

Focus on AI

Alex de Maria Antolinos
Software Engineer
Data Manager@Data Automation Unit
Software Group
ESRF



What is the current status of AI tool usage in the daily operations of SWG?



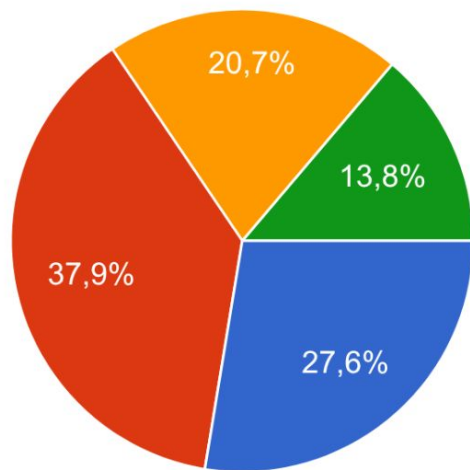
How can AI be used to enhance user experience?

- **Software Group**
 - Inhouse and collaborative projects
 - Open source projects
 - Working on public repositories
 - No confidential data
 - No personal data

Survey: Usage Frequency

How frequently do you use generative AI tools (ChatGPT, Copilot, Claude, etc.)?

29 respuestas

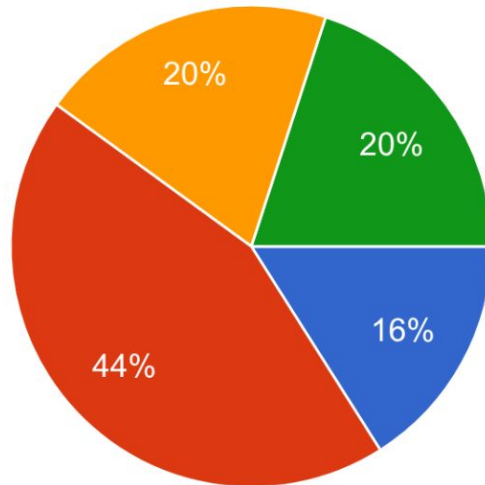


- Never used
- Occasional use (1–2 times per week)
- Frequent use (almost daily)
- Heavy use (multiple times a day)

Survey: Time saving

How much time would you say you save by using these tools?

25 respuestas

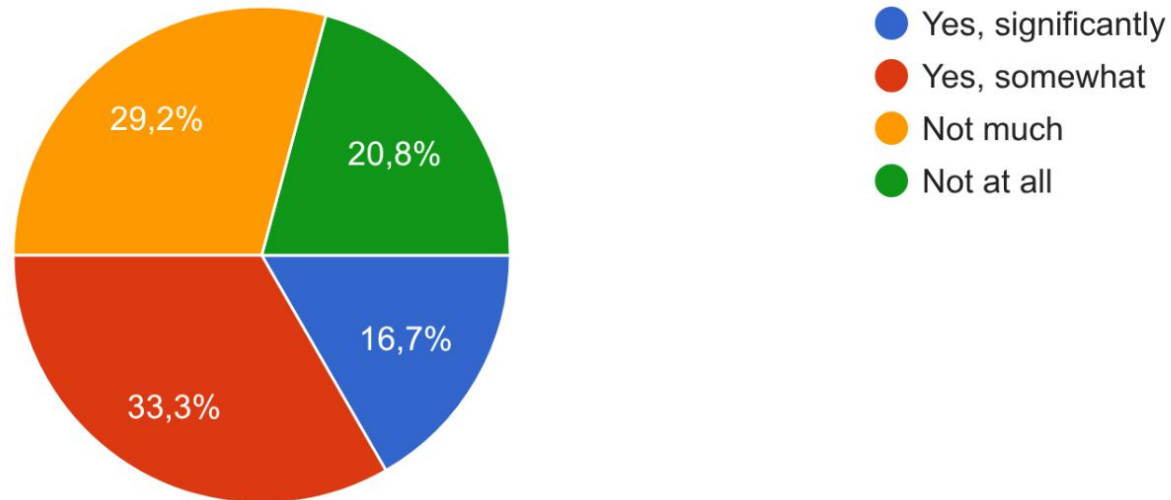


- None
- A little (less than 10%)
- Moderate (10-30%)
- Significant (more than 30%)

Survey: Quality Improvement

Has AI improved the quality of your work (e.g., fewer errors, more clarity, better ideas)?

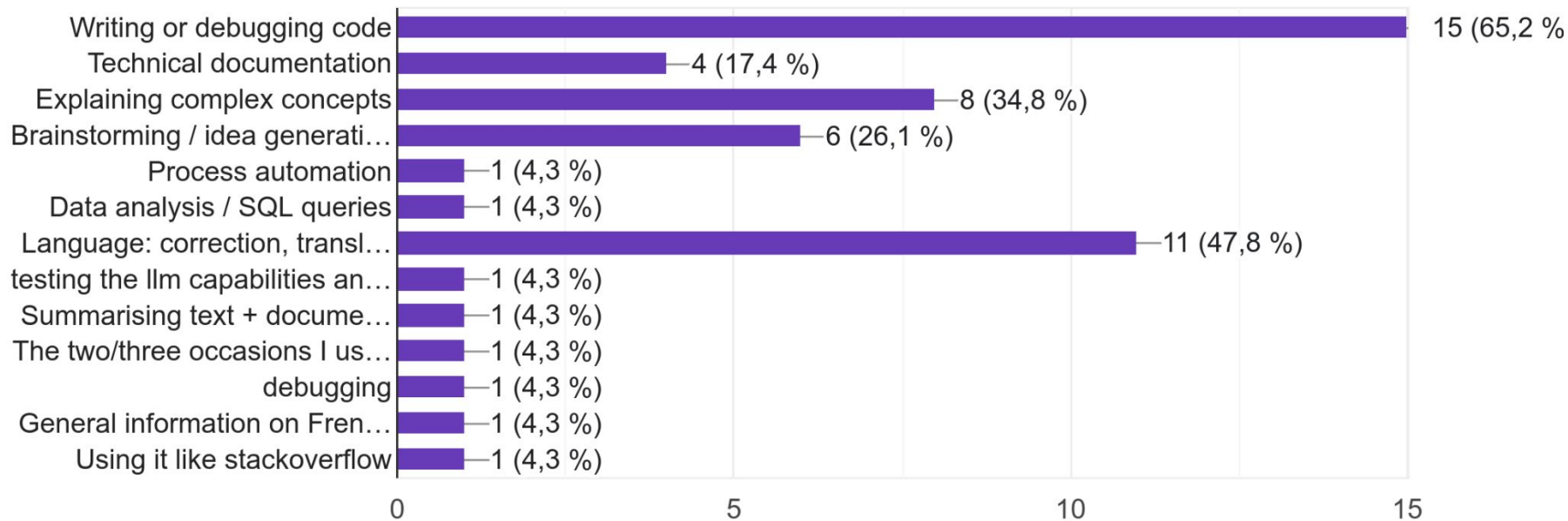
24 respuestas



Survey: Quality Improvement

Which activities do you most often use ChatGPT/LLM for?

