



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2024 – 09:36 AM EST

PDB ID : 3LVH
Title : Crystal structure of a clathrin heavy chain and clathrin light chain complex
Authors : Wilbur, J.D.; Hwang, P.K.; Ybe, J.A.; Lane, M.; Sellers, B.D.; Jacobson, M.P.;
Fletterick, R.J.; Brodsky, F.M.
Deposited on : 2010-02-20
Resolution : 9.00 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

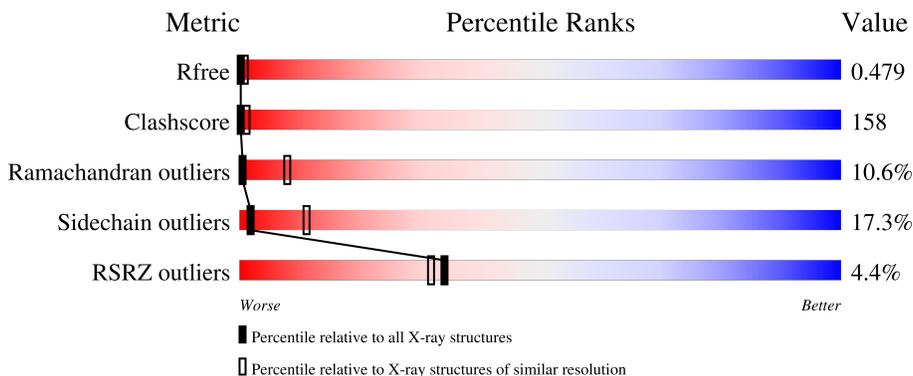
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.00 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.



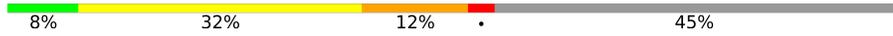
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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	624	
1	B	624	
1	C	624	
2	D	205	
2	E	205	

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Mol	Chain	Length	Quality of chain
2	F	205	 8% 32% 12% . 45%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16020 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 Clathrin heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	554	4550	2901	768	856	25	0	0	0
1	B	554	4550	2901	768	856	25	0	0	0
1	C	554	4550	2901	768	856	25	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1052	MET	-	expression tag	UNP P49951
A	1053	GLY	-	expression tag	UNP P49951
A	1054	SER	-	expression tag	UNP P49951
A	1055	SER	-	expression tag	UNP P49951
A	1056	HIS	-	expression tag	UNP P49951
A	1057	HIS	-	expression tag	UNP P49951
A	1058	HIS	-	expression tag	UNP P49951
A	1059	HIS	-	expression tag	UNP P49951
A	1060	HIS	-	expression tag	UNP P49951
A	1061	HIS	-	expression tag	UNP P49951
A	1062	SER	-	expression tag	UNP P49951
A	1063	SER	-	expression tag	UNP P49951
A	1064	GLY	-	expression tag	UNP P49951
A	1065	LEU	-	expression tag	UNP P49951
A	1066	VAL	-	expression tag	UNP P49951
A	1067	PRO	-	expression tag	UNP P49951
A	1068	ARG	-	expression tag	UNP P49951
A	1069	GLY	-	expression tag	UNP P49951
A	1070	SER	-	expression tag	UNP P49951
A	1071	HIS	-	expression tag	UNP P49951
A	1072	MET	-	expression tag	UNP P49951
A	1073	LEU	-	expression tag	UNP P49951
B	1052	MET	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1053	GLY	-	expression tag	UNP P49951
B	1054	SER	-	expression tag	UNP P49951
B	1055	SER	-	expression tag	UNP P49951
B	1056	HIS	-	expression tag	UNP P49951
B	1057	HIS	-	expression tag	UNP P49951
B	1058	HIS	-	expression tag	UNP P49951
B	1059	HIS	-	expression tag	UNP P49951
B	1060	HIS	-	expression tag	UNP P49951
B	1061	HIS	-	expression tag	UNP P49951
B	1062	SER	-	expression tag	UNP P49951
B	1063	SER	-	expression tag	UNP P49951
B	1064	GLY	-	expression tag	UNP P49951
B	1065	LEU	-	expression tag	UNP P49951
B	1066	VAL	-	expression tag	UNP P49951
B	1067	PRO	-	expression tag	UNP P49951
B	1068	ARG	-	expression tag	UNP P49951
B	1069	GLY	-	expression tag	UNP P49951
B	1070	SER	-	expression tag	UNP P49951
B	1071	HIS	-	expression tag	UNP P49951
B	1072	MET	-	expression tag	UNP P49951
B	1073	LEU	-	expression tag	UNP P49951
C	1052	MET	-	expression tag	UNP P49951
C	1053	GLY	-	expression tag	UNP P49951
C	1054	SER	-	expression tag	UNP P49951
C	1055	SER	-	expression tag	UNP P49951
C	1056	HIS	-	expression tag	UNP P49951
C	1057	HIS	-	expression tag	UNP P49951
C	1058	HIS	-	expression tag	UNP P49951
C	1059	HIS	-	expression tag	UNP P49951
C	1060	HIS	-	expression tag	UNP P49951
C	1061	HIS	-	expression tag	UNP P49951
C	1062	SER	-	expression tag	UNP P49951
C	1063	SER	-	expression tag	UNP P49951
C	1064	GLY	-	expression tag	UNP P49951
C	1065	LEU	-	expression tag	UNP P49951
C	1066	VAL	-	expression tag	UNP P49951
C	1067	PRO	-	expression tag	UNP P49951
C	1068	ARG	-	expression tag	UNP P49951
C	1069	GLY	-	expression tag	UNP P49951
C	1070	SER	-	expression tag	UNP P49951
C	1071	HIS	-	expression tag	UNP P49951
C	1072	MET	-	expression tag	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1073	LEU	-	expression tag	UNP P49951

