



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 03:00 AM UTC

PDB ID : 4O9Y / pdb_00004o9y
Title : Crystal Structure of TcdA1
Authors : Meusch, D.; Gatsogiannis, C.; Efremov, R.G.; Lang, A.E.; Hofnagel, O.; Vetter, I.R.; Aktories, K.; Raunser, S.
Deposited on : 2014-01-03
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

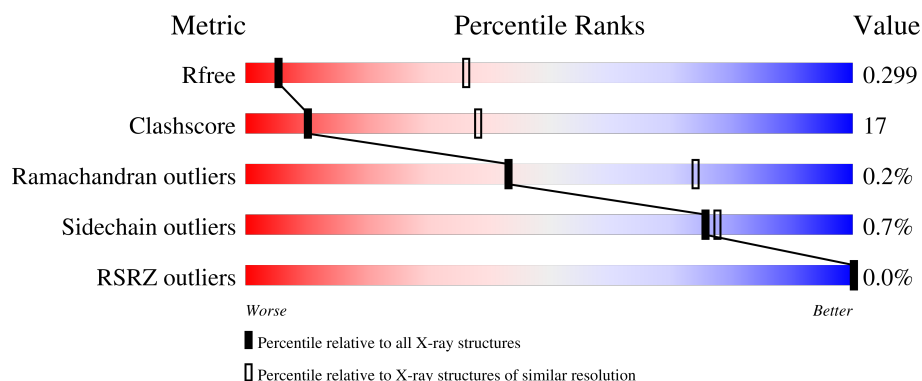
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2516	 62% 36% ..
1	B	2516	 62% 36% ..
1	C	2516	 61% 36% ..
1	D	2516	 63% 35% ..
1	E	2516	 62% 35% ..

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Mol	Chain	Length	Quality of chain
1	F	2516	 62% 36% ..
1	G	2516	 63% 34% ..
1	H	2516	 64% 34% ..
1	I	2516	 62% 36% ..
1	J	2516	 61% 36% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 197663 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

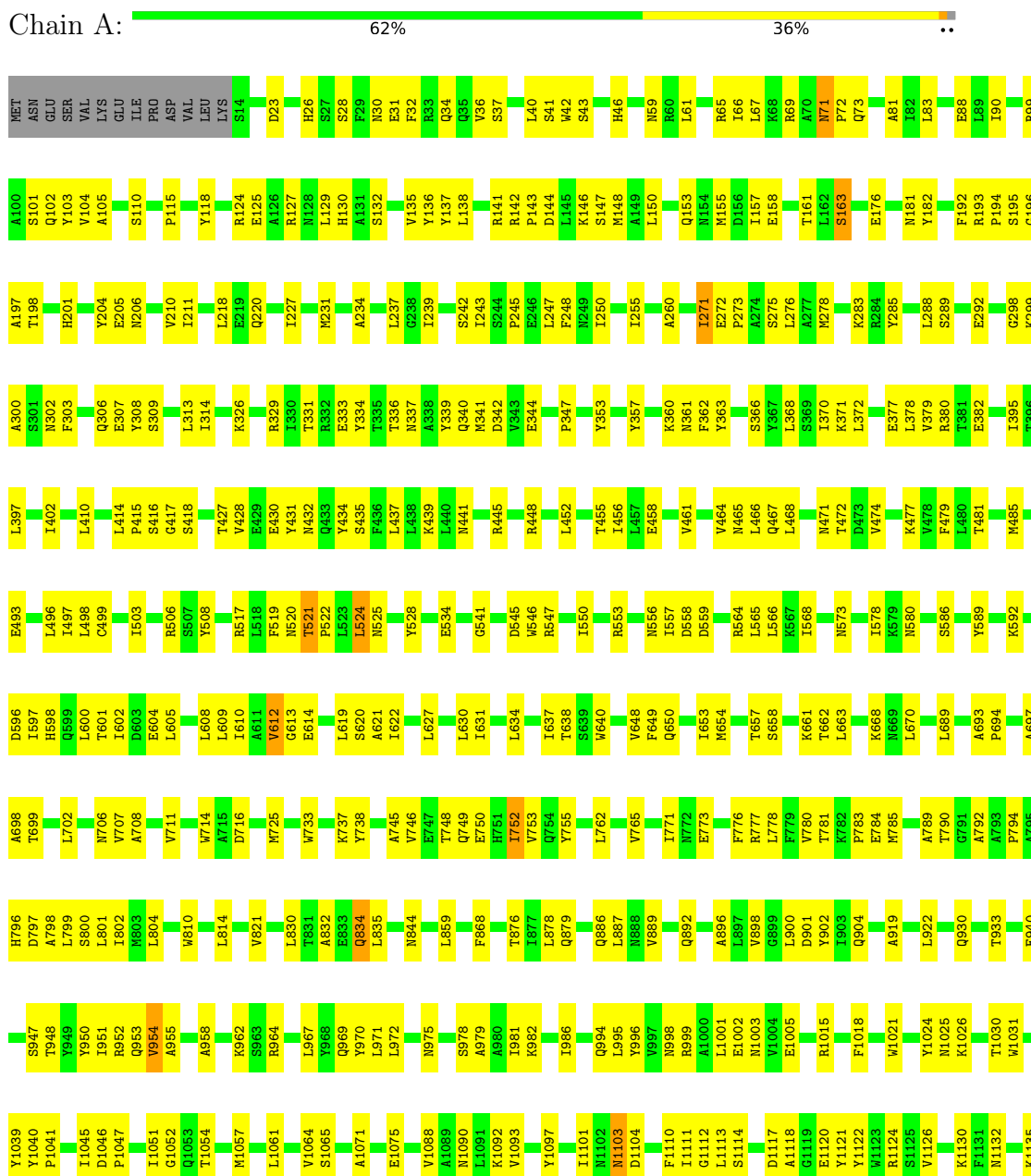
- Molecule 1 is a protein called TcdA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2490	Total 19768	C 12508	N 3364	O 3833	S 63	0	0	0
1	B	2490	Total 19768	C 12508	N 3364	O 3833	S 63	0	0	0
1	C	2490	Total 19768	C 12508	N 3364	O 3833	S 63	0	0	0
1	D	2490	Total 19768	C 12508	N 3364	O 3833	S 63	0	0	0
1	E	2490	Total 19768	C 12508	N 3364	O 3833	S 63	0	0	0
1	F	2490	Total 19768	C 12508	N 3364	O 3833	S 63	0	0	0
1	G	2488	Total 19751	C 12499	N 3359	O 3830	S 63	0	0	0
1	H	2490	Total 19768	C 12508	N 3364	O 3833	S 63	0	0	0
1	I	2490	Total 19768	C 12508	N 3364	O 3833	S 63	0	0	0
1	J	2490	Total 19768	C 12508	N 3364	O 3833	S 63	0	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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





Chain B: 62% 36% ..





