



wwPDB EM Map/Model Validation Report ⓘ

Oct 10, 2016 – 11:35 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 : 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

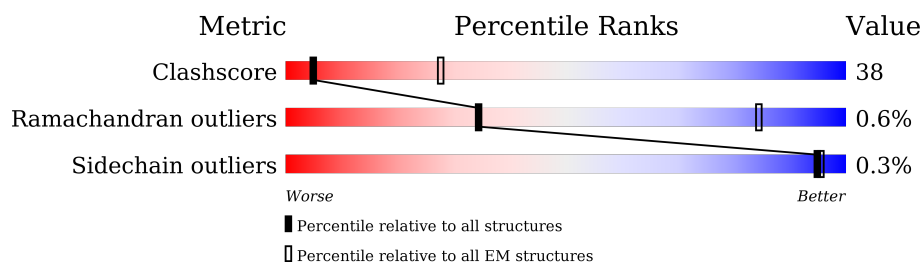
1 Overall quality at a glance

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	
1	B	2516	
1	C	2516	
1	D	2516	
1	E	2516	

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.

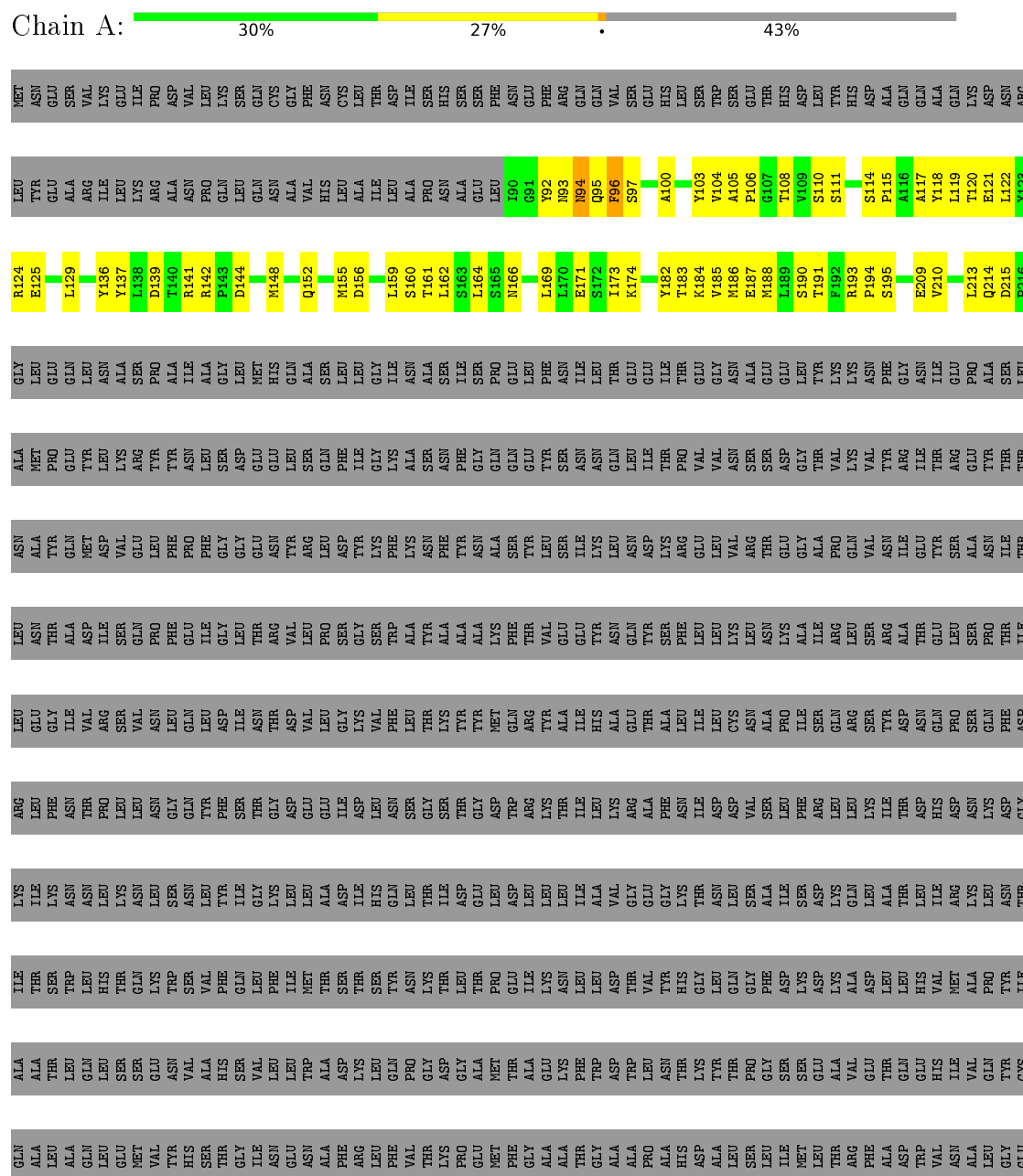
- Molecule 1 is a protein called TcdA1.