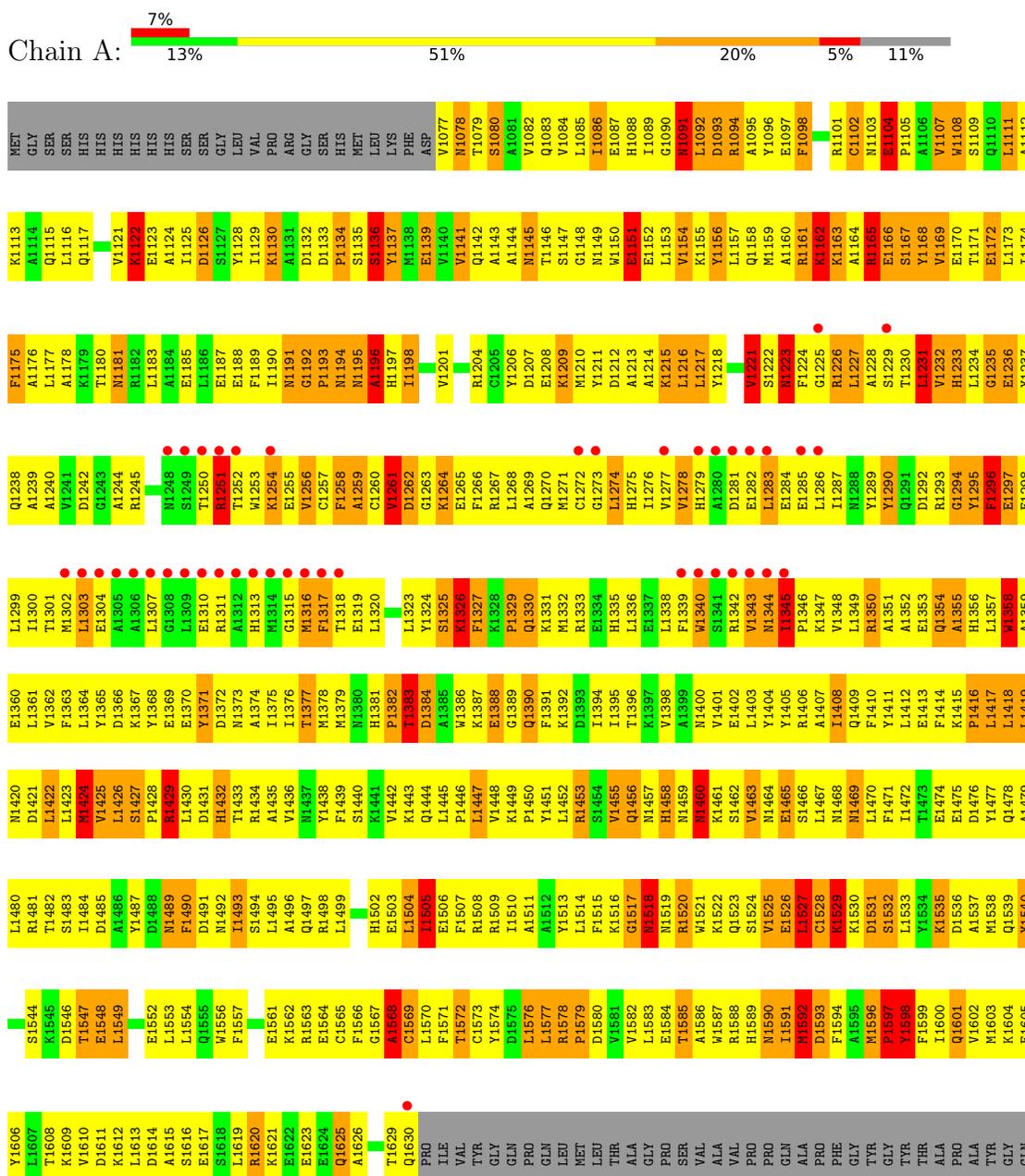
- Molecule 2 is a protein called Clathrin light chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	113	Total	C	N	O	S	0	0	0
			811	489	160	161	1			
2	E	102	Total	C	N	O	S	0	0	0
			753	455	149	148	1			
2	F	112	Total	C	N	O	S	0	0	0
			806	486	159	160	1			