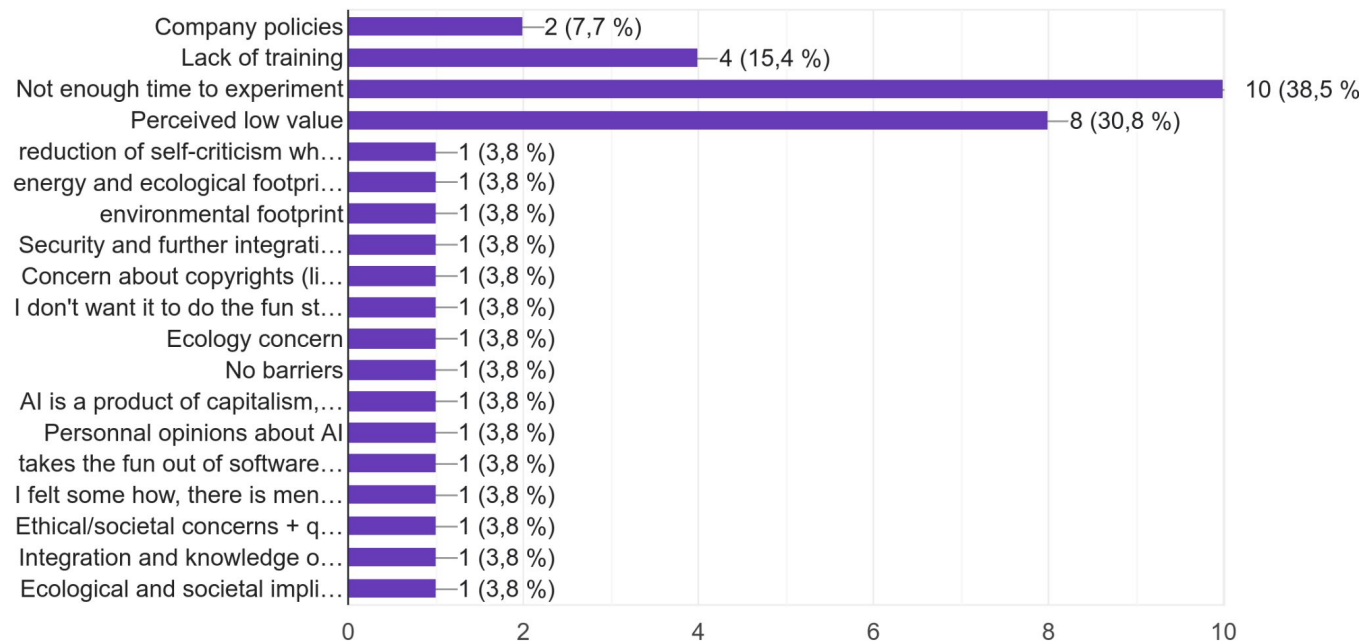
23 respuestas



Survey: Barriers

What barriers prevent you from using these tools more?

26 respuestas

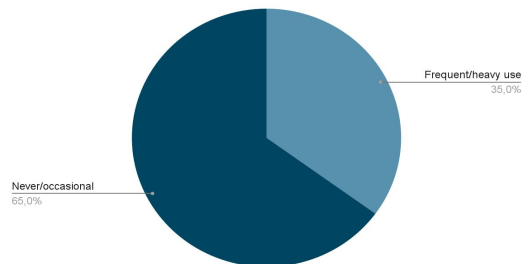


Survey: Barriers

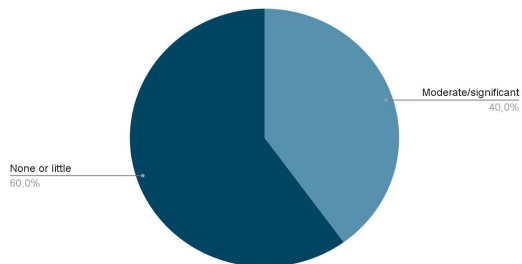
- Ecological, carbon foot concerns (30%)
- Copyrights and license authorship unknowns (10%)
- Unknown medium/long term future business model (10%)
- Risk of losing ability to solve engineering problems (10%)

Survey: Wrap up

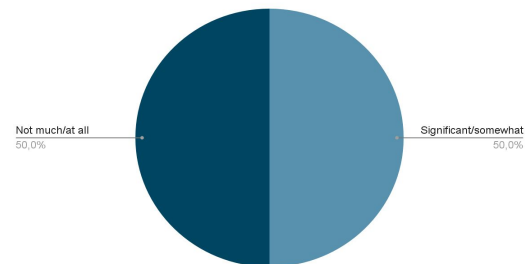
Usage



Time saving



Quality improvement



Main usage:

- Writing and debugging code
- Language correction
- Explaining complex ideas
- Brainstorming
- Producing technical documentation

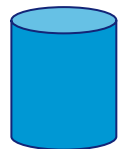
Barriers:

- Not enough time to experiment
- Ecological/ethical concerns
- Perceived low value
- Lack of training

In what ways can AI enhance the user experience?



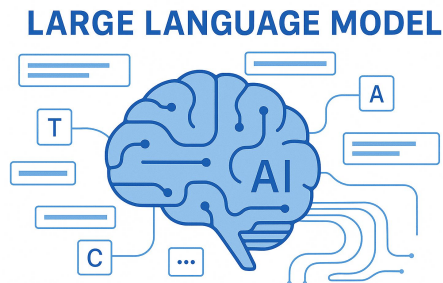
Data Repository
for Advancing open science

