



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:14 AM UTC

PDB ID : 2NYY / pdb_00002nyy
Title : Crystal structure of botulinum neurotoxin type A complexed with monoclonal antibody CR1
Authors : Stevens, R.C.; Arndt, J.W.
Deposited on : 2006-11-21
Resolution : 2.61 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

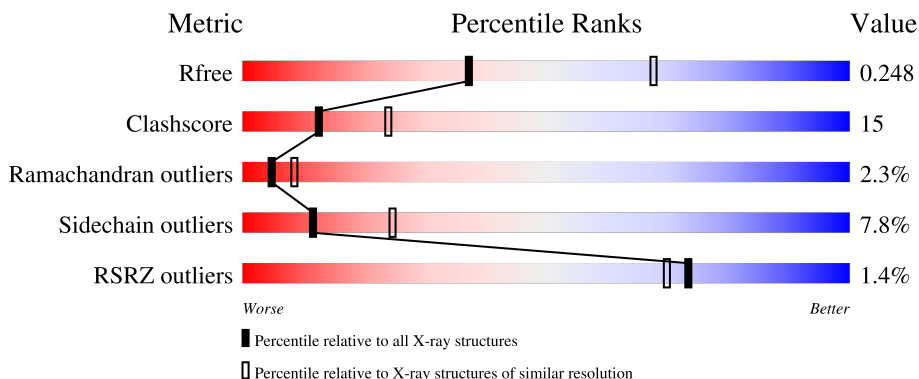
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	1295	% 70% 22% 5% ..
2	C	218	% 70% 24% 5% .
3	D	223	2% 73% 19% 5% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13507 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1267	Total	C	N	O	S	0	0	0
			10211	6549	1691	1940	31			

- Molecule 2 is a protein called CR1 monoclonal antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	216	Total	C	N	O	S	0	0	0
			1657	1039	279	334	5			

- Molecule 3 is a protein called CR1 monoclonal antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	0	0
			1637	1031	270	329	7			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

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.

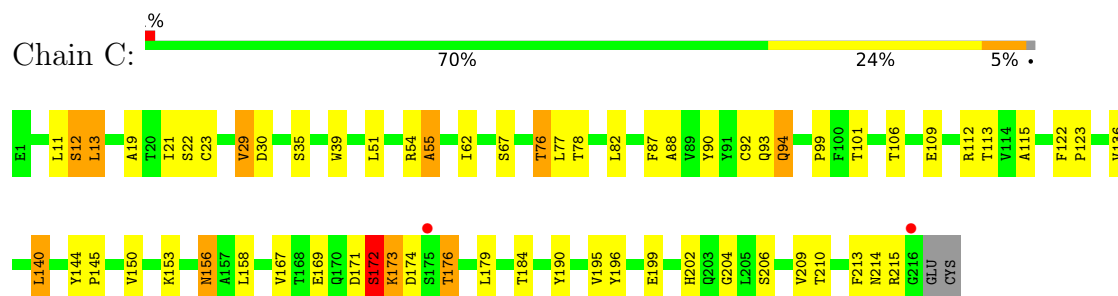
Chain A:

70% 22% 5%

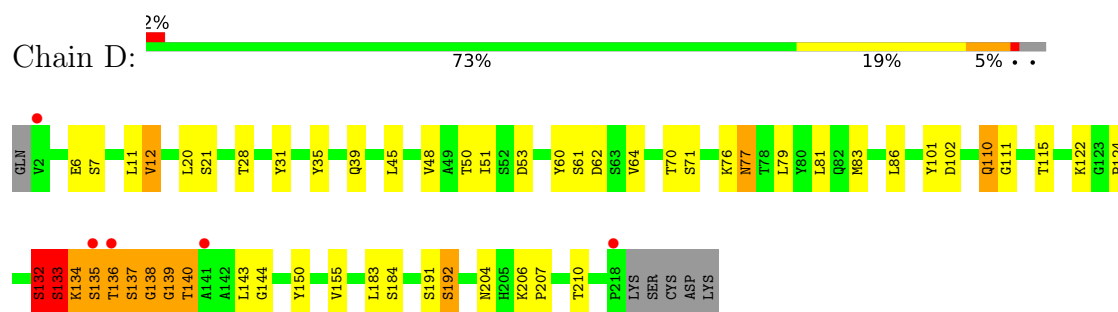
Y1181 Y1184 Y1193 Y1199 Y1206 Y1210 Y1211 Y1212 Y1213 Y1214 Y1226 Y1227 Y1228 Y1229 Y1230 Y1231 Y1232 Y1247 Y1253 Y1254 Y1255 Y1256 Y1257 Y1258 Y1259 Y1260 Y1261 Y1262 Y1265 Y1272 Y1283 Y1284 Y1287 Y1295 LEU

