



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 19, 2017 – 09:01 AM EST

PDB ID : 5M59
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

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

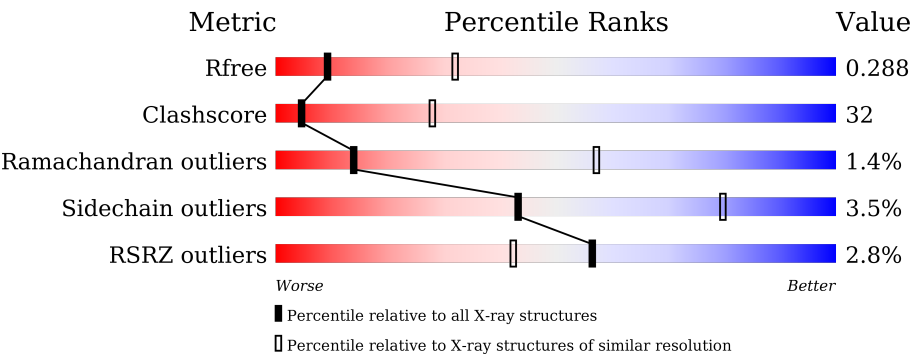
1 Overall quality at a glance i

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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 on the lower 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 $\leq 5\%$. 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	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>45%48% . .</div></div>
1	D	276	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>50%42% . 5%</div></div>
1	F	276	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>50%44% . .</div></div>
1	H	276	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>47%47% . .</div></div>
2	A	1772	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>47%49% . .</div></div>
2	C	1772	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>44%48% . .</div></div>

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Mol	Chain	Length	Quality of chain
2	E	1772	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>49%</div> <div>..</div> </div> </div>
2	G	1772	<div> <div>6%</div> <div> <div></div> <div>44%</div> <div>50%</div> <div>..</div> </div> </div>

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	C	2201	-	-	-	X
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			

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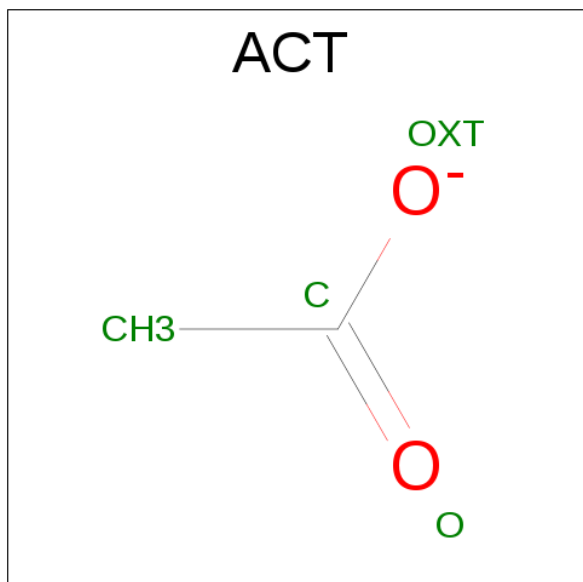
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	1740	Total	C	N	O	S	0	0	0
			13925	8896	2372	2592	65			
2	G	1710	Total	C	N	O	S	0	0	0
			13701	8753	2336	2547	65			

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 (three-letter code: 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

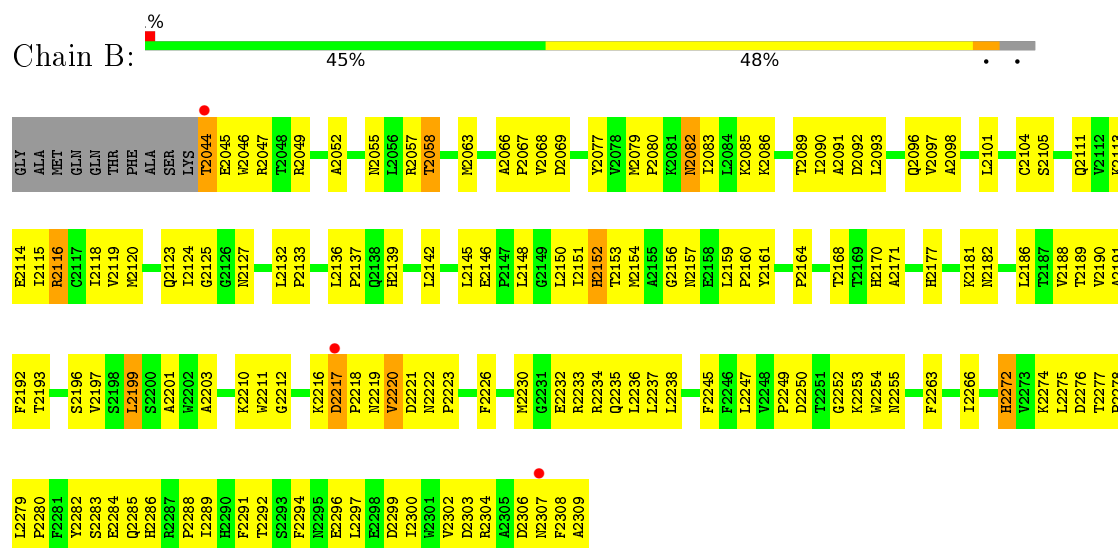
- Molecule 4 is water.

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

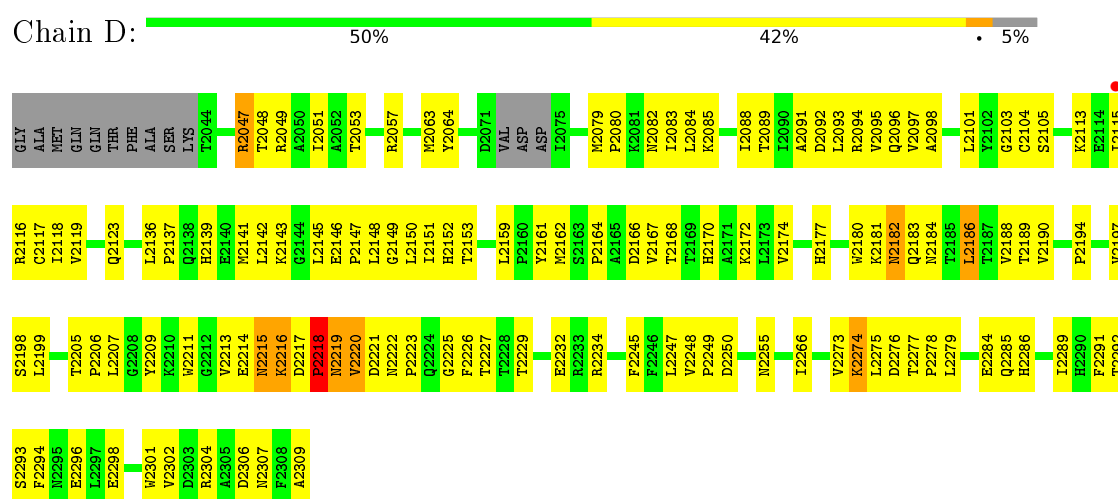
3 Residue-property plots

These plots are drawn for all protein, RNA 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 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