Response	Percentage
Yes	61%
No	36%
Don't know	3%



F1555	D1454	Q1371	M1273	LYS	Q1105	I986	1874	T781	1667	1578	V474	V379	A300	G196
F1558	D1455	C1372	A1274	ASP	F1110	A987	1877	E784	K668	A579	K477	R380	S301	A197
E1559	Y1456	N1373	S1275	GLY	I1111	E988	1878	E785	N669	N580	V478	T381	Q306	T198
E1560	L1374	M1375	M1278	Y1188	L1112	Q994	Q879	A789	L670	S586	F479	I395	Y308	N206
E1561	D1459		M1279	R1195	L1113	L995	W890	T790	T673	Y589	T481	T386	S309	V207
G1562	M1462	Y1378	P1280	Y1196	S1114	Y996				I590		L397		I211
R1563	K1463	G1379		H1202	D1117	E1005	W883	P794	L689	I597	Y484	N398	Q312	Q212
K1564	P1464	K1380	S1283		A1118		Q886	A795	A693	L600	M485	T399	L313	Q215
L1565	D1465	N1381	N1284	I1213	E1119	F1018		H796	P694	L593		I314	D215	
E1568	D1466	G1382	Y1285	Y1285	E1120		A896	A798		I597	Y488	D401	T315	L218
S1569	L1467	D1383	Y1286	Y1217	E1121	W1021			A697	H598	A489	I402		E219
F1570	K1468	F1385	R1287	Y1217	Y1122	D1022	L900	T802	A698	Q599	I490		V318	Q220
	G1478	I1386	D1288				D901	H803	T699	L600		P406		
L1576	T1479	S1390	S1290	K1220	V1126	Y1024	Y902	L804		T601	L496		D322	A223
T1585	A1480	S1391	Y1291	I1221	Y1024	K1025	I903	L804	A707	I602	L497	L410	T324	
H1588	S1484	L1391	Q1292	S1222	K1130	K1026	Q904	A808	A708	D603	L498	V413	V325	I227
N1589	P1485	S1398	D1293	E1223	F1131	W1031	S905	D809	V711	E604	C499	L414	K326	H232
E1590	P1486	S1399	F1294	K1225	N1132		P910	W810	L712	L605		P415	Y327	S235
	V1487	N1400	T1295	K1226	A1138	V1034	T911	H811	L713	G417	R506	S416	Y328	L236
Q1594	T1491	K1401	N1296	K1227	M1139	E1227	Y912	A813	L714	L608		W418	R329	L237
		L1402	N1297	K1228	A1140	Y1039	A913	L814	A715		Y508	W419	T331	G238
Q1597	S1494	P1406	Y1299	A1231	V1141	Y1040	Q914	K817	D716	V612			R332	I239
W1598	P1495	Y1407	R1300	F1232	P1041		L922		Q719	G613	N520	T427	E333	N240
Q1599	A1496	G1408	V1301	G1233	I1045		N927	H821	T720	G615	T521		Y334	
R1602	K1497	Q1409	C1236	I1147	I1045	R1050		L822	G721	K616	P522	Y434	T335	L247
T1603	V1502	Y1410	A1237	I1151	R1050	K1055	Q930	L830	D722	T617	L523	L437	T336	T248
R1604	K1503	G1412	Y1306	N1152	K1055		T933	T831	G723	N618	N525	L438	N337	I249
	A1504	S1411	E1311	P1153	K1056		L934	A832	A724	S620		K439	Y339	I250
T1607	G1505	T1414	T1244	Y1154	M1057			E833	A727	A621	Y528	L440	M341	L251
A1610	D1514	S1415	Y1244	K1155	M1057	L1061	E940	Q834	L734	I622	E534	N441	D342	T252
V1614	K1515	L1416	L1245	I1158	L1061			L835		S623		R445	V343	E253
A1615	Q1520	N1418	L1246	R1159	V1064		S947	A838	T739	Q626	L538	L446	E344	E254
R1616	P1521	G1420	L1247	T948	S1065		T948	M839	A745	L627		T450	P347	I255
A1617	S1522	R1421	F1249	Y954	Q1066			A843	Q749	I631	G541	E451	F348	A260
T1618	Y1333	L1422	Y1250	A958	L1069	L1069		N844	Q751	L634	K548	S453	P273	
I1621	D1336	L1423	Q1253		F1085		A958	L847	H751	I637	L551	P454	Y353	L276
L1625	I1337	F1424	D1254	S1165	E1086		K962		I752	T638	K552	T455	R354	A277
S1626	T1351	H1425	T1255	L1167	Q1087		S963	S850	W753		R553	I456	Y357	M278
M1627	A1534	T1429	D1257	Y1168	V1088		R964	T851	Q754	V648	N556	E458	K360	P279
E1628	L1535	I1438	S1258	L1169	A1089		D965	Q852			I557			E280
T1629	E1536		Y1259	L1170	N1090			A853	Q757	F652	D558	V461	S366	Y281
Q1630	I1537		K1260	L1172	L1091		L971	Q854	A758		D559			
		A1441	N1261	E1173	K1092		N975	P860	L759	T655		V464	I370	Y285
Q1633	L1542	K1442	A1262		V1093		Q976		L762		R564	N465	K371	S289
E1634	T1545	R1443	S1283	T1177	Y1097		T983	T863	L763	Y659	L565	L466	L372	
P1635	N1546	L1445	M1264	T1178	H1098		S978	E763	M764	N660	L566	Q467	N373	E292
Q1636		T1446	G1265	K1179			A979	N866	I771	K661	K567		D374	F296
L1637	A1549	N1447	G1266	THR	T1101		T983	A867	L778	T662	I568	I470	K375	L297
G1638			L1267	GLY	N1102		T984	F868		L663		M471	R376	E378
K1639	D1552	I1452	Y1268	ASN	N1103					T664		T472	G298	
G1640		G1453	D1272	SER	D1104		R985	S873			H571	D473	L378	K299

F1641	L1740	H1843	L1947	R2046	A2176	L2268	Q2364	W2455
Y1642	H1743	D1844	Q1951	Q2047	D2177	A2289	S2367	D2466
I1647	S1755	P1845	I1952	L2056	I2179	V2270	K2468	G2467
Y1650	E1756	H1846	V1955	Q2059	S2182	R2272	L2376	P2471
N1651	L1760	Y1848	M1956	L2063	E2183	C2273	F2377	F2472
L1652	S1761	K1849	M1957	I2064	R2186	D2281	L2387	E2473
S1653	F1761	Y1848	N1958	L2065	R2187	S2287	Q2388	G2474
H1654	N1764	T1852	Y1959	L2068	R2188	D2288	L2475	A2476
H1655	Y1767	L1857	Q1960	L2068	R2189	A2289	F2393	L2477
R1659	F1772	D1858	Q1961	K2073	W2192	R2290	K2397	L2482
W1660	Y1773	R1863	R1966	K2087	Q2195	F2291	L2398	T2483
F1661	Y1774	D1865	L1970	S2088	K2195	L2292	R2399	L2484
K1666	T1775	T1866	R1971	K2089	N2198	P2294	E2400	G17
H1667	P1776	Y1868	H1972	R2095	E2202	T2300	P2403	M2491
V1668	M1777	L1871	N1973	R2095	L2203	Y2301	A2404	K2494
V1669	M1777	L1871	N1974	Y2099	K2204	A2302	S2405	Q2497
I1674	R1782	L1876	I1976	L2102	Q2205	G2303	L2406	L2497
L1675	L1783	Q1885	P1980	D2207	D2207	L2304	R2410	L2501
Q1680	L1784	H1888	L1981	E2105	A2214	L2305	R2411	K2502
N1685	D1790	L1889	Y1982	N2106	V2215	E2308	L2412	T2503
F1691	E1791	L1890	L1983	N2108	R2216	L2311	K2413	D2506
I1692	R1794	G1891	A1990	E2111	R2217	L2312	L2422	R2512
P1693	K1797	D1892	D1991	R2118	L2227	A2315	L2423	L2515
L1694	Y1798	L1898	P1992	A2122	Q2231	Q2316	Q2427	K2516
D1696	W1800	R1906	L1995	E2127	Q2232	E2318	A2431	
H1704	S1801	L1907	S1997	V2128	Q2233	L2326	L2432	
A1705	P1802	A1911	G2006	A2127	T2234	R2327	L2433	
K1706	S1803	A1917	G2007	V2128	Q2235	E2330	G2440	
T1710	G1804	N1917	K2008	P2142	S2236	V2331	L2441	
F1711	Y1805	A1918	S2015	N2143	Q2237	A2442	A2442	
K1712	I1806	H1919	S2015	F2240	F2240	C2445	C2445	
K1713	V1807	D1920	R2018	K2244	K2244	L2448	L2448	
S1714	Q1812	A1922	F2019	G2146	N2247	A2449	A2449	
P1715	W1816	I1923	M2022	F2147	N2247	V2450	S2451	
T1719	N1817	V1924	R2027	G2148	Y2251	N2348	S2451	
W1720	R1819	R1927	G2026	G2149	W2252	Q2349	M2454	
W1721	P1820	Q1928	M2029	G2150	W2253	P2350	N2455	
H1724	L1821	N1929	V2030	G2151	R2256	F2351	D2456	
F1725	L1822	T1932	L2033	A2188	G2257	E2356	S2457	
V1726	L1822	ALA	L2033	T2161	R2257	E2356	Q2458	
K1730	S1829	PRD	L2033	N2165	L2258	K2359	Q2459	
N1736	D1830	PRD	T2039	W2171	I2261	L2360	F2460	
P1737	P1831	LEU	L2040	V2171	Y2266	V2361	Q2461	
K1738	V1835	LEU	I2043	E2175	D2267	L2363	L2462	
S1739	D1838	R1939				Q2363	F2464	