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: Clathrin heavy chain 1



PRO
GLN
PRO
GLY
SER
PHE
GLY
TYR
SER
MET

● Molecule 1: Clathrin heavy chain 1

Chain B: 12% 52% 20% 5% 11%

MET	K1113	F1175	E1236	L1299	V1362	L1422	T1482	T1547	V1610	PHE
GLY	A1114	A1176	Y1237	L1300	F1363	L1423	S1483	E1548	D1611	GLY
PRO	A1117	L1177	Q1238	L1301	F1364	M1424	L1484	L1549	K1612	TYR
GLY	L1116	L1178	A1239	M1302	Y1365	V1425	D1485	D1485	L1613	SER
GLY	Q1117	K1179	D1240	L1303	D1366	L1426	L1486	E1552	D1614	HIS
TYR	V1121	T1180	V1241	E1304	K1367	S1427	Y1487	L1553	S1615	HIS
SER	K1122	M1181	D1242	L1307	Y1368	P1428	D1488	L1554	S1616	HIS
HIS	A1123	L1182	G1243	L1307	E1369	R1429	M1489	Q1555	E1617	HIS
HIS	E1123	L1183	A1244	L1310	I370	L1430	F1490	W1556	S1618	HIS
HIS	A1124	L1184	R1245	R1311	D1371	D1431	D1491	F1557	L1619	HIS
SER	I1125	E1185	R1245	R1311	D1372	H1432	M1492	F1557	R1620	HIS
SER	D1126	E1186	G1245	T1250	M1373	T1433	I1493	E1561	K1621	SER
GLY	S1127	E1187	E1251	H1312	M1374	R1434	A1494	E1562	E1622	GLY
LEU	Y1128	E1188	T1252	H1313	I1375	A1435	L1495	R1563	E1623	LEU
VAL	I1129	F1189	M1253	H1314	I1376	V1436	A1496	C1564	E1624	VAL
PRO	K1130	M1190	K1254	M1316	T1377	T1437	Q1497	C1565	Q1625	VAL
ARG	D1131	M1191	E1255	F1317	M1378	Y1438	F1498	F1566	R1626	PRO
GLY	A1132	M1192	V1256	T1318	M1379	F1439	L1499	G1567	A1626	ARG
SER	D1133	P1193	C1257	E1319	M1380	S1440	L1499	A1568	T1629	SER
SER	F1134	M1194	F1258	L1320	H1381	K1441	H1502	C1569	Q1630	HIS
HIS	S1135	M1195	A1259	L1320	P1382	V1442	L1503	L1570	I1630	HIS
MET	S1135	M1195	A1259	L1320	P1382	V1442	L1503	L1570	Q1630	MET
LEU	S1136	A1196	C1260	L1323	T1383	K1443	L1504	F1571	I1630	LEU
LYS	Y1137	H1197	V1261	Y1324	D1384	Q1444	L1505	T1572	I1630	LEU
PHE	M1138	I1198	D1262	S1325	A1385	L1445	E1506	C1573	T1572	VAL
ASP	E1139	Q1199	G1263	K1326	W1386	P1446	F1507	Y1574	Y1574	TYR
V1077	V1140	Q1200	K1264	F1327	K1387	L1447	R1508	D1575	Y1574	GLY
M1078	V1141	Q1200	K1264	F1327	K1387	L1447	R1508	D1575	Y1574	GLN
T1079	Q1142	Q1200	K1264	F1327	K1387	L1447	R1508	D1575	Y1574	PRO
S1080	A1143	R1204	F1266	K1328	E1388	V1448	R1509	L1576	L1576	PRO
