



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 02:18 AM EDT

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

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

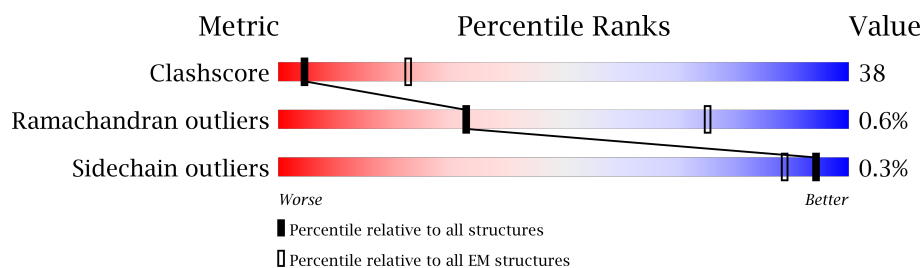
1 Overall quality at a glance

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.



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	 30% 27% . 43%
1	B	2516	 30% 27% . 43%
1	C	2516	 30% 27% . 43%
1	D	2516	 30% 26% . 43%
1	E	2516	 29% 27% . 43%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 55415 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	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0
1	B	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0
1	C	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0
1	D	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0
1	E	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0



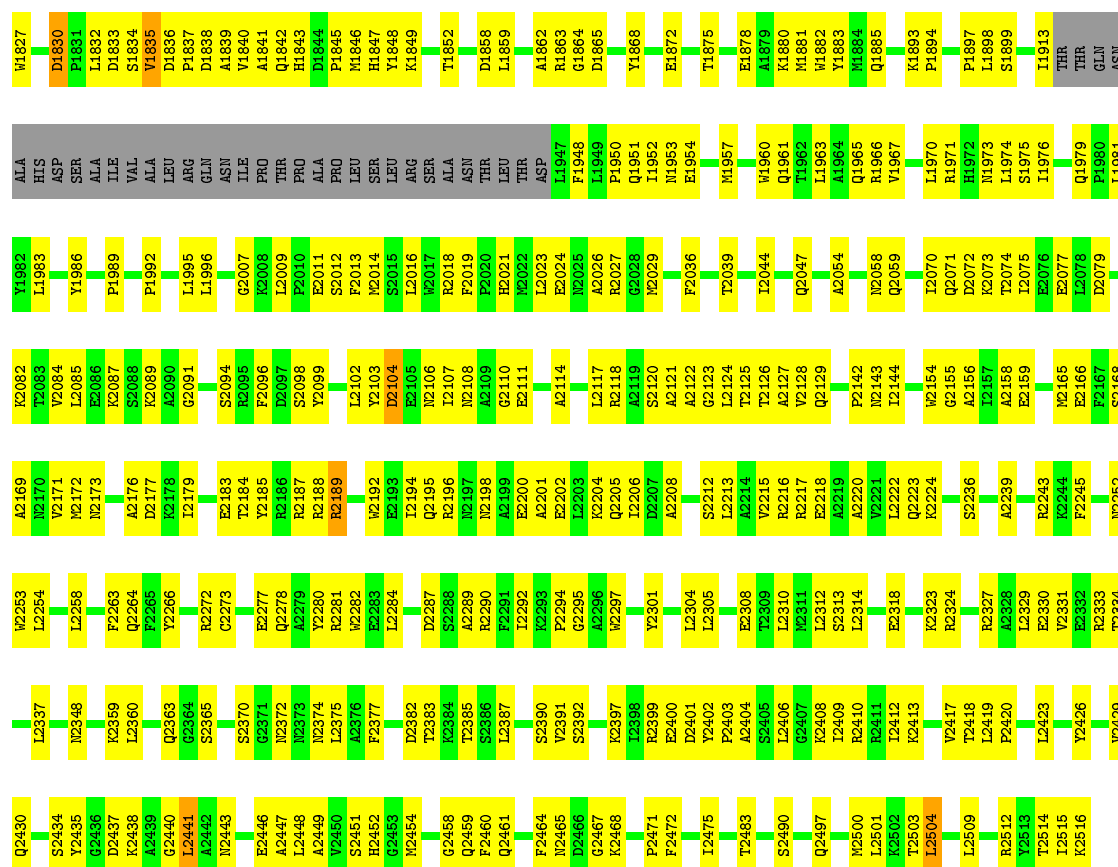

P1989	K2087	A2176	N2252	V2429
P1992	S2088	D2177	W2253	Q2430
L1995	K2089	K2178	L2254	S2434
L1996	G2091	I2179	L2258	Y2435
G2007	S2094	E2183	F2263	G2436
K2008	R2095	T2184	Q2264	D2437
L2009	R2096	Y2185	F2265	K2438
P2010	D2097	Y2186	Y2266	A2439
E2011	S2098	R2187	R2272	G2440
S2012	Y2099	R2188	C2273	L2441
F2013	L2102	R2189	G2277	A2442
M2014	Y2103	W2192	E2277	N2443
S2015	D2104	E2193	Q2278	E2446
L2016	E2105	I2194	A2279	A2447
W2017	N2106	Q2195	L2280	L2448
R2018	I2107	R2196	R2281	L2449
F2019	N2108	R2197	W2282	Y2450
P2020	A2109	N2198	E2283	S2451
H2021	G2110	A2199	E2284	H2452
M2022	E2111	E2200	L2284	M2454
L2023	A2114	A2201	D2287	G2458
E2024	N2025	E2202	S2288	Q2459
N2026	L2117	L2203	A2289	Q2460
R2027	R2118	Q2204	R2290	Q2461
G2028	R2119	Q2205	F2291	
M2029	A2119	I2206	I2292	
F2036	S2120	D2207	K2293	F2464
T2039	A2121	A2208	P2294	N2465
I2044	A2122	Q2209	G2295	D2466
Q2047	G2123	L2210	A2296	G2467
A2054	L2124	K2211	W2297	K2468
N2058	T2125	S2212	Y2301	P2471
Q2059	T2126	L2213	L2305	F2472
I2070	A2127	V2215	E2308	E2473
Q2071	V2128	R2216	T2309	G2474
D2072	Q2129	R2217	L2310	I2475
K2073	P2142	E2218	G2311	T2483
T2074	N2143	A2219	K2312	S2490
I2075	I2144	Y2221	L2313	Q2497
E2076	W2154	L2222	S2313	M2500
E2077	G2155	Q2223	L2314	L2501
L2078	A2156	K2224	E2318	T2503
D2079	I2157	Q2233	K2323	L2504
K2082	E2158	S2236	R2324	L2509
T2083	M2165	A2239	R2327	Y118
V2084	E2166	R2243	A2328	L119
L2085	F2167	R2244	L2329	T120
E2086	S2168	F2245	V2330	G2423
	N2170	L2250	E2332	T2514
	V2171	L2251	T2334	L2515
	M2172			R2333
	N2173			Y2426