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

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






P1989	K2087	A2176	N2252	L2337	V2429
P1992	S2088	D2177	W2253	L2337	Q2430
L1995	A2090	I2179	L2254	N2348	S2434
L1996	G2091	E2183	L2258	K2359	G2436
G2007	S2094	T2184	F2263	L2360	D2437
K2008	R2095	T2185	Q2264	Q2363	K2438
L2009	D2097	Y2185	Y2266	F2265	A2439
P2010	R2186	R2187		S2365	G2440
E2011	S2098	R2188	R2272	S2370	L2441
S2012	Y2099	R2189	C2273	G2371	A2442
F2013	L2102	W2192		N2372	N2443
M2014	D2103	E2193	E2277	N2373	E2446
S2015	D2104	I2194	Q2278	A2279	A2447
L2016	E2105	Q2195	A2279	L2279	L2448
W2017	N2106	Q2196	Y2280	L2375	L2449
R2018	I2107	R2196	R2281	A2376	Y2450
F2019	N2108	R2197	W2282	F2377	S2451
P2020	A2109	N2198	E2283	D2382	H2452
H2021	G2110	A2199	L2284	T2383	G2453
M2022	E2111	E2200		L2384	M2454
L2023		A2201	D2287	T2385	G2458
E2024	A2114	E2202	S2288	S2386	Q2459
N2025		L2203	A2289	L2387	Q2461
A2026	I2117	Q2204	R2290		
R2027	R2118	Q2205	F2291		
G2028	A2119	I2206	I2292		
M2029	S2120	D2207	K2293	S2390	F2464
	A2121	A2208	P2294	S2392	N2465
F2036	A2122	Q2209	G2295		D2466
	G2123	L2210	A2296	K2397	G2467
T2039	L2124	K2211	W2297	I2398	K2468
I2044	T2125	S2212		R2399	
Q2047	T2126	L2213	Y2301	E2400	P2471
	A2127	A2214	L2305	D2401	F2472
A2054	V2128	V2215		Y2402	E2473
N2058	Q2129	R2216	E2308	P2403	G2474
Q2059	P2142	R2217	T2309	A2404	I2475
	N2143	A2218	L2310	S2405	
	I2144	A2219	M2311	G2407	T2483
I2070	W2154	L2222	L2312	K2408	S2490
Q2071	G2155	Q2223	S2313	I2409	Q2497
D2072	A2156	K2224	L2314	R2411	M2500
K2073	I2157			T2412	L2501
T2074	A2158	Q2233	E2318	K2413	M2502
I2075	E2159	S2236	K2323	V2417	T2503
E2076	M2165	A2239	R2324	T2418	L2504
E2077	E2166	R2327		P2420	
L2078	F2167	A2328		L2509	
D2079	S2168	R2243	L2329	Y118	
	A2169	K2244	E2330	L119	
K2082	N2170	F2245	V2331	T120	
T2083	V2171		E2332	G2424	
V2084	M2172	L2250	T2334	T2514	
L2085	N2173			I2515	
E2086				Y2426	
					K2516

• Molecule 1: TcdA1

Chain B:



MET	LEU	R124	P216	LEU	THR	TLE	ASP	GLY
ASN	TYR	E125	GLY	TYR	ALA	ALA	ARG	LYS
GLU	ALA	L129	LEU	GLU	MET	THR	THR	ILE
SER	GLU		GLN	PRO	GLU	ALA	ASN	THR
VAL	ARG	Y136	LEU	GLN	TYR	ASP	THR	ASN
LYS	ILE	Y137	ASN	TYR	LEU	ILE	PRO	LEU
GLU	LYS	L138	ALA	LYS	LEU	SER	LEU	LYS
ILE	PRO	D139	SER	ARG	LYS	GLY	ASP	ASP
PRO	ARG	R140	PRO	TYR	ARG	THR	LEU	THR
ASP	ALA	T141	ASN	TYR	GLU	ASN	GLY	GLY
VAL	VAL	R142	ALA	TYR	PRO	ASN	PRO	ASN
LEU	PRO	P143	ILE	ASN	GLU	PHE	GLN	GLN
LYS	GLN	D144	ALA	LEU	LEU	GLY	THR	THR
SER	LEU	M148	GLY	SER	SER	GLY	PHE	THR
GLN	ASN	A149	LEU	ASP	GLY	GLY	GLY	ILE
CYS	CYS	L150	MET	GLU	GLU	THR	SER	THR
ASN	PHE	L151	HIS	GLU	GLU	ARG	GLY	LYS
CYS	ASN	S151	LEU	GLN	LEU	VAL	ASP	ASP
THR	LEU	Q152	SER	VAL	SER	LEU	GLU	LEU
LEU	ALA	M155	THR	ALA	GLN	GLY	GLU	ALA
ALA	LEU	D156	LEU	PHE	ILE	TYR	ILE	ASP
ILE	ILE	L159	ILE	GLY	LYS	TRP	ASP	HIS
THR	ALA	S160	ILE	TYR	ALA	ALA	ASN	GLN
ASP	ASN	T161	ALA	ASN	SER	ALA	SER	LEU
GLN	GLU	L162	ALA	PHE	ASN	ALA	GLY	THR
PHE	LEU	S163	SER	ILE	ASN	ALA	GLY	THR
GLY	PRO	L164	PRO	GLY	GLY	ALA	ASP	GLY
PHE	GLU	S165	GLU	GLN	GLN	LYS	TRP	ASP
THR	LEU	N166	LEU	TYR	GLU	THR	ARG	LEU
ASN	PHE	L169	PHE	TYR	VAL	VAL	LYS	LEU
GLN	ILE	L170	ASN	SER	GLU	GLU	ILE	LEU
THR	ILE	E171	ILE	ASN	ILE	ILE	THR	THR
GLU	SER	S172	THR	LYS	THR	THR	ASN	ALA
	GLU	I173	GLU	ASN	LEU	GLN	GLN	VAL
	HIS	Y182	GLU	THR	ILE	ASP	THR	THR
	LEU	T183	THR	THR	PRO	LYS	LYS	GLY
	THR	K184	GLU	THR	VAL	GLU	ASN	LYS
	GLY	V185	GLY	GLY	VAL	LEU	LEU	THR
	ASN	M186	ASN	ASN	VAL	LYS	ASN	ASN
	ALA	E187	ALA	SER	ASN	LEU	ASP	SER
	THR	M188	THR	THR	ARG	LEU	VAL	LEU
	THR	L189	THR	GLU	THR	ASN	THR	THR
	GLU	S190	GLU	GLU	GLY	GLY	ASP	ALA
	THR	T191	LEU	LEU	ALA	ILE	PHE	THR
	LYS	F192	TYR	TYR	VAL	THR	ASP	GLN
	LYS	R193	LYS	LYS	GLN	ARG	LEU	ARG
	ASN	P194	ASN	ASN	VAL	LEU	LYS	LEU
	PHE	S195	PHE	PHE	VAL	THR	ILE	LEU
	GLY	E209	GLY	GLY	ILE	THR	THR	ALA
	ASN	V210	ASN	ASN	THR	GLU	ASP	THR
	ILE	L213	ILE	ILE	THR	GLY	HIS	ILE
	GLU	Q214	GLU	THR	ARG	LEU	ASP	ARG
	PRO	D215	PRO	GLU	ALA	SER	ASN	LYS
	ALA		ALA	THR	ASN	GLN	LYS	THR
	SER		SER	THR	ILE	PHE	ASN	ASN

