wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 03:53 PM EDT

PDB ID	:	3PVM
Title	:	Structure of Complement C5 in Complex with CVF
Authors	:	Laursen, N.S.; Andersen, K.R.; Braren, I.; Sottrup-Jensen, L.; Spillner, E.; Andersen, G.R.
Deposited on	:	2010-12-07
Resolution	:	4.30 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 (i) 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 (i)) were used in the production of this report:

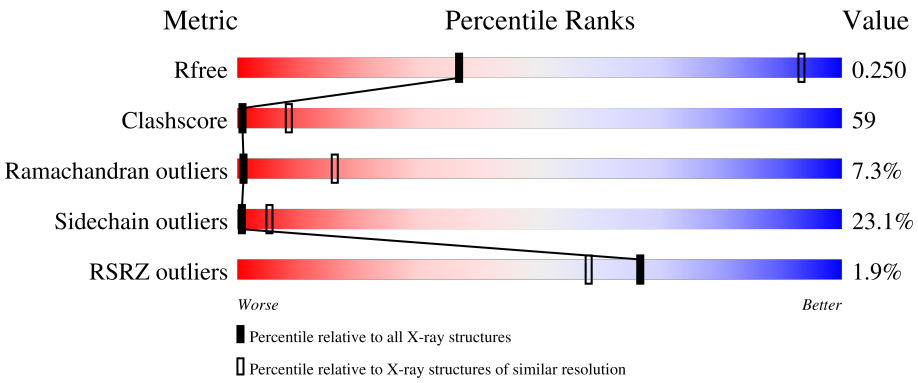
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.30 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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 <=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	1676	2% 24% 52% 20% • •
1	C	1676	2% 24% 52% 20% • •
2	B	1642	2% 23% 38% 13% • 25%
2	D	1642	% 23% 38% 13% • 25%

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	NAG	B	2002	-	-	-	X
3	NAG	D	2002	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 45268 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.

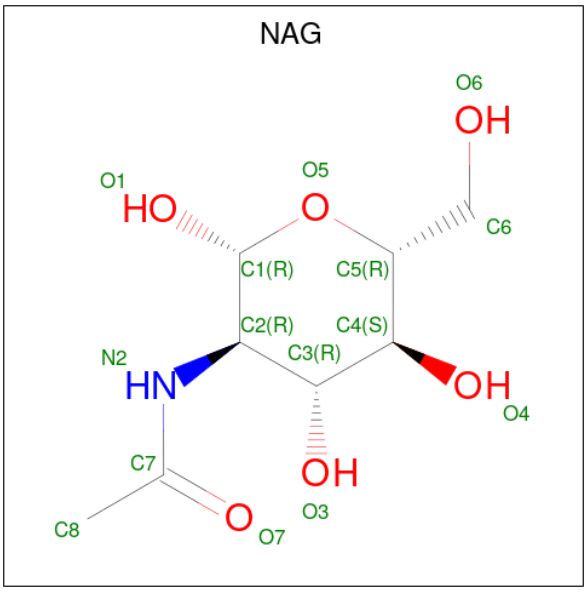
- Molecule 1 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1627	12881	8246	2114	2469	52	0	0	0
1	C	1627	12881	8246	2114	2469	52	0	0	0

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1225	9711	6187	1633	1851	40	0	0	0
2	D	1225	9711	6187	1633	1851	40	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