• Molecule 1: TcdA1

Chain B: 30% 27% 43%

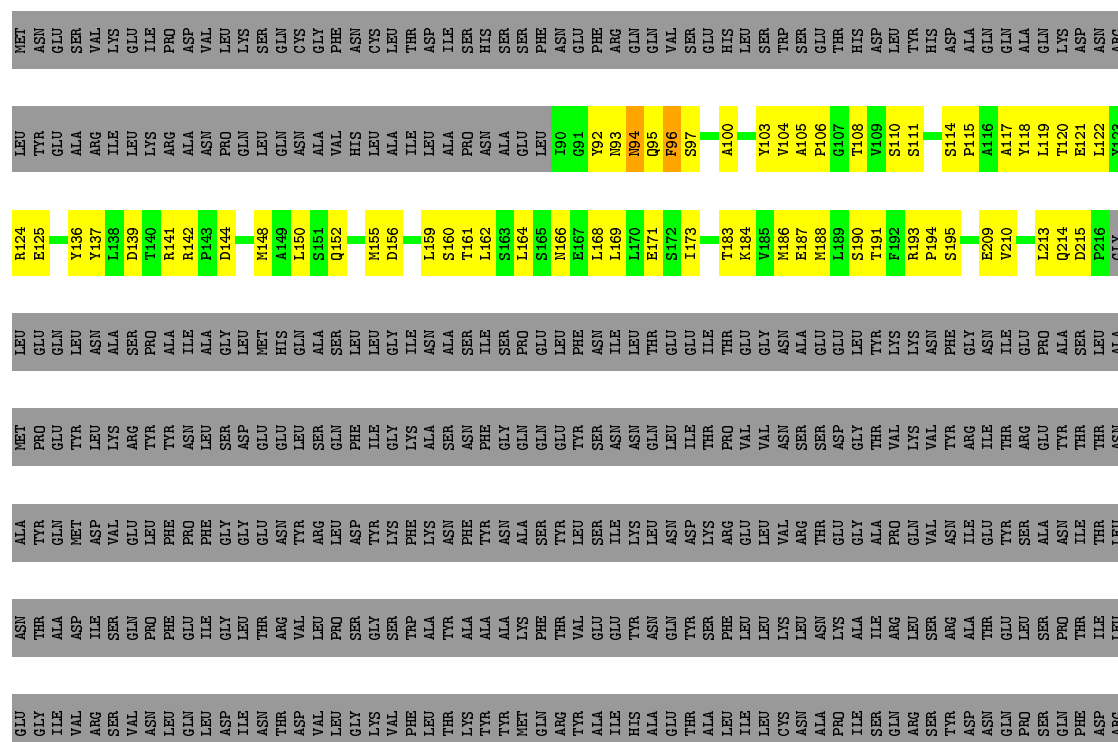
MET	LEU	R124	P216	THR	THR	TLE	ASP	GLY
ASN	TYR	E125	GLY	ALA	LEU	LEU	ARG	LYS
GLU	ALA	L129	LEU	MET	GLU	THR	ASN	ILE
SER	GLU		GLN	PRO	GLU	THR	ASN	THR
VAL	ARG	Y136	LEU	GLN	ASP	ASP	THR	LEU
LYS	ILE	Y137	ASN	TYR	ILE	ILE	PRO	LEU
GLU	LYS	L138	ALA	LEU	SER	SER	LEU	LYS
ILE	PRO	D139	ARG	LYS	ARG	VAL	LEU	ASN
PRO	ARG	R140	TYR	ARG	TYR	GLN	LEU	VAL
ASP	ALA	T141	PRO	TYR	PRO	PRO	ASN	ASN
VAL	VAL	R142	ALA	TYR	GLU	GLU	ASN	LEU
LEU	PRO	P143	ILE	ASN	GLU	ILE	GLN	GLN
LYS	GLN	D144	ALA	LEU	PHE	PHE	LEU	LEU
SER	LEU		GLY	SER	GLY	GLY	ASP	THR
GLN	ASN	M148	LEU	ASP	GLY	GLY	ILE	ILE
CYS	GLN	A149	MET	GLU	GLU	THR	THR	GLY
PHE	ALA	L150	HIS	GLU	GLU	ARG	GLY	LYS
ASN	VAL	S151	GLN	LEU	TYR	ASN	ASP	LEU
CYS	HIS	Q152	ALA	SER	VAL	VAL	GLU	LEU
ILE	LEU	D155	SER	LEU	LEU	LEU	GLU	ALA
ALA	ALA	M156	LEU	PHE	PRO	PRO	ASP	ASP
LEU	LEU		ILE	GLY	GLY	GLY	ILE	ILE
ILE	ILE	L159	ILE	LYS	TRP	TRP	ASN	HIS
THR	LEU	S160	ALA	THR	ASN	ALA	ASN	GLN
ASP	PRO	T161	ASN	LYS	ASN	LYS	SER	LEU
GLY	ALA	L162	ALA	THR	PHE	ALA	GLY	THR
PHE	GLU	S163	SER	GLY	ASN	ALA	THR	ILE
GLU	PRO	L164	PRO	GLN	GLY	ALA	ASP	GLY
PHE	G91	S165	GLU	GLN	ASN	LYS	TRP	ASP
GLU	Y92	N166	LEU	GLY	THR	PHE	ARG	LEU
THR	N93		PHE	TYR	LEU	VAL	LYS	LEU
GLN	N94	L169	ASN	SER	LEU	GLU	THR	LEU
VAL	Q95	L170	ILE	ASN	THR	GLU	PHE	GLY
SER	F96	E171	LEU	LYS	ASN	THR	ASN	LYS
GLU	S97	S172	THR	GLN	LEU	ASN	ASP	THR
	A100	I173	GLU	LEU	ILE	ASN	THR	ARG
	Y103	Y182	THR	ILE	THR	LYS	THR	ALA
	V104	T183	THR	THR	PRO	VAL	ASN	ALA
	TRP	K184	GLU	THR	GLU	VAL	THR	THR
	SER	V185	GLY	GLY	VAL	LEU	THR	LEU
	SER	A105	ASN	ASN	VAL	LYS	LEU	ASN
	GLU	P106	THR	ALA	ASN	LEU	ASP	SER
	THR	G107	ALA	THR	ARG	LEU	VAL	THR
	HIS	V108	GLU	SER	THR	ASN	ASN	LEU
	ASP	L189	LEU	ASP	GLY	GLY	ALA	ALA
	LEU	S190	LEU	GLY	GLY	ILE	PHE	THR
	TYR	T191	LYS	THR	ALA	THR	THR	GLN
	HIS	F192	LYS	VAL	PRO	ARG	LEU	ASN
	ASP	S114	LYS	GLN	GLN	LEU	LEU	GLN
	ALA	P115	VAL	VAL	VAL	LEU	LYS	LEU
	GLN	A116	THR	ASN	THR	ARG	SER	LEU
	ALA	L117	GLY	PHE	ASN	THR	ILE	ALA
	ALA	Y118	ASN	GLY	ILE	ARG	THR	THR
	LYS	L119	LEU	THR	THR	THR	LEU	GLY
	GLN	T120	ILE	THR	THR	THR	GLU	PRO
	LYS	G2423	GLU	ARG	ARG	ARG	LEU	ASN
	ASP	T2514	PRO	ALA	ALA	ALA	SER	LYS
	R2333	L122	TYR	ASN	THR	THR	ASN	LEU
	ARG	K2516	SER	ILE	THR	THR	ASP	ASN