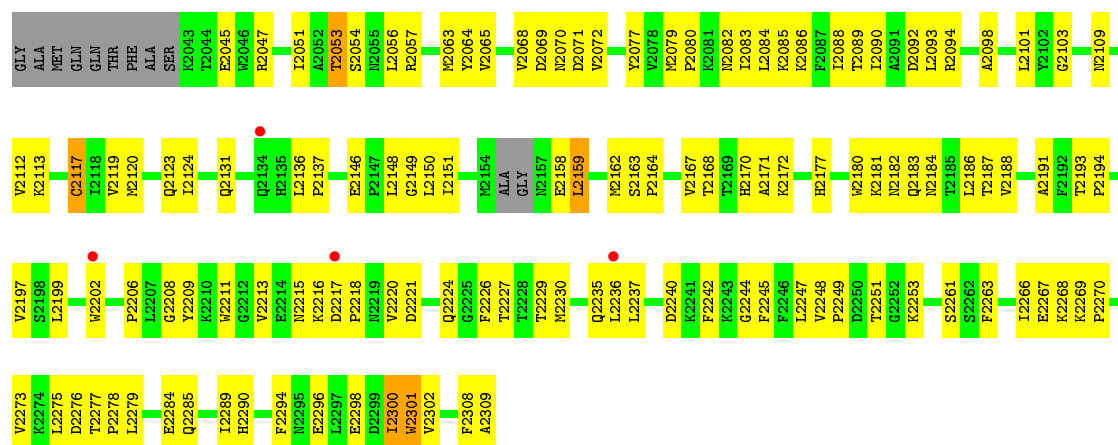


• Molecule 1: Putative pre-mRNA splicing factor

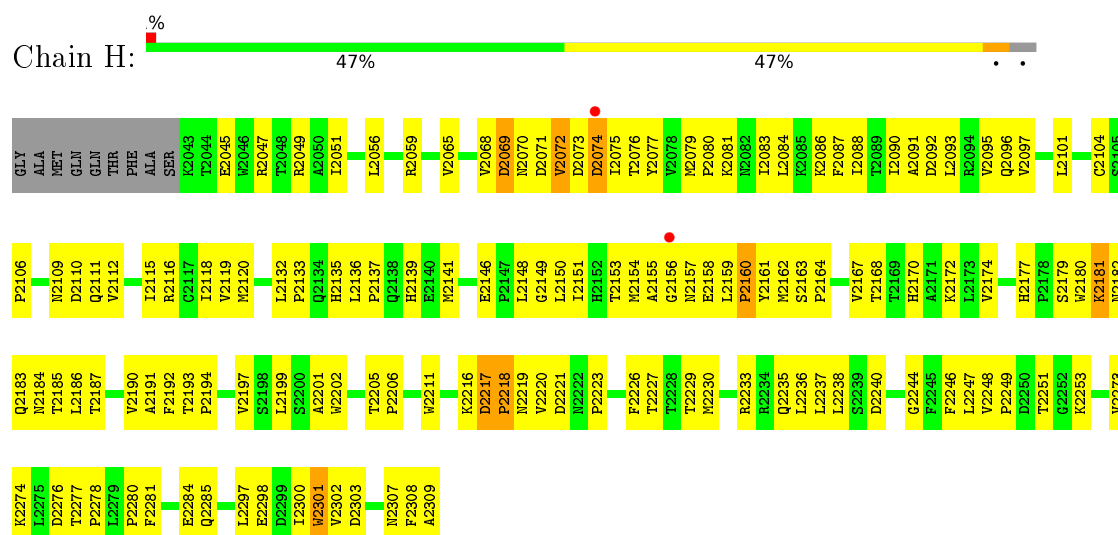


• Molecule 1: Putative pre-mRNA splicing factor

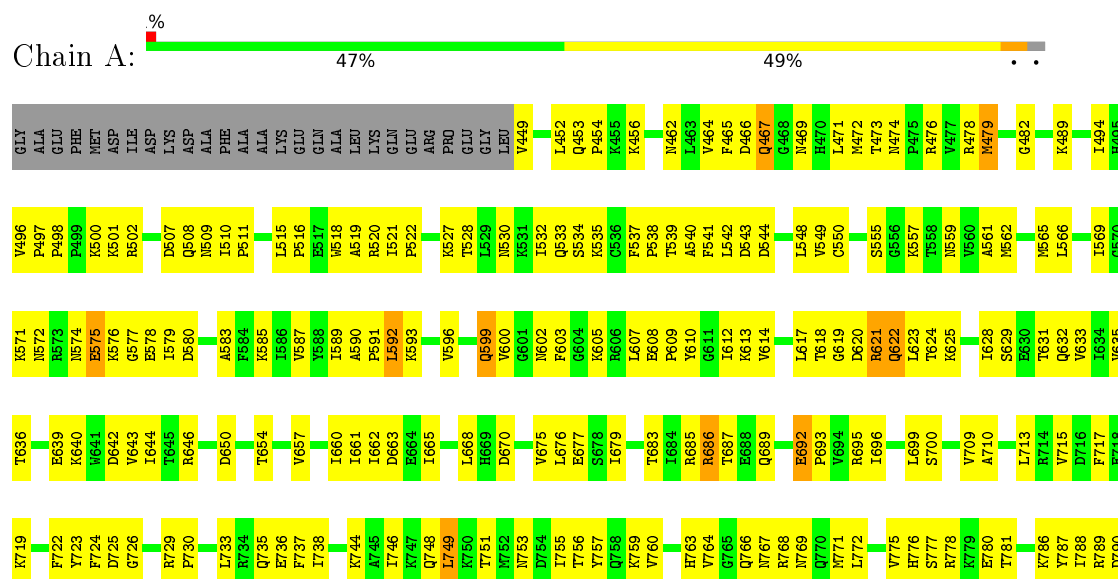




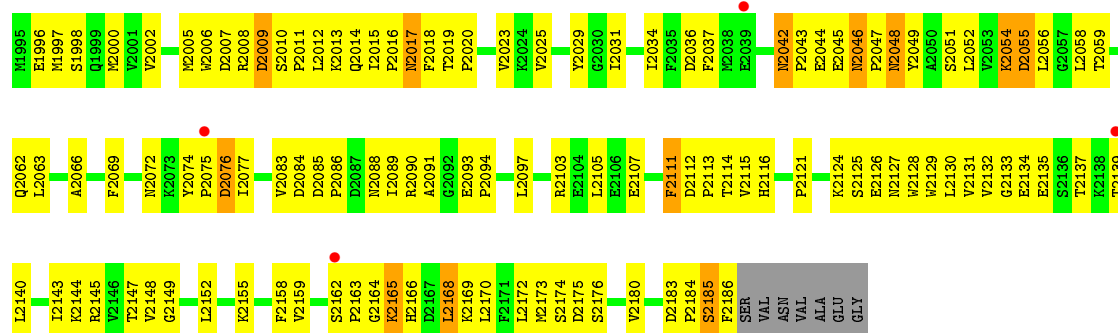
• Molecule 1: Putative pre-mRNA splicing factor