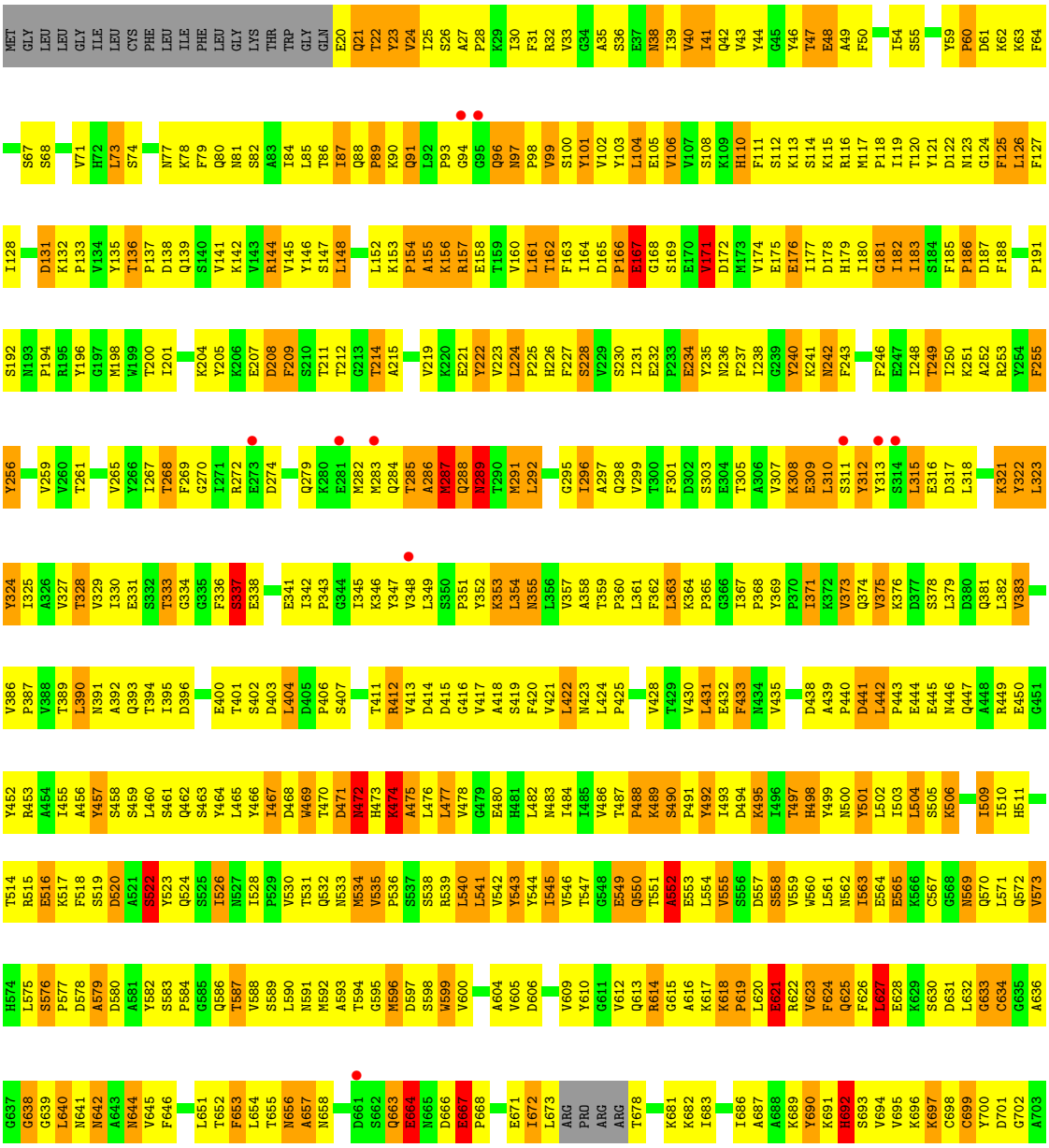
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0