A1081	A1144	R1204	F1266	K1328	E1388	V1448	R1509	L1576	L1576	GLN
V1082	M1145	C1205	R1267	Q1330	Q1390	P1450	A1511	L1577	L1577	GLN
Q1083	T1146	C1205	R1267	Q1330	Q1390	P1450	A1511	L1577	L1577	LEU
V1084	S1147	A1269	D1269	M1332	F1391	Y1451	A1512	P1579	P1579	MET
I1085	E1147	D1270	D1270	R1333	K1392	L1452	Y1513	D1580	D1580	LEU
L1085	E1148	E1208	M1271	R1333	D1393	R1453	Y1514	Y1581	Y1581	THR
I1086	M1149	E1208	M1271	R1333	D1393	R1453	Y1514	Y1581	Y1581	ALA
I1087	V1150	C1272	G1273	H1335	L1394	S1454	F1515	L1582	L1582	ALA
E1088	W1151	M1210	G1273	H1335	L1394	S1454	F1515	L1582	L1582	GLY
I1088	E1151	Y1211	L1274	E1337	K1397	M1457	M1518	T1585	T1585	PRO
I1089	E1152	A1213	H1275	E1337	K1397	M1457	M1519	T1585	T1585	SER
G1090	L1153	A1214	I1276	F1339	A1398	M1459	R1520	W1587	W1587	VAL
M1091	V1154	K1215	V1277	F1340	A1398	M1459	R1520	W1587	W1587	ALA
L1092	K1155	K1215	V1277	F1340	A1398	M1459	R1520	W1587	W1587	VAL
D1093	Y1156	K1216	H1279	S1341	K1461	K1461	K1522	H1589	H1589	PRO
R1094	L1157	L1217	H1279	R1342	E1402	S1462	Q1523	M1590	M1590	PRO
A1095	Q1158	Y1218	D1281	V1343	L1403	V1463	S1524	I1591	I1591	PRO
Y1096	M1159	N1219	E1282	N1344	Y1404	M1464	E1525	M1592	M1592	ALA
E1097	A1160	W1221	L1283	L1346	Y1405	E1465	E1526	F1594	F1594	PRO
F1098	R1161	V1222	L1283	P1346	R1406	S1466	L1527	A1595	A1595	PHE
R1101	K1162	F1224	L1283	P1346	R1406	S1466	L1527	A1595	A1595	GLY
C1102	M1163	N1223	E1284	K1347	L1407	L1467	C1528	M1596	M1596	GLY
M1103	A1164	G1225	E1284	K1347	L1407	L1467	C1528	M1596	M1596	TYR
E1104	A1166	R1226	E1284	K1347	L1407	L1467	C1528	M1596	M1596	TYR
P1105	S1167	L1227	Y1290	E1353	E1412	T1473	Y1534	Q1601	Q1601	PRO
A1106	Y1168	A1228	Q1291	E1353	E1412	T1473	Y1534	Q1601	Q1601	ALA
V1107	V1169	S1229	Q1291	A1355	K1415	E1475	K1536	V1602	V1602	ALA
M1108	E1170	T1230	D1292	A1355	K1415	E1475	K1536	V1602	V1602	TYR
S1109	T1171	V1232	R1293	H1356	P1416	D1476	A1537	K1604	K1604	GLY
Q1110	E1172	H1232	G1294	L1357	L1417	Y1477	M1538	Y1606	Y1606	GLY
L1111	I1173	H1234	Y1295	W1358	L1418	Q1478	Q1539	Y1606	Y1606	PRO
A1112	I1174	G1235	E1298	D1421	L1419	A1479	Y1540	L1607	L1607	PRO

