



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:11 PM UTC

PDB ID : 5M59 / pdb_00005m59
Title : Crystal structure of Chaetomium thermophilum Brr2 helicase core in complex with Prp8 Jab1 domain
Authors : Absmeier, E.; Becke, C.; Wollenhaupt, J.; Santos, K.F.; Wahl, M.C.
Deposited on : 2016-10-20
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Mogul	:	2022.3.0, CSD as543be (2022)
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

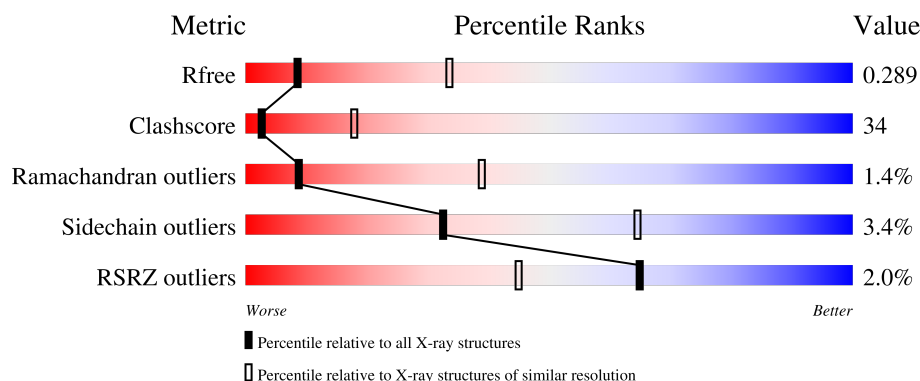
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	B	276	45% 48% • •
1	D	276	48% 45% • 5%
1	F	276	49% 45% • •
1	H	276	2% 46% 48% • •
2	A	1772	46% 49% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	1772	
2	E	1772	
2	G	1772	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	E	2201	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 63679 atoms, of which 12 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 Putative pre-mRNA splicing factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	266	Total	C	N	O	S	0	0	0
			2116	1352	362	392	10			
1	D	263	Total	C	N	O	S	0	0	0
			2093	1339	359	385	10			
1	F	265	Total	C	N	O	S	0	0	0
			2116	1353	362	391	10			
1	H	267	Total	C	N	O	S	0	0	0
			2125	1358	364	393	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2034	GLY	-	expression tag	UNP G0SFL3
B	2035	ALA	-	expression tag	UNP G0SFL3
B	2036	MET	-	expression tag	UNP G0SFL3
D	2034	GLY	-	expression tag	UNP G0SFL3
D	2035	ALA	-	expression tag	UNP G0SFL3
D	2036	MET	-	expression tag	UNP G0SFL3
F	2034	GLY	-	expression tag	UNP G0SFL3
F	2035	ALA	-	expression tag	UNP G0SFL3
F	2036	MET	-	expression tag	UNP G0SFL3
H	2034	GLY	-	expression tag	UNP G0SFL3
H	2035	ALA	-	expression tag	UNP G0SFL3
H	2036	MET	-	expression tag	UNP G0SFL3

- Molecule 2 is a protein called Pre-mRNA splicing helicase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1738	Total	C	N	O	S	0	0	0
			13917	8891	2369	2592	65			
2	C	1702	Total	C	N	O	S	0	0	0
			13628	8709	2319	2536	64			

Continued on next page...

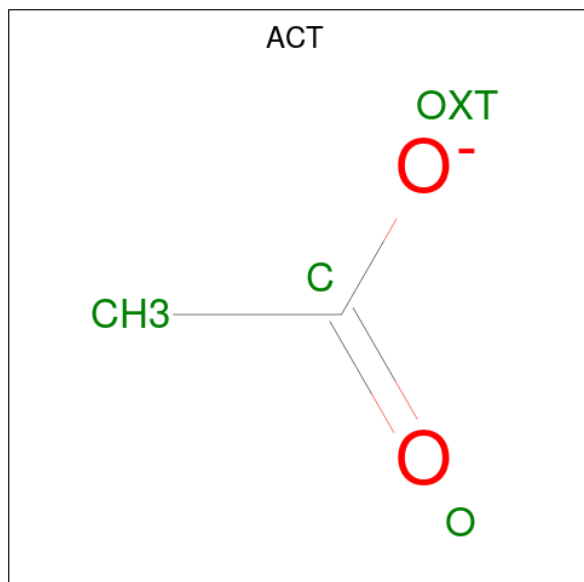
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	1740	Total	C	N	O	S	0	0	0
			13925	8896	2372	2592	65			
2	G	1710	Total	C	N	O	S	0	0	0
			13701	8753	2336	2547	65			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	expression tag	UNP G0S0B9
A	423	ALA	-	expression tag	UNP G0S0B9
A	424	GLU	-	expression tag	UNP G0S0B9
A	425	PHE	-	expression tag	UNP G0S0B9
C	422	GLY	-	expression tag	UNP G0S0B9
C	423	ALA	-	expression tag	UNP G0S0B9
C	424	GLU	-	expression tag	UNP G0S0B9
C	425	PHE	-	expression tag	UNP G0S0B9
E	422	GLY	-	expression tag	UNP G0S0B9
E	423	ALA	-	expression tag	UNP G0S0B9
E	424	GLU	-	expression tag	UNP G0S0B9
E	425	PHE	-	expression tag	UNP G0S0B9
G	422	GLY	-	expression tag	UNP G0S0B9
G	423	ALA	-	expression tag	UNP G0S0B9
G	424	GLU	-	expression tag	UNP G0S0B9
G	425	PHE	-	expression tag	UNP G0S0B9

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 7 2 3 2	0	0
3	C	1	Total C H O 7 2 3 2	0	0
3	E	1	Total C H O 7 2 3 2	0	0
3	G	1	Total C H O 7 2 3 2	0	0