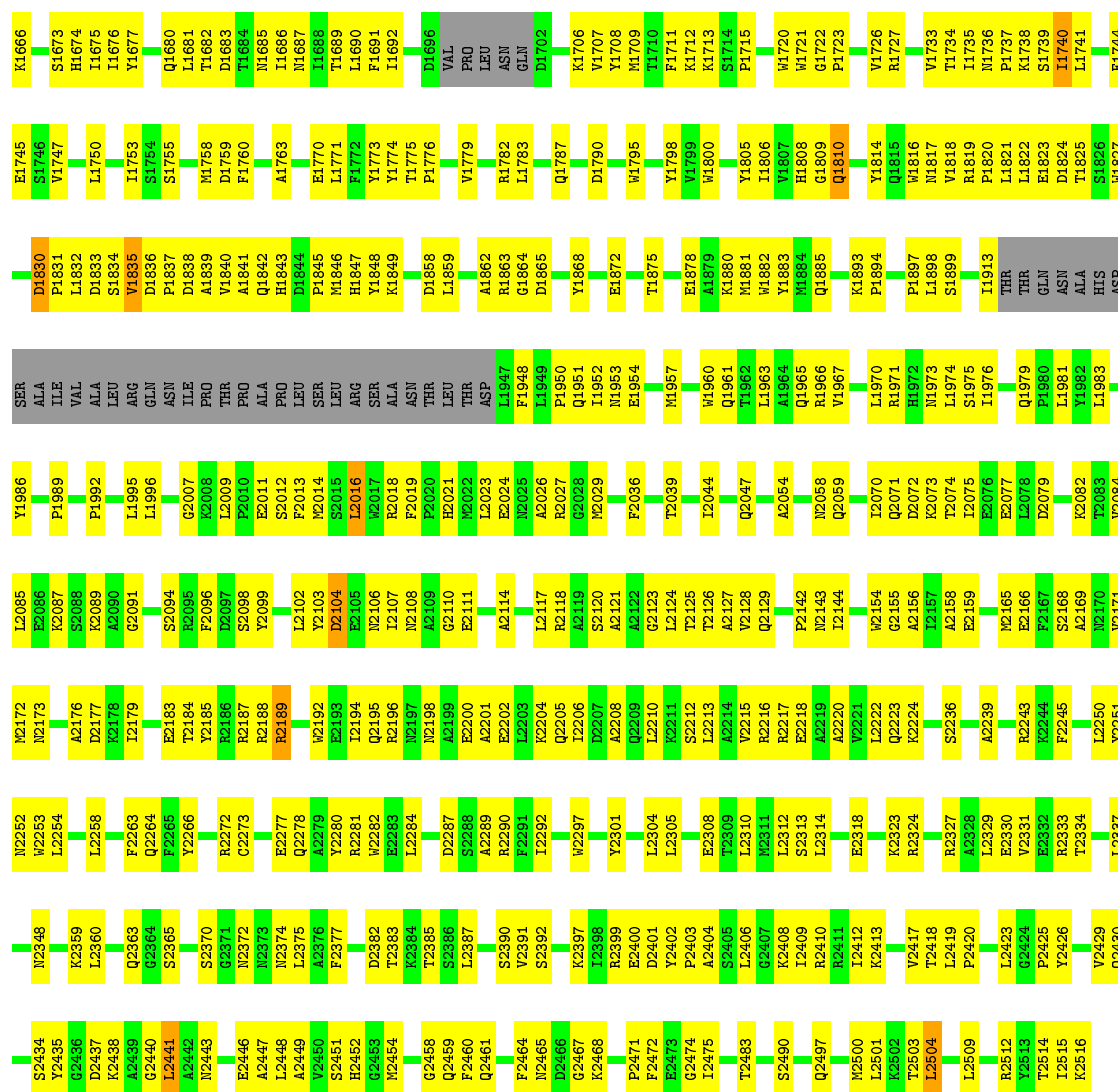



- Molecule 1: TcdA1

Chain C: 30% 27% . 43%

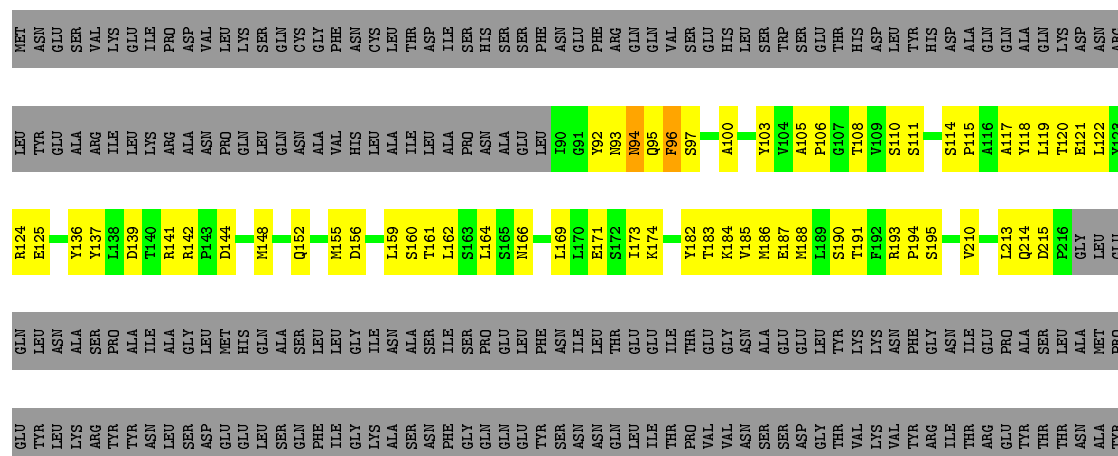


Q1594	MET	LYS	TYR	ASP	V1285	H1202	K1130	Y1044	I973	LEU	ALA	ALA	ALA	THR	THR	ILE	LEU
Y1595	ASN	GLN	GLN	LEU	Y1286	I1203	F1131	I1045	D974	GLN	SER	SER	SER	LEU	SER	LYS	PHE
M1596	GLN	ILE	SER	ILE	R1287	R1204	N1132	D1046	M975	TRP	VAL	VAL	VAL	ALA	TRP	ASN	ASN
Q1597	PHE	PHE	GLY	TYR	S1290	Y1205	D1133		Q976	ASN	ASN	ASN	ASN	LEU	HIS	LYS	PRO
W1598	ASN	MET	ASN	ILE	Y1291	G1207	K1135	R1049	S978	VAL	ALA	ALA	ALA	SER	THR	GLN	LEU
W1599	ALA	THR	THR	SER	Q1292	T1208	F1136	Q1083	I981	GLN	PHE	VAL	VAL	GLU	GLN	ASN	LEU
Q1600	LEU	ASP	SER	PRO	Q1293	W1209	A1137	T1094	K982	GLN	GLU	TYR	TYR	GLU	LYS	SER	ASN
Y1601	GLU	SER	GLY	LYS	F1294	W1295	N1139	K1055	T983	LEU	ALA	HIS	HIS	VAL	TRP	ASN	GLY
R1602	ILE	LYS	LEU	LEU	Q1295		A1140	M1056	T984	ASN	ASN	SER	TYR	ALA	VAL	LEU	GLN
T1603	ASP	GLY	ASN	ARG	T1296	I1213	W1141	M1057	R985	VAL	SER	THR	PHE	HIS	PHE	TYR	PHE
R1604	GLY	THR	GLN	ILE		T1214	S1142	D1058	I986	ALA	THR	ILE	ILE	VAL	GLN	ILE	SER
L1605	SER	ALA	GLY	ARG	F1215		E1143	A1089									THR
W1606	GLY	THR	ARG	HIS			W1144	L1060									THR
A1610	LEU	ASP	LEU	ASN	R1300	N1218	W1145		T990	G899	ALA	ALA	ALA	LEU	THR	ASP	ILE
V1614	ASN	VAL	LEU	GLY	V1302	K1219	H1145		L900	L900	GLN	GLU	GLU	LEU	ILE	LYS	GLY
A1615	ILE	SER	PHE	THR	N1303	K1220	K1146	V1064	S992	D901	GLN	ASN	ASN	TRP	MET	LEU	GLU
R1616	ASN	PRO	ARG	GLY	T1305	I1221	P1153	Q1068	Q994	Y902	LEU	ALA	ALA	THR	SER	ASP	ILE