• Molecule 1: TcdA1

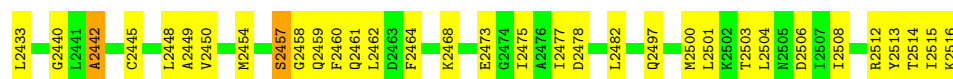
Chain D:  63% 35%

RET	G91	P194	Q306	D401
ASN	Y92	S195	Q306	I402
GLU	N93	G196	S309	L402
SER	A197	T198	Q312	P405
VAL	S101	H201	L313	F406
LYS	Q102	Y204	L314	E407
GLU	Y103	E209	N319	L410
ILE	V104	V210	D322	V413
PRO	A105	T211	R329	L414
ASP	P106	Q212	L330	P415
VAL	G107	L218	T330	S416
LEU	T108	E219	T331	G417
LYS	V109	Q220	R332	S418
S14	Y118	A223	R333	W419
Q15	R124	M231	Y334	S416
C16	Y136	H232	T335	G417
G17	L138	L237	T336	G417
F18	R141	P143	R337	S418
L21	R142	D144	Y339	W419
T22	P143	L145	Q340	K425
D23	D144	K146	R341	F426
H26	L145	S147	D342	T427
S27	S147	Q152	F348	V428
S28	Q152	Q153	Y353	Y434
E31	N154	L154	R354	K437
V36	M155	L164	L355	L438
L40	P156	E167	Y357	K439
S41	E157	L168	K358	K442
W42	E158	L170	K360	L446
S43	T161	S163	N361	L452
E44	L162	L164	L368	S453
N59	E167	E167	S369	L456
R65	L168	L179	T370	V461
I66	L170	F180	K371	V464
L67	L179	N181	L372	N465
K68	F180	T183	N373	L466
A70	N181	I82	K375	Q467
M71	T183	E390	L378	I470
P72	V185	L189	V379	N471
Q73	L189	F192	L389	T472
L74	F192	L395	E390	D473
Q75	L189	T396	L395	V474
A81	F192	L397	L396	K477
I82	L189	N301	L397	V478
L83	L189	N302	L398	F479
N86	L189	N302	L399	L480
A87	F192	N302	L399	T481
E88	L189	N302	L399	K482
L89	L189	N302	L399	L482
R90	L189	N302	L399	M485