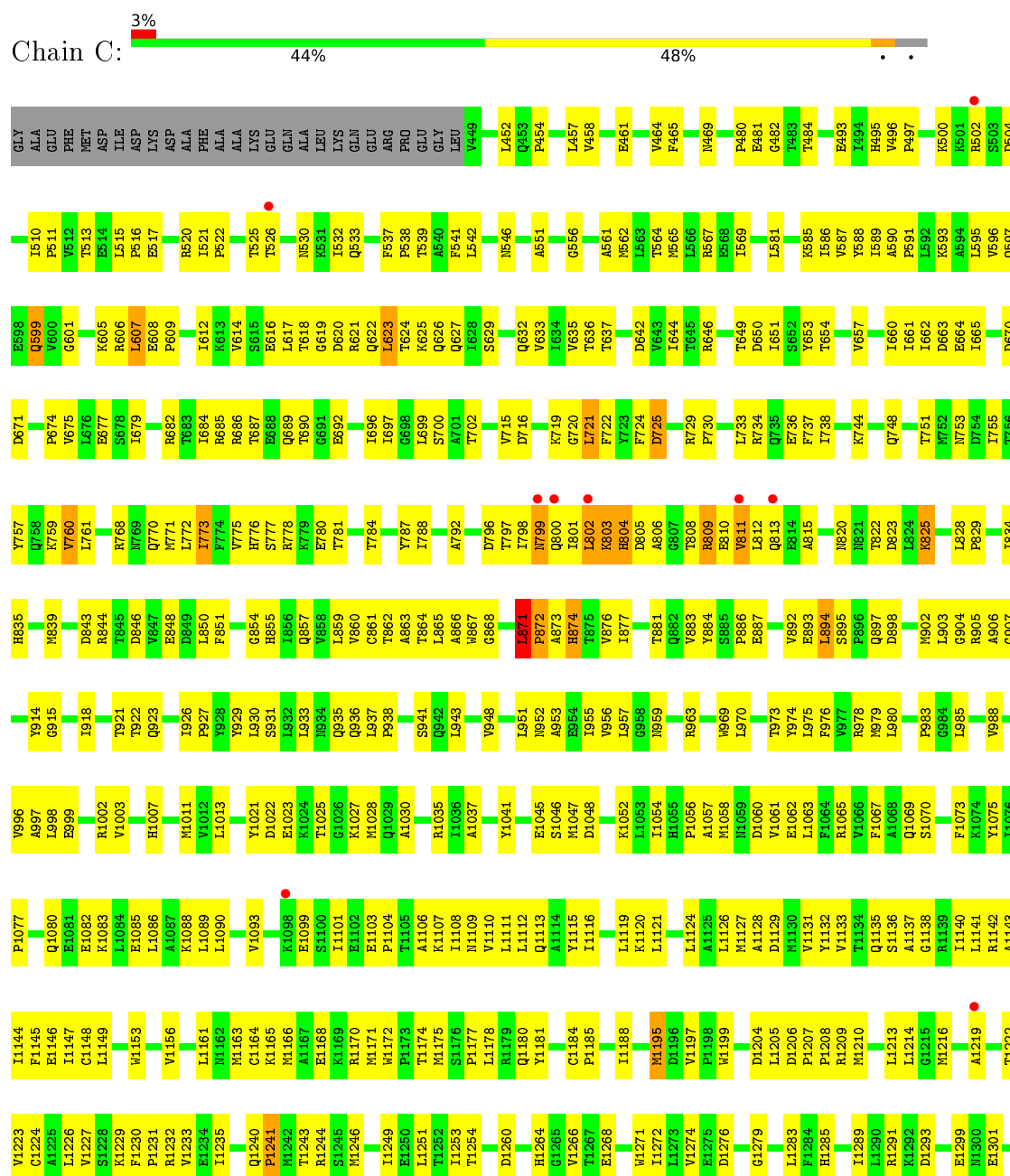
• Molecule 2: Pre-mRNA splicing helicase-like protein

