26%



- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

Chain B: 50% 24% 26%



- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

Chain C: 61% 13% 26%



- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

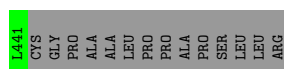
Chain D: 42% 31% 26%



- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

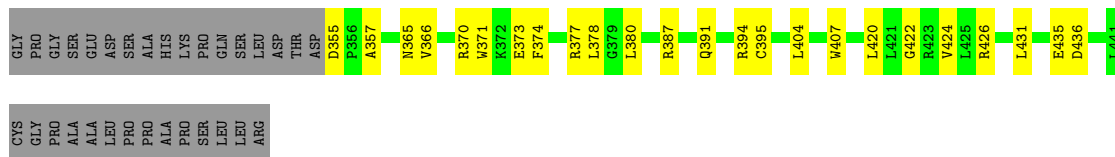
Chain G: 53% 21% 26%





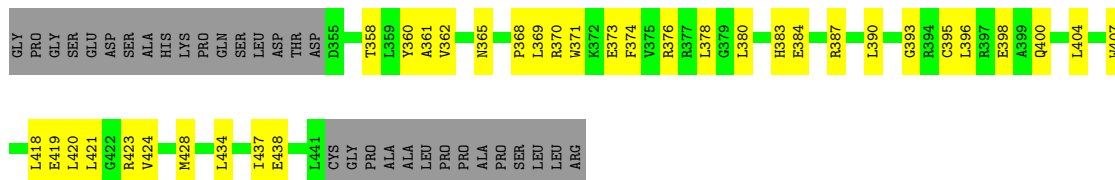
- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

Chain a:  53% 20% 26%



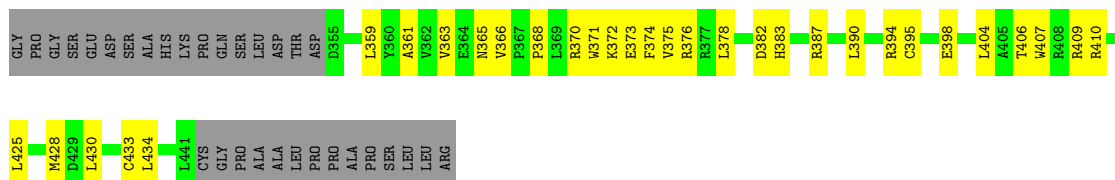
- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

Chain b:  44% 30% 26%



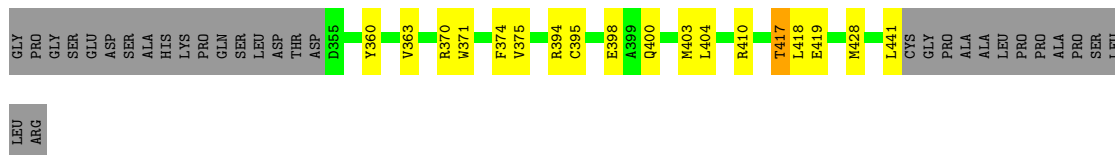
- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

Chain c:  47% 26% 26%



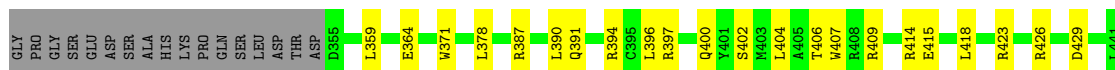
- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

Chain d:  58% 14% 26%



- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form

Chain e:  55% 19% 26%



CYS
GLY
PRO
ALA
ALA
LEU
PRO
PRO
ALA
ALA
PRO
SER
SER
LEU
LEU
ARG

- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form



GLY
PRO
GLY
SER
GLU
ASP
SER
ALA
HIS
LYS
PRO
GLN
SER
LEU
ASP
THR
ASP
D355
Y360
A361
V362
V363
E364
N365
P368
L369
R370
W371
K372
E373
F374
V375
R376
R377
L378
G379
L380
S381
L388
E389
L390
Q391
N392
G393
R397
F398
A399
Q400
Y401
S402
M403
L404
A405
T406
W407
R408

R409
D427
M428
L441
CYS
PRO
GLY
ALA
ALA
LEU
PRO
PRO
ALA
ASP
SER
LEU
LEU
ARG

- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form



GLY
PRO
GLY
SER
GLU
ASP
SER
ALA
HIS
LYS
PRO
GLN
SER
LEU
ASP
THR
ASP
D355
A361
N365
W371
F374
V375
L380
L388
N392
G393
Q400
M403
W407
R410
E419
R423
D429
L430
C433
I437
L441
CYS
GLY
PRO
ALA
ALA