D1622	ALA	VAL	ASP	GLN	ALA	S1222	Y1154	L1069	L995	Q904	ASP	PHE	PHE	THR	THR	ASP	ASP
T1623	ALA	GLU	THR	LYS	GLU	E1223	Y1155			S905	LEU	ARG	ARG	THR	THR	ILE	ASP
I1624	SER	ILE	THR	ARG	ASP	L1225	S1156	D1072	N998	N906	MET	PHE	PHE	TYR	TYR	GLN	ASN
I1625	ASP	ALA	THR	GLN	ILE	L1226			R999	K907	ASN	VAL	VAL	ASN	THR	GLY	SER
S1626	VAL	ILE	LYS	ASN	PRO	E1227	P1160	F1078	A1000	E908	ASP	LYS	LYS	LYS	LYS	THR	SER
T1629	THR	SER	VAL	LYS	PRO	G1283	I1161	M1079	L1001	A918	ALA	PRO	LYS	THR	LEU	ILE	THR
Q1633	PHE	GLN	GLY	GLY	ARG	L1234	I1162	S1080	E1002		ASN	GLU	GLU	THR	THR	GLU	GLY
E1634	ALA	ILE	ALA	LEU	LYS	L1235	Y1171	Y1081	W1003	L922	LEU	MET	MET	PRO	PRO	LEU	ASP
P1635	GLU	ILE	ILE	LEU	ASP	T1244	E1172	K1092	I1013	N932	ILE	THR	THR	LEU	LEU	ALA	ILE
Q1636	GLY	VAL	VAL	LYS	TYR	L1245	Q1174	V1083	S1014	T933	GLN	ASP	ASP	ASP	VAL	VAL	LEU
G1638	ARG	LYS	LYS	ASP	GLY	L1246			R1045	R935	ALA	ALA	ALA	THR	THR	GLY	ARG
K1639	LYS	ALA	ALA	LYS	TRP	V1247	I1177	Y1097	R1016	A936	GLN	PRO	PRO	LEU	VAL	GLU	ALA
G1640	LEU	GLY	LEU	PHE	GLY	M1248	THR	H1098	F1017	F937	ASN	ALA	ALA	ASN	TYR	GLY	PHE
F1641	GLY	THR	THR	ILE	ASP	F1249	LYS	D1099	F1018	L938	HIS	HIS	HIS	THR	HIS	LYS	ASN
Y1642	TYR	LYS	ASN	VAL	ASP	Y1250	GLN	N1100	I1019	D939	GLN	ASP	ASP	LYS	GLY	THR	ILE
A1643	GLU	GLN	GLN	THR	TYR	N1251	THR	I1101	D1020		HIS	ALA	ALA	TYR	LEU	ASN	ASP
F1644	SER	ASN	ASN	THR	LEU		GLY	N1102	W1021	S947	LEU	LEU	LEU	THR	GLN	LEU	ASP
F1645	PHE	ALA	ALA	SER	SER	K1260	ASN	N1103		T948	PRO	SER	SER	PRO	GLY	VAL	VAL