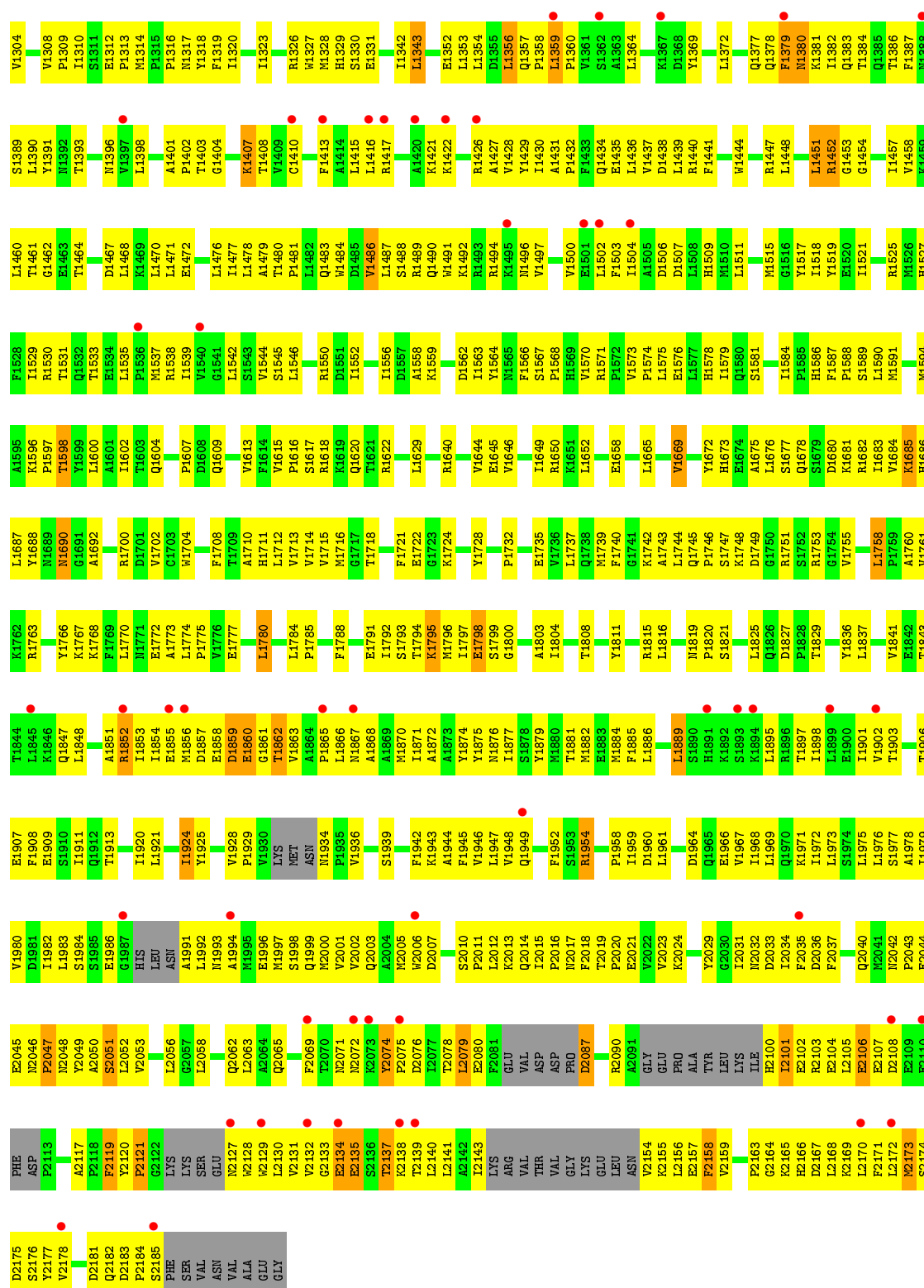


Y1925	D1839	K1748	L1676	S1581	I1504	R1426	T1351	W1271	H1175	E1102	Q1029	I939	A866	V791
D1926	L1840	D1749	S1677	H586	A1505	A1427	E1352	I1272	S1176	E1103	A1030	E940	A866	A792
H1927	T1843	G1750	S1679	F1587	L1508	V1428	L1353	L1273	P1177	P1104	E1032	S941	L871	D796
V1928	T1844	S1752	D1680	P1588	Q1514	A1430	P1359	E1275	Y1181	K1107	R1035	L943	T875	I798
P1929	L1845	R1753	L1681	S1589	M1515	A1431	L1358	D1276	P1182	I1108	I1036	V944	W876	W799
V1930	K1846	G1754	R1682	L1590	M1516	F1432	P1360	C1277	T1183	M1109	A1037	S945	L877	Q800
K1931	Q1847	V1755	L1683	M1591	Y1517	Q1434	V1361	D1278	F1184	V1110	S1038	L947	L878	L801
P1934	L1853	L1756	V1684	L1584	I1518	E1435	S1362	G1279	P1185	L1111	H1039	L947	L878	L802
P1935	T1854	W1757	K1685	M1594	I1519	E1436	L1364	I1282	I1188	Q1113	H1039	N952	T881	K803
V1936	E1855	P1759	Y1688	A1596	E1520	L1436	K1365	L1283	K1191	L1119	Y1041	A953	D882	H804
M1856	M1856	A1760	M1689	P1597	I1521	V1437	K1366	D1286	M1195	K1120	H1044	V956	D884	D805
S1939	G1861	Y1766	L1696	Y1599	V1523	F1441	Y1369	V1287	L1199	L1122	E1045	L957	S885	A806
F1942	V1862	Y1766	S1594	L1595	R1525	L1448	Y1372	F1288	W1199	G1123	S1047	R961	D887	R809
K1944	V1863	L1770	R1700	L1602	T1529	E1456	Y1373	L1289	F1203	A1125	M1047	N962	D888	E810
F1945	P1865	V1701	D1701	Q1609	R1530	E1457	P1374	D1290	D1204	L1126	D1048	R963	G889	Q813
V1946	L1866	L1774	V1702	P1610	T1533	L1457	M1375	A1291	D1206	Y1132	P1056	L970	S895	A816
V1947	L1867	P1775	V1702	P1610	L1535	L1458	W1376	D1293	P1207	V1133	A1057	G971	V819	V819
V1948	A1868	L1780	L1706	V1613	L1536	E1459	Q1377	L1294	P1208	Y1134	H1058	Y972	Q897	T822
Q1949	A1869	L1784	F1708	V1614	L1537	K1460	Q1378	L1294	F1379	Y1133	M1059	T973	D898	D823
A1950	M1870	P1785	A1710	V1615	P1536	T1461	M1380	L1294	M1301	Y1133	P1056	G971	E893	L824
H1951	L1871	P1785	A1710	V1615	P1536	T1461	M1380	L1294	E1301	Y1133	P1056	G971	E893	L824
L1957	M1876	F1788	H1711	R1618	R1538	T1464	K1381	L1294	E1301	Y1133	P1056	G971	E893	L824
P1958	L1877	F1788	H1711	R1618	R1538	T1464	K1381	L1294	E1301	Y1133	P1056	G971	E893	L824
I1959	S1878	V1713	V1713	Q1620	V1540	D1467	T1384	L1294	E1301	Y1133	P1056	G971	E893	L824
D1960	L1879	V1714	V1714	Q1621	G1541	L1468	Q1385	L1294	E1301	Y1133	P1056	G971	E893	L824
L1961	M1880	V1715	V1715	R1622	L1542	K1469	Q1386	L1294	E1301	Y1133	P1056	G971	E893	L824
A1962	M1881	M1796	M1716	R1622	L1543	L1470	T1386	L1294	E1301	Y1133	P1056	G971	E893	L824
Q1965	E1881	W1797	L1471	A1625	V1544	L1471	L1390	L1294	E1301	Y1133	P1056	G971	E893	L824
E1966	E1882	E1798	Q1719	R1626	L1545	E1472	Y1391	L1294	E1301	Y1133	P1056	G971	E893	L824
V1967	L1883	G1800	F1720	T1630	L1546	Q1473	M1392	L1294	E1301	Y1133	P1056	G971	E893	L824
L1968	L1886	E1801	F1721	T1630	L1546	Q1473	M1392	L1294	E1301	Y1133	P1056	G971	E893	L824
Q1970	L1887	L1804	E1722	E1638	L1562	L1476	T1393	L1294	E1301	Y1133	P1056	G971	E893	L824
K1971	K1894	Y1811	G1723	D1639	W1555	L1477	V1397	L1294	E1301	Y1133	P1056	G971	E893	L824
K1972	L1895	F1812	E1725	L1642	L1556	L1478	L1398	L1294	E1301	Y1133	P1056	G971	E893	L824
L1975	L1896	R1812	H1726	L1642	K1569	T1480	V1399	L1294	E1301	Y1133	P1056	G971	E893	L824
L1976	L1898	R1815	R1727	V1646	K1569	T1480	V1399	L1294	E1301	Y1133	P1056	G971	E893	L824
I1979	L1899	L1816	Y1728	Q1648	H1561	V1486	P1402	L1294	E1301	Y1133	P1056	G971	E893	L824
V1980	V1902	L1817	Y1731	D1647	D1562	L1487	K1407	L1294	E1301	Y1133	P1056	G971	E893	L824
D1981	T1903	A1818	P1732	R1650	I1563	S1488	T1408	L1294	E1301	Y1133	P1056	G971	E893	L824
I1982	P1908	P1820	E1735	L1653	M1566	R1489	V1409	L1294	E1301	Y1133	P1056	G971	E893	L824
L1983	F1908	S1821	E1735	L1653	P1567	H1491	C1410	L1294	E1301	Y1133	P1056	G971	E893	L824
S1984	S1985	Q1738	Q1738	E1658	P1568	K1495	E1412	L1294	E1301	Y1133	P1056	G971	E893	L824
S1985	T1911	L1825	M1739	E1663	H1569	K1495	E1412	L1294	E1301	Y1133	P1056	G971	E893	L824
E1986	Q1912	L1826	F1740	E1663	V1570	N1496	L1415	L1294	E1301	Y1133	P1056	G971	E893	L824
G1987	T1913	D1827	G1741	L1497	R1571	V1497	L1416	L1294	E1301	Y1133	P1056	G971	E893	L824
H1988	R1914	P1828	K1742	S1666	P1572	Q1498	R1417	L1294	E1301	Y1133	P1056	G971	E893	L824
A1991	E1917	T1829	L1744	G1670	V1573	T1499	H1418	L1294	E1301	Y1133	P1056	G971	E893	L824
L1992	N1993	H1830	L1744	G1670	V1573	T1499	H1418	L1294	E1301	Y1133	P1056	G971	E893	L824
A1994	L1921	L1837	P1745	V1672	L1577	E1501	W1419	L1294	E1301	Y1133	P1056	G971	E893	L824
		S1838	S1747	F1503	L1577	F1503	D1423	H1350	T1174		I1101	M1028	P938	L865



