



wwPDB EM Map/Model Validation Report ⓘ

Oct 10, 2016 – 11:29 AM EDT

PDB ID : 5LKH
EMDB ID: : EMD-4068
Title : Cryo-EM structure of the Tc toxin TcdA1 in its pore state (obtained by flexible fitting)
Authors : Gatsogiannis, C.; Merino, F.; Prumbaum, D.; Roderer, D.; Leidreiter, F.; Meusch, D.; Raunser, S.
Deposited on : 2016-07-22
Resolution : 3.46 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

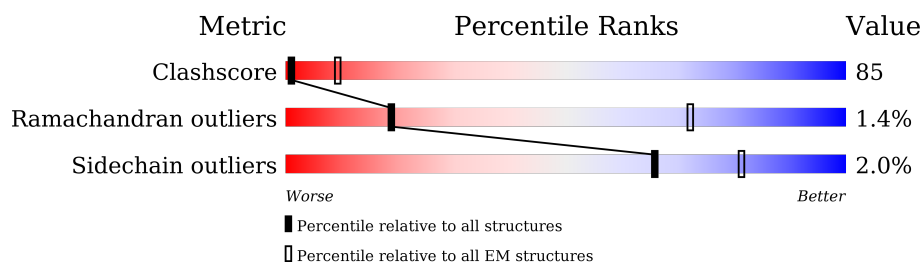
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. 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. 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	2516	12% 24% • 62%
1	B	2516	12% 24% • 62%
1	C	2516	12% 24% • 62%
1	D	2516	12% 24% • 62%
1	E	2516	12% 24% • 62%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 37345 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.

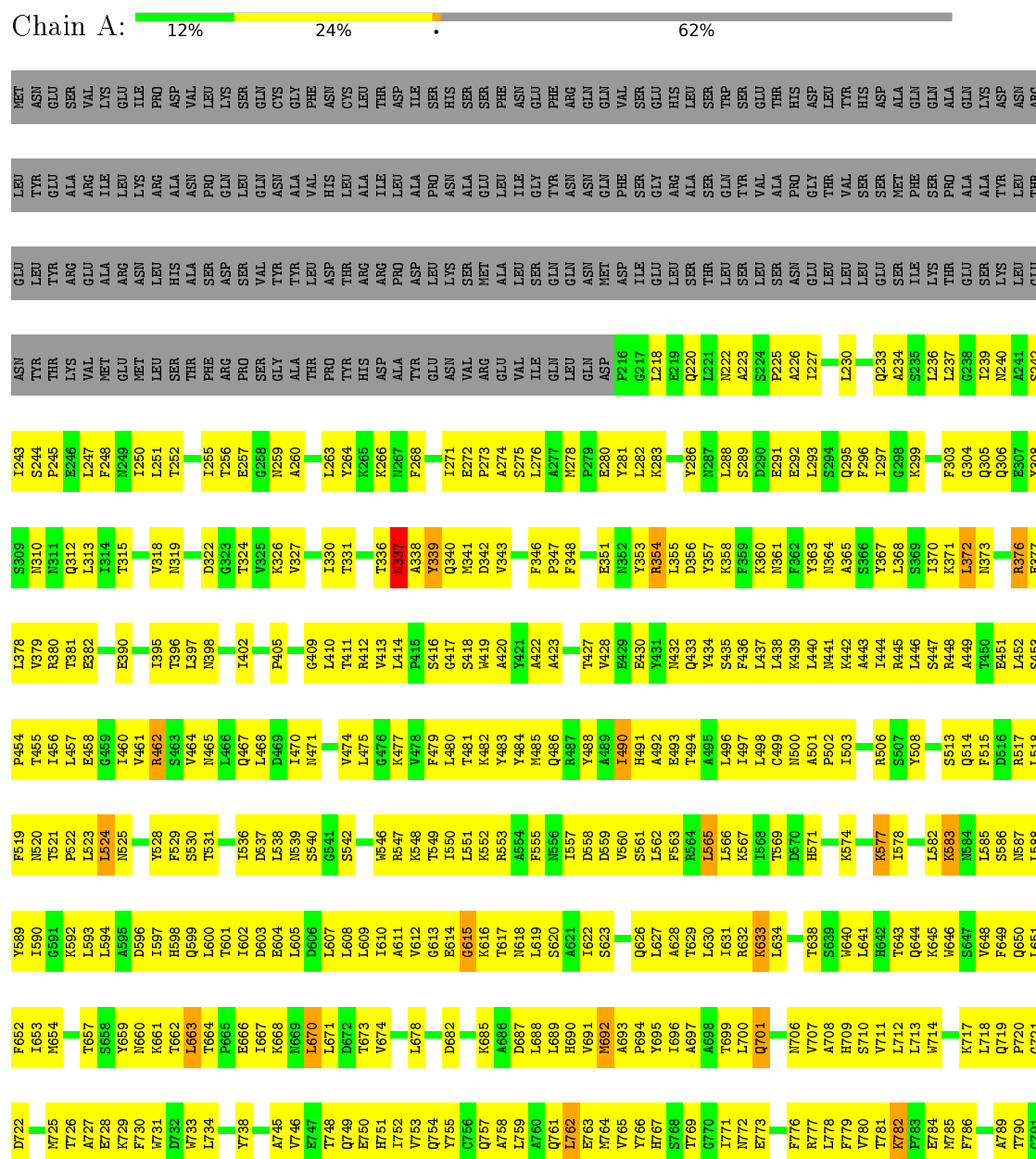
- Molecule 1 is a protein called TcdA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		
1	B	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		
1	C	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		
1	D	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		
1	E	948	Total	C	N	O	S	0	0
			7469	4751	1240	1458	20		