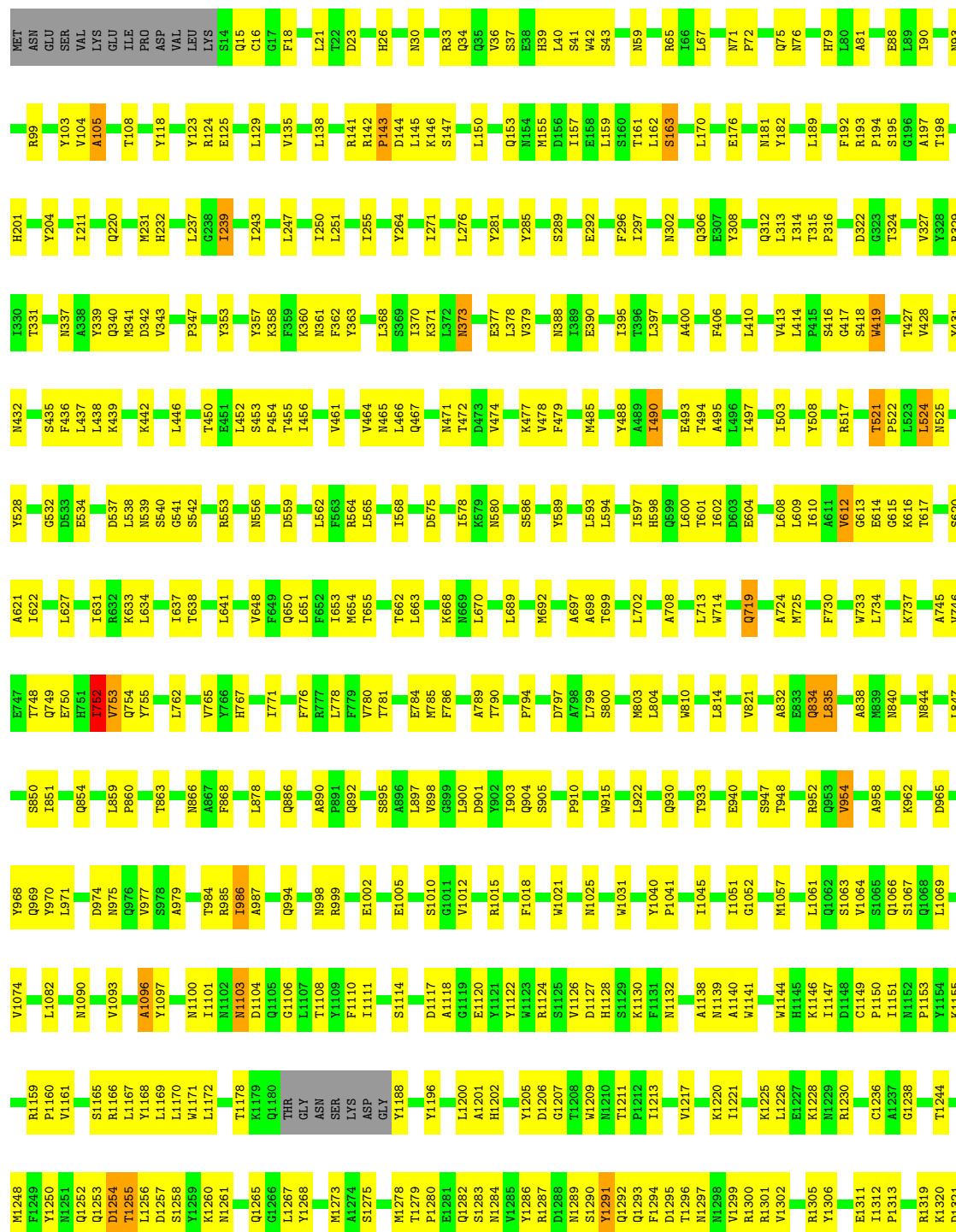


A2315	Q2316	M2317	E2318	D2325	K2326	L2329	E2330	V2331	L2337	N2348	G2349	P2350	F2351	S2352	L2353	E2356	L2360	G2364	L2375	A2376	F2377	G2378	D2382	L2387	Q2388	V2391	S2392	F2393	I2398	Y2402	P2403	A2404	S2405	L2406	G2407	R2410	R2411	I2412	L2422	L2423	Q2430	A2431	I2432																									
L2124	T2125	T2126	A2127	V2128	V2141	P2142	N2143	I2144	F2145	G2146	F2147	A2148	G2149	G2150	G2151	T2151	M2155	F2156	F2157	V2171	M2172	E2175	A2176	D2177	K2178	R2187	R2188	R2189	Q2190	E2191	H2192	E2193	I2194	Q2195	R2196	N2197	N2198	G2199	L2200	K2201	A2202	L2203	K2204	D2207	A2214	G2203	L2204	L2205	A2206	G2207	E2208	K2228	T2229	M2311														
Q2231	E2232	Q2233	Q2237	L2238	A2239	F2240	L2241	K2244	F2245	S2246	N2247	Q2248	A2249	P2250	Y2251	N2252	L2253	R2254	R2255	G2256	R2257	L2258	I2261	A2262	F2263	Y2266	R2272	C2273	Y2280	R2281	A2289	R2290	F2291	L2292	K2293	P2294	G2295	A2296	W2297	T2300	Y2301	A2302	L2303	L2304	L2305	A2306	G2307	E2308	Q2430	A2431	I2432																	
H1888	L1889	D1892	L1896	P1897	L1898	T1901	P1905	R1906	A1911	G1913	H1914	H1915	H1916	H1917	H1918	H1919	I1923	R1927	I1930	P1931	T1932	P1933	ALA	ALA	P1934	ALA	P1935	P1936	P1937	P1938	P1939	P1940	P1941	P1942	P1943	P1944	P1945	P1946	P1947	P1948	P1949	P1950	P1951	P1952	P1953	P1954	P1955	P1956	P1957	P1958	P1959	P1960	P1961	P1962	P1963	P1964	P1965	P1966	P1967	P1968	P1969	P1970	P1971	P1972	P1973	P1974	P1975	P1976
P1980	L1981	L2009	L2016	A2017	F2019	N2025	A2026	R2027	G2028	M2029	V2030	L2033	T2039	L2040	L2043	R2046	Q2047	Q2058	Q2059	L2063	F2064	T2066	L2067	L2068	S2069	L2070	K2087	S2098	Y2099	G2100	K2101	L2102	N2106	T2107	N2108	E2111	L2117	R2118	A2121	T2122	G2123																											
Q1787	D1790	E1791	R1794	H1795	L1796	K1797	Y1798	Y1799	W1800	S1801	P1802	S1803	G1804	Y1805	Q1810	Y1814	Q1815	W1816	R1819	P1820	L1821	L1822	T1825	S1826	W1827	S1828	L1832	V1840	H1843	D1844	P1845	K1849	V1850	T1852	F1853	G1863	D1865	Y1868	M1881	W1882	Q1885																											
V1697	P1698	N1700	S1626	M1627	H1628	T1629	Q1630	Q1633	E1634	F1644	Q1636	L1637	G1638	M1639	G1640	F1641	Y1642	I1647	P1648	Y1650	D1561	G1562	F1563	K1564	L1565	S1569	D1567	E1568	W1660	Y1664	H1665	K1666	V1668	Y1669	D1670	M1671	N1672	S1673	H1674	I1675	Q1680	D1683	T1684	F1691	P1692	P1693	L1694	D1695	D1696																			
Y1530	Q1531	F1532	L1535	E1536	I1537	L1542	F1544	A1549	S1550	I1551	D1552	F1555	T1556	A1557	F1558	E1559	D1561	G1562	F1563	K1564	L1565	S1569	I1572	F1573	Y1574	T1575	T1585	Q1594	Y1595	M1596	Q1597	Y1598	Q1599	R1602	T1603	R1604	L1605	N1606	A1610	R1611	V1614	A1615	R1616	A1617																								
V1434	W1437	I1438	P1439	G1440	A1441	K1442	R1443	S1444	L1445	T1452	G1453	Y1456	D1459	M1462	K1463	P1464	L1467	M1473	T1474	D1475	S1476	K1477	G1478	T1479	A1480	S1484	V1487	E1488	T1491	A1492	N1493	K1497	V1498	Q1499	V1502	K1503	A1504	G1505	D1514	K1515	D1516	V1517	Q1520	F1525																								
L1357	K1368	Q1371	Q1372	M1375	Y1378	K1380	L1381	G1382	D1383	T1389	S1390	M1394	P1395	M1396	N1397	S1398	S1399	N1400	K1401	L1402	Y1405	P1406	Y1407	Y1408	Q1409	Y1410	S1411	G1412	N1413	T1414	S1415	G1416	L1417	M1418	Q1419	G1420	R1421	L1422	F1424	H1425	R1426	D1427	T1428	Y1429	Y1430																							
K1260	N1261	Q1265	G1266	L1267	Y1268	A1271	D1272	M1273	A1274	S1275	M1278	T1279	E1280	P1281	Q1282	S1283	M1284	Y1285	V1286	R1287	D1288	M1289	S1290	Q1291	Q1292	Q1293	F1294	D1295	T1296	M1297	R1300	R1301	Y1306	I1312	D1321	Y1322	Y1327	Y1328	M1334	G1335	D1336	P1338	I1351	Y1352	I1353	S1354	P1355	K1356																				
K1179	Q1180	THR	GLY	ASN	SER	LYS	ASP	GLY	Y1188	Y1196	L1200	A1201	R1204	Y1205	W1209	N1210	T1211	P1212	Y1213	K1220	I1221	L1224	K1225	N1226	E1227	R1230	G1233	L1234	Y1235	C1236	G1238	Y1239	E1242	D1243	T1244	L1245	M1248	F1249	Y1250	N1251	Q1252	Q1253	D1254	Y1255	L1256	D1257	E1258	Y1259																				
V1088	A1089	N1090	L1091	R1092	V1093	Y1097	N1100	M1102	N1103	D1104	G1105	F1110	I1111	G1112	S1114	D1117	E1120	Y1121	Y1122	V1126	K1130	F1131	N1132	A1138	M1139	A1140	W1141	K1146	D1046	P1047	L1151	M1152	P1153	I1158	R1159	P1160	V1161	R1166	V1074	L1167	Y1168	L1169	L1170	W1171	L1172																							
K982	F983	T984	R985	L986	A987	T990	Q993	I994	L995	Y996	F997	N999	L1001	E1002	E1005	S1010	G1011	V1012	R1015	F1018	W1021	Y1024	N1025	K1026	V1034	Y1040	T1045	D1046	P1047	M1057	S1063	V1064	S1065	Q1066	A1071	V1075	L1076	L1082	F1085	E1086	Q1087																											



● Molecule 1: TcdA1

Chain F: 62% 36% ..



Y1322	Q1419	K1503	L1625	Y1708	N1788	H1888	A1994	E2111	E2218	A2302	I2409	N2491
Y1326	H1425	A1504	M1626	M1709	E1791	L1889	L1995	E2117	A2219	G2303	R2410	K2494
Y1327	R1426	G1505	M1627	F1711	E1791	L1890	A1998	R2117	A2220	L2304	G2495	G2495
Y1333	D1427	D1513	E1628	K1712	R1794	G1891	A1999	R2122	V2221	L2305	K2413	K2496
N1334	T1428	D1514	T1629	K1713	M1795	D1892	V2000	A2122	G2223	M2311	P2420	Q2497
G1335	T1429	D1515	Q1630	S1714	L1796	L1896	G2007	T2126	K2224	L2312	A2421	M2500
I1336	Y1430	K1515	D1516	S1715	K1797	P1905	K2008	T2126	T2225	A2315	A2422	L2501
I1337	K1433	D1517	Q1633	S1716	Y1798	R1906	L2009	A2127	S2226	Q2316	L2422	G2496
I1339	K1434	I1518	P1635	G1718	Y1799	L1907	S2012	V2128	K2228	M2317	L2423	L2504
T1340	E1435	Q1520	Q1636	T1719	S1801	D1908	A2136	A2136	T2229	E2318	G2424	N2505
I1351	I1438	S1524	G1638	M1721	S1802	A1911	L2016	N2143	Q2231	K2326	Q2427	D2506
Y1352	A1441	E1527	K1639	V1726	G1804	M1917	R2017	N2144	E2232	L2329	A2431	R2512
I1353	K1442	Y1530	G1640	R1727	I1805	I1918	R2018	F2145	Q2233	E2330	T2441	I2515
S1354	R1443	Q1531	Y1642	K1730	V1807	H1919	F2019	G2146	T2234	G2331	S2434	K2516
P1355	M1447	F1532	V1646	G1731	I1807	I1923	R2027	F2147	Q2235	A2338	Y2435	
K1356	I1452	N1533	I1647	I1732	Q1810	Y1929	G2028	A2148	L2241	Y2341	G2440	
R1358	G1453	N1537	P1648	V1733	I1811	Q1928	M2029	G2149	K2244	A2342	L2441	
I1360	D1454	I1542	P1649	M1736	N1813	N1930	V2030	G2151	A2249	G2343	A2442	
Q1367	D1459	L1542	M1651	P1737	Y1814	I1930	L2033	A2156	N2247	L2344	G2445	
K1368	M1462	F1555	L1652	K1738	Q1815	P1931	T2039	T2157	Q2248	G2344		
L1374	K1463	A1559	L1653	I1743	N1817	T1932	L2040	T2161	L2250	N2348	L2448	
M1375	D1465	K1564	R1659	F1744	R1819	ALA	Q2041	V2164	Y2251	G2349	A2449	
K1380	D1466	L1565	M1660	E1745	P1820	LEU	I2043	M2165	N2252	P2350	V2450	
L1381	L1467	L1569	P1661	M1752	L1821	SER	R2046	E2166	G2256	F2351		
G1382	Y1470	K1662	K1662	S1756	L1822	LEU	L2064	E2167	R2257	S2352	M2454	
D1383	I1471	K1666	K1666	E1756	E1823	R1939	L2065	V2171	T2261	K2359	G2458	
K1384	M1473	P1573	V1669	P1757	S1829	M1942	L2068	E2175	Y2266	L2360	Q2459	
I1386	T1474	T1585	H1674	D1759	D1844	L1947	L2068	A2176	D2267	S2361	Q2461	
L1391	D1475	L1596	H1674	F1760	M1846	M1953	D2072	R2187	L2268	Q2363	F2463	
S1398	S1476	H1587	D1683	S1761	H1847	Y1959	K2073	R2189	A2269	G2364	N2465	
S1399	K1477	Q1594	T1684	M1764	T1852	Y1960	I2075	R2189	R2272	S2367	D2466	
N1400	T1479	Q1597	M1685	M1764	T1856	Q1981	E2081	W2192	C2273	A2368	K2468	
K1401	A1480	W1598	I1686	E1770	T1863	T1982	V2084	Q2195	Y2280	G2369	F2469	
L1402	T1481	Q1599	P1693	Y1774	D1864	L1983	K2087	N2198	R2281	N2374	L2470	
P1406	V1483	R1602	D1695	T1775	D1865	R1966	S2088	E2202	N2285	L2375	F2472	
Y1407	V1487	T1603	D1696	P1776	Y1868	R1972	K2089	E2204	D2266	A2376	E2473	
Y1408	S1494	R1604	D1696	M1777	L1871	N1973	V2084	N2198	D2287	F2377	L2477	
Q1409	P1495	T1607	D1696	M1778	L1876	I1974	R2095	E2204	S2288	D2382	G2480	
G1412	A1496	A1610	L1699	V1779	L1876	I1976	K2099	E2207	D2289	L2387	T2481	
T1414	K1497	R1611	M1700	L1783	W1882	L1981	R2107	D2207	R2291	F2393	T2483	
S1415	Q1499	R1611	H1704	L1784	Q1885	L1981	M2106	L2210	I2292	Y2402	L2484	
G1416	I1500	Y1614	A1705	H1785	A1886	D1991	T2107	A2214	G2295	P2403	S2485	
I1417	I1501	V1616	K1706	E1786	P1992	P1992		R2217		A2404	F2486	
N1418	V1502		V1707	Q1787	L1887	K1993			Y2301	L2406	P2487	