V1646	SER	PHE	THR	ALA	MET	N1261	SER	D1104	M1025		ILE	LEU	LEU	ASP	PHE	SER	SER
I1647	ILE	THR	ILE	ILE	VAL		LYS	Q1105	K1026	T951	VAL	ILE	ILE	ASP	ASP	ALA	LEU
P1648	PRO	ALA	GLY	VAL	TYR	M1264	ASP	G1106	R1027	R952	THR	THR	THR	LYS	LYS	SER	PHE
P1649	VAL	ASP	ASP	ASN	ASN	Q1265	GLY	L1107	Y1028	Q953	PRO	MET	GLU	ASP	ASP	ASP	ARG
Y1650	THR	LYS	ASP	PRO	GLY	G1266	TYR	T1108	S1029	V954	GLU	THR	THR	ALA	LYS	LYS	LEU
N1651	LEU	ASP	TYR	ASN	ASP	L1267	GLN	Y1109	T1030		ASN	ARG	VAL	ALA	ALA	GLN	LEU
L1652	LYS	VAL	ALA	ASN	ILE	Y1268	THR	G1112	W1031	I961	ALA	PHE	THR	ASP	ASP	LYS	LYS
S1653	VAL	SER	THR	SER	PRO	I1269	GLU		A1032	K962	ALA	ALA	ALA	LEU	LEU	ILE	ILE
D1657	SER	ILE	ASP	SER	THR	F1270	THR	Y1122	G1033	S963	SER	ASP	THR	LEU	THR	THR	THR
E1658	GLN	GLN	SER	ASN	ILE	A1271	D1183	W1123	V1034	R964	CYS	TRP	TRP	HIS	VAL	ILE	HIS
R1659	PRO	SER	LEU	LYS	ASN	D1272		R1124		D965	ASN	ASN	ILE	VAL	VAL	ARG	LYS
W1660	SER	ASN	ASN	LYS	TYR		Y1196	S1125	Y1038	D966	THR	THR	THR	ALA	ALA	ASN	ASN
F1661	PRO	LYS	LYS	MET	LYS	S1275	E1197	R1149	Y1039	I967	ILE	THR	PRO	VAL	PRO	LEU	LYS
T1662	SER	PRO	PRO	PHE	ALA		L1198	V1126	Y1040	T968	THR	ILE	GLY	GLN	TYR	LEU	ASN
L1663	PHE	ASP	THR	THR	ALA	Q1282	K1199	D1127	P1041	Q969	ASN	THR	THR	TYR	ILE	THR	GLY
Y1664	ASP	ASP	ASP	PRO	SER	S1283	L1200	H1128	E1042	Y970	THR	THR	CYS	GLN	ALA	THR	THR
H1588	SER	VAL	LEU	VAL	SER	N1284	A1201	S1129	N1043		ILE					ILE	ILE



- Molecule 1: TcdA1

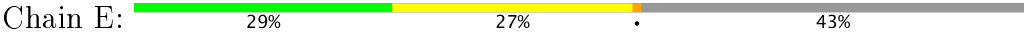
Chain D: 30% 26% • 43%



[illegible]