PHE
GLY
TYR
SER
MET

● Molecule 1: Clathrin heavy chain 1

Chain C: 13% 52% 20% 5% 11%

MET	M1077	M1078	M1079	S1080	V1082	Q1083	I1085	I1086	E1087	H1088	I1089	G1090	M1091	L1092	D1093	R1094	A1095	Y1096	E1097	F1098	R1101	C1102	M1103	E1104	P1105	A1106	V1107	M1108	S1109	Q1110	L1111	A1112
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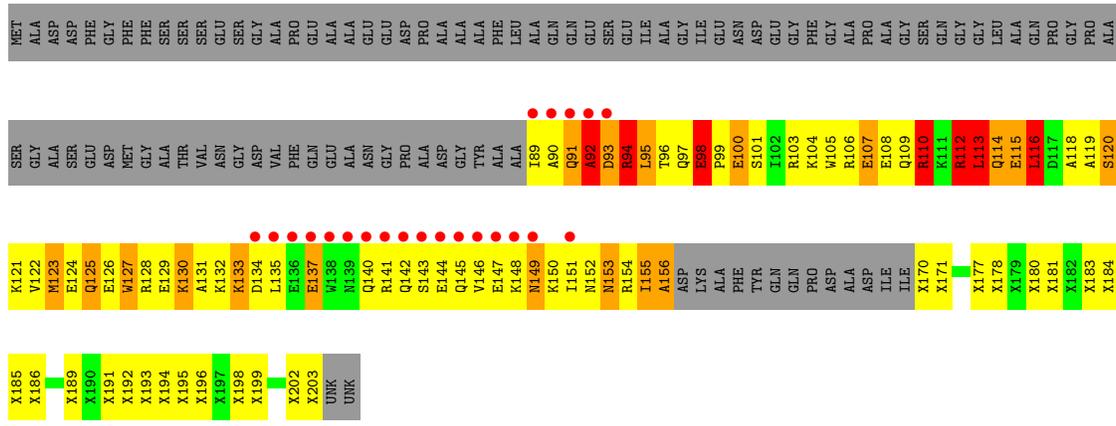
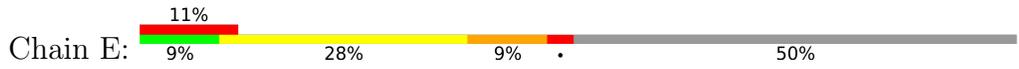
K1113	F1175	Y1237	T1301	F1363	L1423	S1483	E1548	D1611	PHE	SER	K121	X184
A1114	A1176	Q1238	M1302	L1364	M1423	I1484	L1549	K1612	GLY	GLY	V122	X185
Q1115	L1177	A1239	L1303	Y1365	M1426	D1486	E1552	D1613	TYR	ASP	M123	X186
L1116	A1178	A1240	E1304	D1366	L1426	A1486	L1553	D1614	SER	ASP	E124	X187
Q1117	K1179	V1241	A1305	K1367	S1427	Y1487	L1554	A1615	GLY	PHE	Q125	X188
V1121	T1180	D1242	A1306	Y1368	P1428	D1488	L1555	S1616	GLY	ASP	E126	X189
K1122	M1181	G1243	L1307	E1369	R1429	N1489	Q1555	E1617	PHE	MET	M127	X190
E1123	R1182	A1244	E1310	E1370	L1430	F1490	M1556	S1618	PHE	GLY	R128	X191
L1124	L1183	R1245	R1311	Y1371	D1431	D1491	F1557	L1619	ALA	ALA	E129	X192
E1125	A1184	E1126	A1312	D1372	H1432	N1492	N1492	K1620	THR	THR	K130	X193
L1126	E1185	L1127	R1313	M1373	T1433	I1493	E1561	K1621	VAL	VAL	A131	X196
S1127	L1186	T1251	H1314	A1374	R1434	S1494	K1562	E1622	ASN	ASN	K132	X197
Y1128	E1187	T1252	L1314	I1375	A1435	I1495	L1563	E1623	GLY	GLY	K133	X201
I1129	E1188	W1253	G1315	I1376	V1436	A1496	E1564	E1624	GLY	ASP	D134	X202
I1190	F1189	K1254	M1316	T1377	M1437	Q1497	C1565	Q1625	ALA	VAL	L136	X203
I1191	I1190	R1255	F1317	M1378	F1438	R1498	F1566	E1626	PRO	PHE	E137	X204
M1191	G1192	V1256	E1255	M1379	F1439	L1499	G1567	T1627	GLU	GLU	E137	X205
P1193	G1192	C1257	E1319	M1379	S1440	N1380	G1567	T1628	ALA	ALA	E137	X205
P1194	P1193	F1258	L1320	H1381	V1441	H1502	C1569	T1629	ALA	ALA	R141	X205
M1195	M1194	A1259	L1320	P1382	V1442	E1503	L1570	Q1630	GLU	GLU	Q142	X205
S1195	M1195	C1260	L1323	T1383	V1442	L1504	L1571	PRO	GLY	GLY	S143	X205
S1136	A1196	V1261	Y1324	D1384	Q1444	I1505	T1572	ILE	ALA	ASP	E144	X205
Y1137	H1197	D1262	S1325	A1385	L1445	E1506	C1573	VAL	ALA	PRO	Q145	X205
M1138	I1198	G1263	K1326	W1386	F1507	F1507	Y1574	TYR	ALA	ASP	V146	X205
E1139	Q1199	K1264	F1327	K1387	L1447	R1508	D1576	GLY	ALA	ALA	E147	X205
V1140	Q1200	E1285	K1328	E1388	V1448	R1509	L1576	GLN	ALA	ALA	K148	X205