• Molecule 1: TcdA1

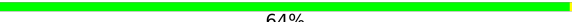
Chain G:  63% 34%

MET	Y1322	Q1419	K1503	L1625	Y1708	N1788	H1888	A1994	E2111	E2218	A2302	I2409	N2491
ASN	Y1326	H1425	A1504	M1626	M1709	E1791	L1889	L1995	E2117	A2219	G2303	R2410	K2494
GLU	Y1327	R1426	G1505	M1627	F1711	E1791	L1890	A1998	R2117	A2220	L2304	G2495	G2495
SER													
VAL													
LYS													
GLU													
ILE													
PRO													
ASP													
VAL													
LEU													
LYS													
S14													
Q15													
C16													
G17													
F18													
N19													
G20													
L21													
T22													
D23													
H26													
S27													
S28													
E31													
V36													
L40													
S41													
W42													
S43													
E44													
L48													
A52													
Q53													
Q56													
L67													
N71													
P72													
A81													
N86													
I90													
F96													
R99													

F1525	F1526	E1527	Y1530	Q1531	F1532	N1533	A1534	L1535	E1536	I1537	L1542	D1552	A1567	E1568	S1569	I1572	P1573	V1574	T1575	K1576	L1577	L1584	T1585	L1586	H1587	H1588	Q1594	Q1597	W1598	Y1601	R1604	R1611	V1614	A1615	R1616	A1617	D1622	M1627	E1628	T1629	Q1630	Q1633	E1634						
R1421	L1422	L1423	R1426	D1427	T1428	I1438	I1453	A1454	E1456	I1457	A1461	A1462	A1463	D1464	D1465	D1466	D1467	I1471	D1475	S1476	G1477	T1478	A1480	V1483	S1484	T1491	S1494	P1495	A1496	V1498	Q1499	T1500	I1501	V1502	K1503	A1504	G1505	D1514	K1515	Q1633	E1634								
G1323	Y1328	D1336	I1337	P1338	Y1352	I1353	S1354	P1355	K1356	L1357	I1358	I1359	I1360	H1361	M1362	G1363	K1368	R1369	M1462	K1463	P1464	L1467	Y1378	G1379	K1380	L1381	G1382	D1383	K1384	F1385	I1386	S1390	S1398	S1399	K1401	L1402	Y1408	Q1409	Y1410	Y1411	G1412	N1413	T1414	S1415	G1416	L1417	T1418	Q1419	G1420
L1245	L1246	V1247	M1248	F1249	N1251	Q1252	Q1253	T1254	T1255	L1256	K1260	L1267	Y1268	A1271	D1272	M1273	A1274	S1275	M1278	T1279	Q1282	S1283	N1284	Y1285	Y1286	D1287	A1288	H1289	S1290	Y1291	Q1292	Q1293	F1294	D1295	T1296	N1297	R1300	R1301	V1302	R1305	Y1306	A1307	Y1310	E1311	I1312	S1317	D1321	Y1322	
M1152	P1153	T1157	I1158	R1159	P1160	Y1163	R1166	Y1168	L1167	L1168	L1169	W1170	W1171	L1172	T1178	K1179	THR	GLY	ASN	SER	LYS	ASP	Y1188	Y1196	L1200	A1201	H1202	Y1205	T1211	P1212	I1213	T1214	I1221	K1225	L1226	E1227	R1230	G1233	C1236	A1237	Y1238	Y1239	E1242	Y1243					
V1064	S1065	Q1066	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151	
T863	N866	A867	F868	C766	Q767	Q761	L762	M763	V765	T769	G770	T771	N772	E773	L778	T781	K782	P783	E784	A789	T790	P794	A795	H796	L804	N812	A813	L814	V821	L822	L830	T831	A832	E833	Q834	L835	A836	N844	L845	L846	L847	S963	R964	D965	P966	L967			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
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L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145	K1146	I1147	I1151			
L971	N975	Q976	V977	S978	A979	A980	K982	I986	I990	A991	K1092	V1093	Y1097	I1101	M1102	N1103	D1104	L1107	F1110	I1111	G1112	L1113	S1114	D1117	G1119	E1120	Y1121	Y1122	W1123	R1124	S1125	V1126	K1130	F1131	N1132	A1138	N1139	A1140	W1141	S1142	E1143	V1144	H1145						

P1635	Q1636	R1727	N1817	SER	L2063	Q2195	P2294	S2405	G2480
Q1637	G1638	K1730	Y1818	A1941	L2064	N2198	G2295	L2406	T2481
K1639	K1731	G1732	P1820	T1943	L2065	A2199	A2296	G2407	L2482
G1640	L1732	L1944	Y1827	T1945	L2068	E2202	W2297	R2408	Q2497
F1641	V1733	T1945	Y1828	D1946	K2073	L2203	T2300	R2410	M2500
Y1642	P1737	P1738	S1829	L1947	K2087	K2204	Y2301	R2411	L2501
V1646	K1738	S1739	D1836	F1948	K2095	L2205	A2302	L2412	K2502
I1647	E1745	E1745	P1837	L1949	R2096	D2207	L2304	K2413	L2504
P1648	S1755	S1755	D1838	M1957	Y2089	E2218	A2306	L2419	L2505
P1649	Y1850	Y1850	P1839	Y1959	L2102	A2219	G2307	A2421	N2506
Y1650	Y1851	Y1851	V1840	W1960	N2107	A2220	M2311	L2422	D2507
Y1651	S1653	S1653	D1844	Y1961	N2108	V2221	L2312	G2424	L2508
S1654	T1654	T1654	Y1848	T1962	E2111	E2223	Q2316	Q2427	R2512
W1660	F1661	F1661	T1852	L1974	L2117	K2224	M2317	D2428	Y2513
F1662	K1662	K1662	T1856	S1975	R2118	K2227	E2330	V2429	T2514
V1668	Y1767	Y1767	L1857	I1976	E2118	T2229	V2331	A2431	L2515
V1669	F1768	F1768	D1858	P1980	A2122	Q2230	T2334	S2434	K2516
D1670	W1769	W1769	D1865	D1991	T2125	Q2231	L2337	G2440	
N1671	E1770	E1770	Y1868	P1992	T2126	E2232	A2338	L2440	
L1672	F1772	F1772	R1869	A1994	Q2128	Q2233	N2348	A2442	
L1675	Y1773	Y1773	Q2004	Q2004	Q2129	L2238	G2349	G2444	
L1676	Y1774	Y1774	G2006	G2006	P2142	L2241	P2350	G2445	
Y1677	T1775	T1775	G2007	G2007	N2143	Q2242	L2360	L2448	
	P1776	P1776	Y1883	G2007	F2145	K2244	S2365	V2450	
	M1777	M1777	L1890	L2009	F2146	N2247	G2366	S2451	
	T1683	T1683	L1898	M2014	F2147	Q2248	G2371	M2454	
	D1684	D1684	L1901	S2015	A2148	Y2251	N2372	G2458	
	I1688	I1688	T1901	L2016	G2149	N2252	N2373	Q2459	
	F1691	F1691	P1905	R2018	G2150	W2253	N2374	F2460	
	I1692	I1692	R1906	F2019	G2151	L2254	N2377	Q2461	
	L1694	L1694	L1907	L1907	T2161	R2255	F2377	L2462	
	H1704	H1704	D1908	M2029	V2164	L2258	D2382	F2464	
	A1705	A1705	R1909	V2030	N2165	Y2262	T2383	N2465	
	K1706	K1706	A1911	L2033	N2166	R2272	S2386	D2466	
	W1800	W1800	T1915	F2036	V2171	C2273	S2390	G2467	
	S1801	S1801	I1930	T2039	E2175	R2281	V2391	K2468	
	F1711	F1711	P1931	L2040	A2176	W2282	F2391	F2469	
	S1803	S1803	T1932	I2043	D2177	R2289	S2392	F2472	
	G1804	G1804	ALA	R2046	R2187	A2289	F2393	E2473	
	K1713	K1713	LEU	Q2047	R2188	R2290	R2389	G2474	
	S1714	S1714	LEU	Q2059	R2189	F2291	P2403	I2475	
	P1715	P1715	ARG		E2191	L2292	A2404	A2476	
	V1807	V1807			K2293			I2477	
	G1718	G1718							
	Q1810	Q1810							
	W1720	W1720							
	W1721	W1721							
	W1726	W1726							