E1745	S1673	Q1594	M1596	I1675	Y1677	S1678	Q1679	Q1680	L1681	T1682	D1683	T1684	N1685	I1686	N1687	I1688	T1689	L1690	F1691	Y1774	T1775	P1776	M1777	L1778	V1779	R1782	L1783	Q1787	D1790	M1795	Y1798	M1799	M1800	Y1805	I1806	Y1807	H1808	G1809	Q1810	Y1814	Q1815	H1816	N1817	V1818	R1819	P1820	L1821	L1822	E1823	D1824	T1825	S1826		
Q1594	Y1595	M1596	Q1597	M1598	Q1599	S1600	Y1601	L1602	T1603	R1604	L1605	M1606	A1610	Y1614	A1615	R1616	D1622	T1623	I1624	G1625	S1626	T1629	Q1633	E1634	P1635	G1636	L1637	G1638	K1639	G1640	F1641	Y1642	T1644	F1645	V1646	I1647	P1648	Y1649	M1650	N1651	L1652	S1653	D1657	M1660	F1661	K1662	L1663	T1664	Y1665	H1666	L1667	F1668		
S1673	H1674	I1675	I1676	Y1677	S1678	G1679	Q1680	L1681	T1682	D1683	T1684	N1685	I1686	N1687	I1688	T1689	L1690	F1691	Y1774	T1775	P1776	M1777	L1778	V1779	R1782	L1783	Q1787	D1790	M1795	Y1798	M1799	M1800	Y1805	I1806	Y1807	H1808	G1809	Q1810	Y1814	Q1815	H1816	N1817	V1818	R1819	P1820	L1821	L1822	E1823	D1824	T1825	S1826			
MET	ASN	THR	GLN	PHE	ASN	ALA	LEU	GLY	ASP	GLY	SER	GLY	GLY	LEU	ASN	PHE	ILE	ASN	ASN	SER	THR	ASN	GLN	ALA	THR	ALA	PHE	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
LYS	GLN	THR	ILE	PHE	MET	THR	ASP	LYS	GLY	THR	GLN	THR	VAL	SER	SER	GLY	PRO	ALA	ILE	THR	ASN	THR	VAL	LYS	VAL	LYS	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
THR	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	LEU	LYS	ILE	THR	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
Y1285	Y1286	R1287	S1290	Y1291	M1292	Q1293	F1294	D1295	T1296	R1300	R1301	V1302	N1303	R1305	THR	ALA	GLU	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
I1203	R1204	Y1205	T1208	M1209	N1210	T1213	T1214	D1215	M1218	K1219	K1220	N1221	E1222	E1223	Y1224	K1225	L1226	E1227	G1233	Y1234	Y1235	G1236	Q1240	G1241	E1242	D1243	L1244	L1245	V1246	M1248	F1249	Y1250	N1251	K1260	N1261	M1264	Q1265	G1266	L1267	Y1268	I1269	T1270	A1271	D1272	S1275	Q1282	S1283	N1284						
F1131	M1132	D1133	G1134	K1135	F1136	A1137	A1138	M1139	M1140	M1141	S1142	E1143	M1144	H1145	K1146	P1153	Y1154	K1155	S1156	P1160	V1161	I1162	Y1163	Y1168	L1169	L1170	M1171	L1172	E1173	Q1174	T1177	THR	LYS	GLN	THR	GLY	ASN	SER	THR	THR	D1193	Y1196	E1197	L1198	K1199	L1200	A1201	H1202						
I1045	D1046	M1049	R1050	Q1053	T1054	K1055	M1056	M1057	D1058	A1059	L1060	V1064	Q1068	L1069	D1072	F1078	M1079	S1080	Y1081	L1082	T1083	V1088	L1091	K1092	V1093	Y1097	H1098	D1099	M1100	T1101	M1102	D1104	Q1105	L1106	T1107	T1108	Y1109	G1112	Y1122	M1123	R1124	S1125	Y1126	D1127	H1128	M1129	K1130							
D974	R975	Q976	Y977	S978	T981	K982	T983	T984	R985	I986	T990	A991	S992	Q993	Q994	I995	Y996	Y997	R998	R999	E1002	H1003	V1004	E1005	E1006	S1010	R1015	Q1016	L1017	R1018	I1019	D1020	M1021	D1022	K1023	Y1024	M1025	K1026	R1027	Y1028	S1029	T1030	M1031	A1032	G1033	V1034	V1038	Y1039	Y1040	P1041	E1042	M1043	Y1044	
THR	ILE	LEU	GLN	TRP	VAL	ASN	VAL	ALA	GLN	LEU	VAL	A990	G899	L900	D901	Y902	N906	K907	E908	A918	L922	Q929	Q930	A931	T933	L934	H935	A936	F937	L938	D939	S947	R952	Q953	Y954	I961	K962	S963	R964	D965	D966	L967	Y968	Q969	Y970	L971	L972	I973						
THR	ILE	ALA	THR	LEU	GLN	LEU	SER	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLY	LYS	ALA	SER	VAL	LEU	ALA	GLU	PHE	GLY	ASN	SER	LEU	THR	ALA	GLN	LEU	ALA	ASP	ASP	ARG	ALA	LEU	LEU	GLN	VAL	THR	GLY	ALA	PRO	GLN	ASN	HIS	GLN	HIS	ALA	LEU	PRO	LEU	THR	ALA	ARG	PHE	ALA	PHE	GLU	THR	GLN	LEU	HIS	VAL	MET	ALA	PRO	THR
CYS	GLN	ALA	LEU	ALA	GLN	LEU	GLU	VAL	THR	HIS	THR	GLY	ILE	ASN	GLU	GLN	LEU	ALA	PHE	ARG	LEU	LEU	VAL	THR	LYS	PRO	THR	GLY	ALA	PRO	GLN	ASN	HIS	GLN	ASP	ALA	LEU	THR	ALA	ARG	PHE	ALA	PHE	GLU	THR	GLN	LEU	HIS	VAL	MET	ALA	PRO	THR	
ILE	ALA	ALA	THR	LEU	GLN	LEU	GLU	VAL	THR	HIS	THR	GLY	ILE	ASN	GLU	GLN	LEU	ALA	PHE	ARG	LEU	LEU	VAL	THR	LYS	PRO	THR	GLY	ALA	PRO	GLN	ASN	HIS	GLN	ASP	ALA	LEU	THR	ALA	ARG	PHE	ALA	PHE	GLU	THR	GLN	LEU	HIS	VAL	MET	ALA	PRO	THR	