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 errors 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: TcdA1






[illegible]

- Molecule 1: TcdA1

Chain B: 12% 24% . 62%

L378	S309	T243	ASN	GLU	LEU	MET
V379	N310	S244	THR	LEU	TYR	ASN
R380	N311	P245	TYR	TYR	GLU	GLY
T381	Q312	E246	LVS	ARG	ALA	SER
E382	L313	L247	VAL	GLU	ARG	ALA
	T314	P248	MET	ALA	ILE	LVS
E390	T315	T249	GLU	ARG	LEU	GLU
			MET	ASN	LVS	ILE
I395	V318	L251	SER	LEU	ARG	ASP
T396	N319	T252	LEU	LEU	ALA	ASP
L397			THR	ALA	ASN	VAL
N398	D322	T255	THR	PHE	LEU	LEU
	G323	T256	ARG	ASP	PRQ	PHE
I402	T324	E257	PRQ	SER	GLN	LVS
	V325	G258	SER	VAL	GLN	SER
P405	K326	K259	GLY	TYR	ASN	CYS
	V327	A260	ALA	TYR	ALA	GLY
			THR	LEU	VAL	PHE
G409	I330	L263	PRQ	ASP	HIS	ASN
L410	T331	Y264	TYR	THR	CYS	LEU
R412		K265	HIS	ARG	ALA	LEU
V413	T336	T266	ASP	ARG	ILE	THR
P415	R337	T267	ALA	PRQ	LEU	ASP
S416	A338	F268	TYR	ASP	ALA	ILE
G417	T339		GLU	LEU	PRQ	SER
S418	Q340	T271	ASN	LVS	ASN	HIS
W419	N341	E272	VAL	SER	ALA	SER
A420	D342	P273	GLU	MET	GLU	SER
	V343	A274	GLU	ALA	LEU	PHE
Y421		S275	VAL	LEU	ILE	ASN
A422	F346	L276	ILE	SER	GLY	GLU
A423	P347	T277	GLN	GLN	TYR	PHE
	F348	T278	LEU	ASN	ASN	ARG
T427		P279	GLN	ASN	GLN	GLN
V428	E351	E280	ASP	MET	GLN	VAL
E429	N352	Y281	P216	ASP	PHE	SER
E430	T353	L282	G217	ILE	SER	SER
Y431	R354	K283	L218	GLU	GLY	GLY
N432	L355		E219	LEU	ARG	HIS
Q433	D356		Q220	SER	ALA	LEU
Y434	T357	Y286	N221	THR	SER	SER
S435	K358	L288	N222	LEU	GLN	TRP
F436	F359	S289	A223	SER	TYR	GLN
L437	K360	D290	S224	LEU	VAL	GLU
L438	N361	E291	A225	SER	ALA	SER
K439	F362	E292	A226	ASN	PRQ	HIS
L440	Y363	L293	I227	GLU	GLY	ASP
N441	N364	S294		LEU	THR	LEU
K442	A365	Q295	T230	LEU	VAL	TYR
A443	S366	F296		GLU	SER	HIS
L444	T367	T297	Q233	GLU	SER	SER
R445	L368	G298	A234	SER	MET	ALA
L446	S369	K298	S235	ILE	PHE	PHE
S447	I370		L236	LVS	SER	GLN
R448	K371	G304	L237	THR	PRQ	GLN
A449	L372	Q305	G238	GLU	ALA	ALA
	N373	Q306	T239	SER	ALA	LVS
			N240	LVS	TYR	ASN
L452	R376	E307	A241	LEU	LEU	THR
P454	P377	Y298	S242	GLU	TYR	ASN