S885 N886 N902 N907 N913 N917 N918 N923 N926 N928 N929 N930 N931 N932 N933 N934 N935 N936 N937 N938 N939 N940 N941 N942 N943 N944 N945 N946 N947 N948 N949 N950 N951 N952 N953 N954 N955 N956 N957 N958 N959 N960 N961 N962 N963 N964 N965 N966 N967 N968 N969 N970 N971 N972 N973 N974 N975 N976 N977 N978 N979 N980 N981 N982 N983 N984 N985 N986 N987 N988 N989 N990 N991 N992 N993 N994 N995 N996 N1006 N1011 N1012 N1013 N1014 N1015 N1016 N1017 N1018 N1019 N1020 N1021 N1022 N1023 N1024 N1025 N1026 N1027 N1028 N1029 N1030 N1031 N1032 N1033 N1034 N1035 N1036 N1037 N1038 N1039 N1040 N1041 N1042 N1043 N1044 N1045 N1046 N1047 N1048 N1049 N1050 N1051 N1052 N1053 N1054 N1055 N1056 N1057 N1058 N1059 N1060 N1061 N1062 N1063 N1064 N1065 N1066 N1067 N1068 N1069 N1070 N1071 N1072 N1073 N1074 N1075 N1076 N1077 N1078 N1079 N1080 N1081 N1082 N1083 N1084 N1085 N1086 N1087 N1088 N1089 N1090 N1091 N1092 N1093 N1094 N1095 N1096 N1097 N1098 N1099 N1100 N1101 N1102 N1103 N1104 N1105 N1106 N1107 N1108 N1109 N1110 N1111 N1112 N1113 N1114 N1115 N1116 N1117 N1118 N1119 N1120 N1121 N1122 N1123 N1124 N1125 N1126 N1127 N1128 N1129 N1130 N1131 N1132 N1133 N1134 N1135 N1136 N1137 N1138 N1139 N1140 N1141 N1142 N1143 N1144 N1145 N1146 N1147 N1148 N1149 N1150 N1151 N1152 N1153 N1154 N1155 N1156 N1157 N1158 N1159 N1160 N1161 N1162 N1163 N1164 N1165 N1166 N1167 N1168 N1169 N1170 N1171 N1172 N1173 N1174 N1175 N1176 N1177 N1178 N1179 N1180 N1181 N1182 N1183 N1184 N1185 N1186 N1187 N1188 N1189 N1190 N1191 N1192 N1193 N1194 N1195 N1196 N1197 N1198 N1199 N1200 N1201 N1202 N1203 N1204 N1205 N1206 N1207 N1208 N1209 N1210 N1211 N1212 N1213 N1214 N1215 N1216 N1217 N1218 N1219 N1220 N1221 N1222 N1223 N1224 N1225 N1226 N1227 N1228 N1229 N1230 N1231 N1232 N1233 N1234 N1235 N1236 N1237 N1238 N1239 N1240 N1241 N1242 N1243 N1244 N1245 N1246 N1247 N1248 N1249 N1250 N1251 N1252 N1253 N1254 N1255 N1256 N1257 N1258 N1259 N1260 N1261 N1262 N1263 N1264 N1265 N1266 N1267 N1268 N1269 N1270 N1271 N1272 N1273 N1274 N1275 N1276 N1277 N1278 N1279 N1280 N1281 N1282 N1283 N1284 N1285 N1286 N1287 N1288 N1289 N1290 N1291 N1292 N1293 N1294 N1295 N1296 N1297 N1298 N1299 N1300 N1301 N1302 N1303 N1304 N1305 N1306 N1307 N1308 N1309 N1310 N1311 N1312 N1313 N1314 N1315 N1316 