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	GLN	TRP	ASN	ASN
Q1597	PHE	PHE	GLY	TYR	S1290	Y1205	D1133	—	Q976	ASN	ALA	ALA	ALA	LEU	HIS	LYS	PRO
W1598	ASN	MET	ASN	ILE	Y1291	G1207	K1135	R1049	S978	VAL	ALA	ALA	ALA	SER	THR	GLN	LEU
Q1599	ALA	THR	THR	SER	Q1292	T1208	F1136	Q1083	I981	GLN	PHE	VAL	VAL	GLU	LYS	ASN	LEU
W1600	LEU	ASP	SER	PRO	Q1293	W1209	A1137	T1094	K982	GLN	GLU	TYR	TYR	GLU	TRP	SER	ASN
Y1601	GLU	SER	GLY	LYS	Q1294	W1295	A1138	K1055	T983	LEU	ALA	HIS	HIS	VAL	TRP	ASN	GLY
R1602	ILE	LYS	LEU	LEU	F1295	—	N1139	M1056	T984	ASN	ASN	SER	VAL	ALA	VAL	LEU	GLN
T1603	ASP	GLY	ASN	ARG	T1296	I1213	W1141	M1057	R985	VAL	SER	THR	HIS	PHE	THR	TYR	PHE
R1604	GLY	THR	GLN	ILE	—	T1214	S1142	D1058	I986	ALA	LEU	GLY	GLY	GLN	ILE	ILE	SER
L1605	SER	ALA	GLY	ARG	F1215	—	E1143	A1089	—	—	THR	ILE	VAL	LEU	LEU	GLY	THR
W1606	GLY	THR	ARG	HIS	—	—	W1144	L1060	—	—	ALA	ALA	ALA	LEU	PHE	LYS	ASP
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	GLU	GLU	GLU	LEU	ILE	LYS	GLY
A1615	PHE	SER	PHE	THR	N1303	K1220	K1146	V1064	S992	D901	GLN	ASN	MET	TRP	ILE	LEU	ASP
R1616	ASN	GLY	HIS	GLU	N1304	I1221	—	Q1068	Q994	Y902	ALA	ALA	ALA	THR	SER	ALA	GLU
D1622	ASN	VAL	ASP	GLY	TYR	S1222	P1153	L1069	L995	Q904	ASP	PHE	PHE	SER	THR	ASP	ILE
T1623	ALA	GLU	THR	LYS	ALA	E1223	Y1154	—	—	Q905	ALA	ARG	ARG	LEU	SER	ILE	ASP
I1624	SER	ILE	THR	ARG	ASP	L1224	K1155	S1080	N998	N906	LEU	PHE	PHE	GLN	TYR	GLN	ASN
I1625	ASP	THR	PRO	GLN	TYR	K1225	S1156	L1082	R999	K907	ASN	VAL	VAL	PRO	ASN	THR	SER
S1626	VAL	ILE	LYS	ASN	ILE	E1227	P1160	Y1083	E1005	E908	GLY	LYS	LYS	GLY	THR	SER	THR
T1629	THR	SER	VAL	ASN	PRO	G1233	I1161	M1079	A1000	—	ASP	LYS	THR	ASP	THR	ILE	ASP
Q1633	PHE	GLN	GLY	GLY	GLU	L1234	I1162	S1080	E1002	A918	ALA	PRO	GLY	GLY	LEU	ASP	THR
E1634	ALA	ILE	ALA	THR	SER	L1235	Y1163	Y1081	W1003	L922	LEU	GLU	ALA	ALA	THR	GLU	GLY
P1635	GLU	ILE	GLY	GLY	ASP	T1244	E1172	K1092	I1013	N932	ILE	THR	THR	THR	LEU	ILE	ILE
Q1636	GLY	VAL	LYS	LEU	TYR	L1245	E1173	V1083	S1014	T933	GLN	ASP	ASP	ASP	VAL	ALA	LEU