Y1141	V1201	F1266	P1329	G1389	L1449	L1510	L1577	PRO	PHE	ALA	M149	X205
Q1142	W1201	R1267	Q1330	Q1390	P1450	A1511	R1578	GLN	ALA	ALA	K150	X205
R1204	R1204	L1268	K1331	K1391	Y1451	E1512	P1579	LEU	ALA	ALA	I151	X205
A1143	C1205	A1144	M1332	K1392	L1452	M1513	D1580	MET	ALA	ALA	M152	X205
M1145	Y1206	A1145	R1333	D1393	L1453	L1514	V1581	LEU	ALA	ALA	M153	X205
T1146	D1207	Q1270	E1334	I1394	S1454	F1515	Y1582	THR	ALA	ALA	Q154	X205
S1147	E1208	C1272	H1335	I1395	V1455	G1516	L1583	ALA	ALA	SER	R155	X205
M1150	M1210	I1274	L1336	T1396	Q1456	M1517	E1584	PRO	GLY	GLY	A156	X205
E1151	Y1211	H1150	E1337	K1397	M1457	H1458	T1585	GLY	ALA	ALA	T96	X205
E1152	D1212	M1150	F1339	A1399	M1459	R1520	W1587	SER	ALA	ALA	Q97	X205
L1153	A1213	E1152	M1340	N1400	H1460	Y1521	R1588	VAL	ALA	ALA	E98	X205
V1154	A1214	L1154	S1341	V1401	K1461	K1522	H1589	VAL	ALA	ALA	P99	X205
K1155	L1216	L1155	V1342	E1402	S1462	Q1523	M1590	PRO	ASN	ASN	E100	X205
Y1156	L1217	Y1156	M1344	L1403	V1463	S1524	I1591	PRO	ASP	ASP	S101	X205
Q1158	Y1218	Q1158	P1345	Y1405	M1464	E1525	M1592	GLN	GLU	GLU	I102	X205
M1159	V1221	E1158	L1283	R1406	E1465	L1526	D1593	ALA	ALA	GLY	R103	X205
A1160	S1222	M1159	K1346	A1407	S1466	C1528	F1594	PRO	PHE	PHE	K104	X205
R1161	R1223	R1161	E1284	I1408	L1467	K1529	A1596	PHE	GLY	GLY	W105	X205
G1225	F1224	G1225	L1286	E1285	M1468	K1529	M1596	GLY	ALA	ALA	R106	X205
A1164	F1224	L1227	R1350	E1285	M1469	K1529	F1597	TYR	PRO	PRO	E107	X205
K1165	G1225	L1227	A1351	L1287	L1470	D1531	Y1598	TYR	ALA	ALA	E108	X205
R1166	R1226	R1227	M1288	M1288	F1471	S1532	F1599	TYR	GLY	GLY	Q109	X205
S1167	L1227	A1228	Y1289	E1413	I1472	L1533	L1600	THR	SER	SER	R110	X205
Y1168	A1228	R1293	Q1354	F1414	T1473	Y1534	Q1601	ALA	GLN	GLN	K111	X205
Y1169	S1229	S1229	Q1355	F1414	E1474	K1535	V1602	PRO	GLY	GLY	R112	X205
E1170	T1230	G1294	H1356	K1415	A1475	D1536	M1603	ALA	ALA	GLY	L113	X205
E1171	T1230	Y1295	H1357	P1416	D1476	A1537	K1604	TYR	LEU	LEU	Q114	X205
T1171	L1231	Y1295	X1558	L1417	Y1477	M1538	E1605	GLY	ALA	ALA	E115	X205
E1172	V1232	E1297	X1558	L1418	Q1478	Q1539	Y1606	GLN	GLN	GLN	L116	X205
L1173	H1233	E1297	X1558	L1419	A1479	Y1540	L1607	PRO	PRO	PRO	D117	X205
L1174	H1233	E1298	X1560	L1420	L1480	D1546	T1608	GLN	GLY	GLY	A118	X205
	G1234	E1298	L1361	L1421	R1481	D1546	K1609	PRO	PRO	PRO	A119	X205
	E1236	I1300	V1362	L1422	T1482	T1547	V1610	GLY	ALA	ALA	S120	X205