● Molecule 1: TcdA1

Chain H:  64%  34% ..

RET	S111	Q220	P347	T455
ASN	S114	A223	Y353	E458
GLU	Y123	N231	R354	R461
VAL	H130	L237	D356	R462
LYS	V135	G236	Y357	S463
ILE	Y137	I239	Y363	V464
PRO	L138	I250	Q467	T471
ASP	R141	E253	N471	T472
LEU	R142	E254	I370	D473
LYS	P143	I255	K371	V474
S14	K146	A260	N373	K477
Q15	S147	T271	D374	V478
C16	M148	E272	K375	F479
T22	Q152	L276	L378	K482
D23	Q153	A277	V379	Y483
H26	S154	M278	R380	Y484
S28	M155	Y281	T381	M485
E31	D156	L282	E382	Q486
F32	E157	K283	N388	R487
R33	E158	A284	A393	Y488
V36	L159	Y285	N394	T497
S37	S160	L288	L498	L498
T161	T161	S289	T395	C499
L40	S163	D290	T396	N500
S41	L170	E291	L397	I503
W42	E171	E292	L402	R506
A52	E176	G298	L410	S507
N59	Y182	K299	L414	Y508
L67	L189	A300	P415	N520
K68	F192	Q306	S417	T521
R69	R193	F307	S418	P522
A70	P194	Y308	T427	L523
F72	S195	S309	V428	L524
Q73	G198	L313	Y434	N525
H79	A197	T331	L437	Y528
L83	T198	K332	L438	E534
I90	R201	E333	K439	G541
R99	A203	T336	K442	K552
Y204	Y204	N337	R448	R553
I211	T211	K338	A449	A554
Y103	L218	Y338	T450	F555
V109	E219	K341	E451	N556
S110		D342	L452	T557
				D558

H1972	G1864	T1775	V1668	K1564	K1477	I1386	F1294	K1220	A1138	Y1040	G899	E773	R568	R564
N1973	D1865	P1776	V1669	L1565	G1478	S1390	D1295	I1221	M1139	P1041	L900	L778	L566	L566
S1975	L1778	M1777	I1675	S1569	A1480	S1390	T1296	L1224	A1140	Y1044	L922	E784	L663	K567
I1976	L1779	V1779	Q1680	S1579	V1483	P1394	N1297	L1226	W1141	I1045	Q930	F786	L870	I568
L1981	L1784	L1784	D1683	S1579	V1483	P1394	R1300	L1227	W1144	M1049	T933	A789	H571	H571
A1994	L1876	W1795	D1684	T1580	S1484	M1396	R1301	K1228	H1145	R1050	T933	T673	I578	I578
L1995	W1882	L1796	T1684	D1581	G1485	M1397	V1302	K1229	H1146	G1052	E940	T790	V674	V674
S2003	Q1885	K1797	I1686	Q1594	V1487	S1398	N1303	R1230	N1147	Q1053	E940	A789	K579	K579
Q2004	Q1885	L1798	N1686	Q1597	T1491	M1400	N1304	L1233	N1151	T1054	S947	P794	L669	N500
L2009	H1888	F1799	F1691	Q1598	A1492	L1402	Y1306	G1233	N1152	T943	T943	A796	S866	S866
R2018	L1889	P1801	I1692	Q1599	P1495	Y1405	T1312	Y1235	P1153	M1057	R952	H796	M682	M682
F2019	S1803	D1695	P1693	R1604	K1496	Y1408	S1317	C1236	Q953	D1058	R952	L799	A693	A693
N2025	G1804	D1696	D1695	N1606	K1497	Q1409	D1321	G1238	V954	A1059	V954	L799	P694	P694
A2026	L1806	V1697	V1697	T1607	Q1499	Y1410	Y1322	D1243	A958	L1060	A958	I802	A698	A698
R2027	T1901	I1806	H1704	L1608	I1500	S1411	Y1322	T1244	I1182	L1069	A958	M603	T699	T699
G2028	W1902	V1807	K1713	T1609	I1501	T1414	D1326	L1245	Y1183	V1074	K962	F807	L702	D596
N2029	R1906	Q1810	M1709	R1610	K1502	S1415	Y1327	M1248	R1166	F1085	L967	A808	N706	I597
V2030	L1907	T1811	T1710	R1611	K1503	G1416	Y1328	F1249	L1167	E1086	L967	A808	N706	I597
L2033	D1908	Q1812	F1711	V1614	A1504	L1417	Y1328	Y1250	Y1168	M1090	N975	L822	L713	Q599
L2039	S1921	M1813	K1712	W1614	G1505	H1418	Y1333	M1251	L1169	V1083	Y970	V811	L714	L600
N2042	W1816	W1816	K1713	T1618	E1508	Q1419	Y1333	K1252	L1170	A1089	Y970	N812	W714	T601
L2043	M1817	N1817	F1715	D1622	D1514	F1424	I1337	Q1253	W1171	K1092	N975	L830	A715	I602
E2045	A1925	Y1818	P1715	D1622	K1515	H1425	I1337	T1255	L1172	K1092	N975	L830	A715	L605
R2046	L1926	R1819	G1717	S1625	D1516	W1437	N1341	D1257	T1178	V1093	S973	T831	D722	L608
N2047	R1927	G1718	G1718	S1625	Q1520	I1438	N1341	S1258	Q1179	A1096	S973	A832	M725	L609
L2052	T1932	T1719	T1719	M1627	Q1520	I1438	N1341	S1258	Q1179	A1096	S973	A832	M725	L609
D2048	T1932	W1721	W1721	Q1630	P1523	A1441	I1351	K1260	THR	Y1097	E933	Q834	T726	V612
L2052	D1836	V1726	R1727	E1634	S1524	S1444	I1352	K1260	GLY	H1098	E933	Q834	T726	G613
L2055	P1837	R1727	R1727	E1634	S1524	S1444	I1352	K1260	ASN	N102	E933	Q834	T726	E614
L2055	D1838	K1730	G1731	K1639	F1525	L1445	Y1352	K1260	LYS	N1103	E933	Q834	T726	G615
L2055	A1839	G1731	G1731	K1640	D1527	L1445	Y1352	K1260	ASP	N1103	E933	Q834	T726	K616
N2058	V1840	I1732	I1732	F1641	E1530	M1447	I1357	D1272	GLY	D1104	E933	Q834	T726	T617
L2063	Q1842	V1733	V1733	I1647	F1532	I1452	I1360	S1275	Y1188	I1111	E933	Q834	T726	N618
L2063	H1843	V1733	V1733	I1647	F1532	I1452	I1360	S1275	Y1188	I1111	E933	Q834	T726	N618
L2063	D1844	P1737	P1737	P1648	L1535	Y1456	H1361	S1275	Y1188	I1111	E933	Q834	T726	N618
L2065	M1846	K1738	K1738	P1649	E1536	D1459	N1362	M1278	L1198	G1112	E933	Q834	T726	N618
L2065	H1847	H1743	H1743	N1651	I1537	D1459	G1363	M1278	L1198	G1112	E933	Q834	T726	N618
L2068	Y1848	H1743	H1743	S1653	L1542	K1462	K1368	Q1282	L1200	L1113	E933	Q834	T726	N618
K2073	K1849	L1750	L1750	T1654	Y1551	D1465	Q1371	S1283	H1202	G1119	E933	Q834	T726	N618
K2073	V1850	E1756	E1756	H1655	Y1551	D1465	Q1371	S1283	H1202	G1119	E933	Q834	T726	N618
K2087	S1851	E1756	E1756	H1655	Y1551	D1465	Q1371	S1283	H1202	G1119	E933	Q834	T726	N618
S2088	F1853	S1761	S1761	D1657	F1555	L1467	M1375	Y1286	W1209	W1123	E933	Q834	T726	N618
R2095	L1857	Y1767	Y1767	V1660	F1558	Q1469	K1380	D1288	N1210	S1125	E933	Q834	T726	N618
Y2099	D1858	Y1767	Y1767	V1661	E1560	M1473	K1382	S1290	N1211	K1026	E933	Q834	T726	N618
Y2099	L1859	E1770	E1770	F1661	E1560	T1474	D1383	Y1291	P1212	G1033	E933	Q834	T726	N618
Y2099	R1863	Y1774	Y1774	Y1664	G1563	S1476	F1385	Q1293	F1215	N1132	E933	Q834	T726	N618