G1638	ARG	LYS	ARG	ASP	GLY	L1246	Q1174	—	R1015	R935	ALA	ALA	ALA	THR	THR	GLY	ARG
K1639	LYS	ALA	SER	LYS	TRP	V1247	I1177	Y1097	R1016	A936	GLN	PRO	VAL	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	THR	THR	HIS	LYS	ASN
Y1642	THR	LYS	ASN	VAL	TYR	Y1250	GLN	N1100	I1019	D939	GLN	ASP	ASP	LYS	GLY	THR	ILE
A1643	GLU	GLN	THR	THR	TYR	N1251	THR	I1101	D1020	—	HIS	ALA	ALA	TYR	LEU	ASN	ASP
F1645	SER	ASN	ALA	THR	LEU	—	GLY	N1102	W1021	S947	LEU	LEU	THR	GLN	GLN	LEU	ASP
V1646	PHE	THR	ALA	SER	SER	K1260	ASN	N1103	—	T948	PRO	SER	GLY	THR	VAL	SER	VAL
I1647	SER	PHE	ALA	LEU	MET	N1261	SER	D1104	M1025	—	ILE	LEU	PHE	ASP	PHE	ALA	SER
P1648	ILE	THR	ILE	GLY	VAL	—	LYS	Q1105	K1026	T951	VAL	ILE	SER	ASP	ASP	ILE	LEU
P1649	PRO	ALA	GLY	VAL	TYR	M1264	ASP	L1106	R1027	R952	THR	MET	SER	LYS	LYS	PHE	PHE
Y1650	VAL	ASP	ASP	ASN	ASN	Q1265	GLY	L1107	Y1028	Q953	THR	LEU	GLU	ASP	ASP	ASP	ARG
N1651	THR	LYS	ASP	PRO	GLY	G1266	TYR	T1108	S1029	V954	GLU	THR	ALA	LYS	LYS	LEU	LEU
L1652	LEU	ASP	TYR	ASN	ILE	L1267	GLN	Y1109	T1030	—	ASN	ARG	VAL	ALA	ALA	GLN	LEU
S1653	LYS	VAL	ALA	ASN	THR	Y1268	THR	G1112	W1031	I961	ALA	PHE	GLU	ASP	ASP	LYS	LYS
D1657	—	SER	THR	SER	PRO	I1269	GLU	—	A1032	K962	THR	ALA	THR	LEU	LEU	ALA	ILE
E1658	—	ILE	ASP	SER	THR	F1270	THR	Y1122	G1033	S963	SER	ASP	GLN	LEU	THR	THR	THR
R1659	PRO	GLN	SER	ASN	ILE	A1271	D1183	W1123	V1034	R964	THR	TRP	GLU	HIS	LEU	ILE	HIS
W1660	ASN	LEU	LEU	LYS	ASN	D1272	—	R1124	—	D965	THR	ASN	ILE	VAL	VAL	ILE	ASP
F1661	SER	SER	ASN	TYR	LYS	—	Y1196	S1125	V1038	D966	SER	THR	THR	ALA	ALA	ARG	ASN
T1584	PRO	LYS	LYS	MET	THR	—	E1197	R1149	Y1039	I967	ILE	SER	VAL	PRO	ALA	LYS	ASN
T1585	SER	PRO	PRO	PHE	ALA	—	L1198	V1126	Y1040	T968	THR	THR	GLY	GLN	THR	LEU	LYS
L1586	PHE	ASP	THR	THR	ALA	Q1282	K1199	D1127	P1041	Q969	ASN	ILE	TYR	TYR	PRO	ASN	ASP
Y1664	ASP	PRO	ASP	PRO	SER	S1283	L1200	H1128	E1042	Y970	THR	THR	CYS	ILE	THR	THR	GLY
I1665	—	GLU	LEU	VAL	SER	N1284	A1201	S1129	N1043	—	ILE	—	GLN	ALA	ALA	ILE	LYS