Molecule 1: TcdA1

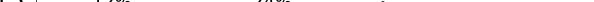
Chain C:

12%

24%

62%

- Molecule 1: TcdA1

Chain C:  12% 24% 62%

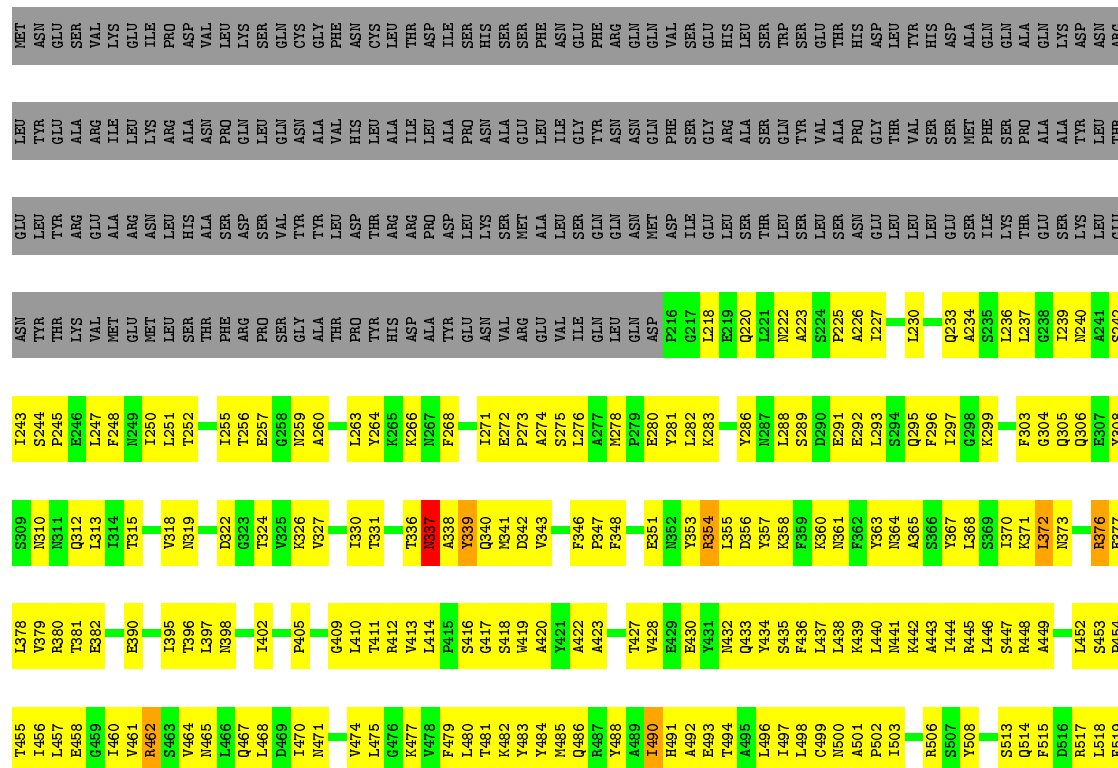
ARG	LEU	GLY	ASP	ILE	LEU	N866	F794	T726	1653	I590	M520	T455	L378	S309	I243	ASN	GLU	LEU	THR
LEU	TYR	THR	PRO	ALA	GLU	A867	A795	A727	M694	G591	T521	I456	V379	S310	S244	TYR	LEU	TYR	LEU
LEU	LEU	THR	MET	ALA	GLN	S868	D797	A728	T657	K392	P522	E458	R380	R311	E245	THR	TYR	ARG	ALA
TRP	ILE	PHE	ARG	ILE	GLN	C870	A798	K729	S658	L594	L523	E459	E382	R312	L247	MET	ALA	ARG	ALA
LEU	GLY	SER	ILE	ALA	ASN	M871	F799	K730	M659	A595	M525	I460	E390	T314	F248	GLU	ARG	LEU	ILE
GLU	LEU	LEU	GLN	ILE	THR	T872	S800	A731	M660	D596	Y528	V461	E390	T315	D249	MET	ASN	ARG	LEU
GLN	THR	LEU	THR	ILE	THR	S873	L801	D732	K661	I597	F529	R462	T395	V318	L250	LEU	LEU	LEU	ARG
LYS	GLU	LYS	THR	GLN	HIS	N875	I802	K733	T662	H598	S530	S463	T396	R319	L251	SER	HIS	LEU	ARG
GLU	THR	THR	MET	LEU	THR	N876	L804	L734	L663	Q999	T531	V464	L397	R397	T252	ALA	ALA	ALA	ASN
ILE	ASP	ASP	MET	VAL	PHE	I877	T805	Y738	T664	L800	Y531	M465	L397	T319	A260	VAL	VAL	VAL	VAL
THR	ALA	THR	ASP	ASN	LEU	L878	P806	Y738	E865	T601	I536	D467	N398	D322	T255	PRO	PHE	PRO	GLN
LYS	GLY	GLY	ALA	ARG	ASP	Q879	F807	A745	E866	L602	D537	L468	I402	T324	E257	ASP	ASP	ASP	GLN
GLN	GLU	GLU	LEU	ALA	GLU	M880	A808	V746	E867	D603	L538	L469	L402	T325	G258	VAL	SER	SER	LEU
GLY	THR	THR	LEU	LEU	SER	N881	D809	E747	E868	B504	M539	L470	P405	V326	G259	TYR	TYR	TYR	GLN
ASN	TRP	TRP	GLN	GLU	ARG	N882	M810	E748	L670	D806	S540	M471	P405	V327	A260	ALA	TYR	ALA	ALA
N883	ASN	ASN	SER	ASN	SER	N883	V811	Q749	L671	G541	G541	G409	G409	V327	T260	THR	LEU	VAL	VAL
ALA	ALA	ALA	ALA	ALA	ALA	Q884	L814	E750	E869	L608	S542	V474	L410	T330	L263	HIS	ASP	HIS	HIS
PRO	PRO	PRO	PRO	PRO	PRO	Q885	L814	H751	T673	L609	S542	L475	T411	T331	Y264	LEU	THR	LEU	LEU
GLN	GLN	GLN	GLN	GLN	GLN	Q886	L814	H752	T674	I610	M546	G476	R412	T336	T265	ALA	ARG	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	N887	V821	V753	E870	A611	K547	K477	V413	R337	K266	ILE	ARG	ILE	ILE
THR	THR	THR	THR	THR	THR	N888	L822	Q754	L678	V612	K548	V478	L414	R337	K267	PRO	PRO	PRO	PRO
LYS	LYS	LYS	LYS	LYS	LYS	V889	A823	Y755	L678	G613	T549	F479	P415	A338	N267	ALA	ASP	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	Q889	F825	Q757	D682	B614	L550	L480	Q417	A338	F268	PRO	LEU	PRO	PRO
GLY	GLY	GLY	GLY	GLY	GLY	Q890	F825	Q757	D682	G615	L551	T481	Q417	A338	F268	ASN	LYS	ASN	ASN
THR	THR	THR	THR	THR	THR	N891	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	N892	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
LEU	LEU	LEU	LEU	LEU	LEU	N893	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	N894	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
TRP	TRP	TRP	TRP	TRP	TRP	N895	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	N896	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	N897	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	N898	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASN	ASN	ASN	ASN	ASN	ASN	N899	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N900	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
PRO	PRO	PRO	PRO	PRO	PRO	N901	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