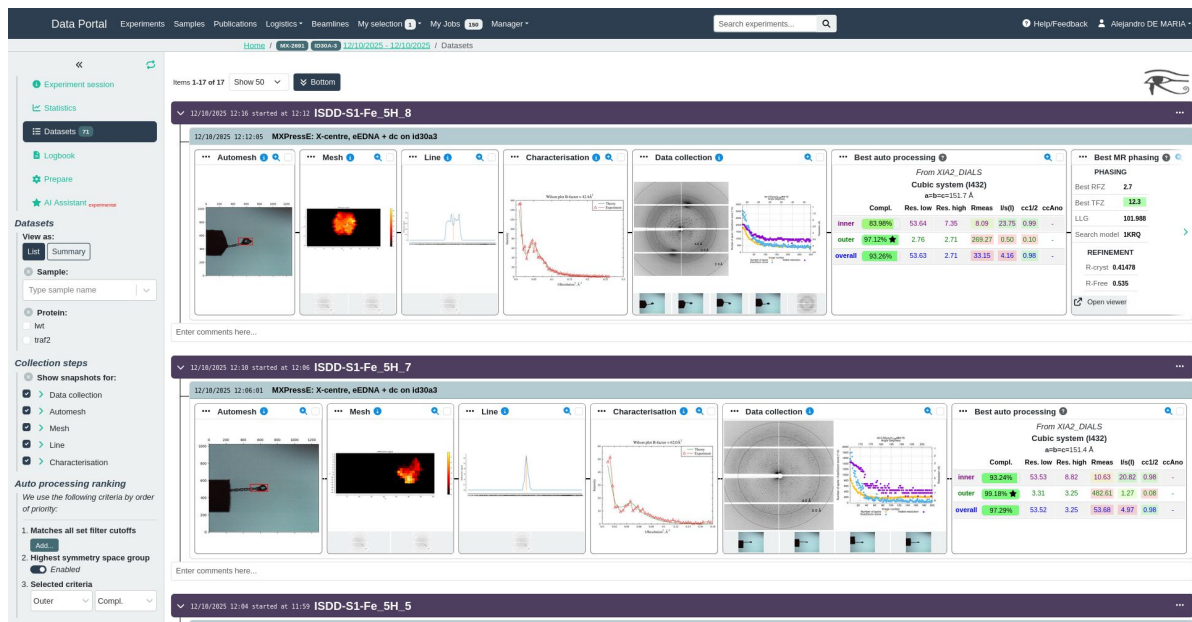


Catalog

- 40k Experiments
- 6M Datasets
- 170M exp. params
- ~30PB of data

Logbook





Example of the Data portal for a MX experiment at ID30A-3

Data portal

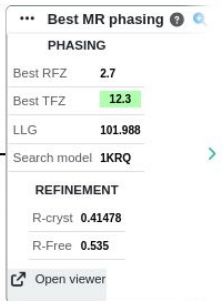
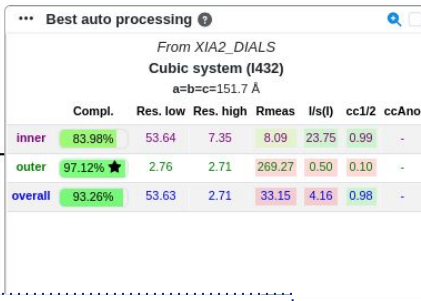
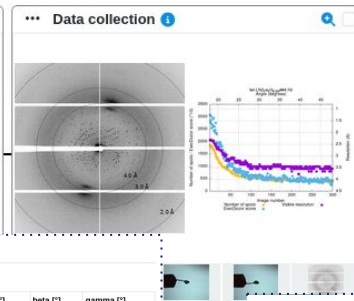
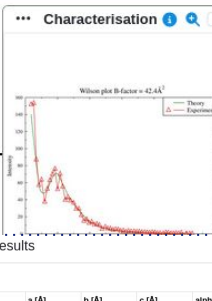
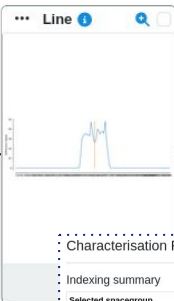
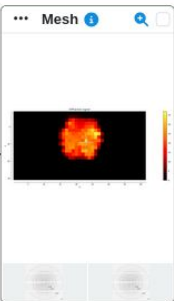
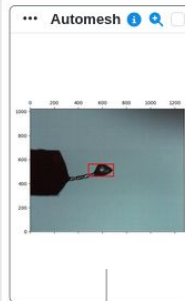
Automatic capture of the metadata
Automatic processing and analysis
Real time quality assessment

MX Experiment

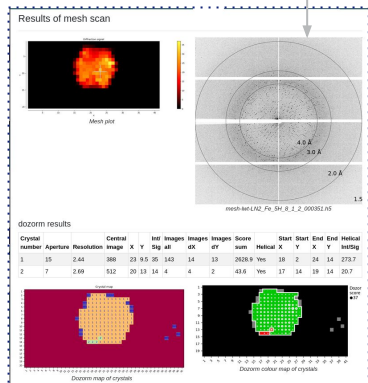
~2 minutes/sample
Hundreds samples/experiment
Thousand of datasets

12/10/2025 12:16 started at 12:12 ISDD-S1-Fe_5H_8

12/10/2025 12:12:05 MXPressE: X-centre. eEDNA + dc on id30a3



Steps x	Steps y	Size x [mm]	Size y [mm]
41	20	0.342	0.175



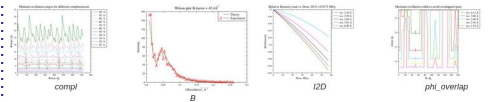
Characterisation Results

- Indexing summary

Selected spacegroup	a [Å]	b [Å]	c [Å]	alpha [°]	beta [°]	gamma [°]
100	151.100	151.100	151.100	90.000	90.000	90.000

- Collection plan strategy: resolution limit is set by the radiation damage

Wedge	Subwedge	Start (°)	Width (°)	No images	Exp time (s)	Max res (Å)	Rel trans (%)	Distance (mm)
1	1	18.00	0.10	300	0.167	2.30	10.00	169.95

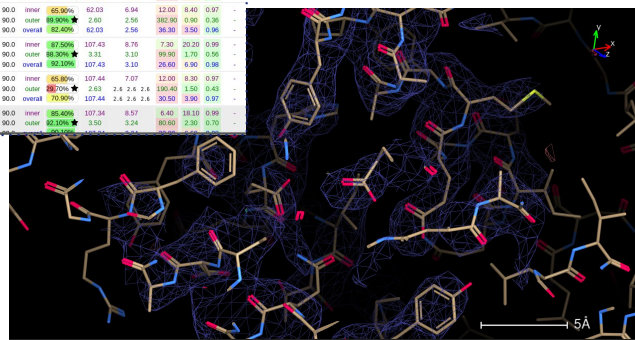


- Diffraction Plan

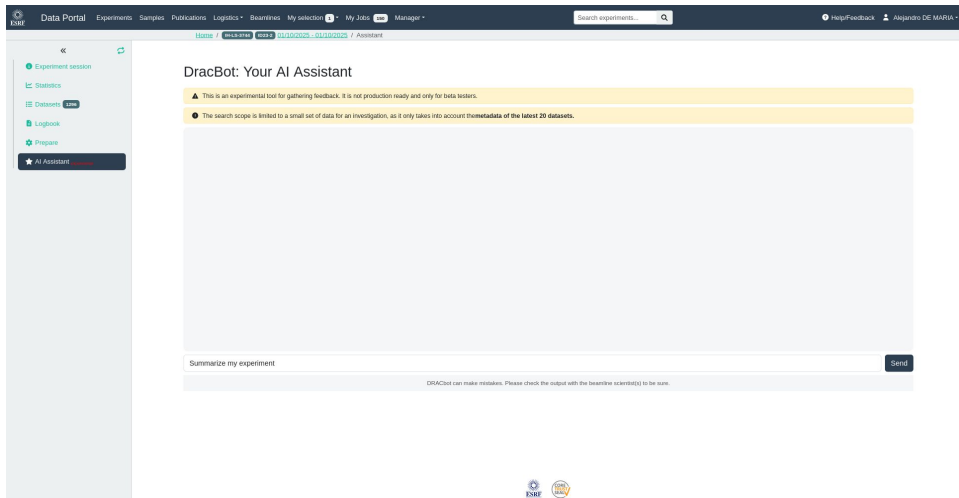
Forced space group	Anomalous data	Aimed multiplicity	Aimed completeness	Aimed I/sigma at highest res.	Aimed resolution (Å)	Min osc. width
--------------------	----------------	--------------------	--------------------	-------------------------------	----------------------	----------------

