



wwPDB EM Validation Summary Report ⓘ

Apr 29, 2026 – 06:17 PM JST

PDB ID : 9VEE / pdb_00009vee
EMDB ID : EMD-65005
Title : The cryo-EM structure of human Piezo2-MDFIC2 complex (composite map)
Authors : Zhang, Y.; Dai, F.; Zhou, Z.; Dai, F.; Cheng, D.; Ma, X.; Omidkhoda, S.F.;
Clarke, J.; Zhang, H.; Laden, M.; Guo, Y.; Li, J.V.; Liu, R.; Wong, E.S.;
Zhang, Y.; Cox, C.D.
Deposited on : 2025-06-09
Resolution : 3.36 Å(reported)

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

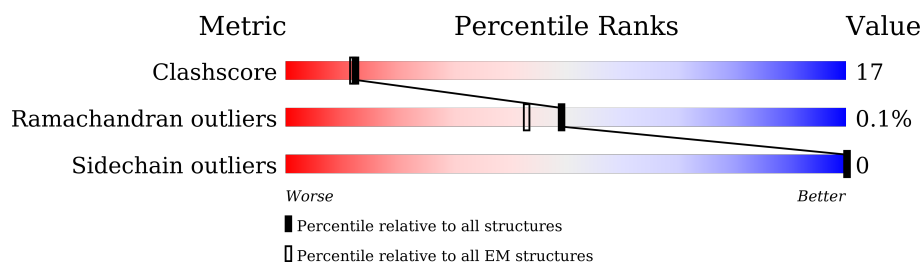
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 3.36 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	A	3020	
1	B	3020	
1	C	3020	
2	D	211	
2	E	211	
2	F	211	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34893 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 Piezo-type mechanosensitive ion channel component 2, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1396	Total	C	N	O	S	0	0
			11465	7568	1851	1969	77		
1	B	1396	Total	C	N	O	S	0	0
			11465	7568	1851	1969	77		
1	C	1396	Total	C	N	O	S	0	0
			11465	7568	1851	1969	77		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2753	SER	-	linker	UNP Q9H5I5
A	2754	ASN	-	linker	UNP Q9H5I5
A	2755	SER	-	linker	UNP Q9H5I5
A	2756	LEU	-	linker	UNP Q9H5I5
A	2757	GLU	-	linker	UNP Q9H5I5
A	2758	VAL	-	linker	UNP Q9H5I5
A	2759	LEU	-	linker	UNP Q9H5I5
A	2760	PHE	-	linker	UNP Q9H5I5
A	2761	GLN	-	linker	UNP Q9H5I5
A	2762	GLY	-	linker	UNP Q9H5I5
A	2763	PRO	-	linker	UNP Q9H5I5
A	2764	THR	-	linker	UNP Q9H5I5
A	2765	ALA	-	linker	UNP Q9H5I5
A	2766	ALA	-	linker	UNP Q9H5I5
A	2767	ALA	-	linker	UNP Q9H5I5
A	2768	ALA	-	linker	UNP Q9H5I5
A	2769	VAL	-	linker	UNP Q9H5I5
A	2832	LEU	PHE	conflict	UNP P42212
A	2833	THR	SER	conflict	UNP P42212
A	2974	LYS	ALA	conflict	UNP P42212
A	2999	LEU	HIS	conflict	UNP P42212
A	3007	SER	-	expression tag	UNP P42212
A	3008	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3009	GLY	-	expression tag	UNP P42212
A	3010	GLY	-	expression tag	UNP P42212
A	3011	HIS	-	expression tag	UNP P42212
A	3012	HIS	-	expression tag	UNP P42212
A	3013	HIS	-	expression tag	UNP P42212
A	3014	HIS	-	expression tag	UNP P42212
A	3015	HIS	-	expression tag	UNP P42212
A	3016	HIS	-	expression tag	UNP P42212
A	3017	HIS	-	expression tag	UNP P42212
A	3018	HIS	-	expression tag	UNP P42212
A	3019	HIS	-	expression tag	UNP P42212
A	3020	HIS	-	expression tag	UNP P42212
B	2753	SER	-	linker	UNP Q9H5I5