LEU	LEU	LEU	LEU	LEU	LEU	N902	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N903	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	N904	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	N905	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	N906	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASN	ASN	ASN	ASN	ASN	ASN	N907	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N908	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
PRO	PRO	PRO	PRO	PRO	PRO	N909	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
LEU	LEU	LEU	LEU	LEU	LEU	N910	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N911	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	N912	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	N913	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	N914	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASN	ASN	ASN	ASN	ASN	ASN	N915	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N916	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
PRO	PRO	PRO	PRO	PRO	PRO	N917	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
LEU	LEU	LEU	LEU	LEU	LEU	N918	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N919	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	N920	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	N921	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	N922	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASN	ASN	ASN	ASN	ASN	ASN	N923	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N924	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
PRO	PRO	PRO	PRO	PRO	PRO	N925	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
LEU	LEU	LEU	LEU	LEU	LEU	N926	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N927	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	N928	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	N929	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	N930	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASN	ASN	ASN	ASN	ASN	ASN	N931	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N932	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
PRO	PRO	PRO	PRO	PRO	PRO	N933	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
LEU	LEU	LEU	LEU	LEU	LEU	N934	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N935	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	N936	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	N937	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	N938	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASN	ASN	ASN	ASN	ASN	ASN	N939	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N940	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
PRO	PRO	PRO	PRO	PRO	PRO	N941	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
LEU	LEU	LEU	LEU	LEU	LEU	N942	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N943	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	N944	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	N945	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	N946	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
ASN	ASN	ASN	ASN	ASN	ASN	N947	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
THR	THR	THR	THR	THR	THR	N948	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
PRO	PRO	PRO	PRO	PRO	PRO	N949	L824	H757	E871	K616	R552	K482	S418	Q340	L271	VAL	SER	ALA	ALA
LEU	LEU	LEU	LEU	LEU	LEU	N950	L824	H757	E871	K616	R552								