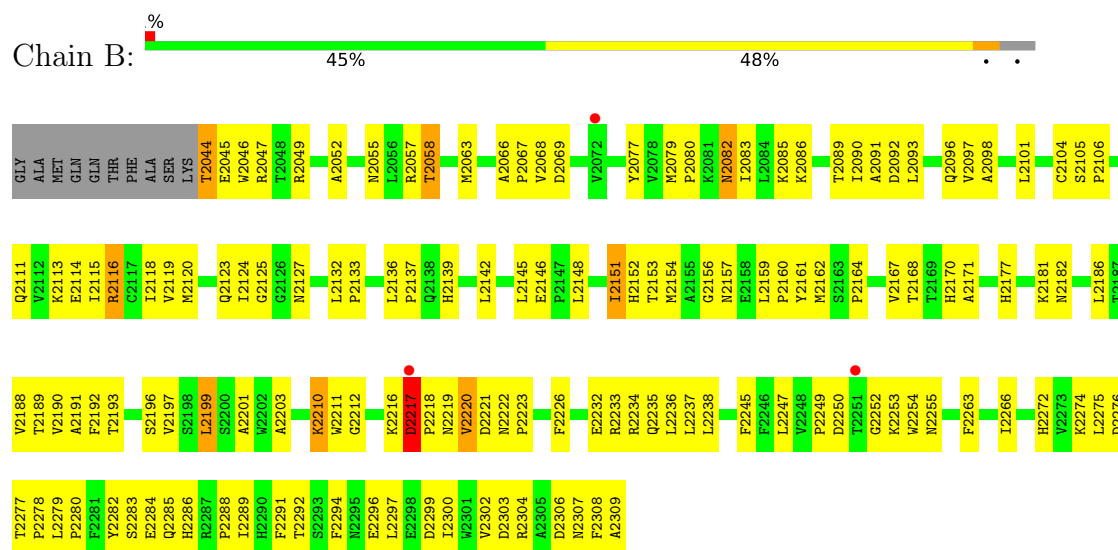
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	D	2	Total O 2 2	0	0
4	C	5	Total O 5 5	0	0
4	F	1	Total O 1 1	0	0
4	E	7	Total O 7 7	0	0
4	G	3	Total O 3 3	0	0

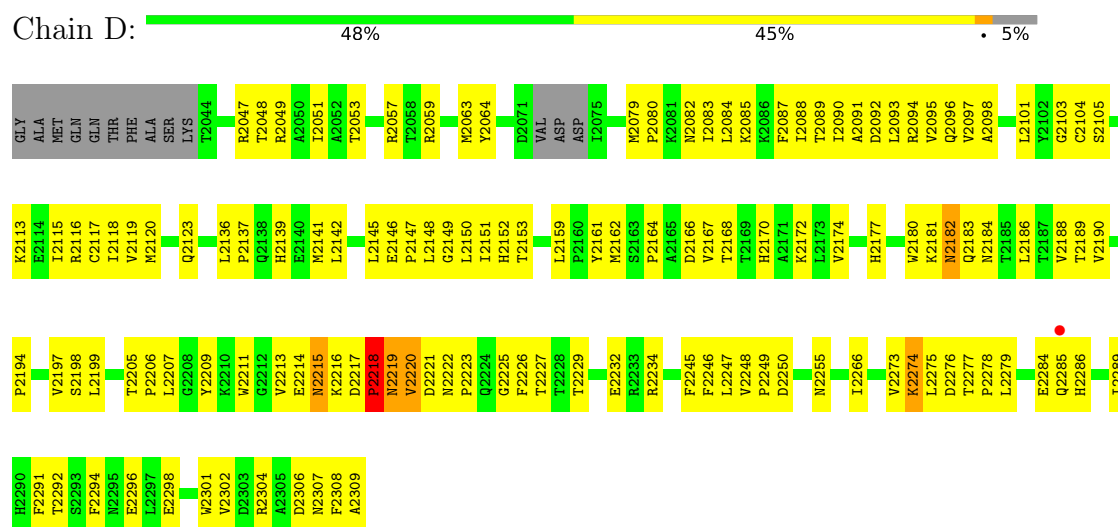
3 Residue-property plots

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: Putative pre-mRNA splicing factor