B	2754	ASN	-	linker	UNP Q9H5I5
B	2755	SER	-	linker	UNP Q9H5I5
B	2756	LEU	-	linker	UNP Q9H5I5
B	2757	GLU	-	linker	UNP Q9H5I5
B	2758	VAL	-	linker	UNP Q9H5I5
B	2759	LEU	-	linker	UNP Q9H5I5
B	2760	PHE	-	linker	UNP Q9H5I5
B	2761	GLN	-	linker	UNP Q9H5I5
B	2762	GLY	-	linker	UNP Q9H5I5
B	2763	PRO	-	linker	UNP Q9H5I5
B	2764	THR	-	linker	UNP Q9H5I5
B	2765	ALA	-	linker	UNP Q9H5I5
B	2766	ALA	-	linker	UNP Q9H5I5
B	2767	ALA	-	linker	UNP Q9H5I5
B	2768	ALA	-	linker	UNP Q9H5I5
B	2769	VAL	-	linker	UNP Q9H5I5
B	2832	LEU	PHE	conflict	UNP P42212
B	2833	THR	SER	conflict	UNP P42212
B	2974	LYS	ALA	conflict	UNP P42212
B	2999	LEU	HIS	conflict	UNP P42212
B	3007	SER	-	expression tag	UNP P42212
B	3008	GLY	-	expression tag	UNP P42212
B	3009	GLY	-	expression tag	UNP P42212
B	3010	GLY	-	expression tag	UNP P42212
B	3011	HIS	-	expression tag	UNP P42212
B	3012	HIS	-	expression tag	UNP P42212
B	3013	HIS	-	expression tag	UNP P42212
B	3014	HIS	-	expression tag	UNP P42212
B	3015	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3016	HIS	-	expression tag	UNP P42212
B	3017	HIS	-	expression tag	UNP P42212
B	3018	HIS	-	expression tag	UNP P42212
B	3019	HIS	-	expression tag	UNP P42212
B	3020	HIS	-	expression tag	UNP P42212
C	2753	SER	-	linker	UNP Q9H5I5
C	2754	ASN	-	linker	UNP Q9H5I5
C	2755	SER	-	linker	UNP Q9H5I5
C	2756	LEU	-	linker	UNP Q9H5I5
C	2757	GLU	-	linker	UNP Q9H5I5
C	2758	VAL	-	linker	UNP Q9H5I5
C	2759	LEU	-	linker	UNP Q9H5I5
C	2760	PHE	-	linker	UNP Q9H5I5
C	2761	GLN	-	linker	UNP Q9H5I5
C	2762	GLY	-	linker	UNP Q9H5I5
C	2763	PRO	-	linker	UNP Q9H5I5
C	2764	THR	-	linker	UNP Q9H5I5
C	2765	ALA	-	linker	UNP Q9H5I5
C	2766	ALA	-	linker	UNP Q9H5I5
C	2767	ALA	-	linker	UNP Q9H5I5
C	2768	ALA	-	linker	UNP Q9H5I5
C	2769	VAL	-	linker	UNP Q9H5I5
C	2832	LEU	PHE	conflict	UNP P42212
C	2833	THR	SER	conflict	UNP P42212
C	2974	LYS	ALA	conflict	UNP P42212
C	2999	LEU	HIS	conflict	UNP P42212
C	3007	SER	-	expression tag	UNP P42212
C	3008	GLY	-	expression tag	UNP P42212
C	3009	GLY	-	expression tag	UNP P42212
C	3010	GLY	-	expression tag	UNP P42212
C	3011	HIS	-	expression tag	UNP P42212
C	3012	HIS	-	expression tag	UNP P42212
C	3013	HIS	-	expression tag	UNP P42212
C	3014	HIS	-	expression tag	UNP P42212
C	3015	HIS	-	expression tag	UNP P42212
C	3016	HIS	-	expression tag	UNP P42212
C	3017	HIS	-	expression tag	UNP P42212
C	3018	HIS	-	expression tag	UNP P42212
C	3019	HIS	-	expression tag	UNP P42212
C	3020	HIS	-	expression tag	UNP P42212