T1556	E1488	T1414	Y1352	T19	LEU	GLY	ASP	ILE	N866	P794	T726	L653	L590	N520
A1557	I1489	S1415	I1353	ARG	LEU	THR	THR	ALA	A867	A795	A727	M654	G591	T521
F1558	N1490		S1354	ASN	LYS	TYR	THR	GLU	F868	D797	E728		K592	P522
A1559	T1491	Q1419	P1355	THR	LEU	TYR	THR	ILE	C870	A798	E729		L593	L523
E1560	A1492	G1420	K1356	ARG	LEU	PHE	ARG	ALA	M871	L799	K729		L594	L524
D1561	A1493	R1421	L1357	THR	LEU	GLY	ILE	SER	T872	S800	F730		A595	N525
G1562	S1494	L1422	R1358	GLN	PRO	LEU	GLN	SER	T873	L401	D732		D596	
A1563	P1495	L1423	I1359	PHE	GLY	LEU	THR	ILE	S874	1802	K661		L597	T528
K1564	A1496	F1424	I1360	THR	LEU	SER	THR	GLN	S875	1803	T662		H598	F529
L1565	K1497	H1425	H1361	ASP	TYR	GLU	LYS	LEU	N875	N803	L663		Q599	S530
G1566	T1498	N1362	N1361	THR	CYS	GLU	THR	TYR	T876	L804	T664		L600	T531
Y1567	Q1499	D1427	G1363	ASN	ILE	ASP	MET	VAL	I877	T805	P665		T601	
	L1500	Y1364	Y1364	GLY	THR	ALA	ASP	ASN	L878	R806	E666		L602	L536
F1570	I1501	T1428	E1365	VAL	LYS	GLY	ALA	ARG	Q879	F807	L667		D603	D537
S1571	P1502	Y1430	G1366	ARG	GLN	GLU	LEU	ALA	M880	A808	T668		E804	L538
I1572	K1503		I1367	VAL	GLY	TYR	THR	LEU	V881	D809	L669		L605	N539
P1573		K1433	K1368	VAL	GLU	GLY	THR	GLN	N882	N810	L670		D606	S540
Y1574	Q1509	Y1434	R1369	ASN	ASP	TRP	SER	ASN	N883	V811	L671		L607	G541
T1575	T1510		N1370	ASN	THR	ARG	VAL	VAL	A884		D672		L608	S542
L1576	F1511	W1437	Q1371	ARG	LEU	SER	SER	GLU	Q885	L814	T673		L609	
K1577	T1512	I1438	C1372	LEU	LEU	VAL	GLN	GLU	Q886	W821	V674		L610	W546
S1579	A1513	G1440	N1373	MET	VAL	ASP	GLY	ASN	L887	L822	L678		A611	R547
		A1441	L1374	PHE	GLN	TYR	HIS	ALA	N888	N822			V612	K548
THR	D1516	K1442	M1375	THR	GLN	SER	GLN	ASN	V859	A824	C755		G613	T549
ASN	V1517	R1443	Y1378	ASN	GLY	PHE	ALA	GLY	PRO	F825	Q757		G615	L551
ALA	S1518		G1379	GLN	ASN	ASN	ASP	VAL	GLN	S829	A758		K616	
LEU	I1519	M1447	K1380	ASP	THR	THR	THR	ILE	GLN	L830	L686		T617	R553
THR	P1521	Q1448	L1381	ASP	TYR	GLY	VAL	SER	VAL	T831	Q761		N618	A554
LEU	S1522		G1382	THR	ARG	LYS	GLU	ARG	SER	A832	A760		L619	F555