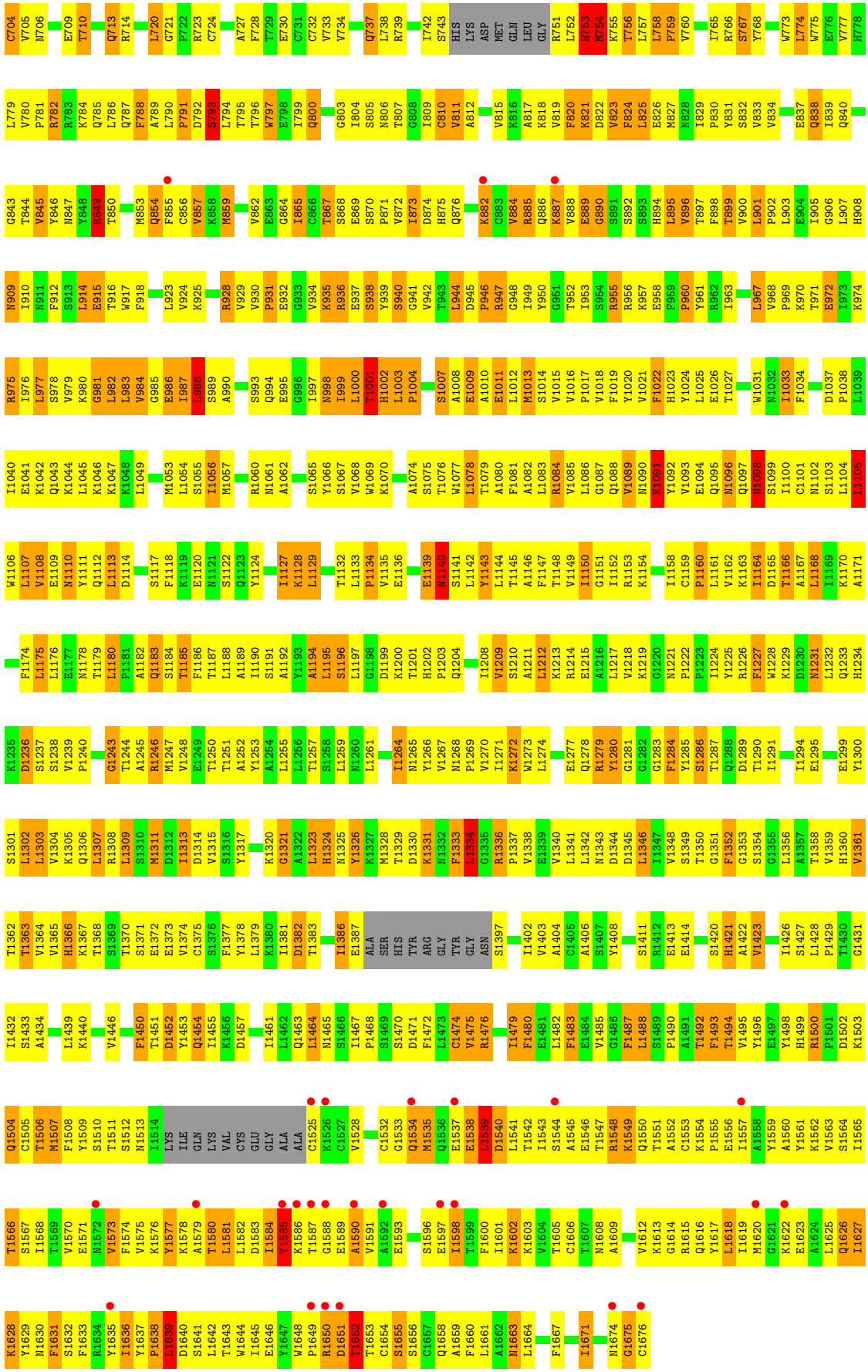
3 Residue-property plots (i)