L2102	Q2205	L2304	K2408	K2502
N2106	I2206	L2305	I2409	T2503
N2107	D2207	A2306	R2410	L2504
N2108	A2214	G2307	R2411	N2505
E2111	A2214	E2308	I2412	D2506
L2117	R2217	L2310	K2413	R2512
A2122	E2218	L2312	Q2414	T2513
V2128	S2226	A2315	L2422	T2514
Q2129	L2227	Q2316	L2423	K2516
A2136	T2228	N2317	D2428	
	Q2230	E2318	Q2430	
	Q2233	K2326	A2431	
	Q2237	L2329	I2432	
F2145	F2240	E2330	S2434	
G2146		V2331	Q2435	
F2147			G2436	
	K2244	V2335	D2437	
G2149	F2245	S2336	A2442	
G2150	S2246	L2337	C2445	
G2151	N2247	A2338	E2446	
	Q2248	E2339	A2447	
A2156	A2249	V2340	L2448	
I2157	Y2251	N2348	V2450	
T2161	W2252	G2349	V2451	
	W2253	P2350	K2454	
V2164	L2254	L2360	N2455	
N2165	G2256	G2364	G2458	
F2167	R2257	S2365	Q2459	
S2168	L2258	G2366	F2460	
	I2261		Q2461	
V2171		L2375	L2462	
	Y2266	A2376	D2463	
E2175	D2267	F2377	F2464	
A2176	L2268	G2378	R2465	
D2177			D2466	
K2178	R2272	D2382	G2467	
	C2273	L2387	K2468	
S2182			F2469	
	R2281	V2391	L2470	
R2186	A2289	S2392	F2471	
R2187		F2393	P2472	
R2188	I2292	L2396	E2473	
R2189	K2293	L2397	G2474	
Q2190	P2294	A2476	I2475	
E2191	G2295	I2477	I2476	
W2192	A2296		I2477	
E2193		P2403	L2482	
I2194	T2300	K2404		
Q2195	Y2301	S2405	Q2497	
	L2203	L2406		
E2202	G2303	G2407	L2501	

• Molecule 1: TcdA1

Chain I:  62% 36% ..

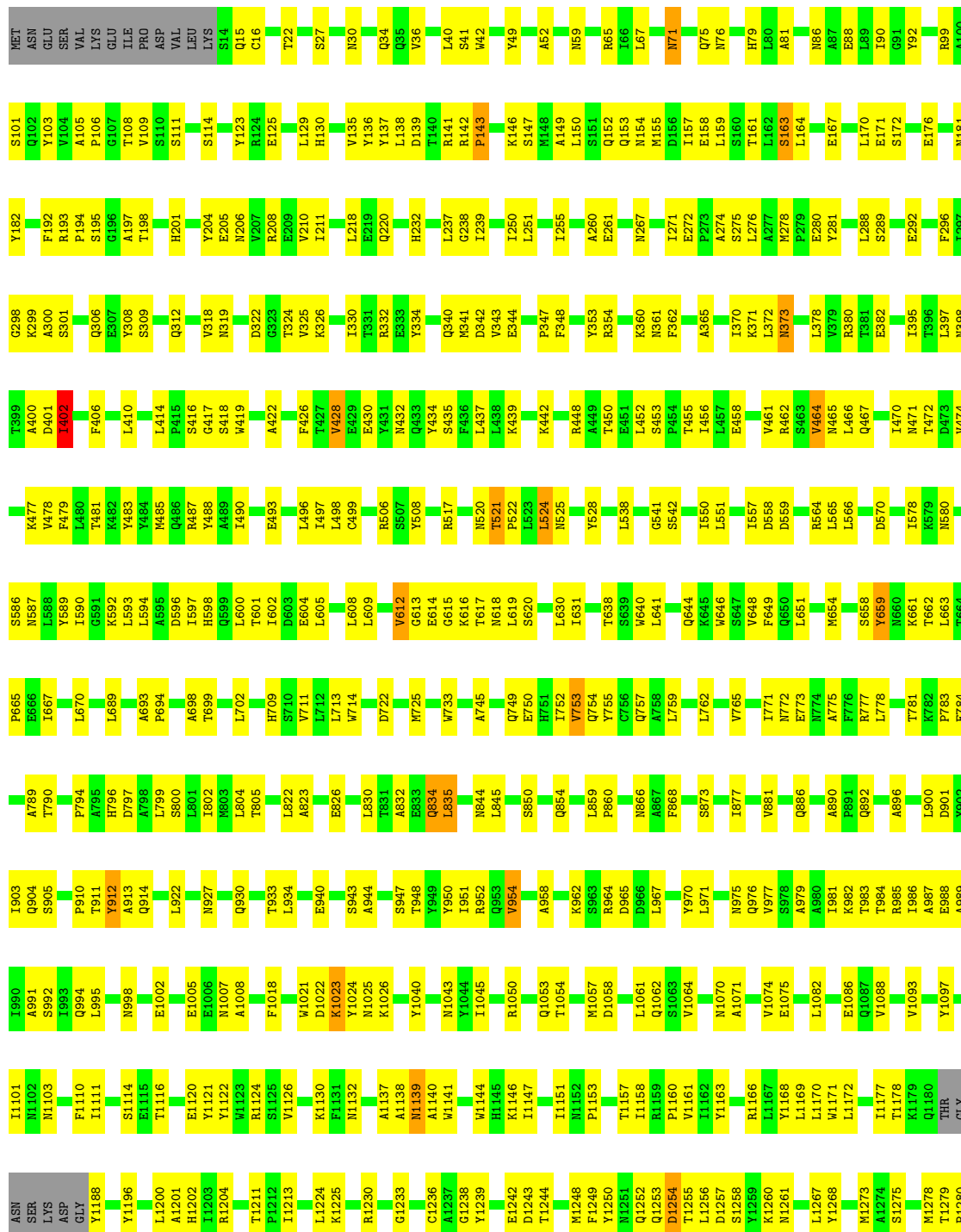
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ASN	E121	L237	V325	L410		K592	A693	F779
GLU	L122	G238	K326			L593	P694	
SER	L123	I239	R329	L414		L594	P783	P783
VAL	R124	N240	R330	P415		A595	E784	E784
LYS			T331	S416		L498	T699	M785
GLU	S132	I243	R332			C499	L702	A789
ILE	V135	L247	E333	W419		R506	Q599	T790
PRO	Y136		T336	A423		Q514	V707	P794
ASP	Y137	I250	N337			B517	H709	
LEU	R141	L251	A338	P426		L516	S710	L799
LYS	R142	I255	Y339	T427		F519	V711	
S14	P143	N259	Q340			N520	D606	T802
C16	K146	E261	K341	E430		P521	L713	N803
D23	S147	L263	E344	Y431		L523	W714	L804
H26	Q153	N267	F348	N432		E524	A715	
S27	M155	I271	E351	O433		L524	D716	L814
S28	D156	E272	R352	Y434		N525	K717	
E31	I157	P273	R353	S435		Y528	L718	W821
F32	E158	L276	K354	L437		E534	Q719	L822
R33	T161	K277	L355			S540	D722	P825
S37	L162	L278	K358	N441		G541	W725	L830
S41	S163	E279	F359	K442		S542	T726	T831
W42	E176	E280	K360	O445		R547	A727	A832
S43	L179	Y281	N361	L446		K548	W733	Q834
N59	L181	K283	F362	S447		T549	L739	L835
L67	Y182	Y285	Y363			L550	P740	N840
K68	T183	L288	I370	T450		R553	A745	L841
R69	K184	S289	K371	E451		L556	E746	N844
A70	L189	E292	L372	L452		D558	E747	L845
N71	P194	L293	L373	S453		D559	T748	L846
P72	S195	A300	R376	T456		L560	Q749	S850
Q73	G196	S301	E377	L457		S561	E750	S851
	T198	N302	L378	E458		L562	H751	Q852
	P199	E292	Y379	S461		F563	I752	A853
H79	S195	L293	R380	V461		R564	W753	Q854
L80	G196	A300	T381	V464		X567	Q754	
A81	T198	E292	E382	L466		L568	Y755	
L83	P199	L293	Y387	Q467		F569	A758	P860
	Q212	Q306	E390	T470		L578	L762	V862
R99	L218	Y308	T391	M471		N580	E763	N866
A100	E219	L313	S392	T472		N581	W764	A867
Q102	Q220	I314	L397	D473		L582	V765	P868
Y103	A223	Y318	N398	V474		L585	S768	S873
A105	T227	G322	T399	K477		S586	L771	N880
M112		G323	A400	V478		Y589	W772	Q886
			D401	P479		L590	A775	L887
			L402	K482				