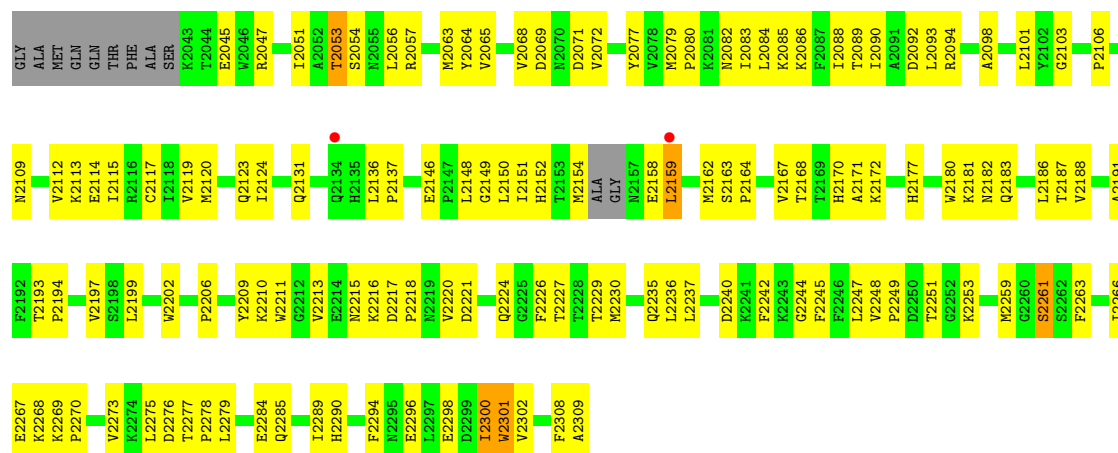


• Molecule 1: Putative pre-mRNA splicing factor

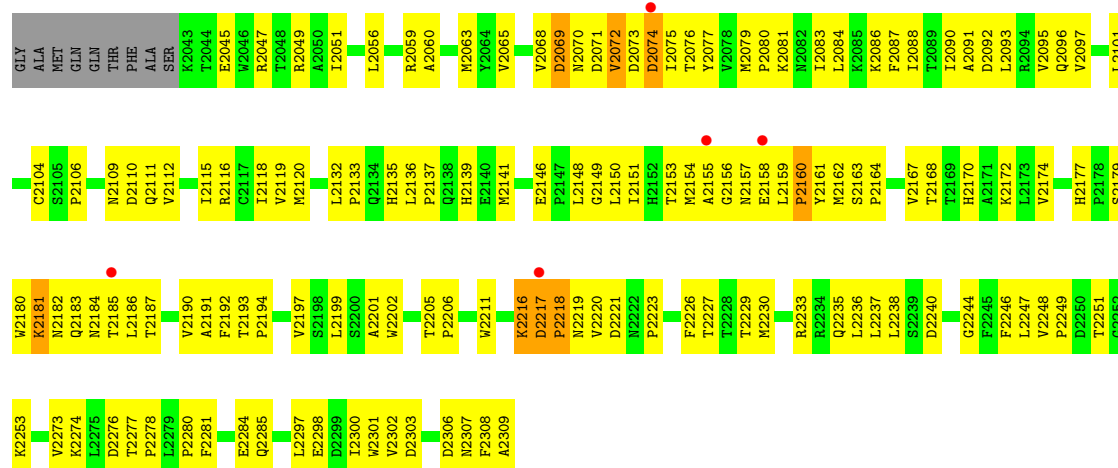


• Molecule 1: Putative pre-mRNA splicing factor

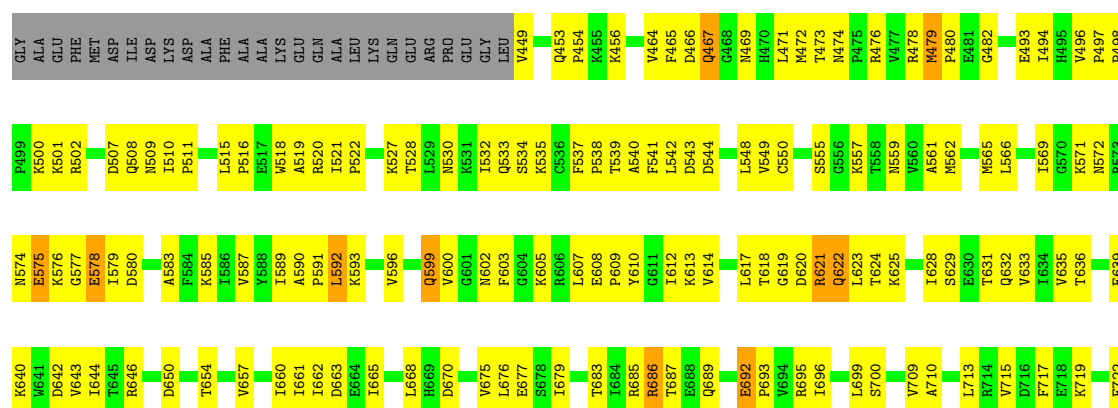




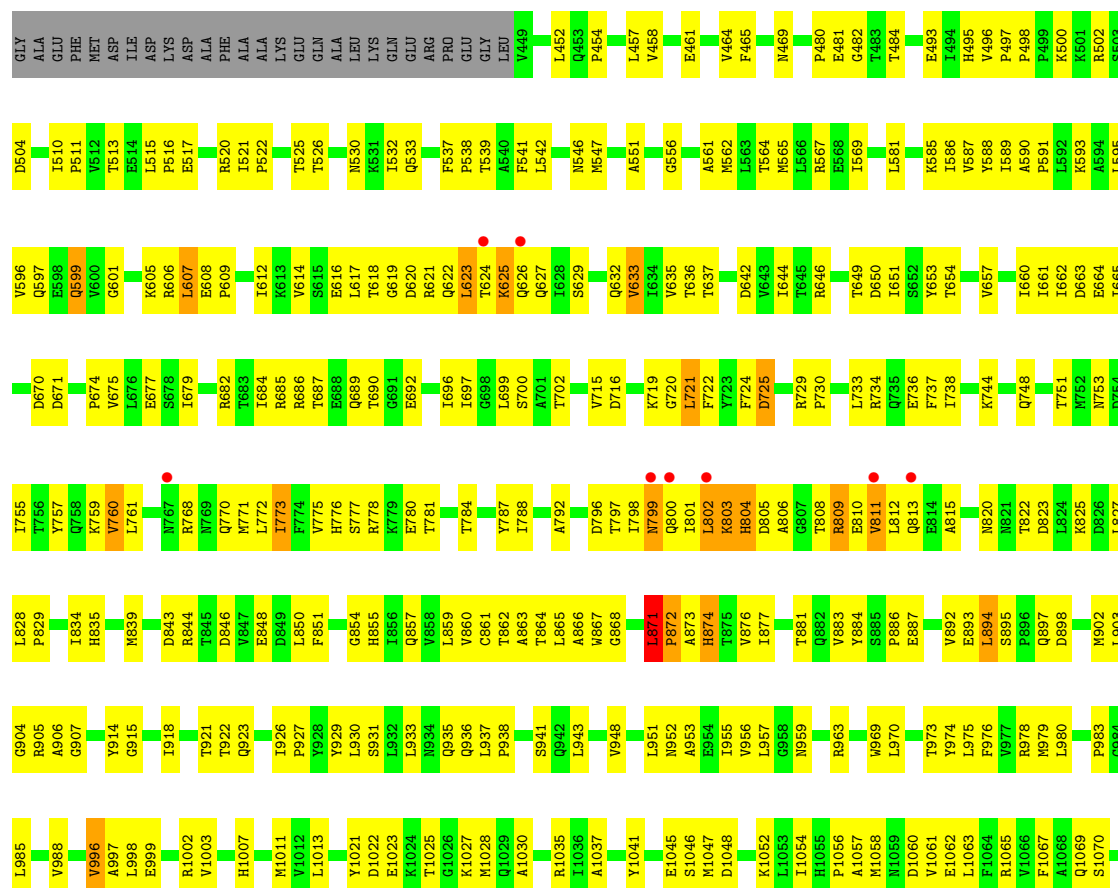
• Molecule 1: Putative pre-mRNA splicing factor