Atom positions				Motor positions for moving to sample positions		
No.	X	Y	Image file	Decor score	Decor resolution	Motor positions for moving to sample positions
1	59	16	inlet IMZ_FH_SH_1_000000.tif	47.921	2.3	samps = -0.054 mm, sampy = 0.658 mm, phis = 0.346 mm
2	59	16	inlet IMZ_FH_SH_1_000000.tif	47.234	2.3	samps = -0.220 mm, sampy = 0.658 mm, phis = 0.346 mm
3	59	64	inlet IMZ_FH_SH_1_000004.tif	39.981	2.5	samps = -0.242 mm, sampy = 0.658 mm, phis = 0.346 mm
4	59	64	inlet IMZ_FH_SH_1_000004.tif	39.27	2.5	samps = -0.255 mm, sampy = 0.658 mm, phis = 0.346 mm
5	59	68	inlet IMZ_FH_SH_1_000006.tif	38.007	2.5	samps = -0.254 mm, sampy = 0.658 mm, phis = 0.346 mm
6	59	65	inlet IMZ_FH_SH_1_000005.tif	37.773	2.5	samps = -0.239 mm, sampy = 0.658 mm, phis = 0.346 mm
7	59	67	inlet IMZ_FH_SH_1_000007.tif	37.406	2.5	samps = -0.180 mm, sampy = 0.658 mm, phis = 0.346 mm
8	59	69	inlet IMZ_FH_SH_1_000009.tif	35.611	2.5	samps = -0.230 mm, sampy = 0.658 mm, phis = 0.346 mm
9	59	65	inlet IMZ_FH_SH_1_000005.tif	35.595	2.5	samps = -0.130 mm, sampy = 0.658 mm, phis = 0.346 mm