• Molecule 2: Clathrin light chain B



MET	SER	K121	X184
ALA	GLY	V122	X185
ASP	TYR	M123	X186
PHE	SER	E124	X187
GLY	ASP	A125	X188
THR	GLY	Q126	X189
ALA	MET	M127	X190
ALA	GLY	R128	X191
ALA	ALA	E129	X192
GLU	THR	K130	X193
GLU	VAL	A131	X196
GLY	ASN	K132	X197
GLY	GLY	E133	X201
GLY	ASP	D134	X202
ALA	VAL	L136	X203
ALA	PHE	E137	X204
ALA	GLU	E137	X205
ALA	ALA	R141	X205
GLU	ASN	Q142	X205
GLY	GLY	S143	X205
PRO	PRO	E144	X205
PRO	ASP	Q145	X205
ALA	ALA	V146	X205
ALA	ALA	E147	X205
ALA	TYR	K148	X205
ALA	ALA	M149	X205
ALA	ALA	K150	X205
ALA	LEU	I151	X205
ALA	ILE	M152	X205
ALA	ALA	M153	X205
GLU	GLU	Q154	X205
SER	SER	R154	X205
GLU	GLY	I155	X205
GLY	GLY	A156	X205
ALA	ALA	R157	X205
ALA	ALA	K158	X205
ALA	ALA	T96	X205
ALA	ALA	Q97	X205
ALA	ALA	E98	X205
ALA	ALA	P99	X205
ALA	ASN	E100	X205
ALA	ASP	S101	X205
ALA	GLU	I102	X205
ALA	GLY	R103	X205
ALA	PHE	K104	X205
ALA	GLY	W105	X205
ALA	ALA	R106	X205
ALA	PRO	E107	X205
ALA	ALA	E108	X205
ALA	ALA	Q109	X205
ALA	SER	R110	X205
ALA	GLN	K111	X205
ALA	GLY	R112	X205
ALA	GLY	L113	X205
ALA	LEU	Q114	X205
ALA	ALA	X176	X205
ALA	ALA	X177	X205
ALA	ALA	X178	X205
ALA	GLN	X179	X205
PRO	PRO	X180	X205
GLN	GLY	A118	X205
PRO	PRO	X182	X205
ALA	ALA	X183	X205

• Molecule 2: Clathrin light chain B



• Molecule 2: Clathrin light chain B



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	229.71Å 229.71Å 512.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 9.00 86.66 – 9.00	Depositor EDS
% Data completeness (in resolution range)	78.7 (500.00-9.00) 78.9 (86.66-9.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 8.41Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.473 , 0.487 0.483 , 0.479	Depositor DCC
R_{free} test set	430 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	604.9	Xtrriage
Anisotropy	0.404	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	16020	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.04% 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 i

5.1 Standard geometry i

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	0.48	3/4645 (0.1%)	1.41	104/6276 (1.7%)
1	B	0.36	2/4645 (0.0%)	1.38	101/6276 (1.6%)
1	C	0.36	2/4645 (0.0%)	1.38	101/6276 (1.6%)
2	D	0.74	0/647	1.15	8/866 (0.9%)
2	E	0.69	0/589	1.24	5/785 (0.6%)
2	F	0.77	0/642	1.20	8/859 (0.9%)
All	All	0.46	7/15813 (0.0%)	1.37	327/21338 (1.5%)

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	7
1	B	0	6
1	C	0	6
2	F	0	1
All	All	0	20

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1196	ALA	C-N	-21.36	0.84	1.34
1	C	1136	SER	C-N	-13.41	1.03	1.34
1	B	1136	SER	C-N	-13.39	1.03	1.34
1	A	1136	SER	C-N	-13.36	1.03	1.34
1	B	1592	MET	C-N	-10.33	1.10	1.34

The worst 5 of 327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	1136	SER	C-N-CA	22.64	178.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1136	SER	C-N-CA	22.63	178.27	121.70
1	A	1136	SER	C-N-CA	22.58	178.15	121.70
1	A	1196	ALA	CB-CA-C	21.84	142.86	110.10
1	C	1196	ALA	CB-CA-C	21.79	142.78	110.10

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1136	SER	Mainchain
1	A	1196	ALA	Peptide,Mainchain
1	A	1223	ASN	Peptide
1	A	1326	LYS	Peptide
1	A	1429	ARG	Peptide

5.2 Too-close contacts [i](#)

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	4550	0	4457	1578	23
1	B	4550	0	4456	1511	40
1	C	4550	0	4461	1420	30
2	D	811	0	641	286	0
2	E	753	0	615	220	0
2	F	806	0	640	345	35
All	All	16020	0	15270	4959	70

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 158.