N1317 N1318 N1319 N1320 N1321 N1322 N1323 N1324 N1325 N1326 N1327 N1328 N1329 N1330 N1331 N1332 N1333 N1334 N1335 N1336 N1337 N1338 N1339 N1340 N1341 N1342 N1343 N1344 N1345 N1346 N1347 N1348 N1349 N1350 N1351 N1352 N1353 N1354 N1355 N1356 N1357 N1358 N1359 N1360 N1361 N1362 N1363 N1364 N1365 N1366 N1367 N1368 N1369 N1370 N1371 N1372 N1373 N1374 N1375 N1376 N1377 N1378 N1379 N1380 N1381 N1382 N1383 N1384 N1385 N1386 N1387 N1388 N1389 N1390 N1391 N1392 N1393 N1394 N1395 N1396 N1397 N1398 N1399 N1400 N1401 N1402 N1403 N1404 N1405 N1406 N1407 N1408 N1409 N1410 N1411 N1412 N1413 N1414 N1415 N1416 N1417 N1418 N1419 N1420 N1421 N1422 N1423 N1424 N1425 N1426 N1427 N1428 N1429 N1430 N1431 N1432 N1433 N1434 N1435 N1436 N1437 N1438 N1439 N1440 N1441 N1442 N1443 N1444 N1445 N1446 N1447 N1448 N1449 N1450 N1451 N1452 N1453 N1454 N1455 N1456 N1457 N1458 N1459 N1460 N1461 N1462 N1463 N1464 N1465 N1466 N1467 N1468 N1469 N1470 N1471 N1472 N1473 N1474 N1475 N1476 N1477 N1478 N1479 N1480 N1481 N1482 N1483 N1484 N1485 N1486 N1487 N1488 N1489 N1490 N1491 N1492 N1493 N1494 N1495 N1496 N1497 N1498 N1499 N1500 N1501 N1502 N1503 N1504 N1505 N1506 N1507 N1508 N1509 N1510 N1511 N1512 N1513 N1514 N1515 N1516 N1517 N1518 N1519 N1520 N1521 N1522 N1523 N1524 N1525 N1526 N1527 N1528 N1529 N1530 N1531 N1532 N1533 N1534 N1535 N1536 N1537 N1538 N1539 N1540 N1541 N1542 N1543 N1544 N1545 N1546 N1547 N1548 N1549 N1550 N1551 N1552 N1553 N1554 N1555 N1556 N1557 N1558 N1559 N1560 N1561 N1562 N1563 N1564 N1565 N1566 N1567 N1568 N1569 N1570 N1571 N1572 N1573 N1574 N1575 N1576 N1577 N1578 N1579 N1580 N1581 N1582 N1583 N1584 N1585 N1586 N1587 N1588 N1589 N1590 N1591 N1592 N1593 N1594 N1595 N1596 N1597 N1598 N1599 N1600 N1601 N1602 N1603 N1604 N1605 N1606 N1607 N1608 N1609 N1610 N1611 N1612 N1613 N1614 N1615 N1616 N1617 N1618 N1619 N1620 N1621 N1622 N1623 N1624 N1625 N1626 N1627 N1628 N1629 N1630 N1631 N1632 N1633 N1634 N1635 N1636 N1637 N1638 N1639 N1640 N1641 N1642 N1643 N1644 N1645 N1646 N1647 N1648 N1649 N1650 N1651 N1652 N1653 N1654 N1655 N1656 N1657 N1658 N1659 N1660 N1661 N1662 N1663 N1664 N1665 N1666 N1667 N1668 N1669 N1670 N1671 N1672 N1673 N1674 N1675 N1676 N1677 N1678 N1679 N1680 N1681 N1682 N1683 N1684 N1685 N1686 N1687 N16