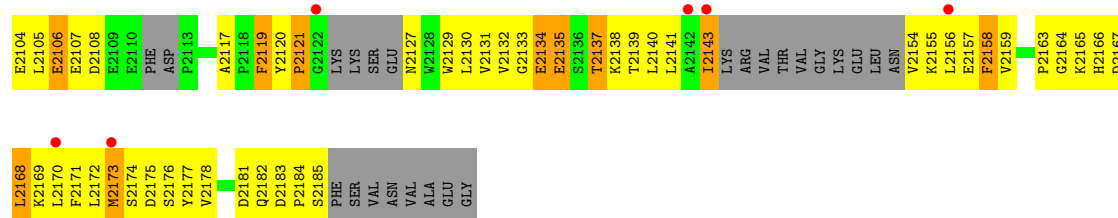
• Molecule 2: Pre-mRNA splicing helicase-like protein



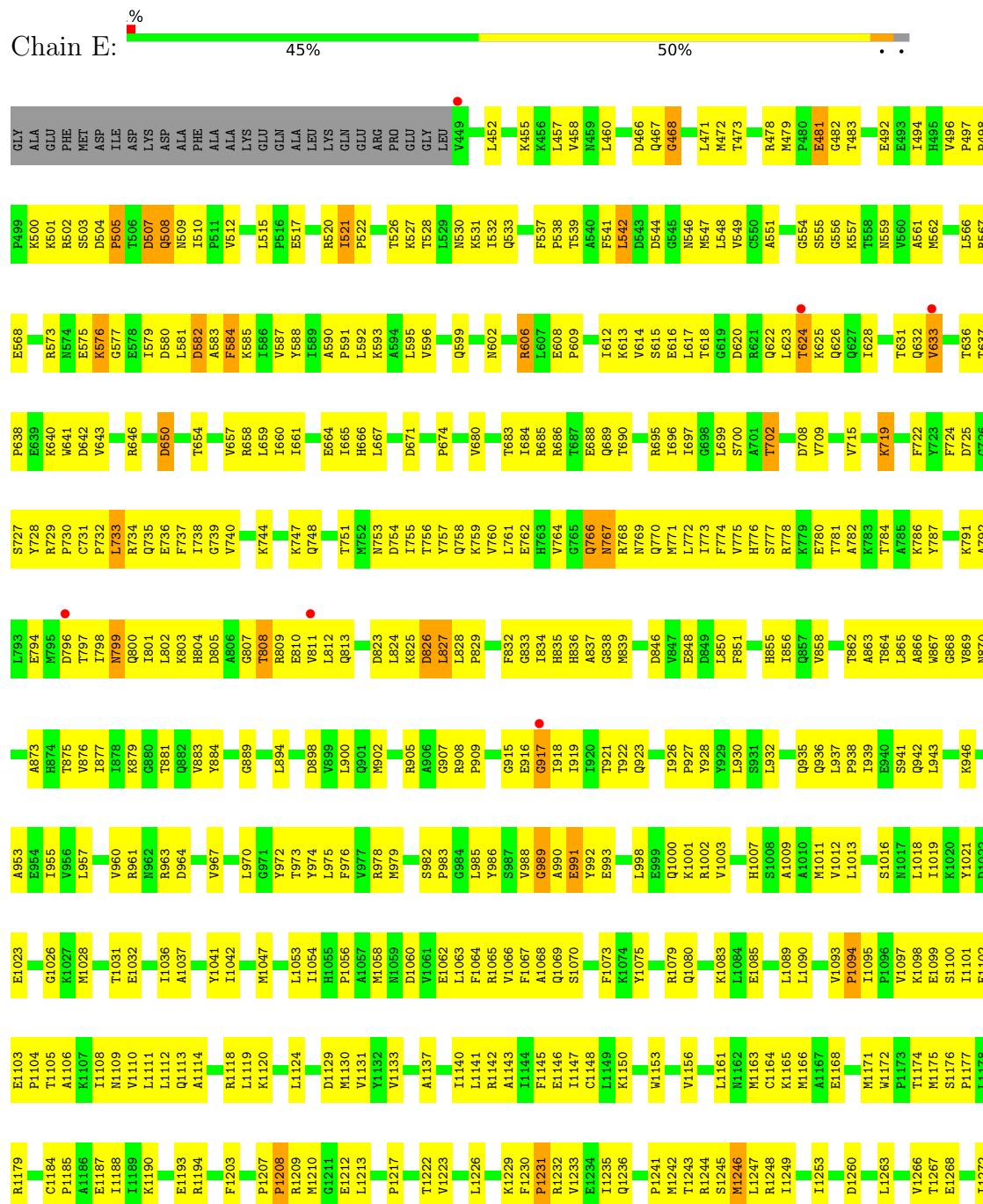


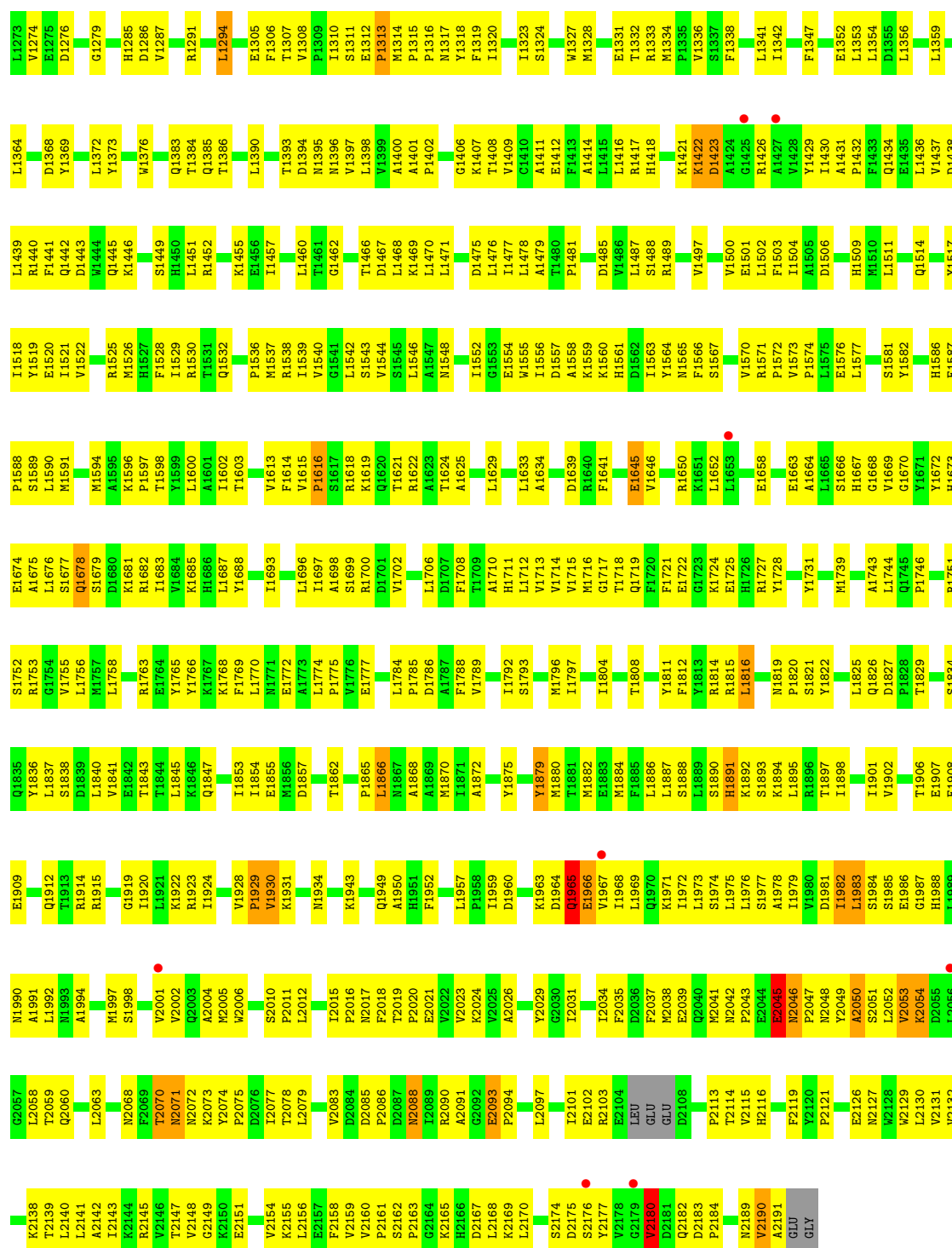


F2037	L1973	L1899	Q1826	V1755	K1681	S1589	G1454	Q1385	E1299	A1219	L1140	F1073
M2041	S1974	E1900	D1827	L1756	R1682	L1590	I1457	T1386	M1300	A1219	L1141	K1074
N2042	L1976	I1901	P1828	M1758	I1683	M1591	V1458	F1387	E1301	T1222	R1142	I1076
P2043	S1977	V1902	T1829	V1684	V1684	M1594	K1459	N1388	V1304	C1224	A1143	P1077
E2044	A1978	T1903	Y1836	P1759	K1685	M1594	L1460	L1390	T1307	C1224	F1145	Q1080
E2045	L1979	A1905	L1837	P1761	H1686	K1596	T1461	Y1391	T1307	A1295	E1146	E1081
N2046	V1980	T1906	L1837	K1762	L1687	P1597	E1462	N1392	V1308	V1227	C1147	E1082
P2047	D1981	E1907	V1841	R1763	Y1688	T1598	G1463	T1393	P1309	V1226	C1148	K1083
N2048	L1982	F1908	T1843	Y1766	N1689	L1599	T1464	N1396	I1310	K1229	L1149	L1084
A2049	L1983	F1908	K1768	K1767	G1691	L1600	D1467	N1397	F1230	V1230	W1153	E1085
A2050	S1985	I1911	Q1847	K1768	A1602	I1602	L1468	L1398	E1312	P1231	W1153	L1086
S2051	E1986	Q1912	L1846	P1769	T1603	T1603	K1489	L1398	P1231	R1232	V1156	A1087
L2052	E1987	T1913		L1770	R1700	Q1604	L1470	A1401	P1313	V1233	V1156	K1088
V2053	HIS		A1851	L1770	D1701	Q1604	L1470	T1403	P1315	V1233	V1156	L1089
L2056	ASN	I1920	R1852	E1772	V1702	P1607	E1472	G1404	P1316	I1235	M1163	L1090
G2057	L1921	L1921	I1853	E1773	W1704	D1608	L1476	K1407	M1317	Q1240	K1164	V1093
L2058	L1921	L1921	I1854	P1775	F1708	Q1609	I1477	T1408	F1319	P1241	K1165	K1098
Q2062	I1924	Y1925	E1855	V1776	T1709	V1613	I1477	C1410	I1323	P1241	M1166	E1099
L2063	Y1925	D1926	R1856	E1777	A1710	F1614	T1479			T1243	M1166	S1100
A2064	H1927	H1927	D1857	E1777	H1711	P1616	T1480			R1244	E1168	I1101
E1996	V1928	V1928	D1859	L1774	L1712	S1617	P1481			S1245	K1169	E1102
M1997	P1929	P1929	E1860	L1780	V1713	S1617	P1481			S1245	K1169	E1102
S1998	V1930	V1930	G1861	P1775	V1714	R1618	Q1483			M1246	R1170	E1103
P1999	LVS	LVS	L1784	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
M2000	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
V2001	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
Q2003	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
L2004	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
M2005	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
P2006	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
D2007	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
S2010	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
P2011	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
L2012	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
K2013	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
Q2014	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
L2015	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
P2016	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
N2017	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
F2018	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
T2019	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
P2020	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
E2021	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
L2022	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
V2023	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
K2024	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
Y2029	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
G2030	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
L2031	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
N2032	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
D2033	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
L2034	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
F2035	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
E2102	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103
R2103	ASN	ASN	P1785	P1785	R1618	R1618	Q1483			M1246	R1170	E1103