- Molecule 2 is a protein called MyoD family inhibitor domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	21	Total 166	C 100	N 26	O 36	S 4	0	0
2	D	21	Total 166	C 100	N 26	O 36	S 4	0	0
2	E	21	Total 166	C 100	N 26	O 36	S 4	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-21	MET	-	initiating methionine	UNP A0A1B0GVS7
F	-20	ASP	-	expression tag	UNP A0A1B0GVS7
F	-19	TYR	-	expression tag	UNP A0A1B0GVS7
F	-18	LYS	-	expression tag	UNP A0A1B0GVS7
F	-17	ASP	-	expression tag	UNP A0A1B0GVS7
F	-16	ASP	-	expression tag	UNP A0A1B0GVS7
F	-15	ASP	-	expression tag	UNP A0A1B0GVS7
F	-14	ASP	-	expression tag	UNP A0A1B0GVS7
F	-13	LYS	-	expression tag	UNP A0A1B0GVS7
F	-12	GLY	-	expression tag	UNP A0A1B0GVS7
F	-11	LEU	-	expression tag	UNP A0A1B0GVS7
F	-10	GLU	-	expression tag	UNP A0A1B0GVS7
F	-9	VAL	-	expression tag	UNP A0A1B0GVS7
F	-8	LEU	-	expression tag	UNP A0A1B0GVS7
F	-7	PHE	-	expression tag	UNP A0A1B0GVS7
F	-6	GLN	-	expression tag	UNP A0A1B0GVS7
F	-5	GLY	-	expression tag	UNP A0A1B0GVS7
F	-4	PRO	-	expression tag	UNP A0A1B0GVS7
F	-3	GLY	-	expression tag	UNP A0A1B0GVS7
F	-2	SER	-	expression tag	UNP A0A1B0GVS7
F	-1	SER	-	expression tag	UNP A0A1B0GVS7
F	0	THR	-	expression tag	UNP A0A1B0GVS7
D	-21	MET	-	initiating methionine	UNP A0A1B0GVS7
D	-20	ASP	-	expression tag	UNP A0A1B0GVS7
D	-19	TYR	-	expression tag	UNP A0A1B0GVS7
D	-18	LYS	-	expression tag	UNP A0A1B0GVS7
D	-17	ASP	-	expression tag	UNP A0A1B0GVS7
D	-16	ASP	-	expression tag	UNP A0A1B0GVS7
D	-15	ASP	-	expression tag	UNP A0A1B0GVS7
D	-14	ASP	-	expression tag	UNP A0A1B0GVS7
D	-13	LYS	-	expression tag	UNP A0A1B0GVS7
D	-12	GLY	-	expression tag	UNP A0A1B0GVS7
D	-11	LEU	-	expression tag	UNP A0A1B0GVS7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	GLU	-	expression tag	UNP A0A1B0GVS7
D	-9	VAL	-	expression tag	UNP A0A1B0GVS7
D	-8	LEU	-	expression tag	UNP A0A1B0GVS7
D	-7	PHE	-	expression tag	UNP A0A1B0GVS7
D	-6	GLN	-	expression tag	UNP A0A1B0GVS7
D	-5	GLY	-	expression tag	UNP A0A1B0GVS7
D	-4	PRO	-	expression tag	UNP A0A1B0GVS7
D	-3	GLY	-	expression tag	UNP A0A1B0GVS7
D	-2	SER	-	expression tag	UNP A0A1B0GVS7
D	-1	SER	-	expression tag	UNP A0A1B0GVS7
D	0	THR	-	expression tag	UNP A0A1B0GVS7
E	-21	MET	-	initiating methionine	UNP A0A1B0GVS7
E	-20	ASP	-	expression tag	UNP A0A1B0GVS7
E	-19	TYR	-	expression tag	UNP A0A1B0GVS7
E	-18	LYS	-	expression tag	UNP A0A1B0GVS7
E	-17	ASP	-	expression tag	UNP A0A1B0GVS7
E	-16	ASP	-	expression tag	UNP A0A1B0GVS7
E	-15	ASP	-	expression tag	UNP A0A1B0GVS7
E	-14	ASP	-	expression tag	UNP A0A1B0GVS7
E	-13	LYS	-	expression tag	UNP A0A1B0GVS7
E	-12	GLY	-	expression tag	UNP A0A1B0GVS7
E	-11	LEU	-	expression tag	UNP A0A1B0GVS7
E	-10	GLU	-	expression tag	UNP A0A1B0GVS7
E	-9	VAL	-	expression tag	UNP A0A1B0GVS7
E	-8	LEU	-	expression tag	UNP A0A1B0GVS7
E	-7	PHE	-	expression tag	UNP A0A1B0GVS7
E	-6	GLN	-	expression tag	UNP A0A1B0GVS7
E	-5	GLY	-	expression tag	UNP A0A1B0GVS7
E	-4	PRO	-	expression tag	UNP A0A1B0GVS7
E	-3	GLY	-	expression tag	UNP A0A1B0GVS7
E	-2	SER	-	expression tag	UNP A0A1B0GVS7
E	-1	SER	-	expression tag	UNP A0A1B0GVS7
E	0	THR	-	expression tag	UNP A0A1B0GVS7