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: Complement C5

Chain A: 2% 24% 52% 20%

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L779 V780 P781 R782 R783 K784 Q785 L786 Q787 F788 A789 L790 P791 D792 S793 L794 T795 T796 W797 E798 I799 Q800 G803 I804 S805 N806 T807 G808 I809 C810 V811 A812 V815 K816 A817 K818 V819 F820 K821 D822 V823 F824 L825 E826 M827 N828 I829 P830 Y831 S832 V833 V834 E837 Q838 I839 Q840
G843 T844 V845 Y846 N847 Y848 R849 T850 M853 Q854 F855 C856 V857 K858 M859 V862 E863 G864 I865 C866 T867 S868 E869 S870 P871 V872 I873 D874 H875 Q876 K882 C883 V884 R885 Q886 K887 V888 E889 G890 S891 S892 S893 H894 L895 V896 T897 F898 T899 V900 L901 P902 L903 E904 I905 G906 L907 H908
N909 I910 N911 F912 S913 L914 E915 T916 W917 F918 L923 V924 K925 R928 V929 V930 P931 E932 G933 V934 K935 R936 E937 S938 Y939 S940 G941 V942 T943 L944 D945 P946 R947 G948 I949 Y950 G951 T952 I953 S954 R955 R956 K957 E958 P959 P960 Y961 R962 I963 L967 V968 P969 K970 T971 E972 I973 K974
R975 I976 L977 S978 V979 K980 G981 L982 L983 V984 G985 E986 I987 L988 S989 A990 S993 Q994 E995 G996 I997 N998 I999 L1000 T1001 H1002 L1003 P1004 S1007 A1008 E1009 A1010 E1011 L1012 M1013 S1014 V1015 V1016 P1017 V1018 F1019 Y1020 V1021 F1022 H1023 Y1024 L1025 E1026 T1027 W1031 N1032 T1033 F1034 D1037 P1038 L1039