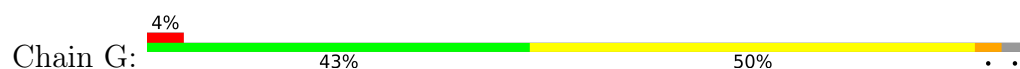


● Molecule 2: Pre-mRNA splicing helicase-like protein





• Molecule 2: Pre-mRNA splicing helicase-like protein



G1516	L1451	V1304	P1208	V1131	P1056	W969	E887	T808	L738	D650	L581	S503
Y1517	R1452	E1305	R1209	Y1132	A1057	L970	W892	R809	G739	L651	D582	D504
I1518	T1386	F1307	L1213	V1133	N1058	T973	E892	E810	V740	T654	A583	P505
V1522	K1455	V1306	L1216	G1138	D1060	Y974	E893	W811	L812	T654	F584	T506
V1523	I1457	P1309	P1217	I1140	E1062	L975	E894	L813	D742	V657	K585	D507
S1524	V1391	I1310	R1216	L1141	L1063	F976	D898	E814	I746	R658	K586	K508
R1525	N1392	S1311	R1219	E1064	L063	Y977	W902	S817	W749	L659	V587	N509
M1526	K1458	I1312	A1219	R1142	F1064	R978	M902	S818	K750	L660	F588	V512
F1527	L1460	E1312	A1219	R1142	R1065	M979	L903	W819	T751	L661	A590	T513
F1528	D1394	P1313	V1223	L1144	P1066	L980	G904	N820	W753	L662	P591	E514
E1463	M1395	M1314	C1224	F1145	F1067	R981	G905	N821	W753	L665	L592	L515
I1529	N1396	V1318	V1227	E1146	A1068	L985	A906	T822	D754	L665	K593	P516
R1530	V1397	F1319	V1227	L1147	Q1069	Y986	G907	L823	I755	L666	A594	E517
T1531	L1398	I1320	P1231	C1148	E1072	Y992	R908	L824	W755	L667	L595	W518
Q1532	V1399	S1321	R1232	L1149	F1073	E993	E912	K825	V759	L668	A590	T513
T1533	A1400	I1322	R1232	L1149	K1074	E993	D912	N825	W760	L669	P591	E514
K1468	P1401	I1323	I1235	W1153	E1075	D984	G917	L827	K761	L670	L592	L515
L1470	T1403	M1328	Q1236	S1155	I1076	E999	E917	L828	E762	L671	K593	P516
L1471	G1404	S1405	Q1236	V1156	P1077	E999	E918	P829	W763	L672	A594	E517
G1474	S1405	E1331	Q1240	L1159	V1078	Q1000	E919	F832	W764	L673	L595	W518
D1475	G1406	P1334	P1241	L1159	V1078	K1001	E920	F832	G765	L674	L596	A519
L1476	T1407	M1334	M1242	A1160	Q1080	R1002	E921	F832	W766	L675	Q597	E514
L1477	T1408	P1335	T1243	L1161	E1081	V1003	E922	H835	W767	L676	L597	L515
L1478	V1409	V1336	R1244	W1162	E1082	D1004	E923	H836	W768	L677	L598	P516
S1545	G1410	S1337	S1245	M1163	K1083	E999	E924	H836	W769	L678	L599	E517
A1479	A1411	F1338	M1246	L1163	E1084	H1007	E925	H839	W770	L679	L606	T526
A1547	F1413	L1343	L1247	K1165	E1085	E999	E926	N840	W771	L680	L607	T526
N1548	L1482	L1343	R1248	E1168	L1089	M1011	E927	R841	W772	L681	L608	T527
D1551	L1415	E1352	I1249	E1169	L1090	S1016	E928	N842	W773	L682	L609	T528
I1552	L1416	L1353	E1250	R1170	L1090	M1017	E929	R843	W774	L683	L610	L529
W1555	R1417	L1354	L1251	M1171	V1093	L1018	E930	R844	W775	L684	L611	M530
L1487	W1419	L1355	N1256	P1172	E1102	E1018	E931	R845	W776	L685	L612	A531
S1488	A1420	L1356	E1262	P1173	E1103	Y1021	E932	T846	W777	L686	L613	Q533
R1489	K1421	Q1357	E1262	T1174	K1098	E1021	E933	W847	W778	L687	L614	T532
Q1490	K1422	P1358	V1266	M1175	S1100	K1027	E934	E848	W779	L688	L615	F537
W1491	D1423	L1359	V1267	S1176	E1101	M1028	E935	D843	W780	L689	L616	P538
K1492	A1424	P1360	T1267	P1177	E1102	Q1029	E936	R844	W781	L690	L617	T539
R1493	G1425	V1361	E1271	E1173	E1103	E1032	E937	T845	W782	L691	L618	A540
K1494	R1426	S1362	W1271	Q1180	P1104	E1032	E938	W847	W783	L692	L619	F541
K1495	A1427	L1363	L1272	V1181	A1106	L1033	E939	E848	W784	L693	L620	L542
N1496	V1428	L1364	L1273	P1182	T1105	L1033	E940	D843	W785	L694	L621	L542
V1497	Y1429	K1365	V1274	T1183	K1107	I1036	E941	R844	W786	L695	L622	L542
Q1498	I1430	A1366	L1283	C1184	L1111	A1037	E942	R845	W787	L696	L623	M547
T1499	A1431	K1367	F1284	P1185	L1112	S1038	E943	T862	W788	L697	L624	L548
V1500	F1433	D1368	H1285	E1186	Q1113	H1039	E944	A863	W789	L698	L625	L549