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

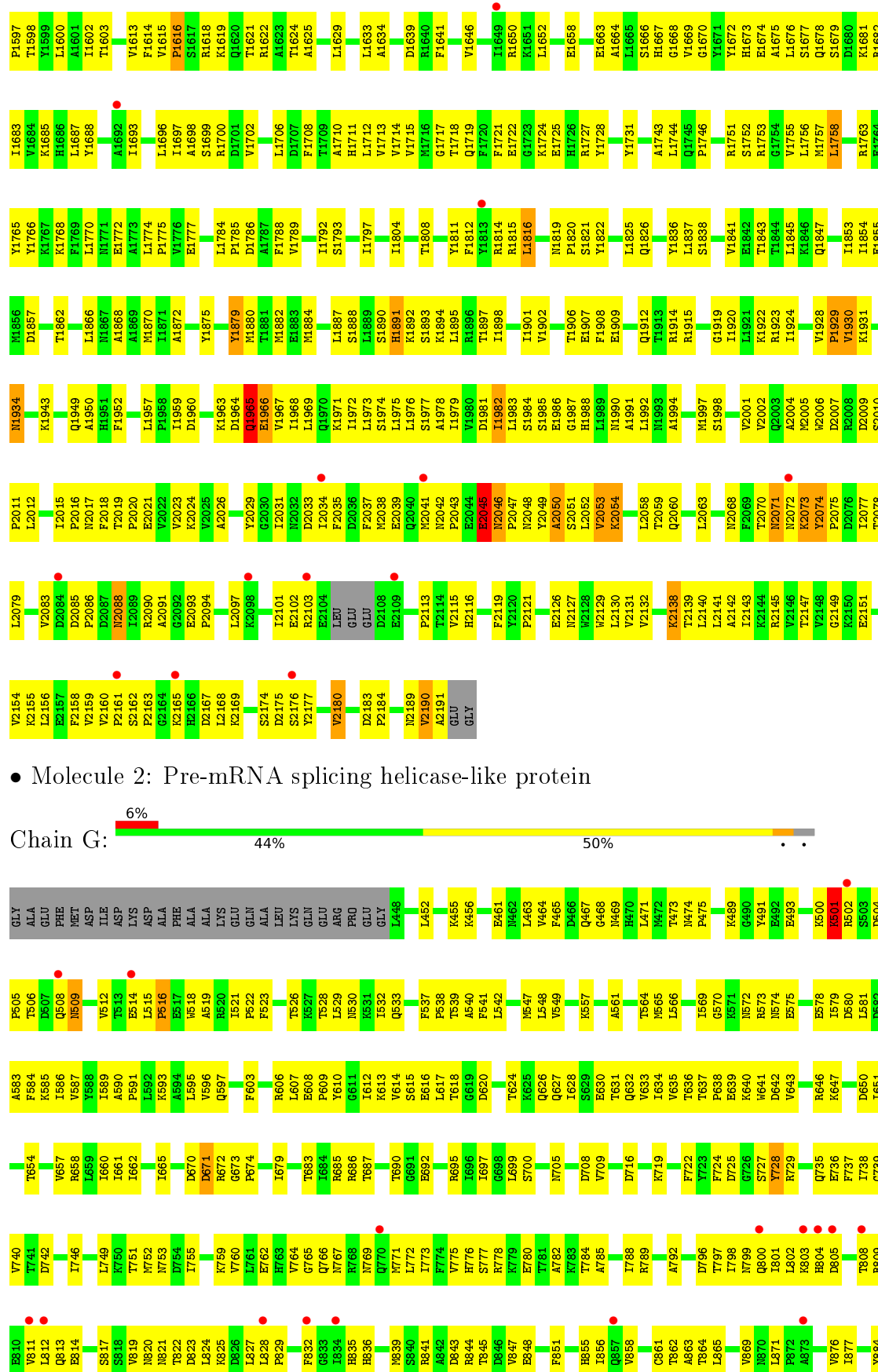




• Molecule 2: Pre-mRNA splicing helicase-like protein

Chain E: 46% 49%

M1526	Q1442	L1273	L1178	I1101	E1023	A953	H874	E794	Y728	E639	E568	P499	GLY
H1527	D1443	V1274	R1179	E1102	G1026	E954	T875	H795	R729	H640	E568	K500	ALA
F1528	V1444	E1275	C1184	E1103	K1027	V955	H876	D796	P730	H641	R573	R501	GLU
I1529	Q1445	D1276	P1185	P1104	K1028	V956	L877	T797	C731	D642	H574	R502	PHE
R1530	K1446	G1279	P1185	T1105	M1028	L957	L878	I798	L733	V643	E575	S503	MET
T1531	L1372	G1279	L1188	A1106	T1031	V960	K879	N799	L733	H646	K576	D504	ASP
Q1532	Y1373	G1279	L1188	A1106	T1031	V960	K879	Q800	R734	H646	G577	P605	ILE
P1536	W1376	H1285	L1189	L1108	E1032	R961	K880	Q801	Q735	H646	T806	T506	ASP
M1537	L1451	D1286	K1190	M1109	E1032	R962	T881	L802	E736	D650	D607	D507	LYS
R1538	Q1384	V1287	L1190	M1109	E1032	R962	T881	L802	E736	D650	D607	Q508	ASP
I1539	Q1385	L1191	E1193	L1110	I1036	R963	H883	K803	F737	H654	L581	N509	ALA
V1540	T1386	R1194	E1193	L1111	A1037	D964	Y884	H804	I738	H654	A583	I510	PHE
E1541	L1390	L1294	F1203	Q1113	S1038	V967	G889	D805	G739	V657	F584	P511	ALA
L1542	L1390	L1294	F1203	Q1113	S1038	V967	G889	D805	G739	V657	F584	P511	ALA
S1543	T1393	E1305	P1207	R1118	Y1041	L970	L894	T808	K744	H658	K585	V512	ALA
V1544	D1394	F1306	P1207	R1118	Y1041	L970	L894	T808	K744	H658	K585	V512	ALA
G1545	L1461	F1306	P1207	R1118	Y1041	L970	L894	T808	K744	H658	K585	V512	ALA
L1546	G1462	T1307	P1208	L1119	M1047	T972	D898	R809	K747	H660	I585	L515	LYS
L1547	G1462	V1308	M1210	L1124	M1047	T972	D898	R809	K747	H660	I585	L515	LYS
A1547	T1466	P1309	G1211	L1124	M1047	T972	D898	R809	K747	H660	I585	L515	LYS
D1467	D1467	I1310	E1212	D1129	L1053	L975	L901	L812	T751	I665	A590	R520	LYS
L1468	L1468	S1311	P1217	M1130	I1054	F976	L901	L812	T751	I665	A590	R520	LYS
K1469	A1400	E1312	P1217	V1131	P1056	R978	R905	D823	N753	H666	L592	I521	GLN
L1470	A1401	P1313	T1222	Y1132	A1057	H979	A906	K825	I755	D671	A594	P522	GLU
L1471	P1402	M1314	T1222	Y1132	A1057	H979	A906	K825	I755	D671	A594	P522	GLU
D1475	G1406	P1315	V1223	A1137	H1059	S982	R908	L827	Y757	P674	V596	T528	PRO
L1476	K1407	P1316	L1226	A1137	H1059	S982	R908	L827	Y757	P674	V596	T528	PRO
I1477	T1408	M1317	L1226	A1137	H1059	S982	R908	L827	Y757	P674	V596	T528	PRO