• Molecule 1: TcdA1

Chain J: 61% 36% 3%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	303.25Å 320.73Å 667.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	78.3 (20.00-3.50) 78.3 (20.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.39	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.243 , 0.295 0.248 , 0.299	Depositor DCC
R_{free} test set	19006 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 11.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	197663	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.53	0/20194	1.02	59/27427 (0.2%)
1	B	0.53	0/20194	1.02	77/27427 (0.3%)
1	C	0.52	0/20194	1.01	74/27427 (0.3%)
1	D	0.53	0/20194	1.01	65/27427 (0.2%)
1	E	0.54	0/20194	1.03	88/27427 (0.3%)
1	F	0.51	1/20194 (0.0%)	1.00	72/27427 (0.3%)
1	G	0.53	0/20177	1.01	67/27405 (0.2%)
1	H	0.51	0/20194	1.01	59/27427 (0.2%)
1	I	0.51	0/20194	1.00	54/27427 (0.2%)
1	J	0.51	0/20194	1.02	69/27427 (0.3%)
All	All	0.52	1/201923 (0.0%)	1.01	684/274248 (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	C	0	2
1	D	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	2450	VAL	CA-CB	5.34	1.60	1.54

The worst 5 of 684 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1647	ILE	CA-C-N	17.43	132.21	119.66
1	D	1647	ILE	C-N-CA	17.43	132.21	119.66
1	E	1647	ILE	CA-C-N	13.46	129.49	119.66
1	E	1647	ILE	C-N-CA	13.46	129.49	119.66
1	I	1291	TYR	N-CA-C	-13.30	90.79	109.95

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1730	LYS	Peptide
1	C	1730	LYS	Peptide
1	C	521	THR	Peptide
1	D	1730	LYS	Peptide
1	F	1730	LYS	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	19768	0	19307	722	0
1	B	19768	0	19307	726	0
1	C	19768	0	19307	734	0
1	D	19768	0	19307	730	0
1	E	19768	0	19307	731	0
1	F	19768	0	19307	716	0
1	G	19751	0	19289	692	0
1	H	19768	0	19307	685	0
1	I	19768	0	19307	729	0
1	J	19768	0	19307	728	0
All	All	197663	0	193052	6693	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 6693 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:1653:SER:H	1:A:1713:LYS:HE3	1.13	1.09
1:J:1653:SER:H	1:J:1713:LYS:HE3	1.22	1.04
1:C:1117:ASP:H	1:D:1211:THR:HG21	1.21	1.03
1:J:1250:TYR:HE2	1:J:1294:PHE:HB3	1.20	1.03
1:E:1250:TYR:HE2	1:E:1294:PHE:HB3	1.26	1.01

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 X-ray entries followed by that with respect to entries of similar resolution.

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	2484/2516 (99%)	2384 (96%)	94 (4%)	6 (0%)	43	74
1	B	2484/2516 (99%)	2397 (96%)	82 (3%)	5 (0%)	43	74
1	C	2484/2516 (99%)	2394 (96%)	85 (3%)	5 (0%)	43	74
1	D	2484/2516 (99%)	2390 (96%)	90 (4%)	4 (0%)	43	74
1	E	2484/2516 (99%)	2387 (96%)	92 (4%)	5 (0%)	43	74
1	F	2484/2516 (99%)	2389 (96%)	90 (4%)	5 (0%)	43	74
1	G	2482/2516 (99%)	2393 (96%)	84 (3%)	5 (0%)	43	74
1	H	2484/2516 (99%)	2393 (96%)	86 (4%)	5 (0%)	43	74
1	I	2484/2516 (99%)	2393 (96%)	86 (4%)	5 (0%)	43	74
1	J	2484/2516 (99%)	2395 (96%)	84 (3%)	5 (0%)	43	74
All	All	24838/25160 (99%)	23915 (96%)	873 (4%)	50 (0%)	43	74

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1651	ASN
1	C	522	PRO
1	D	954	VAL

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Mol	Chain	Res	Type
1	F	954	VAL
1	F	1651	ASN

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 X-ray entries followed by that with respect to entries of similar resolution.

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	2134/2157 (99%)	2120 (99%)	14 (1%)	76	78
1	B	2134/2157 (99%)	2124 (100%)	10 (0%)	81	80
1	C	2134/2157 (99%)	2116 (99%)	18 (1%)	73	77
1	D	2134/2157 (99%)	2116 (99%)	18 (1%)	73	77
1	E	2134/2157 (99%)	2120 (99%)	14 (1%)	76	78
1	F	2134/2157 (99%)	2122 (99%)	12 (1%)	78	79
1	G	2132/2157 (99%)	2119 (99%)	13 (1%)	78	79
1	H	2134/2157 (99%)	2117 (99%)	17 (1%)	73	77
1	I	2134/2157 (99%)	2116 (99%)	18 (1%)	73	77
1	J	2134/2157 (99%)	2121 (99%)	13 (1%)	78	79
All	All	21338/21570 (99%)	21191 (99%)	147 (1%)	76	78

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2261	ILE
1	J	2171	VAL
1	I	752	ILE
1	I	1814	TYR
1	D	1146	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 340 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1843	HIS

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Mol	Chain	Res	Type
1	I	1419	GLN
1	H	94	ASN
1	H	1961	GLN
1	I	2248	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2490/2516 (98%)	-1.30	0 100 100	11, 61, 112, 209	0
1	B	2490/2516 (98%)	-1.27	1 (0%) 100 100	19, 63, 114, 190	0
1	C	2490/2516 (98%)	-1.28	0 100 100	14, 67, 116, 184	0
1	D	2490/2516 (98%)	-1.29	0 100 100	10, 64, 115, 186	0
1	E	2490/2516 (98%)	-1.29	0 100 100	11, 58, 112, 186	0
1	F	2490/2516 (98%)	-1.24	0 100 100	8, 71, 134, 210	0
1	G	2488/2516 (98%)	-1.24	0 100 100	6, 67, 128, 210	0
1	H	2490/2516 (98%)	-1.23	0 100 100	13, 68, 128, 194	0
1	I	2490/2516 (98%)	-1.22	0 100 100	10, 68, 127, 195	0
1	J	2490/2516 (98%)	-1.22	0 100 100	8, 69, 130, 197	0
All	All	24898/25160 (98%)	-1.26	1 (0%) 100 100	6, 65, 123, 210	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.