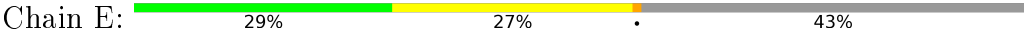
Chain D:  30% 26% . 43%






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	T1603	T1682	M1759	D1839	ILE	G2007	R2095	Y2184	R2272	N2371	N2443
GLY	L1604	R1604	T1683	F1760	V1840	PRO	K2008	R2096	Y2185	C2273	N2372	E2446
SER	L1605	L1605	T1683	A1763	Q1841	THR	L2009	D2097	E2186	Q2277	N2373	A2447
GLY	M1606	M1606	T1684	M1685	Q1842	PRO	P2010	S2098	R2187	E2278	L2374	L2448
LEU	A1610	A1610	I1686	E1770	H1843	ALA	E2011	Y2099	R2188	Q2278	N2375	A2449
ASN	A1611	A1611	M1687	E1771	D1844	PRO	S2012	L2102	R2189	Y2280	F2376	V2450
PHE	A1614	A1614	I1688	E1772	P1845	LEU	F2013	Y2103	E2192	Y2281	F2377	H2452
ILE	A1615	A1615	T1689	F1773	M1846	SER	M2014	D2104	E2193	W2282	D2382	G2453
ASN	A1616	A1616	L1690	Y1774	H1847	LEU	S2015	E2105	I2194	E2283	T2383	M2454
SER	A1616	A1616	F1691	I1692	K1849	ANG	L2016	E2106	Q2195	E2284	T2384	G2458
ALA	I1621	I1621	M1696	M1777	T1852	SER	W2017	N2106	Q2196	D2287	K2385	Q2459
ALA	D1622	D1622	L1778	M1778	T1852	ASN	F2019	N2108	R2197	S2288	T2386	F2460
ILE	T1623	T1623	L1779	V1779	D1858	THR	P2020	A2109	E2198	A2289	L2387	Q2461
ASP	L1624	L1624	PRO	LEU	A1862	LEU	H2021	G2110	A2199	R2290	S2390	F2464
VAL	S1626	S1626	ASN	GLN	R1863	ASP	L2022	E2111	E2200	F2291	V2391	N2465
THR	T1629	T1629	D1702	R1782	G1864	LEU	E2024	A2114	E2202	I2292	S2392	D2466
THR	A1633	A1633	K1706	Q1787	D1865	THR	N2025	L2117	L2203	W2297	K2397	G2467
PHE	E1634	E1634	I1707	D1790	Y1868	THR	G2026	R2118	K2204	Y2301	I2398	K2468
ALA	P1635	P1635	Y1708	M1795	E1872	ASP	M2029	A2119	Q2205	Y2301	R2399	P2471
GLU	Q1636	Q1636	M1709	M1795	E1872	ASP	P2029	S2120	R2207	L2304	E2400	F2472
GLY	L1637	L1637	T1710	M1800	Y1875	LEU	G2028	R2118	I2206	L2305	D2401	E2473
ARG	K1639	K1639	F1711	Y1798	T1875	LEU	P2027	R2119	Q2206	L2305	Y2402	G2474
LYS	Q1640	Q1640	K1712	Y1798	T1875	LEU	G2028	G2123	S2212	E2308	A2404	I2475
LEU	F1641	F1641	K1713	W1800	E1878	LEU	L2044	L2124	E2214	T2309	S2405	T2483
GLY	A1642	A1642	P1715	Y1805	A1879	LEU	T2044	T2125	W2215	L2310	L2406	G2407
TYR	Y1643	Y1643	P1715	Y1806	K1880	LEU	Q2047	A2127	R2216	M2311	K2408	L2407
SER	T1644	T1644	W1721	V1807	M1881	LEU	Q2047	W2128	R2217	L2312	G2408	I2409
PHE	F1645	F1645	G1722	H1808	W1882	LEU	A2054	Q2129	E2218	S2313	I2409	R2410
SER	V1646	V1646	P1723	G1809	Y1883	LEU	Q2054	P2142	E2219	L2314	R2410	R2411
ILE	I1647	I1647	Q1810	Q1809	Q1885	LEU	N2058	N2143	A2220	E2318	E2411	L2412
PRO	P1648	P1648	V1726	G1809	Q1885	LEU	Q2059	I2144	L2222	K2323	K2413	K2413
VAL	P1649	P1649	R1727	Y1814	K1893	LEU	T2070	W2154	K2224	R2324	V2417	T2418
THR	M1651	M1651	V1733	Q1815	P1894	LEU	Q2071	G2155	K2224	R2324	T2418	L2419
LEU	L1652	L1652	T1734	M1816	P1897	LEU	D2072	A2156	S2236	L2327	L2419	P2420
LYS	S1653	S1653	I1735	M1818	L1898	LEU	K2073	E2157	A2239	L2329	L2423	G2424
VAL	D1657	D1657	M1736	R1819	S1899	LEU	T2074	E2159	R2243	V2331	P2425	Y2426
SER	W1660	W1660	P1737	P1820	T1913	LEU	I2075	E2159	R2243	E2332	G2424	P2425
A1583	F1661	F1661	K1738	L1821	THR	LEU	E2077	M2165	K2244	R2333	Y2426	Y2426
L1584	K1662	K1662	S1739	L1822	THR	LEU	D2078	E2166	F2245	T2334	V2429	Q2430
T1586	Y1664	Y1664	I1740	E1823	GLN	LEU	K2082	S2168	L2250	L2337	Q2430	Q2430
H1587	K1666	K1666	L1741	T1825	ASN	LEU	T2084	A2169	Y2251	N2348	S2434	Y2435
H1588	F1744	F1744	F1744	W1827	ALA	LEU	V2084	N2170	N2252	N2348	Y2435	Y2435
H1589	S1746	S1746	S1746	W1827	ASP	LEU	L2085	N2171	W2253	N2348	G2436	D2437
Q1594	Q1666	Q1666	D1830	D1830	SER	LEU	E2086	N2172	L2254	K2359	G2436	K2438
Y1595	S1673	S1673	P1831	P1831	ALA	LEU	K2087	A2176	L2258	L2360	D2437	K2438
M1596	H1674	H1674	L1750	L1832	VAL	LEU	S2088	D2177	F2263	Q2363	A2439	A2439
Q1597	I1676	I1676	I1753	S1834	ALA	LEU	K2089	D2177	F2263	Q2363	A2439	A2439