K1478	V1409	F1319	K1229	L1141	E1062	L985	Y911	R832	V760	V680	N802	K531	ARG
A1479	G1410	I1320	P1230	R1142	F1064	Y986	Y911	R832	V760	V680	N802	K531	ARG
T1480	A1411	I1320	P1230	R1142	F1064	Y986	Y911	R832	V760	V680	N802	K531	ARG
P1481	A1411	I1320	P1230	R1142	F1064	Y986	Y911	R832	V760	V680	N802	K531	ARG
D1485	F1413	S1324	V1233	F1145	F1067	A990	E917	H835	V764	H686	R606	Q533	LYS
V1486	L1415	M1327	I1235	F1145	F1067	A990	E917	H835	V764	H686	R606	Q533	LYS
L1487	L1416	M1328	Q1236	I1147	A1068	E991	E917	H835	V764	H686	R606	Q533	LYS
S1488	R1417	M1328	Q1236	I1147	A1068	E991	E917	H835	V764	H686	R606	Q533	LYS
V1570	R1418	E1331	Q1240	K1150	F1073	L998	Q923	D846	N769	H695	V614	L542	LYS
R1571	K1421	T1332	P1241	W1153	K1074	E999	Q923	D846	N769	H695	V614	L542	LYS
P1572	K1422	M1333	T1242	W1153	K1074	E999	Q923	D846	N769	H695	V614	L542	LYS
V1573	D1423	M1334	T1242	W1153	K1074	E999	Q923	D846	N769	H695	V614	L542	LYS
P1574	D1423	M1334	T1242	W1153	K1074	E999	Q923	D846	N769	H695	V614	L542	LYS
L1502	R1426	V1336	S1245	V1156	Q1080	R1002	Y928	F851	F774	L699	G619	M547	LYS
F1503	A1427	F1338	M1246	L1161	K1083	H1007	L930	H855	H776	A701	R621	V549	LYS
L1504	Y1429	F1338	M1246	L1161	K1083	H1007	L930	H855	H776	A701	R621	V549	LYS
A1505	I1430	I1342	L1247	M1162	L1084	S1008	S931	I856	S777	T702	Q622	A551	LYS
D1506	I1430	I1342	L1247	M1162	L1084	S1008	S931	I856	S777	T702	Q622	A551	LYS
H1509	P1431	F1347	I1253	K1165	L1089	M1011	Q935	T862	E760	D708	K625	G554	LYS
F1587	P1432	F1347	I1253	K1165	L1089	M1011	Q935	T862	E760	D708	K625	G554	LYS
P1588	F1433	E1362	D1260	A1167	L1090	V1012	L937	A863	A782	V715	Q626	S555	LYS
S1589	Q1434	L1353	L1263	M1171	P1094	S1016	L937	A863	A782	V715	Q626	S555	LYS
L1518	E1435	L1354	L1263	M1171	P1094	S1016	L937	A863	A782	V715	Q626	S555	LYS
Y1519	L1436	D1355	L1263	M1171	P1094	S1016	L937	A863	A782	V715	Q626	S555	LYS
E1520	V1437	L1356	V1266	P1172	I1095	L1017	S941	A866	F722	K719	T631	N559	LYS
M1591	D1438	L1356	V1266	P1172	I1095	L1017	S941	A866	F722	K719	T631	N559	LYS
T1521	D1438	L1356	V1266	P1172	I1095	L1017	S941	A866	F722	K719	T631	N559	LYS
V1522	L1439	L1359	E1288	M1175	K1098	I1019	L943	G868	Y787	F724	V633	M562	LYS
M1594	R1440	L1364	I1272	S1176	E1099	Y1021	R946	N870	K791	D725	T636	V496	LYS
A1595	R1440	L1364	I1272	S1176	E1099	Y1021	R946	N870	K791	D725	T636	V496	LYS
K1596	F1441	L1364	I1272	S1176	E1099	Y1021	R946	N870	K791	D725	T636	V496	LYS