ALA	LEU	Q1599	Y1677	S1754	V1835	LEU	L1995	A2090	K2178	Q2264	Q2364	G2440
LEU	GLU	S1600	Q1680	S1755	D1835	ARG	L1996	G2091	I2179	F2265	S2365	L2441
ILE	I1601	R1602	L1681	M1758	D1838	GLN	L1996	S2094	E2183	Y2266	S2370	A2442
ASP	T1603	R1603	T1682	M1759	D1839	ILE	G2007	F2096	T2184	R2272	N2371	N2443
GLY	L1604	T1604	D1683	F1760	V1840	PRO	K2008	D2097	Y2185	C2273	N2372	E2446
SER	L1605	L1605	T1683	A1763	Q1841	THR	L2009	S2098	R1866	Q2277	N2373	L2446
GLY	M1606	M1606	M1685	A1763	Q1842	PRO	P2010	S2099	R1867	E2278	L2374	A2449
LEU	A1610	A1610	M1686	E1770	H1843	ALA	E2011	Y2099	R1868	Q2278	N2375	A2449
ASN	P1614	P1614	M1687	E1771	D1844	PRO	S2012	L2102	W2192	Y2280	D2382	S2451
PHE	A1615	A1615	M1688	F1772	M1845	LEU	F2013	Y2103	E2193	R2281	T2383	H2452
ILE	A1616	A1616	T1689	Y1773	M1846	SER	M2014	D2104	I2194	W2282	T2384	G2453
ASN	R1616	R1616	L1690	Y1774	H1847	LEU	S2015	E2105	I2194	E2283	T2385	M2454
SER	I1621	I1621	F1691	T1775	Y1848	ANG	L2016	E2106	Q2196	E2284	K2386	G2458
ALA	T1622	T1622	I1692	P1776	K1849	SER	W2017	N2106	R2197	L2284	T2387	Q2459
ILE	D1623	D1623	M1777	M1777	T1852	ASN	F2019	N2108	N2198	D2287	L2387	F2460
ASP	L1624	L1624	V1779	L1778	D1858	THR	P2020	A2109	A2199	A2288	S2390	Q2461
VAL	S1626	S1626	VAL	D1702	A1862	LEU	H2021	G2110	A1999	A2289	S2390	F2464
THR	T1629	T1629	LEU	R1782	R1863	ASP	E2022	E2111	E2200	F2291	V2391	N2465
THR	A1633	A1633	ASN	L1783	G1864	THR	N2025	A2114	L2203	I2292	S2392	D2466
PHE	E1634	E1634	GLN	Q1787	D1865	THR	A2026	L2117	K2204	W2297	K2397	G2467
ALA	E1635	E1635	K1706	D1790	Y1868	THR	G2028	R2118	Q2205	Y2301	I2398	K2468
GLU	Q1636	Q1636	Y1707	M1795	E1872	ASP	M2029	A2119	I2206	Y2301	R2399	P2471
ASP	L1637	L1637	M1708	M1795	E1872	ASP	E1954	S2120	D2207	L2304	E2400	F2472
ARG	G1638	G1638	T1710	M1800	T1875	LEU	P1950	R2118	L2206	L2305	D2401	G2473
GLY	K1639	K1639	F1711	Y1798	T1875	LEU	P1950	R2118	L2206	L2305	Y2402	P2474
LYS	Q1640	Q1640	K1712	Y1798	T1875	LEU	P1950	R2118	L2206	L2305	P2403	I2475
LEU	F1641	F1641	K1713	Y1798	T1875	LEU	P1950	R2118	L2206	L2305	A2404	L2475
GLY	T1642	T1642	S1714	Y1800	E1878	LEU	P1950	R2118	L2206	L2305	S2405	T2483
THR	A1643	A1643	P1715	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	K2406	G2407
GLU	T1644	T1644	P1715	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
SER	V1645	V1645	W1721	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
PHE	V1646	V1646	W1722	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
SER	I1647	I1647	P1723	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
ILE	P1648	P1648	W1726	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
PRO	P1649	P1649	R1727	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
THR	M1651	M1651	V1733	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
LEU	L1652	L1652	T1734	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
LYS	S1653	S1653	I1735	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
VAL	D1657	D1657	M1736	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
SER	T1580	T1580	P1737	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
A1583	W1660	W1660	K1738	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
L1584	F1661	F1661	L1740	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
T1586	K1662	K1662	L1741	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
L1587	L1663	L1663	S1739	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
H1588	Y1664	Y1664	I1741	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
K1589	L1665	L1665	F1744	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
Q1594	K1666	K1666	W1745	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
Y1595	S1673	S1673	S1746	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
M1596	H1674	H1674	W1747	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
Q1597	L1675	L1675	L1750	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407
W1598	I1676	I1676	I1753	Y1800	A1879	LEU	P1950	R2118	L2206	L2305	L2406	G2407