I1040 E1041 K1042 Q1043 K1044 L1045 K1046 K1047 K1048 L1049 M1053 L1054 S1055 I1056 M1057 R1060 N1061 A1062 S1065 Y1066 S1067 V1068 W1069 K1070 A1074 S1075 T1076 W1077 L1078 T1079 A1080 F1081 A1082 L1083 R1084 V1085 L1086 G1087 Q1088 V1089 N1090 K1091 Y1092 V1093 E1094 Q1095 N1096 Q1097 N1098 S1099 I1100 C1101 N1102 S1103 L1104 L1105
W1106 L1107 V1108 E1109 N1110 Y1111 Q1112 L1113 D1114 S1117 F1118 K1119 E1120 N1121 S1122 Q1123 Y1124 I1127 K1128 L1129 T1132 L1133 P1134 V1135 E1136 E1139 N1140 S1141 L1142 Y1143 L1144 T1145 A1146 F1147 T1148 V1149 I1150 G1151 I1152 R1153 K1154 I1158 C1159 P1160 L1161 V1162 K1163 I1164 D1165 T1166 A1167 L1168 T1169 K1170 A1171
F1174 L1175 L1176 E1177 N1178 T1179 L1180 P1181 A1182 Q1183 S1184 T1185 F1186 T1187 L1188 A1189 I1190 S1191 A1192 Y1193 A1194 L1195 S1196 L1197 G1198 D1199 K1200 T1201 H1202 P1203 Q1204 I1208 V1209 S1210 A1211 L1212 K1213 R1214 E1215 A1216 L1217 V1218 K1219 G1220 N1221 P1222 P1223 I1224 Y1225 R1226 F1227 W1228 K1229 D1230 N1231 L1232 Q1233 H1234
K1235 D1236 S1237 S1238 V1239 P1240 G1243 T1244 A1245 R1246 M1247 V1248 E1249 T1250 T1251 A1252 Y1253 A1254 L1255 L1256 T1257 S1258 L1259 N1260 L1261 I1264 N1265 Y1266 V1267 N1268 P1269 V1270 I1271 K1272 W1273 L1274 E1277 Q1278 R1279 Y1280 G1281 G1282 G1283 F1284 Y1285 S1286 T1287 Q1288 D1289 T1290 I1291 I1294 E1295 E1299 Y1300
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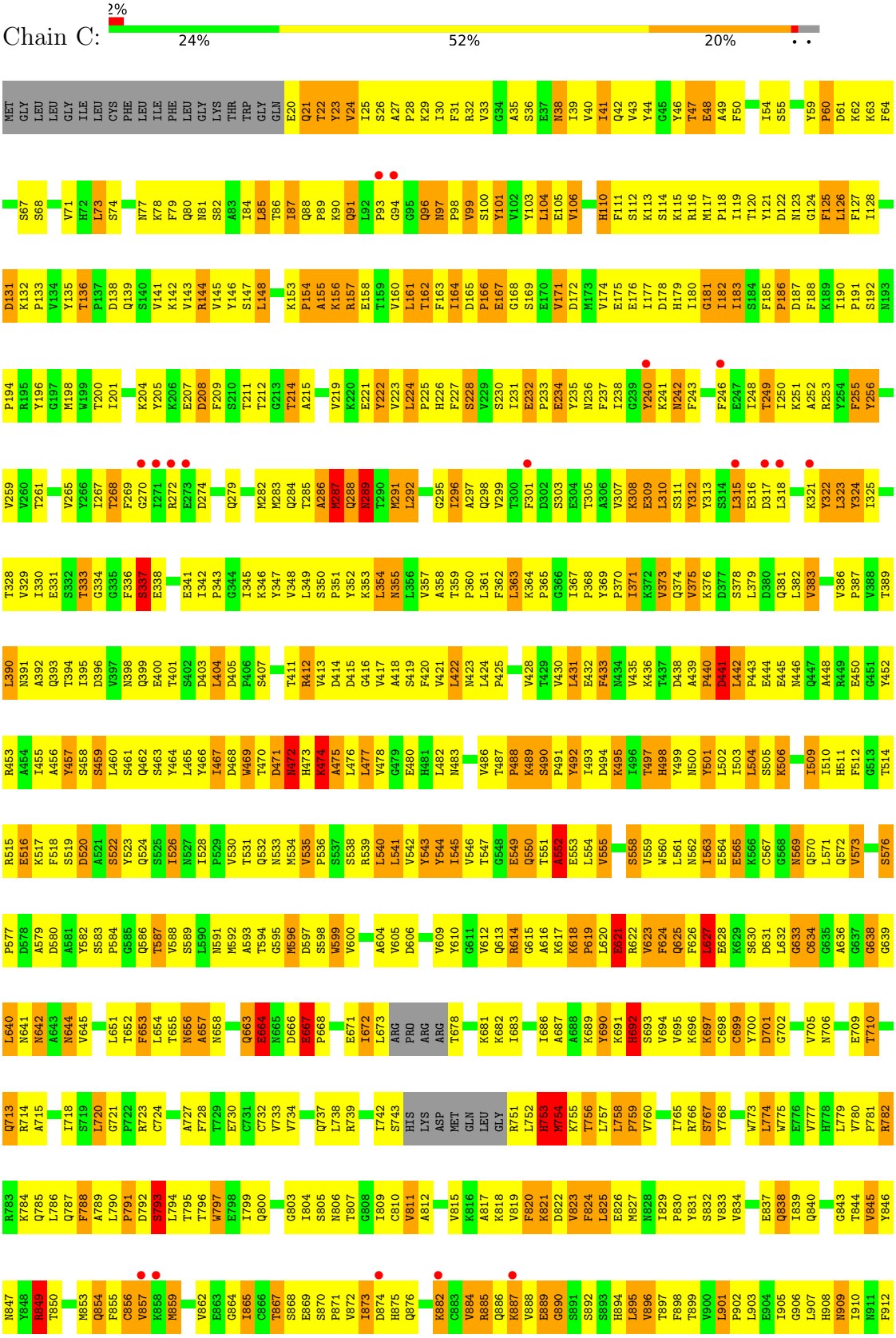
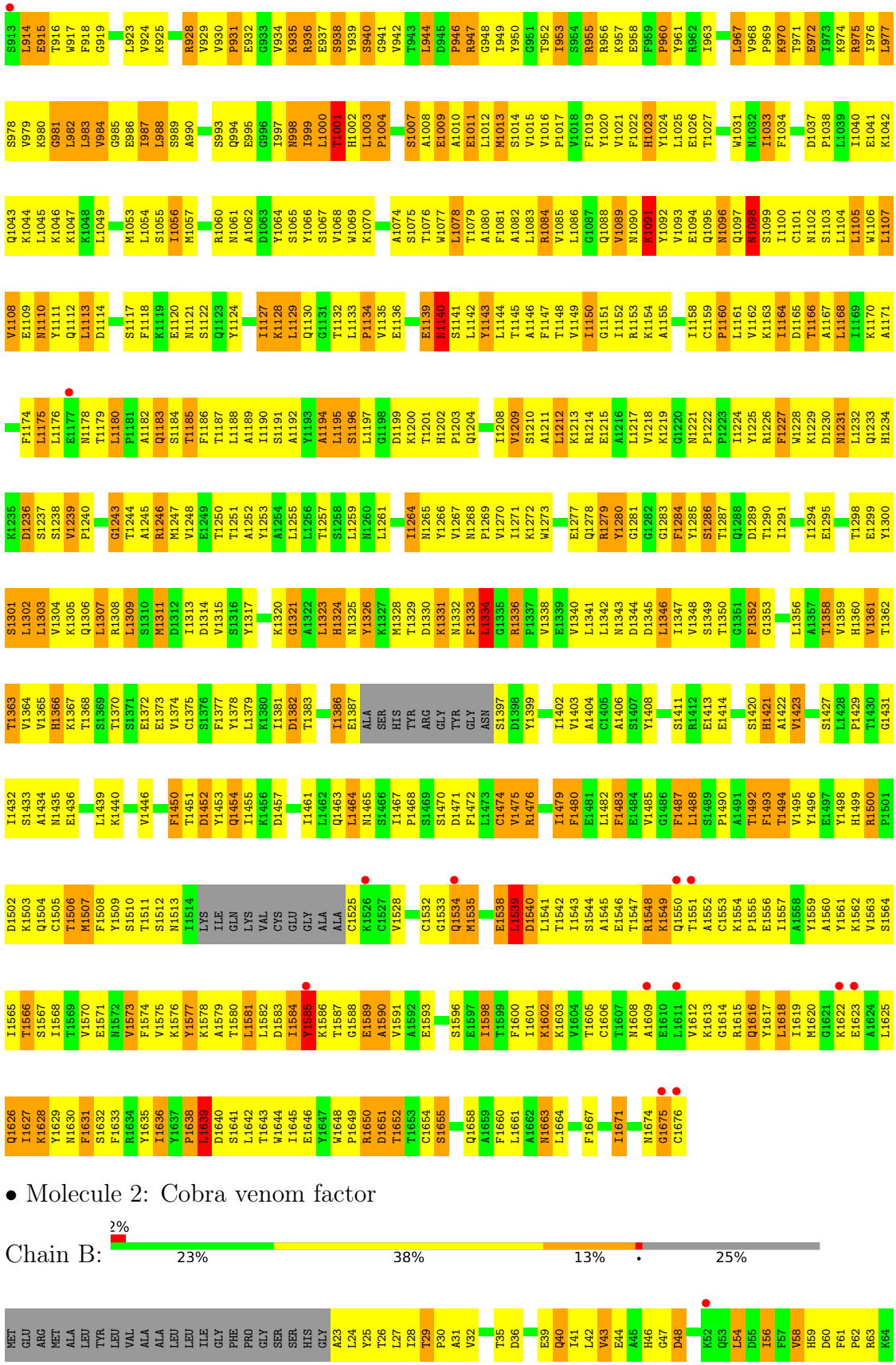