G1987	H1988	E1917	Q1847	L1774	M1689	S1524	I1457	L1390	F1306	L1213	Y1132	P1056	E968	E887
H1989	L1848	E1918	L1848	P1775	M1690	R1525	V1488	T1391	T1307	L1213	V1133	A1057	H969	
L1989	S1849	G1919	H1850		I1693	H1526	K1459	M1392	V1308		G1138	H1058	L970	
A1991	A1851		G1694	S1778	I1693	F1528	T1460	T1393	T1309	M1216	G1138	H1059		H892
L1992	L1854	E1923	L1695	H1779	Q1604	L1529	T1461	D1394	I1310	T1217	I1139	V1061	T973	E893
M1993	L1855	E1923	L1696	H1781	S1606	R1530	E1463	D1395	S1311	K1218	I1140	V1060	T974	L894
A1994	H1856	E1924	L1697		P1607	T1531	T1464	M1396	E1312	A1219	L1141	E1062	L975	S895
E1995	M1857	Y1925	L1784		D1608	Q1532	T1465	V1397	P1313	V1223	R1142	F1063	F976	
E1996	D1857	P1785	P1785		Q1609	T1533	T1466	L1398	M1314	C1224	R1143	F1064	H977	D898
S1997	E1858	F1788	F1788		E1705	I1539	D1467	V1399	Y1318	V1227	T1144	R1065	H978	
S1998	E1859	L1706	L1706		L1705	V1539	L1468	A1401	F1319	F1145	E1146	V1066	H979	H902
V1930	E1860	F1789	F1789		L1707	G1541	K1469	P1402	I1320	V1227	E1147	F1067	L980	L903
K1931	G1861	T1790	F1708		F1709	G1541	L1470	T1403	S1321	P1231	C1148	A1068	L981	G904
	L1862	E1791	L1709		L1710	L1542	G1404	G1405	I1322	R1232	L1149	Q1069		H905
V2001	H1863	I1792	A1710		H1711	S1543	L1472	L1405	I1323					
Q2003	A1864	S1793	H1711		L1712	V1544	G1473	G1406		I1236	M1153	E1072	H985	
A2004	P1865	T1794	L1712		L1713	S1546	D1475		M1328	Q1240	M1153	F1073	H986	
M2005	L1866	K1795	V1713		V1714	L1547	L1476		E1381	P1241	V1156	Y1075	H987	
M2006	L1867	A1625				A1547	L1476		E1381	Q1240	V1156	I1076	H988	
D2007	A1868	L1629			L1718	M1548	L1477		E1381	P1241	M1153	F1074	H989	
R2008	A1869	L1630			L1719	D1551	L1478		E1381	P1241	M1153	F1074	H990	
S2010	M1870	T1630			T1719	I1552	L1478		E1381	P1241	M1153	F1074	H991	
L2011	L1871	G1800			F1720	A1631	A1479		E1381	P1241	M1153	F1074	H992	
L2012	L1871	E1801			F1721	C1632	T1480		E1381	P1241	M1153	F1074	H993	
Q2013	Y1874	D1802			E1722	D1639	L1481		E1381	P1241	M1153	F1074	H994	
H2014	Y1875	A1803			G1723	D1640	L1482		E1381	P1241	M1153	F1074	H995	
L2015	L1877	L1804			F1641	F1641	L1483		E1381	P1241	M1153	F1074	H996	
P2016	S1878	F1809			R1727	F1809	D1485		E1381	P1241	M1153	F1074	H997	
M2017	L1879	F1812			Y1728	K1560	L1487		E1381	P1241	M1153	F1074	H998	
P2018	M1880	L1812			L1729	H1561	S1483		E1381	P1241	M1153	F1074	H999	
P2019		L1813			P1732	F1566	R1489		E1381	P1241	M1153	F1074	H1000	
P2020	E1883	R1814			L1652	L1652	L1490		E1381	P1241	M1153	F1074	H1001	
V2023	L1884	R1815			L1653	L1653	L1491		E1381	P1241	M1153	F1074	H1002	
K1963	F1885	L1816			D1654	D1654	K1492		E1381	P1241	M1153	F1074	H1003	
D1964	L1886	E1735			H1655	H1655	R1493		E1381	P1241	M1153	F1074	H1004	
Q1965	L1887	A1743			V1656	V1656	A1427		E1381	P1241	M1153	F1074	H1005	
E1966	S1888	P1820			Q1657	Q1657	L1428		E1381	P1241	M1153	F1074	H1006	
V1967	L1889	L1821			E1658	E1658	L1430		E1381	P1241	M1153	F1074	H1007	
P1968	S1890	Y1822			P1746	P1746	A1431		E1381	P1241	M1153	F1074	H1008	
L1969	H1891	S1747			G1670	G1670	Q1498		E1381	P1241	M1153	F1074	H1009	
Q1970	K1892	D1748			Y1671	Y1671	T1499		E1381	P1241	M1153	F1074	H1010	
K1971	S1893	D1749			H1672	H1672	V1500		E1381	P1241	M1153	F1074	H1011	
L1972	K1894	G1750			H1673	H1673	E1501		E1381	P1241	M1153	F1074	H1012	
F2035	L1895	R1751			A1674	A1674	L1502		E1381	P1241	M1153	F1074	H1013	
D2036	R1896	S1752			A1675	A1675	F1503		E1381	P1241	M1153	F1074	H1014	
S1974	T1897	T1829			L1676	L1676	V1504		E1381	P1241	M1153	F1074	H1015	
L1975	L1898	S1677			S1677	S1677			E1381	P1241	M1153	F1074	H1016	
M2038	L1899	V1755			Q1684	Q1684			E1381	P1241	M1153	F1074	H1017	
E2039	Q1835	L1758			Q1678	Q1678			E1381	P1241	M1153	F1074	H1018	
Q2040	L1837	L1758			S1679	S1679			E1381	P1241	M1153	F1074	H1019	
M2041	S1838	Y1766			D1680	D1680	Q1514		E1381	P1241	M1153	F1074	H1020	
N2042	D1839	K1767			M1591	M1591	M1515		E1381	P1241	M1153	F1074	H1021	
P2043	L1840	R1682			L1592	L1592	G1516		E1381	P1241	M1153	F1074	H1022	
E2044	V1841	I1683			A1593	A1593	L1451		E1381	P1241	M1153	F1074	H1023	
E2045	F1908	F1769			L1584	L1584	R1452		E1381	P1241	M1153	F1074	H1024	
N2046	L1770	L1770			K1685	K1685	G1453		E1381	P1241	M1153	F1074	H1025	
P2047	M1771	M1771			L1686	L1686	G1454		E1381	P1241	M1153	F1074	H1026	
N2048	L1912	L1913			L1687	L1687	K1455		E1381	P1241	M1153	F1074	H1027	
	S1985	E1772			P1597	P1597	V1522		E1381	P1241	M1153	F1074	H1028	
	R1914	K1846			A1773	T1598	V1523		E1381	P1241	M1153	F1074	H1029	