- Molecule 2: CR1 monoclonal antibody



- Molecule 3: CR1 monoclonal antibody



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.05Å 148.25Å 196.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 50.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.61) 89.5 (50.00-2.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.246 0.211 , 0.248	Depositor DCC
R_{free} test set	3912 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13507	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: CA, ZN

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	0.79	0/10428	0.90	8/14115 (0.1%)
2	C	0.68	0/1695	0.86	0/2303
3	D	0.63	0/1678	0.82	2/2287 (0.1%)
All	All	0.76	0/13801	0.88	10/18705 (0.1%)

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	46
2	C	0	2
3	D	0	5
All	All	0	53

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	GLY	CA-C-N	7.06	126.58	119.24
1	A	638	GLY	C-N-CA	7.06	126.58	119.24
1	A	870	ILE	CB-CA-C	-6.59	103.25	112.14
1	A	154	ILE	CB-CA-C	-6.49	101.55	110.90
1	A	603	PHE	N-CA-C	-5.62	105.07	111.14

There are no chirality outliers.

5 of 53 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Peptide
1	A	118	TRP	Peptide
1	A	532	PRO	Peptide
1	A	534	ILE	Peptide
1	A	6	LYS	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	10211	0	10013	313	0
2	C	1657	0	1595	38	0
3	D	1637	0	1562	58	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
All	All	13507	0	13170	409	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 15.

The worst 5 of 409 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:578:ASN:HB3	1:A:579:PRO:C	1.38	1.48
1:A:1228:ASP:HB3	1:A:1229:GLN:CB	1.51	1.38
1:A:578:ASN:HB3	1:A:579:PRO:CA	1.48	1.33
3:D:139:GLY:N	3:D:140:THR:HB	1.40	1.32
1:A:604:LEU:N	1:A:605:GLY:HA3	1.55	1.15

There are no symmetry-related clashes.

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	1259/1295 (97%)	1112 (88%)	117 (9%)	30 (2%)	4	8
2	C	214/218 (98%)	198 (92%)	13 (6%)	3 (1%)	9	17
3	D	215/223 (96%)	193 (90%)	17 (8%)	5 (2%)	5	8
All	All	1688/1736 (97%)	1503 (89%)	147 (9%)	38 (2%)	5	8

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	560	GLU
1	A	566	ILE
1	A	576	LEU
1	A	578	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1126/1178 (96%)	1038 (92%)	88 (8%)	11	25
2	C	186/190 (98%)	169 (91%)	17 (9%)	9	18
3	D	181/189 (96%)	169 (93%)	12 (7%)	15	32
All	All	1493/1557 (96%)	1376 (92%)	117 (8%)	11	25

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	814	SER
3	D	71	SER
1	A	1026	ASN
3	D	62	ASP
2	C	176	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	202	HIS
3	D	5	GLN
3	D	176	GLN
1	A	722	ASN
1	A	609	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1267/1295 (97%)	-0.24	17 (1%) 75 71	2, 10, 33, 45	0
2	C	216/218 (99%)	-0.08	2 (0%) 81 78	2, 14, 31, 38	0
3	D	217/223 (97%)	-0.32	5 (2%) 61 56	2, 17, 29, 30	0
All	All	1700/1736 (97%)	-0.23	24 (1%) 73 70	2, 11, 32, 45	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	ALA	5.7
1	A	644	GLY	4.9
2	C	216	GLY	4.2
3	D	218	PRO	3.8
1	A	1260	LYS	2.8

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	1297	1/1	0.72	0.09	63,63,63,63	0
4	ZN	A	1	1/1	1.00	0.15	3,3,3,3	0

6.5 Other polymers [i](#)

There are no such residues in this entry.