	Acquisition	Scan	Sample
Product name	run_01_09_040306036	Remission	2.300 Å
Product date	13/05/2018 12:51:21	Wavelength	0.97
Product		Overlap	0.87
Product		Axis start/end	507.146/7.0
Product	MPD0000	Exposure Time	0.001 s
Product	h0, h1, h2, h3, h4, h5, h6, h7, h8, h9, h10, h11, h12, h13, h14, h15, h16, h17, h18, h19, h20, h21, h22, h23, h24, h25, h26, h27, h28, h29, h30, h31, h32, h33, h34, h35, h36, h37, h38, h39, h40, h41, h42, h43, h44, h45, h46, h47, h48, h49, h50, h51, h52, h53, h54, h55, h56, h57, h58, h59, h60, h61, h62, h63, h64, h65, h66, h67, h68, h69, h70, h71, h72, h73, h74, h75, h76, h77, h78, h79, h80, h81, h82, h83, h84, h85, h86, h87, h88, h89, h90, h91, h92, h93, h94, h95, h96, h97, h98, h99, h100, h101, h102, h103, h104, h105, h106, h107, h108, h109, h110, h111, h112, h113, h114, h115, h116, h117, h118, h119, h120, h121, h122, h123, h124, h125, h126, h127, h128, h129, h130, h131, h132, h133, h134, h135, h136, h137, h138, h139, h140, h141, h142, h143, h144, h145, h146, h147, h148, h149, h150, h151, h152, h153, h154, h155, h156, h157, h158, h159, h160, h161, h162, h163, h164, h165, h166, h167, h168, h169, h170, h171, h172, h173, h174, h175, h176, h177, h178, h179, h180, h181, h182, h183, h184, h185, h186, h187, h188, h189, h190, h191, h192, h193, h194, h195, h196, h197, h198, h199, h200, h201, h202, h203, h204, h205, h206, h207, h208, h209, h210, h211, h212, h213, h214, h215, h216, h217, h218, h219, h220, h221, h222, h223, h224, h225, h226, h227, h228, h229, h230, h231, h232, h233, h234, h235, h236, h237, h238, h239, h240, h241, h242, h243, h244, h245, h246, h247, h248, h249, h250, h251, h252, h253, h254, h255, h256, h257, h258, h259, h260, h261, h262, h263, h264, h265, h266, h267, h268, h269, h270, h271, h272, h273, h274, h275, h276, h277, h278, h279, h280, h281, h282, h283, h284, h285, h286, h287, h288, h289, h290, h291, h292, h293, h294, h295, h296, h297, h298, h299, h300, h301, h302, h303, h304, h305, h306, h307, h308, h309, h310, h311, h312, h313, h314, h315, h316, h317, h318, h319, h320, h321, h322, h323, h324, h325, h326, h327, h328, h329, h330, h331, h332, h333, h334, h335, h336, h337, h338, h339, h340, h341, h342, h343, h344, h345, h346, h347, h348, h349, h350, h351, h352, h353, h354, h355, h356, h357, h358, h359, h360, h361, h362, h363, h364, h365, h366, h367, h368, h369, h370, h371, h372, h373, h374, h375, h376, h377, h378, h379, h380, h381, h382, h383, h384, h385, h386, h387, h388, h389, h390, h391, h392, h393, h394, h395, h396, h397, h398, h399, h400, h401, h402, h403, h404, h405, h406, h407, h408, h409, h410, h411, h412, h413, h414, h415, h416, h417, h418, h419, h420, h421, h422, h423, h424, h425, h426, h427, h428, h429, h430, h431, h432, h433, h434, h435, h436, h437, h438, h439, h440, h441, h442, h443, h444, h445, h446, h447, h448, h449, h450, h451, h452, h453, h454, h455, h456, h457, h458, h459, h460, h461, h462, h463, h464, h465, h466, h467, h468, h469, h470, h471, h472, h473, h474, h475, h476, h477, h478, h479, h480, h481, h482, h483, h484, h485, h486, h487, h488, h489, h490, h491, h492, h493, h494, h495, h496, h497, h498, h499, h500, h501, h502, h503, h504, h505, h506, h507, h508, h509, h510, h511, h512, h513, h514, h515, h516, h517, h518, h519, h520, h521, h522, h523, h524, h525, h526, h527, h528, h529, h530, h531, h532, h533, h534, h535, h536, h537, h538, h539, h540, h541, h542, h543, h544, h545, h546, h547, h548, h549, h550, h551, h552, h553, h554, h555, h556, h557, h558, h559, h560, h561, h562, h563, h564, h565, h566, h567, h568, h569, h570, h571, h572, h573, h574, h575, h576, h577, h578, h579, h580, h581, h582, h583, h584, h585, h586, h587, h588, h589, h590, h591, h592, h593, h594, h595, h596, h597, h598, h599, h600, h601, h602, h603, h604, h605, h606, h607, h608, h609, h610, h611, h612, h613, h614, h615, h616, h617, h618, h619, h620, h621, h622, h623, h624, h625, h626, h627, h628, h629, h630, h631, h632, h633, h634, h635, h636, h637, h638, h639, h640, h641, h642, h643, h644, h645, h646, h647, h648, h649, h650, h651, h652, h653, h654, h655, h656, h657, h658, h659, h660, h661, h662, h663, h664, h665, h666, h667, h668, h669, h670, h671, h672, h673, h674, h675, h676, h677, h678, h679, h680, h681, h682, h683, h684, h685, h686, h687, h688, h689, h690, h691, h692, h693, h694, h695, h696, h697, h698, h699, h700, h701, h702, h703, h704, h705, h706, h707, h708, h709, h710, h711, h712, h713, h714, h715, h716, h717, h718, h719, h720, h721, h722, h723, h724, h725, h726, h727, h728, h729, h730, h731, h732, h733, h734, h735, h736, h737, h738, h739, h740, h741, h742, h743, h744, h745, h746, h747, h748, h749, h750, h751, h752, h753, h754, h755, h756, h757, h758, h759, h760, h761, h762, h763, h764, h765, h766, h767, h768, h769, h770, h771, h772, h773, h774, h775, h776, h777, h778, h779, h780, h781, h782, h783, h784, h785, h786, h787, h788, h789, h790, h791, h792, h793, h794, h795, h796, h797, h798, h799, h800, h801, h802, h803, h804, h805, h806, h807, h808, h809, h810, h811, h812, h813, h814, h815, h816, h817, h818, h819, h820, h821, h822, h823, h824, h825, h826, h827, h828, h829, h830, h831, h832, h833, h834, h835, h836, h837, h838, h839, h840, h841, h842, h843, h844, h845, h846, h847, h848, h849, h850, h851, h852, h853, h854, h855, h856, h857, h858, h859, h860, h861, h862, h863, h864, h865, h866, h867, h868, h869, h870, h871, h872, h873, h874, h875, h876, h877, h878, h879, h880, h881, h882, h883, h884, h885, h886, h887, h888, h889, h890, h891, h892, h893, h894, h895, h896, h897, h898, h899, h900, h901, h902, h903, h904, h905, h906, h907, h908, h909, h910, h911, h912, h913, h914, h915, h916, h917, h918, h919, h920, h921, h922, h923, h924, h925, h926, h927, h928, h929, h930, h931, h932, h933, h934, h935, h936, h937, h938, h939, h940, h941, h942, h943, h944, h945, h946, h947, h948, h949, h950, h951, h952, h953, h954, h955, h956, h957, h958, h959, h960, h961, h962, h963, h964, h965, h966, h967, h968, h969, h970, h971, h972, h973, h974, h975, h976, h977, h978, h979, h980, h981, h982, h983, h984, h985, h986, h987, h988, h989, h990, h991, h992, h993, h994, h995, h996, h997, h998, h999, h1000, h1001, h1002, h1003, h1004, h1005, h1006, h1007, h1008, h1009, h1010, h1011, h1012, h1013, h1014, h1015, h1016, h1017, h1018, h1019, h1020, h1021, h1022, h1023, h1024, h1025, h1026, h1027, h1028, h1029, h1030, h1031, h1032, h1033, h1034, h1035, h1036, h1037, h1038, h1039, h1040, h1041, h1042, h1043, h1044, h1045, h1046, h1047, h1048, h1049, h1050, h1051, h1052, h1053, h1054, h1055, h1056, h1057, h1058, h1059, h1060, h1061, h1062, h1063, h1064, h1065, h1066, h1067, h1068, h1069, h1070, h1071, h1072, h1073, h1074, h1075, h1076, h1077, h1078, h1079, h1080, h1081, h1082, h1083, h1084, h1085, h1086, h1087, h1088, h1089, h1090, h1091, h1092, h1093, h1094, h1095, h1096, h1097, h1098, h1099, h1100, h1101, h1102, h1103, h1104, h1105, h1106, h1107, h1108, h1109, h1110, h1111, h1112, h1113, h1114, h1115, h1116, h1117, h1118, h1119, h1120, h1121, h1122, h1123, h1124, h1125, h1126, h1127, h1128, h1129, h1130, h1131, h1132, h1133, h1134, h1135, h1136, h1137, h1138, h1139, h1140, h1141, h1142, h1143, h1144, h1145, h1146, h1147, h1148, h1149, h1150, h1151, h1152, h1153, h1154, h1155, h1156, h1157, h1158, h1159, h1160, h1161, h1162, h1163, h1164, h1165, h1166, h1167, h1168, h1169, h1170, h1171, h1172, h1173, h1174, h1175, h1176, h1177, h1178, h1179, h1180, h1181, h1182, h1183, h1184, h1185, h1186, h1187, h1188, h1189, h1190, h1191, h1192, h1193, h1194, h1195, h1196, h1197, h1198, h1199, h1200, h1201, h1202, h1203, h1204, h1205, h1206, h1207, h1208, h1209, h1210, h1211, h1212, h1213, h1214, h1215, h1216, h1217, h1218, h1219, h1220, h1221, h1222, h1223, h1224, h1225, h1226, h1227, h1228, h1229, h1230, h1231, h1232, h1233, h1234, h1235, h1236, h1237, h1238, h1239, h1240, h1241, h1242, h1243, h1244, h1245, h1246, h1247, h1248, h1249, h1250, h1251, h1252, h1253, h1254, h1255, h1256, h1257, h1258, h1259, h1260, h1261, h1262, h1263, h1264, h1265, h1266, h1267, h1268, h1269, h1270, h1271, h1272, h1273, h1274, h1275, h1276, h1277, h1278, h1279, h1280, h1281, h1282, h1283, h1284, h1285, h1286, h1287, h1288, h1289, h1290, h1291, h1292, h1293, h1294, h1295, h1296, h1297, h1298, h1299, h1300, h1301, h1302, h1303, h1304, h1305, h1306, h1307, h1308, h1309, h1310, h1311, h1312, h1313, h1314, h1315, h1316, h1317, h1318, h1319, h1320, h1321, h1322, h1323, h1324, h1325, h1326, h1327, h1328, h1329, h1330, h1331, h1332, h1333, h1334, h1335, h1336, h1337, h1338, h1339, h1340, h1341, h1342, h1343, h1344, h1345, h1346, h1347, h1348, h1349, h1350, h1351, h1352, h1353, h1354, h1355, h1356, h1357, h1358, h1359, h1360, h1361, h1362, h1363, h1364, h1365, h1366, h1367, h1368, h1369, h1370, h1371, h1372, h1373, h1374, h1375, h1376, h1377, h1378, h1379, h1380, h1381, h1382, h1383, h1384, h1385, h1386, h1387, h1388, h1389, h1390, h1391, h1392, h1393, h1394, h1395, h1396, h1397, h1398, h1399, h1400, h1401, h1402, h1403, h1404, h1405, h1406, h1407, h1408, h1409, h1410, h1411, h1412, h1413, h1414, h1415, h1416, h1417, h1418, h1419, h1420, h1421, h1422, h1423, h1424, h1425, h1426, h1427, h1428, h1429, h1430, h1431, h1432, h1433, h1434, h1435, h1436, h1437, h1438, h1439, h1440, h1441, h1442, h1443, h1444, h1445, h1446, h1447, h1448, h1449, h1450, h1451, h1452, h1453, h1454, h1455, h1456, h1457, h1458, h1459, h1460, h1461, h1462, h1463, h1464, h1465, h1466, h1467, h1468, h1469, h1470, h1471, h1472, h1473, h1474, h1475, h1476, h1477, h1478, h1479, h1480, h1481, h1482, h1483, h1484, h1485, h1486, h1487, h1488, h1489, h1490, h1491, h1492, h1493, h1494, h1495, h1496, h1497, h1498, h1499, h1500, h1501, h1502, h1503, h1504, h1505, h1506, h1507, h1508, h1509, h1510, h1511, h1512, h1513, h1514, h1515, h1516, h1517, h1518, h1519, h1520, h1521, h1522, h1523, h1524, h1525, h1526, h1527, h1528, h1529, h1530, h1531, h1532, h1533, h1534, h1535, h1536, h1537, h1538, h1539, h1540, h1541, h1542, h1543, h1544, h1545, h1546, h1547, h1548, h1549, h1550, h1551, h1552, h1553, h1554, h1555, h1556, h1557, h1558, h1559, h1560, h1561, h1562, h1563, h1564, h1565, h1566, h1567, h1568, h1569, h1570, h1571, h1572, h1573, h1574, h1575, h1576, h1577, h1578, h1579, h1580, h1581, h1582, h1583, h1584, h1585, h1586, h1587, h1588, h1589, h1590, h1591, h1592, h1593, h1594, h1595, h1596, h1597, h1598, h1599, h1600, h1601, h1602, h1603, h1604, h1605, h1606, h1607, h1608, h1609, h1610, h1611, h1612, h1613, h1614, h1615, h1616, h1617, h1618, h1619, h1620, h1621, h1622, h1623, h1624, h1625, h1626, h1627, h1628, h1629, h1630, h1631, h1632, h1633, h1634, h1635, h1636, h1637, h1638, h1639, h1640, h1641, h1642, h1643, h1644, h1645, h1646, h1647, h1648, h1649, h1650, h1651, h1652, h1653, h1654, h1655, h1656, h1657, h1658, h1659, h1660, h1661, h1662, h1663, h1664, h1665, h1666, h1667, h1668, h1669, h1670, h1671, h1672, h1673, h1674, h1675, h1676, h1677, h1678, h1679, h1680, h1681, h1682, h1683, h1684, h1685, h1686, h1687, h1688, h1689, h1690, h1691, h1692, h1693, h1694, h1695, h1696, h1697, h1698, h1699, h1700, h1701, h1702, h1703, h1704, h1705, h1706, h1707, h1708, h1709, h1710, h1711, h1712, h1713, h1714, h1715, h1716, h1717, h1718, h1719, h1720, h1721, h1722, h1723, h1724, h1725, h1726, h1727, h1728, h1729, h1730, h1731, h1732, h1733, h1734, h1735, h1736, h1737, h1738, h1739, h1740, h1741, h1742, h1743, h1744, h1745, h1746, h1747, h1748, h1749, h1750, h1751, h1752, h1753, h1754, h1755, h1756, h1757, h1758, h1759, h1760, h1761, h1762, h1763, h1764, h1765, h1766, h1767, h1768, h1769, h1770, h1771, h1772, h1773, h1774, h1775, h1776, h1777, h1778, h1779, h1780, h1781, h1782, h1783, h1784, h1785, h1786, h1787, h1788, h1789, h1790, h1791, h1792, h1793, h1794, h1795, h1796, h1797, h1798, h1799, h1800, h1801, h1802, h1803, h1804, h1805, h1806, h1807, h1808, h1809, h1810, h1811, h1812, h1813, h1814, h1815, h1816, h1817, h1818, h1819, h1820, h1821, h1822, h1823, h1824, h1825, h1826, h1827, h1828, h1829, h1830, h1831, h1832, h1833, h1834, h1835, h1836, h1837, h1838, h1839, h1840, h1841, h1842, h1843, h1844, h1845, h1846, h1847, h1848, h1849, h1850, h1851, h1852, h1853, h1854, h1855, h1856, h1857, h1858, h1859, h1860, h1861, h1862, h1863, h1864, h1865, h1866, h1867, h1868, h1869, h1870, h1871, h1872, h1873, h1874, h1875, h1876, h1877, h1878, h1879, h1880, h1881, h1882, h1883, h1884, h1885, h1886, h1887, h1888, h1889, h1890, h1891, h1892, h1893, h1894, h1895, h1896, h1897, h1898, h1899, h1900, h1901, h1902, h1903, h1904, h1905, h1906, h1907, h1908, h1909, h1910, h1911, h1912, h1913, h1914, h1915, h1916, h1917, h1918, h1919, h1920, h1921, h1922, h1923, h1924, h1925, h1926, h1927, h1928, h1929, h1930, h1931, h1932, h1933, h1934, h1935, h1936, h1937, h1938, h1939, h1940, h1941, h1942, h1943, h1944, h1945, h1946, h1947, h1948, h1949, h1950, h1951, h1952, h1953, h1954, h1955, h1956, h1957, h1958, h1959, h1960, h1961, h1962, h1963, h1964, h1965, h1966, h1967, h1968, h1969, h1970, h1971, h1972, h1973, h1974, h1975, h1976, h1977, h1978, h1979, h1980, h1981, h1982, h1983, h1984, h1985, h1986, h1987, h1988, h1989, h1990, h1991, h1992, h1993, h1994, h1995, h1996, h1997, h1998, h1999, h2000, h2001, h2002, h2003, h2004, h2005, h2006, h2007, h2008, h2009, h2010, h2011, h2012, h2013, h2014, h2015, h2016, h2017, h2018, h2019, h2020, h2021, h2022, h2023, h2024, h2025, h2026, h2027, h2028, h2029, h2030, h2031, h2032, h2033, h2034, h2035, h2036, h2037, h2038, h2039, h2040, h2041, h2042, h2043, h2044, h2045, h2046, h2047, h2048, h2049, h2050, h2051, h2052, h2053, h2054, h2055, h2056, h2057, h2058, h2059, h2060, h2061, h2062, h2063, h2064, h2065, h2066, h2067, h2068, h2069, h2070, h2071, h2072, h2073, h2074, h2075, h2076, h2077, h2078, h2079, h2080, h2081, h2082, h2083, h2084, h2085, h2086, h2087, h2088, h2089, h2090, h2091, h2092, h2093, h2094, h2095, h2096, h2097, h2098, h2099, h2100, h2101, h2102, h2103, h2104, h2105, h2106, h2107, h2108, h2109, h2110, h2111, h2112, h2113, h2114, h2115, h2116, h2117, h2118, h2119, h2120, h2121, h2122, h2123, h2124, h2125, h2126, h2127, h2128, h2129, h2130, h2131, h2132, h2133, h2134, h2135, h2136, h2137, h2138, h2139, h2140, h2141, h2142, h2143, h2144, h2145, h2146, h2147, h2148, h2149, h2150, h2151, h2152, h2153, h2154, h2155, h2156, h2157, h2158, h2159, h2160, h2161, h2162, h2163, h2164, h2165, h2166, h2167, h2168, h2169, h2170, h2171, h2172, h2173, h2174, h2175, h2176, h2177, h2178, h2179, h2180, h2181, h2182, h2183, h2184, h2185, h2186, h2187, h2188, h2189, h2190, h2191, h2192, h2193, h2194, h2195, h2196, h2197, h2198, h2199, h2200, h2201, h2202, h2203, h2204, h2205, h2206, h220		