WORLDWIDE
PDB
PROTEIN DATA BANK





- Molecule 1: Piezo-type mechanosensitive ion channel component 2, Green fluorescent protein

Response	Percentage
Yes	29%
No	17%
Don't know	54%



K2482	M2404	S2306	D2197	SER	ALA	L1948	ARG	GLU	ALA	ALA	ASN	ILE	THR	GLU	R1193
M2483	V2410	C2312	I2202	PHE	ARG	I1949	MET	ALA	THR	THR	ILE	THR	ASP	GLU	D1194
F2485	L2411	V2318	G2207	SER	VAL	F1950	ALA	VAL	GLY	GLY	LEU	ASP	ASP	ASP	Y1196
E2487	L2412	L2319	R1962	ASN	SER	R1962	SER	PRO	TYR	TYR	W1666	THR	GLU	GLU	P1196
N2488	I2413	L2319	R1962	ARG	ASP	R1962	ASP	ASP	VAL	VAL	W1666	THR	ARG	ARG	W1197
Y2489	I2415	S2326	F1970	SER	ASP	I1969	ASP	ASP	GLY	GLY	I1670	ALA	GLU	GLU	F1199
E2490	V2416	S2326	V1970	GLN	GLU	V1970	ASP	ASP	VAL	VAL	I1670	LEU	ALA	ALA	F1204
K2491	W2417	S2326	I1971	ARG	LEU	I1971	SER	SER	ALA	ALA	E1673	ARG	ASP	ASP	N1205
V2496	W2417	S2326	T1972	GLY	SER	T1972	THR	THR	GLY	GLY	E1673	ARG	GLN	GLN	D1206
L2499	F2418	S2326	E1973	THR	GLY	E1973	ASP	ASP	ALA	ALA	I1677	HIS	LYS	LYS	N1207
E2500	L2426	S2326	Y1980	THR	HIS	Y1980	LYS	LYS	GLU	GLU	S1678	LYS	ALA	ALA	I1208
G2501	L2426	S2326	F1981	THR	GLY	F1981	LEU	LEU	GLU	GLU	T1679	GLY	LYS	LYS	I1209
N2504	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	V1680	LYS	GLY	GLY	K1210
S2505	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	I1681	LYS	LYS	LYS	D1216
L2506	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	F1217
W2507	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	I1218
T2508	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	I1219
D2509	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	P1223
S2510	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	L1226
P2511	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	F1230
P2512	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	R1240
S2513	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	M1254
K2514	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	E1255
K2515	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	G1256
K2516	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	D1257
N2517	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	M1263
L2522	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	A1268
D2523	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	N1274
P2524	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	F1275
N2525	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	V1276
S2526	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	I1280
S2527	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	H1281
F2528	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	C1282
S2529	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	R1283
V2530	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	D1287
S2533	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	K1290
V2534	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	F1294
S2535	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	F1298
I2536	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	V1301
Q2537	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	I1304
S2538	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	I1305
A2544	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	F1306
E2547	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	
I2548	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	
A2549	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	
A2549	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	
D2550	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	
T2551	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	
K2552	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	
L2553	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	
P2556	L2426	S2326	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	R1682	ARG	LYS	LYS	