E1501	P1432	Y1369	D1286	E1187	A1114	Y1040	E945	T864	W790	L699	L626	K557
L1502	Q1434	L1372	V1287	L1188	A1114	Y1041	E946	L865	W791	L700	L627	K557
F1503	E1435	L1372	F1288	Y1115	Y1115	I1042	E947	L865	W792	L701	L628	A561
I1504	V1437	Y1373	I1289	L1116	L1116	I1042	E948	W869	W793	L702	L629	A561
A1505	D1438	P1374	L1290	R1118	R1118	M1047	E949	N870	W794	L703	L630	T564
H1509	F1441	Q1377	K1291	M1195	L1126	T1049	E950	L871	W795	L704	L631	T564
M1510	Q1442	N1380	R1292	V1197	L1127	K1052	E951	L871	W796	L705	L632	M565
L1511	Q1445	K1381	D1293	L1205	M1127	L1053	E952	L871	W797	L706	L633	L566
Q1514	Q1445	I1382	L1294	D1206	A1128	L1053	E953	L871	W798	L707	L634	L566
M1515	Q1445	Q1383	T1303	P1207	M1130	H1055	E954	L871	W799	L708	L635	L566
							E955	L871	W800	L709	L636	L566
							E956	L871	W801	L710	L637	L566
							E957	L871	W802	L711	L638	L566
							E958	L871	W803	L712	L639	L566
							E959	L871	W804	L713	L640	L566
							E960	L871	W805	L714	L641	L566
							E961	L871	W806	L715	L642	L566
							E962	L871	W807	L716	L643	L566
							E963	L871	W808	L717	L644	L566
							E964	L871	W809	L718	L645	L566
							E965	L871	W810	L719	L646	L566
							E966	L871	W811	L720	L647	L566
							E967	L871	W812	L721	L648	L566
							E968	L871	W813	L722	L649	L566
							E969	L871	W814	L723	L650	L566
							E970	L871	W815	L724	L651	L566
							E971	L871	W816	L725	L652	L566
							E972	L871	W817	L726	L653	L566
							E973	L871	W818	L727	L654	L566
							E974	L871	W819	L728	L655	L566
							E975	L871	W820	L729	L656	L566
							E976	L871	W821	L730	L657	L566
							E977	L871	W822	L731	L658	L566
							E978	L871	W823	L732	L659	L566
							E979	L871	W824	L733	L660	L566
							E980	L871	W825	L734	L661	L566
							E981	L871	W826	L735	L662	L566
							E982	L871	W827	L736	L663	L566
							E983	L871	W828	L737	L664	L566
							E984	L871	W829	L738	L665	L566
							E985	L871	W830	L739	L666	L566
							E986	L871	W831	L740	L667	L566
							E987	L871	W832	L741	L668	L566
							E988	L871	W833	L742	L669	L566
							E989	L871	W834	L743	L670	L566
							E990	L871	W835	L744	L671	L566
							E991	L871	W836	L745	L672	L566
							E992	L871	W837	L746	L673	L566
							E993	L871	W838	L747	L674	L566
							E994	L871	W839	L748	L675	L566
							E995	L871	W840	L749	L676	L566
							E996	L871	W841	L750	L677	L566
							E997	L871	W842	L751	L678	L566
							E998	L871	W843	L752	L679	L566
							E999	L871	W844	L753	L680	L566
							E1000	L871	W845	L754	L681	L566
							E1001	L871	W846	L755	L682	L566
							E1002	L871	W847	L756	L683	L566
							E1003	L871	W848	L757	L684	L566
							E1004	L871	W849	L758	L685	L566
							E1005	L871	W850	L759	L686	L566
							E1006	L871	W851	L760	L687	L566
							E1007	L871	W852	L761	L688	L566
							E1008	L871	W853	L762	L689	L566
							E1009	L871	W854	L763	L690	L566
							E1010	L871	W855	L764	L691	L566
							E1011	L871	W856	L765	L692	L566
							E1012	L871	W857	L766	L693	L566
							E1013	L871	W858	L767	L694	L566
							E1014	L871	W859	L768	L695	L566
							E1015	L871	W860	L769	L696	L566
							E1016	L871	W861	L770	L697	L566
							E1017	L871	W862	L771	L698	L566
							E1018	L871	W863	L772	L699	L566
							E1019	L871	W864	L773	L700	L566
							E1020	L871	W865	L774	L701	L566
							E1021	L871	W866	L775	L702	L566
							E1022	L871	W867	L776	L703	L566
							E1023	L871	W868	L777	L704	L566
							E1024	L871	W869	L778	L705	L566
							E1025	L871	W870	L779	L706	L566
							E1026	L871	W871	L780	L707	L566