DRACBot: AI Assistant



POC

- A proof of concept deployed on 16th Oct
- Accessible to ESRF beamline staff only

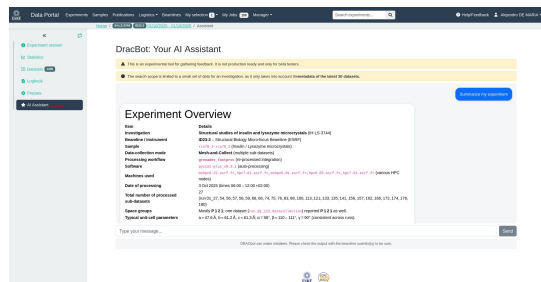
RAG (Retrieval Augmented Generation)

- Limited context send to the LLM
 - Metadata of latest datasets
- LLM installed by TID: gpt-oss

Evaluation purposes only

- Gather feedback
- Inspiration about use cases

DRACBot: Example of “summarize my experiment”



Data-quality Summary (representative values)

Metric	Typical range across runs
Overall completeness	7 % – 15 % (most runs 12-15 %)
Overall $\langle I/\sigma(I) \rangle$	0.8 – 2.5 (inner shells often much higher, up to ~40 for the best runs)
Overall CC $\frac{1}{2}$	0.96 – 0.998 (inner shells often > 0.99)
Overall R _{merge}	0 – 30 % (many runs report 0, a few high values up to ~95 % for low-resolution shells)
Overall R _{meas}	0 – 65 % (some anomalously large negative values indicate statistical noise in very low-count data)
Overall R _{pim}	0 – 27 % (most ≤ 12 %)
Overall multiplicity	1.0 – 1.3 (generally low, as expected for single-crystal mesh scans)
Resolution limits	High-resolution shell typically 1.63 – 1.66 Å; low-resolution cut-off varies from ~18 Å to > 40 Å depending on crystal quality.
Anomalous signal	Generally absent (overall anomalous multiplicity = 0, anomalous completeness = 0 – 0.3 %).