LEU
PRO
PRO
ALA
PRO
SER
LEU
LEU
ARG

- Molecule 3: Tumor necrosis factor receptor superfamily member 1A, membrane form



GLY
PRO
GLY
SER
GLU
ASP
SER
ALA
HIS
LYS
PRO
GLN
SER
LEU
ASP
THR
ASP
D355
P356
A357
T358
L359
Y360
A361
V362
N365
V366
P367
P368
L369
R370
W371
K372
E373
F374
V375
R376
R377
L378
E389
R394
C396
L396
R397
Q400
Y401
S402
M403
L404
A405
T406
R410
L421

V424
L425
R426
D429
L430
L431
G432
C433
L434
I437
E438
L441
CYS
PRO
ALA
ALA
LEU
PRO
PRO
ALA
SER
LEU
LEU
ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k 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	E	0.14	0/879	0.33	0/1183
1	F	0.15	0/879	0.33	0/1183
1	N	0.13	0/879	0.32	0/1183
1	V	0.13	0/879	0.30	0/1183
1	W	0.15	0/879	0.32	0/1183
2	i	0.13	0/829	0.30	0/1113
2	j	0.13	0/829	0.31	0/1113
2	k	0.14	0/829	0.26	0/1113
2	l	0.14	0/829	0.26	0/1113
2	m	0.14	0/829	0.26	0/1113
2	n	0.13	0/835	0.24	0/1121
2	o	0.14	0/829	0.28	0/1113
2	p	0.16	0/835	0.38	0/1121
2	q	0.15	0/829	0.36	0/1113
2	r	0.14	0/829	0.28	0/1113
2	s	0.13	0/829	0.23	0/1113
2	t	0.13	0/829	0.26	0/1113
2	u	0.11	0/835	0.31	0/1121
3	A	0.11	0/729	0.31	0/985
3	B	0.13	0/729	0.36	0/985
3	C	0.12	0/729	0.28	0/985
3	D	0.12	0/729	0.30	0/985
3	G	0.12	0/729	0.29	0/985
3	a	0.12	0/729	0.27	0/985
3	b	0.12	0/729	0.34	0/985
3	c	0.11	0/729	0.30	0/985
3	d	0.11	0/729	0.24	0/985
3	e	0.14	0/729	0.35	0/985
3	f	0.16	0/729	0.40	0/985
3	g	0.13	0/729	0.30	0/985
3	h	0.17	0/729	0.35	0/985
All	All	0.13	0/24667	0.31	0/33213

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	E	867	0	877	15	0
1	F	867	0	877	16	0
1	N	867	0	877	19	0
1	V	867	0	877	20	0
1	W	867	0	877	18	0
2	i	815	0	817	11	0
2	j	815	0	817	17	0
2	k	815	0	817	14	0
2	l	815	0	817	7	0
2	m	815	0	817	16	0
2	n	818	0	822	13	0
2	o	815	0	817	19	0
2	p	818	0	820	18	0
2	q	815	0	817	17	0
2	r	815	0	817	16	0
2	s	815	0	817	14	0
2	t	815	0	817	9	0
2	u	818	0	820	17	0
3	A	718	0	726	21	0
3	B	718	0	726	22	0
3	C	718	0	726	13	0
3	D	718	0	726	33	0
3	G	718	0	726	18	0
3	a	718	0	726	16	0
3	b	718	0	726	33	0
3	c	718	0	726	30	0
3	d	718	0	726	11	0
3	e	718	0	726	19	0
3	f	718	0	726	33	0
3	g	718	0	726	17	0
3	h	718	0	726	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	24273	0	24455	506	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 506 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)
3:c:394:ARG:HH22	3:f:393:GLY:HA3	1.49	0.77
3:c:371:TRP:O	3:c:374:PHE:HB3	1.84	0.76
2:i:593:ASN:HB2	2:i:661:LEU:HD21	1.66	0.76
3:a:380:LEU:HD11	3:a:407:TRP:HB2	1.69	0.75
3:D:392:ASN:HB2	3:D:399:ALA:HB2	1.69	0.74