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.54Å 269.59Å 231.69Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	49.13 – 3.20 49.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.13-3.20) 99.0 (49.13-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.244 , 0.287 0.249 , 0.289	Depositor DCC
R_{free} test set	9222 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	63679	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	B	0.25	0/2175	0.73	2/2962 (0.1%)
1	D	0.27	0/2151	0.71	0/2927
1	F	0.26	0/2174	0.72	0/2958
1	H	0.26	0/2184	0.72	0/2973
2	A	0.27	0/14227	0.72	1/19296 (0.0%)
2	C	0.26	0/13925	0.73	1/18882 (0.0%)
2	E	0.26	0/14234	0.71	4/19306 (0.0%)
2	G	0.28	0/13998	0.74	7/18976 (0.0%)
All	All	0.27	0/65068	0.73	15/88280 (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	D	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	504	ASP	CA-C-N	7.53	129.25	119.84
2	G	504	ASP	C-N-CA	7.53	129.25	119.84
1	B	2217	ASP	CA-C-N	-7.40	114.17	121.65
1	B	2217	ASP	C-N-CA	-7.40	114.17	121.65
2	G	1417	ARG	CA-C-N	6.77	130.20	120.79

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2217	ASP	Peptide
2	E	1965	GLN	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	B	2116	0	2075	144	0
1	D	2093	0	2057	131	0
1	F	2116	0	2079	137	0
1	H	2125	0	2088	134	0
2	A	13917	0	13956	899	0
2	C	13628	0	13674	1001	0
2	E	13925	0	13970	918	0
2	G	13701	0	13768	1027	0
3	A	4	3	3	1	0
3	C	4	3	3	1	0
3	E	4	3	3	4	0
3	G	4	3	3	0	0
4	A	12	0	0	0	0
4	C	5	0	0	0	0
4	D	2	0	0	0	0
4	E	7	0	0	0	0
4	F	1	0	0	0	0
4	G	3	0	0	1	0
All	All	63667	12	63679	4303	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 34.

The worst 5 of 4303 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)
2:E:521:ILE:HD12	2:E:522:PRO:HD3	1.22	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:874:HIS:HA	2:C:907:GLY:HA2	1.28	1.13
2:G:515:LEU:HB3	2:G:516:PRO:HD2	1.18	1.10
2:C:2040:GLN:HA	2:C:2046:ASN:HB3	1.29	1.10
2:G:1574:PRO:HB2	2:G:1751:ARG:HG2	1.31	1.09

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	B	264/276 (96%)	241 (91%)	19 (7%)	4 (2%)	8	37
1	D	259/276 (94%)	239 (92%)	13 (5%)	7 (3%)	4	25
1	F	261/276 (95%)	237 (91%)	22 (8%)	2 (1%)	16	50
1	H	265/276 (96%)	243 (92%)	13 (5%)	9 (3%)	3	20
2	A	1736/1772 (98%)	1619 (93%)	105 (6%)	12 (1%)	18	52
2	C	1686/1772 (95%)	1537 (91%)	130 (8%)	19 (1%)	11	43
2	E	1736/1772 (98%)	1580 (91%)	127 (7%)	29 (2%)	7	35
2	G	1698/1772 (96%)	1537 (90%)	131 (8%)	30 (2%)	6	34
All	All	7905/8192 (96%)	7233 (92%)	560 (7%)	112 (1%)	9	39

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2217	ASP
1	B	2220	VAL
2	A	575	GLU
2	A	1748	LYS
1	D	2218	PRO

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	B	234/241 (97%)	226 (97%)	8 (3%)	32	64
1	D	231/241 (96%)	226 (98%)	5 (2%)	45	71
1	F	235/241 (98%)	229 (97%)	6 (3%)	40	69
1	H	235/241 (98%)	231 (98%)	4 (2%)	53	75
2	A	1534/1562 (98%)	1476 (96%)	58 (4%)	29	62
2	C	1503/1562 (96%)	1433 (95%)	70 (5%)	23	57
2	E	1537/1562 (98%)	1488 (97%)	49 (3%)	34	65
2	G	1511/1562 (97%)	1470 (97%)	41 (3%)	39	68
All	All	7020/7212 (97%)	6779 (97%)	241 (3%)	32	64

5 of 241 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1795	LYS
2	G	1502	LEU
1	F	2172	LYS
2	G	1499	THR
2	G	2138	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	1396	ASN
2	G	1496	ASN
2	G	2003	GLN
1	F	2152	HIS
1	F	2111	GLN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	C	2201	-	3,3,3	0.82	0	3,3,3	1.35	0
3	ACT	E	2201	-	3,3,3	0.82	0	3,3,3	1.35	0
3	ACT	A	2201	-	3,3,3	0.83	0	3,3,3	1.34	0
3	ACT	G	2201	-	3,3,3	0.82	0	3,3,3	1.35	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2201	ACT	1	0
3	E	2201	ACT	4	0
3	A	2201	ACT	1	0

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	B	266/276 (96%)	0.13	3 (1%) 78 61	54, 76, 110, 128	0
1	D	263/276 (95%)	-0.02	1 (0%) 88 79	56, 73, 101, 130	0
1	F	265/276 (96%)	0.08	2 (0%) 82 67	53, 83, 117, 143	0
1	H	267/276 (96%)	0.07	5 (1%) 66 46	54, 77, 111, 132	0
2	A	1738/1772 (98%)	0.02	20 (1%) 76 58	39, 73, 123, 171	0
2	C	1702/1772 (96%)	0.28	48 (2%) 55 35	49, 86, 159, 209	0
2	E	1740/1772 (98%)	0.11	14 (0%) 82 67	48, 80, 132, 205	0
2	G	1710/1772 (96%)	0.34	66 (3%) 43 27	48, 92, 171, 209	0
All	All	7951/8192 (97%)	0.17	159 (1%) 65 45	39, 81, 154, 209	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1971	LYS	5.5
2	G	2172	LEU	4.7
2	G	2143	ILE	4.6
2	C	813	GLN	4.5
2	C	1504	ILE	4.2

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	C	2201	4/4	0.28	0.18	80,91,97,98	0
3	ACT	E	2201	4/4	0.65	0.19	87,92,111,111	0
3	ACT	G	2201	4/4	0.67	0.11	84,89,104,104	0
3	ACT	A	2201	4/4	0.82	0.12	63,68,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.