HIS	P1523	I1452	N1383	LEU	TYR	PHE	ASP	GLN	ALA	E833	L762		S620	N566
ASN	S1524		K1384	ASP	GLU	ALA	ALA	PHE	LEU	B333	E763		L631	L557
ASN	F1525	Y1456	F1385	SER	LEU	ALA	PHE	PHE	VAL	Q834	M764		L622	D558
ASN	D1526		L1386	TYR	LEU	ASN	MET	ILE	GLY	L835	V765		S623	D559
GLY	E1527	D1459	V1387	ASN	ALA	ALA	SER	ASP	LEU		Y766			V560
ALA	M1528		Y1322	ASN	ALA	TRP	TYR	TRP	ASP	W839	H767		Q626	S561
GLN	M1529	M1462	G1323	ALA	HIS	SER	LEU	ASP	TYR	D842	T769		L627	L562
GLN	Y1530	K1463	W1324	SER	ILE	GLU	THR	LYS	ILE	A843	L696		A628	F563
TYR	Q1531	P1464	G1325	MET	ARG	TRP	SER	TYR	GLN	N844	A697		T629	R564
MET	F1532	D1465	D1326	GLN	TYR	HIS	PHE	ASN	SER	L845	I771		L630	L565
GLN		D1466	Y1327	GLY	ASP	LYS	GLU	LYS	MET	L346	N772		R631	L566
TRP	E1536	L1467	P1395	LEU	GLY	ILE	GLN	ARG	LYS	L847	E773		R632	K567
GLN	I1537	K1468	Y1328	TYR	THR	ASP	VAL	TYR	GLU	Q848	Q701		K633	L568
SER	D1538	Q1469	N1397	ILE	TRP	CYS	ALA	SER	THR	A849	F776		L634	T569
TYR	G1539	Y1470	S1398	PHE	ASN	PRO	ASN	THR	PRO	Q849	K777		D570	
ARG	S1540	I1471	S1399	ALA	THR	ILE	ASN	THR	THR	A849	L778		T638	H571
THR	F1541	F1472	N1400	ASP	PRO	LEU	LYS	ALA	TYR	S850	V707		S639	
ARG	G1542	M1473	I1337	MET	ILE	GLY	VAL	GLY	F779	T851	A708		W640	K574
LEU	L1543	T1474	K1401	ALA	THR	ILE	THR	VAL	V780	Q852	H709		L641	
ASN	F1544		L1402	SER	PHE	LYS	SER	SER	T781	A853	S710		W642	
THR		G1478	M1403	LYS	ASP	SER	ALA	GLN	K782	Q854	V711		H642	
LEU	M1547	T1479	Y1405	VAL	VAL	THR	TYR	LEU	F783	L712	L712		T643	L578
PHE	S1548	A1480	P1406	ASN	THR	ILE	TYR	VAL	E784	L713	Q644		Q644	L582
ALA	A1549	T1481	Y1342	MET	LYS	ARG	ASP	ALA	M785	W714	K645		W646	K583
ARG	S1550	D1482	Y1408	PRO	LYS	PRO	ASN	ALA	F786	L859	K646		S647	N584
GLN	L1551	Y1483	Q1409	GLU	ILE	VAL	ILE	ALA	A789	P860	V648		S647	L585
LEU	D1552	S1484	Y1410	SER	THR	ILE	ASN	GLY	T780	L718	V648		F649	S586
VAL	V1553	G1485	G1411	SER	GLU	TYR	ASN	VAL	A791	P720	Q650		Q650	N587
ALA	T1554	P1486	G1412	ASN	LEU	THR	ASP	THR	G792	L651	L651		L651	L588
ARG	F1555	V1487	M1413	VAL	LYS	SER	GLN	ILE	A793	D722	F652		F652	Y589