• Molecule 1: TcdA1



MET	ASN	LEU	TYR	E125
GLU	SER	GLU	ALA	L129
VAL	LYS	ILE	ARG	Y136
GLU	GLU	LEU	ILE	Y137
ILE	LYS	LYS	LEU	L138
PRO	ASP	ARG	LYS	D139
ALA	ASP	ALA	ARG	T140
ASN	ASP	ASN	ALA	R141
LYS	LEU	PRO	ASN	P143
SER	SER	LEU	GLN	D144
GLN	GLN	GLN	GLN	M148
CYS	CYS	ASN	ASN	A149
GLY	GLY	ALA	ALA	L150
PHE	PHE	VAL	VAL	S151
ASN	ASN	HIS	HIS	Q152
CYS	CYS	LEU	LEU	M155
LEU	LEU	ALA	ALA	D156
ILE	ILE	LEU	LEU	L159
ASP	ASP	ALA	ALA	S160
ALA	ALA	PRO	PRO	T161
ILE	ILE	ASN	ASN	L162
THR	THR	ALA	ALA	S163
ASP	ASP	LEU	LEU	L164
ALA	ALA	ILE	ILE	S165
ILE	ILE	GLY	GLY	M166
THR	THR	PHE	PHE	E167
PHE	PHE	ARG	ARG	L168
GLY	GLY	GLN	GLN	L169
LYS	LYS	GLY	GLY	Q170
LEU	LEU	VAL	VAL	E171
G11	G11	S97	S97	S172
Y92	Y92	A100	A100	I173
N93	N93	Y182	Y182	Y182
N94	N94	T183	T183	T183
F95	F95	K184	K184	K184
V171	V171	V185	V185	V185
S97	S97	M186	M186	M186
A100	A100	E187	E187	E187
Y103	Y103	M188	M188	M188
V104	V104	L189	L189	L189
A105	A105	S110	S110	S110
T108	T108	S111	S111	S111
V109	V109	S114	S114	S114
ASP	ASP	P115	P115	P115
LEU	LEU	A116	A116	A116
THR	THR	A117	A117	A117
ASP	ASP	Y118	Y118	Y118
ASP	ASP	L119	L119	L119
ASP	ASP	ALA	ALA	Y209
ASP	ASP	LYS	LYS	T210
ASP	ASP	ASP	ASP	E121
ASP	ASP	ASN	ASN	L122
ASP	ASP	ARG	ARG	Q123
ASP	ASP	ARG	ARG	D215




V2429	N2346	L2254	N2170	T2083	L1983	ASN	D1830	V1747	S1673	Q1594	ASN	GLN
Q2430	N2348	L2258	V2171	V2084	Y1986	ALA	P1631	L1750	H1674	Y1595	TYR	TYR
S2434	D2358	L2263	M2172	E2086	Y1986	HIS	L1832	L1750	I1675	M1596	GLN	GLY
G2435	K2359	F2263	N2173	E2086	P1989	ASP	D1833	L1750	I1675	Q1597	PHE	PHE
D2437	L2360	Q2264	A2176	K2087	P1989	SER	S1834	I1753	I1677	W1598	ASN	THR
K2438	S2363	Q2265	D2177	S2088	P1992	ALA	V1835	S1755	S1678	Q1599	ALA	THR
A2439	Q2363	F2266	D2178	K2089	P1992	ILE	D1836	S1755	G1679	S1600	LEU	SER
G2440	Q2364	Y2267	I2179	A2090	L1996	VAL	P1837	M1758	Q1680	Y1601	GLU	GLY
L2441	S2365	R2272	E2183	G2091	L1996	LEU	D1838	D1759	I1681	R1602	ILE	LYS
A2442	C2273	C2273	T2184	S2094	L1996	ARG	A1839	F1760	T1682	T1603	GLY	THR
N2443	E2277	Q2278	Y2185	S2094	G2007	GLN	A1841	A1763	T1684	L1605	SER	ALA
E2446	Q2278	Q2278	T2184	R2095	K2008	ASN	A1842	A1763	I1685	M1606	GLY	ARG
A2447	Y2279	Q2279	R2187	F2096	G2008	ILE	H1843	E1770	I1686	M1606	LEU	THR
L2448	Y2280	R2281	R2188	S2098	P2010	PRO	D1844	E1770	I1688	A1610	ASP	VAL
A2449	R2282	Y2282	R2189	Y2099	E2011	THR	M1846	F1772	I1689	V1614	PHE	SER
Y2450	F2283	Y2283	E2192	L2102	S2012	PRO	H1847	Y1773	L1690	A1615	ILE	GLY
S2451	L2284	L2284	E2193	Y2103	F2013	ALA	Y1848	Y1774	L1691	R1616	ASN	VAL
H2452	L2284	L2284	E2193	D2104	M2014	PRO	K1849	P1776	I1692	R1616	SER	THR
M2454	D2287	S2288	I2194	E2105	S2015	LEU	T1852	P1776	D1696	D1622	ALA	ILE
G2458	K2384	A2289	Q2195	F2096	M2016	SER	L1857	L1777	VAL	T1623	ASN	TYR
Q2459	T2385	R2290	R2196	S2098	R2018	ARG	D1858	L1778	PRO	I1624	SER	THR
F2460	S2386	F2291	R2197	N2108	F2019	SER	L1859	Y1779	LEU	L1625	ALA	LYS
Q2461	L2387	F2292	E2199	G2110	P2020	ALA	L1859	R1782	ASN	S1626	VAL	VAL
F2464	S2390	P2294	E2200	E2111	H2021	ASN	A1862	L1783	GLN	T1629	THR	THR
L2465	S2392	Q2295	E2202	E2111	H2021	THR	R1863	L1783	D1702	P1633	PHE	ALA
L2466	K2397	W2297	K2204	L2117	A2026	ASP	G1864	Q1787	K1706	E1634	PHE	VAL
G2467	L2398	Y2301	Q2205	R2118	R2027	F1948	D1865	D1790	W1707	P1635	ALA	GLN
K2468	R2399	L2305	L2206	A2119	G2028	P1949	Y1868	W1795	Y1708	Q1636	GLU	ILE
P2471	E2400	L2401	S2212	S2120	M2029	P1950	E1872	Y1798	M1709	G1638	ASP	ILE
F2472	D2401	L2402	V2215	A2121	F2036	Q1951	T1875	W1800	F1711	K1639	GLY	VAL
G2474	P2403	S2405	R2216	G2123	F2036	I1952	E1878	Y1805	K1712	L1640	LYS	LYS
L2475	A2404	M2311	A2127	L2124	R2036	N1953	K1880	I1806	K1713	F1641	ALA	SER
T2483	L2406	S2313	R2218	L2124	T2039	E1954	W1881	V1807	G1722	Y1642	LEU	LEU
S2490	K2407	L2314	E2218	Q2129	A2054	Q1961	Y1883	Q1810	P1723	I1647	GLY	THR
Q2497	L2409	E2318	A2220	P2142	N2058	Q1965	H1894	Y1814	V1726	P1643	TYR	ASN
M2500	R2411	K2323	L2222	N2143	R1966	R1966	Q1885	Q1815	R1727	Y1650	GLN	GLN
K2502	L2412	R2324	K2224	I2144	Q2059	V1967	L1889	W1816	V1733	M1651	THR	ALA
T2503	K2413	R2324	K2224	W2154	L2070	L1970	L1889	W1817	T1734	L1652	LYS	VAL
L2509	V2417	R2327	S2236	G2155	Q2071	R1971	K1893	N1817	I1735	S1653	VAL	THR
R2512	T2418	A2328	A2239	A2156	D2072	H1972	P1894	V1818	I1736	D1657	SER	ASP
Y2513	L2419	L2329	A2239	L2157	K2073	N1973	P1897	P1820	P1737	W1660	GLN	GLN
L2509	P2420	E2330	E2330	A2158	L2074	L1974	L1821	K1738	K1738	F1661	PRO	LEU
R2512	L2423	P2332	R2244	E2159	T2075	S1975	L1822	S1739	I1740	K1662	PRO	LYS
Y2513	G2424	R2333	F2245	M2165	E2077	L1976	S1899	D1824	L1741	L1663	SER	LYS
T2514	P2425	T2334	F2245	E2166	L2076	Q1979	I1913	T1825	F1744	Y1664	PHE	ASP
L2515	Y2426	L2337	N2252	F2167	D2079	P1980	THR	S1826	E1745	I1665	ASP	GLY
K2516	L2337	L2337	W2253	A2169	K2082	Y1982	GLN	W1827	S1746	K1666	MET	LYS