• Molecule 1: TcdA1



MET	ASN	LEU	TYR	E125
GLU	GLU	TYR	GLU	L129
SER	ALA	ALA	ALA	Y136
VAL	VAL	ILE	ILE	Y137
LYS	LYS	LEU	LEU	L138
GLU	GLU	LYS	LYS	D139
ILE	ILE	ARG	ARG	T140
PRO	PRO	ALA	ALA	R141
ASP	ASP	ASN	ASN	R142
VAL	VAL	PRO	PRO	P143
LEU	LEU	GLN	GLN	D144
SER	SER	LEU	LEU	M148
GLN	GLN	GLN	GLN	A149
CYS	CYS	ASN	ASN	L150
THR	THR	ALA	ALA	S151
ASP	ASP	VAL	VAL	Q152
ILE	ILE	HIS	HIS	M155
ASN	ASN	LEU	LEU	D156
CYS	CYS	ALA	ALA	L159
LEU	LEU	LEU	LEU	S160
ALA	ALA	ILE	ILE	T161
THR	THR	LEU	LEU	L162
ASP	ASP	LEU	LEU	S163
ALA	ALA	LEU	LEU	L164
ILE	ILE	LEU	LEU	S165
GLY	GLY	G11	G11	M166
PHE	PHE	Y92	Y92	E167
ARG	ARG	N93	N93	L168
GLN	GLN	N94	N94	L169
GLY	GLY	Q95	Q95	L170
VAL	VAL	F96	F96	E171
SER	SER	S97	S97	S172
GLU	GLU	A100	A100	I173
HIS	HIS	Y103	Y103	Y182
SER	SER	V104	V104	T183
THR	THR	T2503	T2503	K184
GLU	GLU	A105	A105	V185
THR	THR	T108	T108	M186
HIS	HIS	V109	V109	E187
ASP	ASP	S110	S110	M188
LEU	LEU	S111	S111	L189
THR	THR	S114	S114	R2512
ASP	ASP	P115	P115	Y2513
ALA	ALA	A116	A116	T2514
GLN	GLN	A117	A117	I2515
ALA	ALA	Y118	Y118	K2516
LYS	LYS	L119	L119	L2509
ASN	ASN	T120	T120	R2512
ARG	ARG	E121	E121	Y2513
		L122	L122	T2514
		R124	R124	I2515