4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	13000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	Not provided	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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.89	0/7627	1.14	20/10362 (0.2%)
1	B	0.89	0/7627	1.14	20/10362 (0.2%)
1	C	0.89	0/7627	1.14	20/10362 (0.2%)
1	D	0.89	0/7627	1.14	20/10362 (0.2%)
1	E	0.89	0/7627	1.14	20/10362 (0.2%)
All	All	0.89	0/38135	1.14	100/51810 (0.2%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1541	GLY	C-N-CA	9.54	145.55	121.70
1	B	1541	GLY	C-N-CA	9.53	145.53	121.70
1	E	1541	GLY	C-N-CA	9.52	145.49	121.70
1	A	1541	GLY	C-N-CA	9.51	145.49	121.70
1	D	1541	GLY	C-N-CA	9.51	145.47	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	615	GLY	Peptide
1	B	615	GLY	Peptide
1	C	615	GLY	Peptide
1	D	615	GLY	Peptide
1	E	615	GLY	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	7469	0	7341	1262	0
1	B	7469	0	7341	1262	0
1	C	7469	0	7341	1271	0
1	D	7469	0	7341	1254	0
1	E	7469	0	7341	1268	0
All	All	37345	0	36705	6317	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 85.

The worst 5 of 6317 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:C:557:ILE:HD11	1:C:592:LYS:HD2	1.21	1.21
1:C:218:LEU:HD21	1:C:239:ILE:HG21	1.19	1.18
1:A:1406:PRO:HG3	1:A:1473:MET:HE1	1.22	1.17
1:A:557:ILE:HD11	1:A:592:LYS:HD2	1.21	1.17
1:E:227:ILE:HD13	1:E:883:VAL:HB	1.26	1.16

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	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	14	56
1	B	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	14	56
1	C	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	14	56
1	D	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	14	56
1	E	944/2516 (38%)	899 (95%)	32 (3%)	13 (1%)	14	56
All	All	4720/12580 (38%)	4495 (95%)	160 (3%)	65 (1%)	19	56

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ARG
1	A	525	ASN
1	A	1346	SER
1	A	1381	LEU
1	A	1542	LEU

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	817/2157 (38%)	801 (98%)	16 (2%)	63	86
1	B	817/2157 (38%)	801 (98%)	16 (2%)	63	86
1	C	817/2157 (38%)	801 (98%)	16 (2%)	63	86
1	D	817/2157 (38%)	801 (98%)	16 (2%)	63	86
1	E	817/2157 (38%)	801 (98%)	16 (2%)	63	86
All	All	4085/10785 (38%)	4005 (98%)	80 (2%)	66	86

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	583	LYS
1	C	1306	TYR
1	E	762	LEU
1	C	633	LYS
1	C	701	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	340	GLN
1	C	1361	HIS
1	E	767	HIS
1	C	441	ASN
1	C	650	GLN

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.