The worst 5 of 4959 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:1253:TRP:CZ3	1:A:1276:ILE:HG22	1.19	1.67
1:B:1253:TRP:CZ3	1:B:1276:ILE:HG22	1.19	1.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1253:TRP:CZ3	1:C:1276:ILE:HG22	1.19	1.67
2:E:203:UNK:C	2:E:203:UNK:CA	1.76	1.62
1:B:1108:TRP:CH2	1:B:1129:ILE:HB	1.34	1.61

The worst 5 of 70 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1198:ILE:N	2:F:103:ARG:NH1[5_545]	0.57	1.63
1:B:1199:GLN:N	2:F:103:ARG:NH2[5_545]	0.64	1.56
1:A:1097:GLU:OE1	1:C:1094:ARG:CG[8_465]	0.90	1.30
1:A:1097:GLU:CD	1:C:1094:ARG:CG[8_465]	0.92	1.28
1:B:1198:ILE:CD1	2:F:103:ARG:CB[5_545]	0.98	1.22

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	552/624 (88%)	332 (60%)	164 (30%)	56 (10%)	0	9
1	B	552/624 (88%)	332 (60%)	166 (30%)	54 (10%)	0	10
1	C	552/624 (88%)	332 (60%)	166 (30%)	54 (10%)	0	10
2	D	77/205 (38%)	50 (65%)	16 (21%)	11 (14%)	0	4
2	E	66/205 (32%)	35 (53%)	21 (32%)	10 (15%)	0	4
2	F	76/205 (37%)	42 (55%)	20 (26%)	14 (18%)	0	2
All	All	1875/2487 (75%)	1123 (60%)	553 (30%)	199 (11%)	0	8

5 of 199 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1086	ILE

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Mol	Chain	Res	Type
1	A	1122	LYS
1	A	1193	PRO
1	A	1231	LEU
1	A	1251	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	486/541 (90%)	410 (84%)	76 (16%)	2	14
1	B	486/541 (90%)	409 (84%)	77 (16%)	2	13
1	C	486/541 (90%)	410 (84%)	76 (16%)	2	14
2	D	62/128 (48%)	45 (73%)	17 (27%)	0	3
2	E	61/128 (48%)	42 (69%)	19 (31%)	0	2
2	F	62/128 (48%)	42 (68%)	20 (32%)	0	2
All	All	1643/2007 (82%)	1358 (83%)	285 (17%)	2	11

5 of 285 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	106	ARG
2	D	123	MET
2	E	133	LYS
1	B	1198	ILE
1	B	1175	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1468	ASN
1	C	1489	ASN
2	D	149	ASN
1	B	1103	ASN

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Mol	Chain	Res	Type
1	B	1091	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2
1	C	2

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1592:MET	C	1593:ASP	N	1.10
1	B	1592:MET	C	1593:ASP	N	1.10
1	C	1592:MET	C	1593:ASP	N	1.10
1	A	1136:SER	C	1137:TYR	N	1.03

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1136:SER	C	1137:TYR	N	1.03

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	554/624 (88%)	0.03	43 (7%) 13 15	50, 50, 132, 133	0
1	B	554/624 (88%)	-0.28	2 (0%) 92 87	50, 50, 132, 133	0
1	C	554/624 (88%)	-0.39	11 (1%) 65 58	50, 50, 132, 133	0
2	D	79/205 (38%)	0.13	4 (5%) 28 27	298, 298, 298, 298	0
2	E	68/205 (33%)	1.32	22 (32%) 0 2	314, 314, 314, 314	0
2	F	78/205 (38%)	-0.19	1 (1%) 77 68	339, 339, 339, 339	0
All	All	1887/2487 (75%)	-0.14	83 (4%) 34 32	50, 50, 314, 339	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1313	HIS	6.8
1	A	1306	ALA	6.2
1	A	1341	SER	6.2
1	A	1312	ALA	6.1
1	A	1279	HIS	5.8

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 monosaccharides 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.