ASP	CYS	ARG	HIS	ALA	MET
CYS	ASP	ASP	ARG	ASP	TYR
ASP	MET	THR	THR	LYS	LYS
ASP	ASP	GLU	GLU	PRO	ASP
CYS	GLU	GLU	GLU	ILE	ASP
SER	GLU	CYS	CYS	ASN	ASP
LEU	LEU	CYS	ALA	ILE	ASP
PHE	PHE	ALA	SER	VAL	GLY
GLU	GLU	LEU	LEU	ILE	LYS
S169	E172	ILE	ILE	ASN	LEU
E173	T173	LEU	LEU	VAL	GLU
A180	M181	ALA	CYS	VAL	VAL
E182	E182	LEU	PHE	ASP	GLN
I183	I183	CYS	CYS	PHE	GLY
S184	S184	GLN	PHE	ASN	PRO
E185	E185	THR	THR	THR	GLY
E186	E186	ASP	ASP	GLY	THR
E187	E187	CYS	CYS	PRO	MET
E188	E188	LEU	LEU	ALA	SER
E189	E189	LEU	LEU	LYS	GLU
E190	E190	MET	MET	GLU	THR
E191	E191	LEU	LEU	ASN	GLU
E192	E192	PRO	PRO	PRO	LEU
E193	E193	GLY	GLY	ASN	GLU
E194	E194	THR	THR	GLU	LYS
E195	E195	CYS	CYS	LYS	ILE
E196	E196	GLU	GLU	LEU	VAL
E197	E197	THR	THR	SER	ARG
E198	E198	CYS	CYS	GLU	THR
E199	E199	LYS	LYS	SER	ALA
E200	E200	MET	MET	THR	HIS
E201	E201	CYS	CYS	SER	LEU
E202	E202	GLU	GLU	LEU	GLU
E203	E203	PRO	PRO	SER	ASN
E204	E204	SER	SER	SER	ASP
E205	E205	ARG	ARG	LEU	LYS
E206	E206	THR	THR	GLU	ASN
E207	E207	TYR	TYR	GLU	ASN
E208	E208	HIS	HIS	CYS	ILE
E209	E209	THR	THR	GLN	SER
E210	E210	SER	SER	THR	TRP
E211	E211	ASP	ASP	PHE	LEU
E212	E212	GLU	GLU	THR	LEU
E213	E213	ASN	ASN	TYR	GLN
E214	E214	HIS	HIS	LEU	THR
E215	E215	SER	SER	GLN	ASN
E216	E216	THR	THR	THR	THR
E217	E217	ASN	ASN	ASP	ASN
E218	E218	ASP	ASP	THR	ALA
E219	E219	CYS	CYS	VAL	ALA
E220	E220	THR	THR	THR	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203045	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 ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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	0.40	1/11775 (0.0%)	0.52	4/15965 (0.0%)
1	B	0.40	1/11775 (0.0%)	0.52	4/15965 (0.0%)
1	C	0.40	1/11775 (0.0%)	0.52	4/15965 (0.0%)
2	D	0.32	0/167	0.74	0/223
2	E	0.32	0/167	0.74	0/223
2	F	0.32	0/167	0.74	0/223
All	All	0.40	3/35826 (0.0%)	0.53	12/48564 (0.0%)

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	2
1	C	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2509	ILE	C-N	-6.48	1.24	1.33
1	C	2509	ILE	C-N	-6.44	1.24	1.33
1	A	2509	ILE	C-N	-6.43	1.24	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2509	ILE	CA-C-N	8.51	133.61	120.68
1	C	2509	ILE	C-N-CA	8.51	133.61	120.68
1	A	2509	ILE	CA-C-N	8.48	133.56	120.68
1	A	2509	ILE	C-N-CA	8.48	133.56	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2509	ILE	CA-C-N	8.47	133.56	120.68

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2630	TRP	Peptide
1	A	2642	ASN	Peptide
1	B	2630	TRP	Peptide
1	B	2642	ASN	Peptide
1	C	2630	TRP	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	11465	0	11592	424	0
1	B	11465	0	11592	415	0
1	C	11465	0	11592	411	0
2	D	166	0	153	14	0
2	E	166	0	153	16	0
2	F	166	0	153	14	0
All	All	34893	0	35235	1185	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 17.

The worst 5 of 1185 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:A:2630:TRP:HZ2	1:B:2512:PRO:HD2	1.34	0.93
1:A:2630:TRP:CZ2	1:B:2512:PRO:HD2	2.08	0.88
1:A:2003:PRO:HD2	1:A:2004:PRO:HD2	1.55	0.88
1:C:1204:PHE:HB3	1:C:1209:ILE:HD11	1.56	0.88
1:C:2003:PRO:HD2	1:C:2004:PRO:HD2	1.55	0.88

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	1378/3020 (46%)	1254 (91%)	122 (9%)	2 (0%)	48	76
1	B	1378/3020 (46%)	1255 (91%)	121 (9%)	2 (0%)	48	76
1	C	1378/3020 (46%)	1255 (91%)	121 (9%)	2 (0%)	48	76
2	D	19/211 (9%)	18 (95%)	1 (5%)	0	100	100
2	E	19/211 (9%)	18 (95%)	1 (5%)	0	100	100
2	F	19/211 (9%)	18 (95%)	1 (5%)	0	100	100
All	All	4191/9693 (43%)	3818 (91%)	367 (9%)	6 (0%)	49	76

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2556	PRO
1	B	2556	PRO
1	C	2556	PRO
1	A	1025	PRO
1	B	1025	PRO

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	1268/2707 (47%)	1268 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1268/2707 (47%)	1268 (100%)	0	100	100
1	C	1268/2707 (47%)	1268 (100%)	0	100	100
2	D	20/198 (10%)	20 (100%)	0	100	100
2	E	20/198 (10%)	20 (100%)	0	100	100
2	F	20/198 (10%)	20 (100%)	0	100	100
All	All	3864/8715 (44%)	3864 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1542	HIS
1	C	2598	ASN
1	B	2484	GLN
1	C	1713	ASN
1	B	1713	ASN

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.