Note: Many parameters are reported as **0** for outer shells (e.g., R_{merge}, R_{meas}) because the corresponding reflections are either absent or have intensities below the detection threshold.

Key Observations

- Consistent crystal lattice** – All processed sub-datasets share nearly identical unit-cell dimensions, confirming that the same crystal (or identical crystals) were used throughout the mesh-and-collect experiment.
- High inner-shell data quality** – The inner resolution shells routinely show very high $\langle I/\sigma(I) \rangle$ (up to ~40) and CC $\frac{1}{2}$ > 0.99, indicating that the diffraction spots are strong and well measured.
- Low overall completeness** – Because each mesh-and-collect sub-dataset only samples a small portion of reciprocal space, overall completeness per sub-dataset is modest (7–15 %). The full experiment (combining all sub-datasets) would be expected to reach a much higher completeness.
- Resolution** – The majority of runs reach a high-resolution limit of ~1.64 Å, sufficient for detailed atomic modelling of insulin and lysozyme.
- Anomalous signal** – No significant anomalous signal was detected, which is typical for native protein crystals without heavy-atom derivatization.
- Processing consistency** – All datasets were processed with the same pipeline (`grenades_fastproc` → `pyicat-plus_v0.9.1`) on ESRF HPC resources, ensuring comparable statistical treatment.

Conclusion

The mesh-and-collect experiment on the ID23-2 beamline generated a large set of high-resolution diffraction sub-datasets from insulin/lysozyme microcrystals. While each individual sub-dataset has limited completeness, the data quality within the measured resolution shells is excellent (high CC $\frac{1}{2}$, strong $\langle I/\sigma(I) \rangle$, and low R_{merge}/R_{meas}). When merged, these data should provide a robust structural model of the target proteins at ~1.6 Å resolution.

All information extracted from the dataset metadata supplied (27 re-processed integration datasets, IDs 2260453301 – 2260552388).

DRACBot: Utils

write a list of scp command line that will copy the data to demariaa@myhome:/data

Below are the **scp** commands you can run (one per dataset) to copy each processed-data folder to the remote host **demariaa@myhome** under **/data**. Each command uses the **-r** flag to copy the directory recursively.

```
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_36_datacollection/;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_88_datacollection/;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_76_datacollection/;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_133_datacollection;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_54_datacollection/;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_56_datacollection/;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_113_datacollection;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_156_datacollection;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_59_datacollection/;
```

Type your message...

Send

DRACbot can make mistakes. Please check the output with the beamline scientist(s) to be sure.

write a list of scp command lines that copies the data to demariaa@myhome:/data for the crystals that are not diffracting or resolution between 2 and 3 amstrongs

SCP commands for the datasets that show little or no diffraction (overall $I/\sigma(I) < 1$)

```
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_68_datacollection/;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_74_datacollection/;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_135_datacollection;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_59_datacollection/;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_56_datacollection/;
scp -r /data/visitor/ihls3744/id23eh2/20251001/PROCESSED_DATA/rco78_2/rco78_2-rco78_2/run_01_MeshAndCollect/run_01_88_datacollection/;
```

Type your message...

Send

DRACbot can make mistakes. Please check the output with the beamline scientist(s) to be sure.

do a python script that will plot the resolution of the crystal correlated with the exposure time

Below is a **stand-alone Python script** that

- reads the JSON you posted (or any similar list of dataset dictionaries),
- extracts the **overall high resolution limit** (`MXAutoprocIntegrationScaling_overall_resolution_limit_high`) and the **exposure time** (`__elapsedTime` – reported in seconds),
- skips any dataset that does not contain both values,
- creates a scatter plot **resolution (Å) vs. exposure time (s)**, adds a linear regression line for a quick trend, and
- saves the figure as `resolution_vs_exposure.png` and also shows it on screen.

You can copy-paste the script into a file (e.g. `plot_resolution_vs_exposure.py`) and run it with a standard Python 3 installation that has `matplotlib`, `numpy`, and `scipy` installed.

```
```python
#!/usr/bin/env python3
"""
```