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	E	105/118 (89%)	103 (98%)	2 (2%)	0	100	100
1	F	105/118 (89%)	100 (95%)	5 (5%)	0	100	100
1	N	105/118 (89%)	100 (95%)	5 (5%)	0	100	100
1	V	105/118 (89%)	101 (96%)	4 (4%)	0	100	100
1	W	105/118 (89%)	98 (93%)	7 (7%)	0	100	100
2	i	98/116 (84%)	94 (96%)	4 (4%)	0	100	100
2	j	98/116 (84%)	96 (98%)	2 (2%)	0	100	100
2	k	98/116 (84%)	97 (99%)	1 (1%)	0	100	100
2	l	98/116 (84%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	m	98/116 (84%)	98 (100%)	0	0	100	100
2	n	99/116 (85%)	98 (99%)	1 (1%)	0	100	100
2	o	98/116 (84%)	97 (99%)	1 (1%)	0	100	100
2	p	99/116 (85%)	95 (96%)	4 (4%)	0	100	100
2	q	98/116 (84%)	94 (96%)	4 (4%)	0	100	100
2	r	98/116 (84%)	97 (99%)	1 (1%)	0	100	100
2	s	98/116 (84%)	98 (100%)	0	0	100	100
2	t	98/116 (84%)	97 (99%)	1 (1%)	0	100	100
2	u	99/116 (85%)	98 (99%)	1 (1%)	0	100	100
3	A	85/118 (72%)	81 (95%)	4 (5%)	0	100	100
3	B	85/118 (72%)	82 (96%)	3 (4%)	0	100	100
3	C	85/118 (72%)	82 (96%)	3 (4%)	0	100	100
3	D	85/118 (72%)	83 (98%)	2 (2%)	0	100	100
3	G	85/118 (72%)	84 (99%)	1 (1%)	0	100	100
3	a	85/118 (72%)	83 (98%)	2 (2%)	0	100	100
3	b	85/118 (72%)	82 (96%)	3 (4%)	0	100	100
3	c	85/118 (72%)	83 (98%)	2 (2%)	0	100	100
3	d	85/118 (72%)	84 (99%)	1 (1%)	0	100	100
3	e	85/118 (72%)	83 (98%)	2 (2%)	0	100	100
3	f	85/118 (72%)	82 (96%)	3 (4%)	0	100	100
3	g	85/118 (72%)	81 (95%)	4 (5%)	0	100	100
3	h	85/118 (72%)	84 (99%)	1 (1%)	0	100	100
All	All	2907/3632 (80%)	2831 (97%)	76 (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 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	E	90/96 (94%)	90 (100%)	0	100	100
1	F	90/96 (94%)	90 (100%)	0	100	100
1	N	90/96 (94%)	88 (98%)	2 (2%)	45	63
1	V	90/96 (94%)	89 (99%)	1 (1%)	65	73
1	W	90/96 (94%)	90 (100%)	0	100	100
2	i	89/101 (88%)	89 (100%)	0	100	100
2	j	89/101 (88%)	88 (99%)	1 (1%)	65	73
2	k	89/101 (88%)	89 (100%)	0	100	100
2	l	89/101 (88%)	89 (100%)	0	100	100
2	m	89/101 (88%)	89 (100%)	0	100	100
2	n	90/101 (89%)	90 (100%)	0	100	100
2	o	89/101 (88%)	89 (100%)	0	100	100
2	p	90/101 (89%)	89 (99%)	1 (1%)	65	73
2	q	89/101 (88%)	88 (99%)	1 (1%)	65	73
2	r	89/101 (88%)	89 (100%)	0	100	100
2	s	89/101 (88%)	89 (100%)	0	100	100
2	t	89/101 (88%)	89 (100%)	0	100	100
2	u	90/101 (89%)	90 (100%)	0	100	100
3	A	77/101 (76%)	76 (99%)	1 (1%)	61	71
3	B	77/101 (76%)	76 (99%)	1 (1%)	61	71
3	C	77/101 (76%)	77 (100%)	0	100	100
3	D	77/101 (76%)	77 (100%)	0	100	100
3	G	77/101 (76%)	77 (100%)	0	100	100
3	a	77/101 (76%)	77 (100%)	0	100	100
3	b	77/101 (76%)	77 (100%)	0	100	100
3	c	77/101 (76%)	77 (100%)	0	100	100
3	d	77/101 (76%)	76 (99%)	1 (1%)	61	71
3	e	77/101 (76%)	77 (100%)	0	100	100
3	f	77/101 (76%)	77 (100%)	0	100	100
3	g	77/101 (76%)	77 (100%)	0	100	100
3	h	77/101 (76%)	77 (100%)	0	100	100
All	All	2611/3106 (84%)	2602 (100%)	9 (0%)	84	84

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	369	LEU
3	d	417	THR
2	j	637	MET
2	p	605	LEU
2	q	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	p	611	GLN
3	G	365	ASN
2	r	593	ASN
3	b	365	ASN
2	k	600	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.