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	13000	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 ($e^-/\text{\AA}^2$)	15.4	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k 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 > 2$	RMSZ	# $ Z > 2$
1	A	0.66	1/11313 (0.0%)	0.65	4/15367 (0.0%)
1	B	0.66	1/11313 (0.0%)	0.65	3/15367 (0.0%)
1	C	0.66	1/11313 (0.0%)	0.65	5/15367 (0.0%)
1	D	0.66	1/11313 (0.0%)	0.65	4/15367 (0.0%)
1	E	0.66	1/11313 (0.0%)	0.65	3/15367 (0.0%)
All	All	0.66	5/56565 (0.0%)	0.65	19/76835 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1830	ASP	C-N	-16.99	1.01	1.34
1	D	1830	ASP	C-N	-16.98	1.01	1.34
1	C	1830	ASP	C-N	-16.96	1.02	1.34
1	B	1830	ASP	C-N	-16.95	1.02	1.34
1	A	1830	ASP	C-N	-16.92	1.02	1.34

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2441	LEU	CA-CB-CG	5.75	128.53	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2441	LEU	CA-CB-CG	5.75	128.51	115.30
1	B	2441	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	2441	LEU	CA-CB-CG	5.74	128.50	115.30
1	E	2441	LEU	CA-CB-CG	5.73	128.48	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1005	GLU	Peptide
1	B	1005	GLU	Peptide
1	C	1005	GLU	Peptide
1	D	1005	GLU	Peptide
1	E	1005	GLU	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	11083	0	10580	1079	0
1	B	11083	0	10579	1079	0
1	C	11083	0	10579	1084	0
1	D	11083	0	10580	1096	0
1	E	11083	0	10579	1092	0
All	All	55415	0	52897	4117	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 38.

The worst 5 of 4117 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:2176:ALA:CB	1:D:2117:LEU:HD22	1.13	1.59
1:D:2176:ALA:CB	1:E:2117:LEU:HD22	1.13	1.59
1:D:2169:ALA:CB	1:E:2124:LEU:HD22	1.29	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2169:ALA:HB2	1:B:2124:LEU:CD2	1.14	1.58
1:A:2117:LEU:HD22	1:E:2176:ALA:CB	1.16	1.58

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	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	28	70
1	B	1415/2516 (56%)	1297 (92%)	110 (8%)	8 (1%)	28	70
1	C	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	28	70
1	D	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	28	70
1	E	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	28	70
All	All	7075/12580 (56%)	6489 (92%)	546 (8%)	40 (1%)	33	70

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PHE
1	A	954	VAL
1	A	1810	GLN
1	A	2144	ILE
1	B	96	PHE

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	1135/2157 (53%)	1132 (100%)	3 (0%)	94	98
1	B	1135/2157 (53%)	1132 (100%)	3 (0%)	94	98
1	C	1135/2157 (53%)	1132 (100%)	3 (0%)	94	98
1	D	1135/2157 (53%)	1132 (100%)	3 (0%)	94	98
1	E	1135/2157 (53%)	1132 (100%)	3 (0%)	94	98
All	All	5675/10785 (53%)	5660 (100%)	15 (0%)	94	98

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	94	ASN
1	C	2104	ASP
1	E	94	ASN
1	B	2189	ARG
1	D	2189	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1265	GLN
1	C	2452	HIS
1	E	2059	GLN
1	C	1588	HIS
1	C	1847	HIS

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
1	D	1
1	C	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1830:ASP	C	1831:PRO	N	1.02
1	B	1830:ASP	C	1831:PRO	N	1.02
1	C	1830:ASP	C	1831:PRO	N	1.02
1	D	1830:ASP	C	1831:PRO	N	1.02
1	E	1830:ASP	C	1831:PRO	N	1.02