L2172	L2173	S2174	D2175	S2176	S2177	D2181	Q2182	D2183	P2184	S2185	PHE	SER	VAL	ASN	VAL	ALA	GLU	GLY	GLU	PHE	ASP	P2113	T2114	V2115	H2116	A2117	P2118	F2119	Y2120	P2121	S2125	E2126	N2127	V2128	TRP	LEU	VAL	VAL	GLY	GLU	E2135	S2136	T2137	K2138	T2139	L2140	L2141	A2142	T2143	K2144	R2145	V2146	THR	VAL	GLY	LYS	E2151	L2152	N2153	V2154	K2155	L2156	E2157	F2158	V2159	VAL	PRO	SER	PRO	GLY	LYS	HIS	D2167	L2168	K2169	L2170	F2171	GLU	F2081	E2082	V2083	D2084	D2085	P2086	E2087	N2088	T2089	R2090	A2091	G2092	E2093	P2094	A2095	Y2096	L2097	K2098	L2099	H2100	T2101	E2102	R2103	E2104	L2105	E2106	E2107	ASP	GLU	S2051	L2052	V2053	K2054	D2055	L2056	G2057	L2058	T2059	Q2060	A2061	Q2062	L2063	A2064	Q2065	A2066	A2067	N2068	F2069	T2070	N2071	N2072	F2073	Y2074	PRO	ASP	ILE	THR	LEU	GLU	F2081	E2082	V2083	D2084	D2085	P2086	E2087	N2088	T2089	R2090	A2091	G2092	E2093	P2094	A2095	Y2096	L2097	K2098	L2099	H2100	T2101	E2102	R2103	E2104	L2105	E2106	E2107	ASP	GLU
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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 49.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.13-3.20) 99.0 (49.52-3.20)	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 (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.244 , 0.287 0.246 , 0.288	Depositor DCC
R_{free} test set	9214 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.4	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	0.20	0/2175	0.38	0/2962
1	D	0.22	0/2151	0.39	0/2927
1	F	0.21	0/2174	0.39	0/2958
1	H	0.21	0/2184	0.37	0/2973
2	A	0.21	0/14227	0.37	0/19296
2	C	0.21	0/13925	0.38	0/18882
2	E	0.21	0/14234	0.38	0/19306
2	G	0.22	0/13998	0.39	0/18976
All	All	0.21	0/65068	0.38	0/88280

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.

There are no bond angle outliers.

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	139	0
1	D	2093	0	2057	120	0
1	F	2116	0	2079	124	0
1	H	2125	0	2088	127	0
2	A	13917	0	13956	862	0
2	C	13628	0	13674	959	0
2	E	13925	0	13970	867	0
2	G	13701	0	13768	973	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	4086	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 32.

The worst 5 of 4086 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
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:A:835:HIS:HA	2:A:839:MET:HE1	1.31	1.10
2:C:2040:GLN:HA	2:C:2046:ASN:HB3	1.29	1.10

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%)	13	55
1	D	259/276 (94%)	239 (92%)	13 (5%)	7 (3%)	6	39
1	F	261/276 (95%)	237 (91%)	22 (8%)	2 (1%)	24	69
1	H	265/276 (96%)	243 (92%)	13 (5%)	9 (3%)	5	31
2	A	1736/1772 (98%)	1619 (93%)	105 (6%)	12 (1%)	26	72
2	C	1686/1772 (95%)	1537 (91%)	130 (8%)	19 (1%)	17	62
2	E	1736/1772 (98%)	1580 (91%)	127 (7%)	29 (2%)	11	52
2	G	1698/1772 (96%)	1537 (90%)	131 (8%)	30 (2%)	11	51
All	All	7905/8192 (96%)	7233 (92%)	560 (7%)	112 (1%)	14	57

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%)	225 (96%)	9 (4%)	40	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	231/241 (96%)	224 (97%)	7 (3%)	48	82
1	F	235/241 (98%)	227 (97%)	8 (3%)	44	80
1	H	235/241 (98%)	231 (98%)	4 (2%)	68	90
2	A	1534/1562 (98%)	1475 (96%)	59 (4%)	40	78
2	C	1503/1562 (96%)	1439 (96%)	64 (4%)	35	75
2	E	1537/1562 (98%)	1486 (97%)	51 (3%)	45	81
2	G	1511/1562 (97%)	1469 (97%)	42 (3%)	51	84
All	All	7020/7212 (97%)	6776 (96%)	244 (4%)	43	80

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1645	GLU
2	C	2135	GLU
2	G	1639	ASP
2	C	1758	LEU
2	C	1977	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	2184	ASN
2	E	800	GLN
2	G	1988	HIS
1	F	2290	HIS
2	E	769	ASN

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

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	A	2201	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ACT	C	2201	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ACT	E	2201	-	0,3,3	0.00	-	0,3,3	0.00	-
3	ACT	G	2201	-	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	A	2201	-	-	0/0/0/0	0/0/0/0
3	ACT	C	2201	-	-	0/0/0/0	0/0/0/0
3	ACT	E	2201	-	-	0/0/0/0	0/0/0/0
3	ACT	G	2201	-	-	0/0/0/0	0/0/0/0

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	A	2201	ACT	1	0
3	C	2201	ACT	1	0
3	E	2201	ACT	4	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.05	3 (1%) 82 72	54, 76, 110, 128	0
1	D	263/276 (95%)	-0.06	1 (0%) 93 90	56, 73, 101, 130	0
1	F	265/276 (96%)	-0.02	4 (1%) 76 63	53, 83, 117, 143	0
1	H	267/276 (96%)	-0.01	2 (0%) 89 83	54, 77, 111, 132	0
2	A	1738/1772 (98%)	0.01	26 (1%) 76 63	39, 73, 123, 171	0
2	C	1702/1772 (96%)	0.12	60 (3%) 48 32	49, 86, 159, 209	0
2	E	1740/1772 (98%)	0.06	23 (1%) 79 67	48, 80, 132, 205	0
2	G	1710/1772 (96%)	0.27	106 (6%) 24 13	48, 92, 171, 209	0
All	All	7951/8192 (97%)	0.09	225 (2%) 56 42	39, 81, 154, 209	0

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	2171	PHE	4.8
2	G	2142	ALA	4.7
2	C	2170	LEU	4.6
2	G	2088	ASN	4.5
2	A	1985	SER	4.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	ACT	C	2201	4/4	0.63	0.35	3.22	80,91,97,98	0
3	ACT	E	2201	4/4	0.85	0.27	0.84	87,92,111,111	0
3	ACT	G	2201	4/4	0.85	0.25	0.84	84,89,104,104	0
3	ACT	A	2201	4/4	0.88	0.20	-0.33	63,68,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.