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	ILE
G2435	K2359	F2263	N2173	E2086	Y1986	ASP	D1833	L1750	I1675	Q1597	PHE	GLY
D2437	Q2264	F2263	A2176	K2087	P1989	SER	S1834	I1753	I1677	W1598	ASN	THR
K2438	S2362	F2265	D2177	K2088	P1992	ALA	V1835	S1755	S1678	Q1599	ALA	THR
A2439	Q2363	F2266	D2178	A2090	P1992	ILE	D1836	S1755	G1679	S1600	LEU	SER
G2440	Q2363	F2266	D2177	A2090	P1992	VAL	P1837	S1755	Q1680	Y1601	GLU	GLY
L2441	S2365	R2272	I2179	G2091	L1996	ALA	D1838	M1758	L1681	R1602	ILE	LYS
A2442	C2273	R2272	E2183	S2094	L1996	LEU	A1839	D1759	T1682	T1603	ASP	ASN
N2443	C2273	C2273	E2183	S2094	L1996	ARG	V1840	F1760	D1683	G1604	GLY	THR
E2446	E2277	E2277	T2184	R2095	G2007	GLN	A1841	A1763	T1684	L1605	SER	ALA
A2447	Q2278	Q2278	Y2185	F2096	K2008	ASN	H1842	A1763	N1685	M1606	GLY	ARG
L2448	Q2279	Q2279	R2187	D2097	L2009	ILE	H1843	A1763	I1686	M1606	LEU	THR
A2449	Y2280	Y2280	R2188	S2098	P2010	PRO	D1844	E1770	I1688	A1610	ASP	VAL
V2450	R2281	R2281	R2189	Y2099	E2011	THR	H1846	L1771	I1688	I1614	PHE	SER
S2451	V2282	V2282	R2189	Y2099	S2012	PRO	M1847	F1773	L1690	V1615	ILE	GLY
H2452	W2283	W2283	R2189	Y2099	F2013	ALA	Y1848	Y1774	L1691	R1616	ASN	VAL
M2454	F2283	F2283	R2189	Y2099	M2014	PRO	K1849	P1776	I1692	D1622	SER	THR
G2458	L2284	L2284	E2192	D2104	S2015	LEU	T1852	P1776	D1696	T1623	ALA	ILE
Q2459	D2287	D2287	E2193	E2105	L2016	SER	L1857	P1776	VAL	I1623	THR	ASN
F2460	S2288	S2288	Q2195	E2105	W2017	LEU	D1858	L1778	PRO	L1625	ASP	ALA
S2461	A2289	A2289	R2196	E2105	R2018	ARG	L1859	L1778	LEU	S1626	VAL	LYS
F2464	R2290	R2290	N2197	E2105	F2019	SER	L1859	V1779	ASN	T1629	THR	VAL
L2465	F2291	F2291	A2199	E2105	H2021	ALA	A1862	R1782	PHE	Q1633	ALA	LYS
L2466	L2292	L2292	E2200	E2105	P2020	ASN	R1863	L1783	ALA	P1635	PHE	ILE
G2467	K2293	K2293	A2201	E2105	L2023	THR	R1864	Q1787	THR	Q1637	GLY	ILE
K2468	P2294	P2294	E2202	E2105	E2024	LEU	G1865	Q1787	ALA	G1638	ASP	VAL
P2471	Q2295	Q2295	E2202	E2105	A2026	ASP	D1865	D1790	LYS	K1639	ARG	LYS
F2472	W2297	W2297	K2204	L2203	R2027	F1948	Y1868	W1795	ILE	G1640	LYS	ALA
E2473	Y2301	Y2301	Q2205	A2119	G2028	F1949	E1872	Y1798	GLY	F1641	LEU	GLY
G2474	L2305	L2305	Q2205	A2119	M2029	P1950	T1875	W1800	S1714	Y1642	GLY	THR
L2475	E2308	E2308	L2213	L2124	F2036	N1953	E1878	Y1805	P1715	A1643	TYR	ASN
S2483	T2309	T2309	A2214	L2124	T2039	E1954	K1880	I1806	T1715	T1644	GLU	GLN
T2483	M2311	M2311	R2216	A2127	L2044	M1957	M1881	V1807	W1721	F1645	SER	ASN
S2490	S2313	S2313	E2218	Q2129	Q2047	W1960	W1882	G1809	G1722	V1646	PHE	THR
Q2497	L2314	L2314	A2219	Q2129	A2054	Q1961	Y1883	Q1810	P1723	I1647	SER	ALA
M2500	E2318	E2318	A2220	P2142	N2058	Q1965	H1894	Y1814	V1726	P1649	PRO	ILE
K2502	K2323	K2323	L2222	N2143	Q2059	R1966	Q1885	Q1815	R1727	Y1650	VAL	ALA
L2503	R2324	R2324	K2224	I2144	Q2059	V1967	L1889	W1816	I1735	M1651	THR	LYS
L2509	R2327	R2327	S2236	W2154	L2070	L1970	K1893	W1817	T1734	L1652	LYS	VAL
R2512	A2328	A2328	A2239	G2155	Q2071	R1971	P1894	V1817	I1735	S1653	VAL	THR
Y2513	L2329	L2329	A2239	A2156	D2072	H1972	P1897	R1819	M1736	D1657	SER	ASP
L2515	E2330	E2330	R2243	L2157	K2073	N1973	L1821	P1820	P1737	W1660	GLN	GLN
R2516	V2331	V2331	R2243	E2159	L2075	L1974	L1898	L1822	K1738	F1661	PRO	LYS
L2516	F2332	F2332	K2244	M2165	E2076	I1976	S1899	E1823	I1740	K1662	PRO	LYS
L2516	R2333	R2333	F2245	E2166	L2076	Q1979	I1913	T1825	L1741	Y1664	SER	ASP
L2516	Y2426	Y2426	N2252	F2167	D2079	P1980	THR	E1744	F1744	I1665	ASP	ASP
L2516	L2337	L2337	W2253	A2169	K2082	L1981	GLN	S1746	E1745	H1588	GLU	LYS

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	0.66	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%)	30	74
1	B	1415/2516 (56%)	1297 (92%)	110 (8%)	8 (1%)	30	74
1	C	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	30	74
1	D	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	30	74
1	E	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	30	74
All	All	7075/12580 (56%)	6489 (92%)	546 (8%)	40 (1%)	34	74

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	99
1	B	1135/2157 (53%)	1132 (100%)	3 (0%)	94	99
1	C	1135/2157 (53%)	1132 (100%)	3 (0%)	94	99
1	D	1135/2157 (53%)	1132 (100%)	3 (0%)	94	99
1	E	1135/2157 (53%)	1132 (100%)	3 (0%)	94	99
All	All	5675/10785 (53%)	5660 (100%)	15 (0%)	95	99

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