```
Plot crystal resolution (high-resolution limit) versus exposure time
for a collection of ESRF "grenades_fastproc" datasets.
```

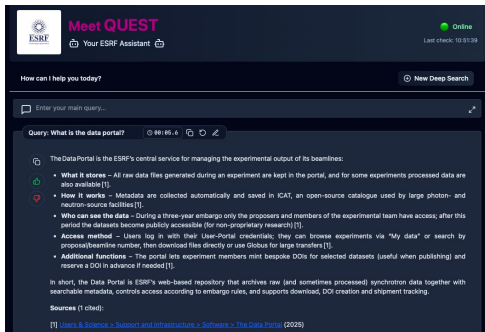
```
The script expects a JSON file that contains a list of dataset objects
exactly like the one you posted. It extracts:
```

Type your message...

Send

DRACbot can make mistakes. Please check the output with the beamline scientist(s) to be sure.

# Related developments

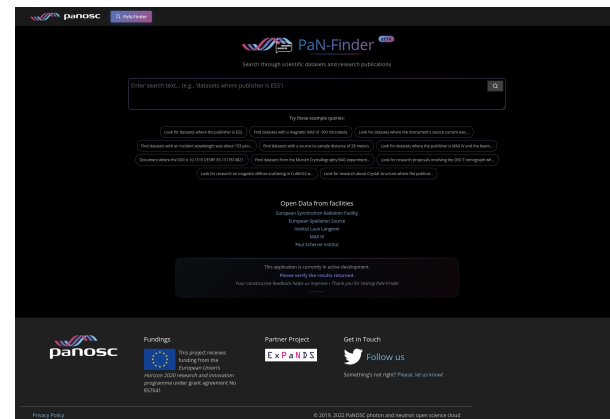


## Quest

- QUEST is ESRF's AI assistant for scientific and administrative support.
- Uses Retrieval-Augmented Generation to deliver accurate, factual answers with inline references.
- Draws information from the ESRF extranet and 40,000+ publications in the PUMA corpus.
- Currently under evaluation BDO + UO

## PaN-Finder

- AI-powered search tool from the OSCARS project that enhances the PaNOSC Data Portal
- Retrieval-Augmented Generation to provide intelligent, prompt-based searches with summaries and references.
- Developed by the European Spallation Source (ESS) team





### What is the current status of AI tool usage in the daily operations of SWG?

- The use of AI, LLMs, and chatbots is modest.
- The perceived usefulness appears to be slightly higher than actual usage.
- Lack of time to experiment, along with ethical and ecological concerns, is the most important barrier.



### How can AI be used to enhance user experience?

- A proof of concept (POC) has been implemented to gather feedback.
- The amount of metadata available at the ESRF, together with increasingly powerful LLMs, may provide a valuable tool for users.
- The implementation or adoption of other solutions will likely require several years of development if we aim to fully leverage them, but they could ultimately be a game changer



**THANKS**

## Lower Artificial Intelligence Literacy Predicts Greater AI Receptivity

Journal of Marketing  
1-20  
© American Marketing Association 2025  
Article reuse guidelines:  
[sagepub.com/journals-permissions](https://sagepub.com/journals-permissions)  
DOI: 10.1177/00222429251314491  
[journals.sagepub.com/home/jmx](https://journals.sagepub.com/home/jmx)

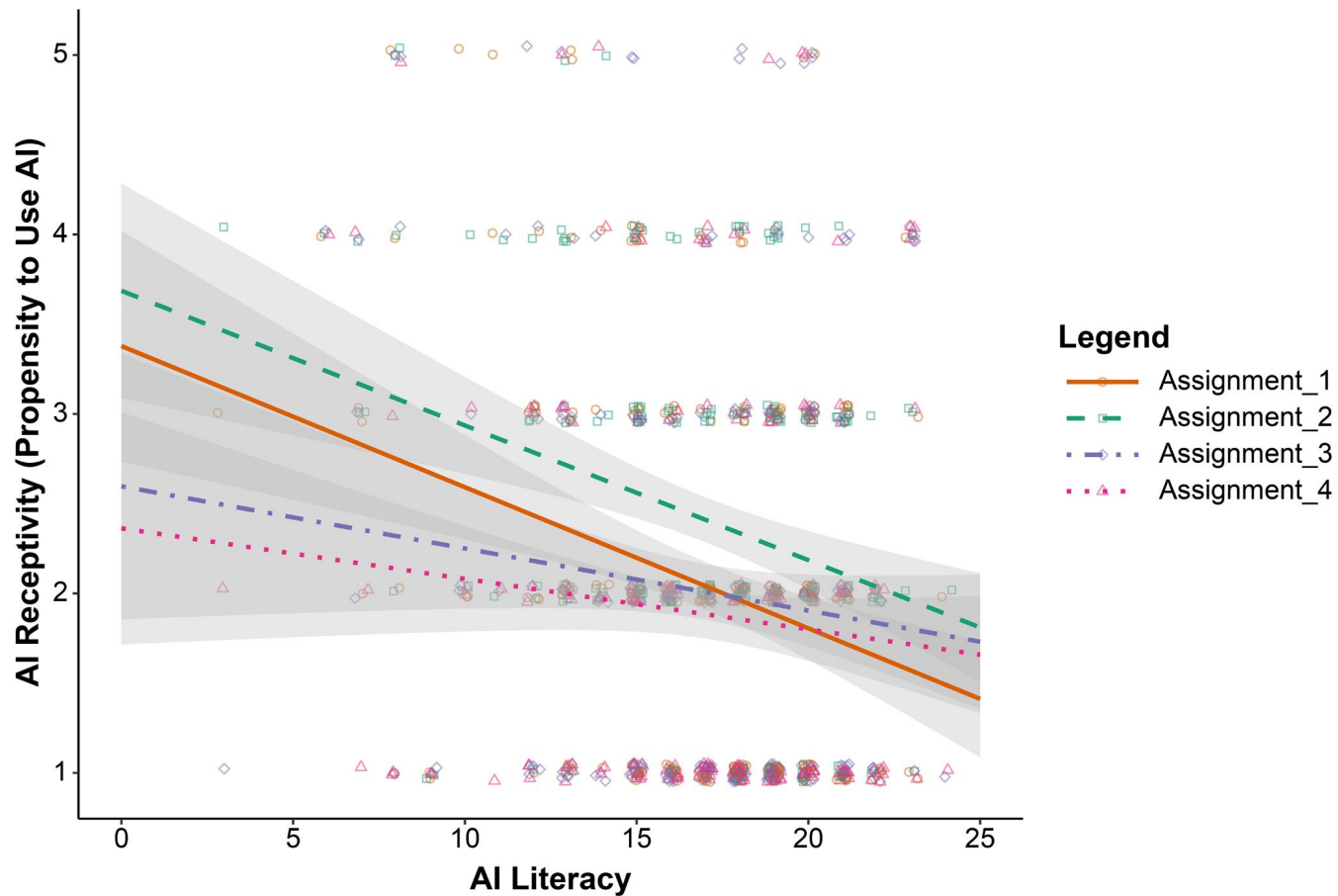


Stephanie M. Tully , Chiara Longoni , and Gil Appel 

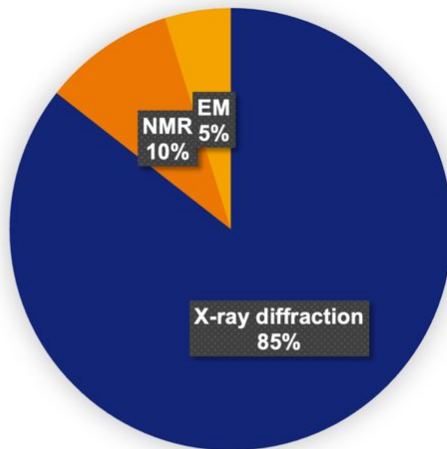
### Abstract

As artificial intelligence (AI) transforms society, understanding factors that influence AI receptivity is increasingly important. The current research investigates which types of consumers have greater AI receptivity. Contrary to expectations revealed in four surveys, cross-country data and six additional studies find that people with lower AI literacy are typically more receptive to AI. This lower literacy–greater receptivity link is not explained by differences in perceptions of AI’s capability, ethicality, or feared impact on humanity. Instead, this link occurs because people with lower AI literacy are more likely to perceive AI as magical and experience feelings of awe in the face of AI’s execution of tasks that seem to require uniquely human attributes. In line with this theorizing, the lower literacy–higher receptivity link is mediated by perceptions of AI as magical and is moderated among tasks not assumed to require distinctly human attributes. These findings suggest that companies may benefit from shifting their marketing efforts and product development toward consumers with lower AI literacy. In addition, efforts to demystify AI may inadvertently reduce its appeal.

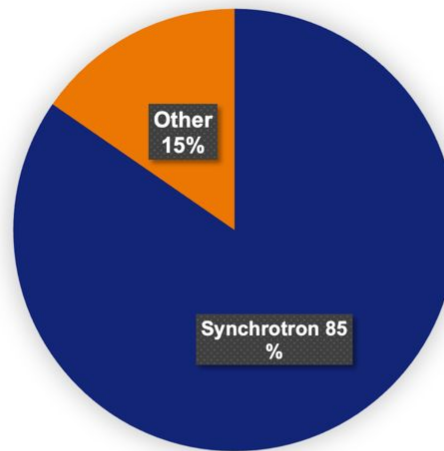
# Acceptancy



Sources of training PDBs, **All**



Sources of training PDBs, **X-ray**



## Fun Facts:

- 8.8 % of training set structures are from the ESRF (10% of X-ray structures)
- 7.8 %(62 million) of all training set atoms are from the ESRF (11% of X-ray atoms)
- 11.2 % (481 million) of all training set (total) reflections are from the ESRF