T1362 T1363 V1364 V1365 H1366 K1367 T1368 S1369 T1370 S1371 E1372 E1373 V1374 C1375 S1376 F1377 Y1378 L1379 K1380 I1381 D1382 T1383 I1386 E1387 ALA SER HIS TYR ARG GLY TYR GLY ASN S1397 I1402 V1403 A1404 C1405 A1406 S1407 Y1408 S1411 H1412 E1413 E1414 S1420 H1421 A1422 V1423 I1426 S1427 L1428 P1429 T1430 G1431
I1432 S1433 A1434 L1439 K1440 V1446 F1450 T1451 D1452 Y1453 Q1454 I1455 K1456 D1457 I1461 L1462 Q1463 L1464 N1465 S1466 I1467 P1468 S1469 S1470 D1471 F1472 L1473 C1474 V1475 R1476 I1479 F1480 E1481 L1482 F1483 E1484 E1486 V1485 G1486 F1487 L1488 S1489 P1490 A1491 T1492 F1493 T1494 V1495 Y1496 E1497 Y1498 H1499 R1500 P1501 D1502 K1503
Q1504 C1505 T1506 M1507 F1508 Y1509 S1510 T1511 S1512 N1513 I1514 LYS ILE GLN LYS VAL CYS GLU GLY ALA ALA C1525 K1526 C1527 V1528 C1532 G1533 Q1534 M1535 Q1536 E1537 E1538 L1539 D1540 L1541 T1542 I1543 S1544 A1545 E1546 T1547 R1548 K1549 Q1550 T1551 A1552 C1553 K1554 P1555 E1556 I1557 A1558 Y1559 A1560 Y1561 K1562 V1563 S1564 I1565
T1566 S1567 I1568 T1569 V1570 E1571 N1572 V1573 F1574 V1575 K1576 Y1577 K1578 A1579 T1580 L1581 L1582 D1583 Y1584 Y1585 K1586 T1587 G1588 E1589 A1590 V1591 A1592 E1593 S1596 E1597 I1598 T1599 F1600 I1601 K1602 K1603 V1604 T1605 C1606 T1607 N1608 A1609 V1612 K1613 G1614 R1615 Q1616 Y1617 L1618 I1619 M1620 G1621 K1622 E1623 A1624 L1625 Q1626 I1627
K1628 Y1629 N1630 F1631 S1632 F1633 R1634 Y1635 I1636 Y1637 P1638 L1639 D1640 S1641 L1642 T1643 W1644 I1645 E1646 Y1647 W1648 P1649 R1650 D1651 T1652 T1653 C1654 S1655 S1656 C1657 Q1658 A1659 F1660 L1661 A1662 N1663 L1664 F1667 I1671 N1674 G1675 C1676

- Molecule 1: Complement C5

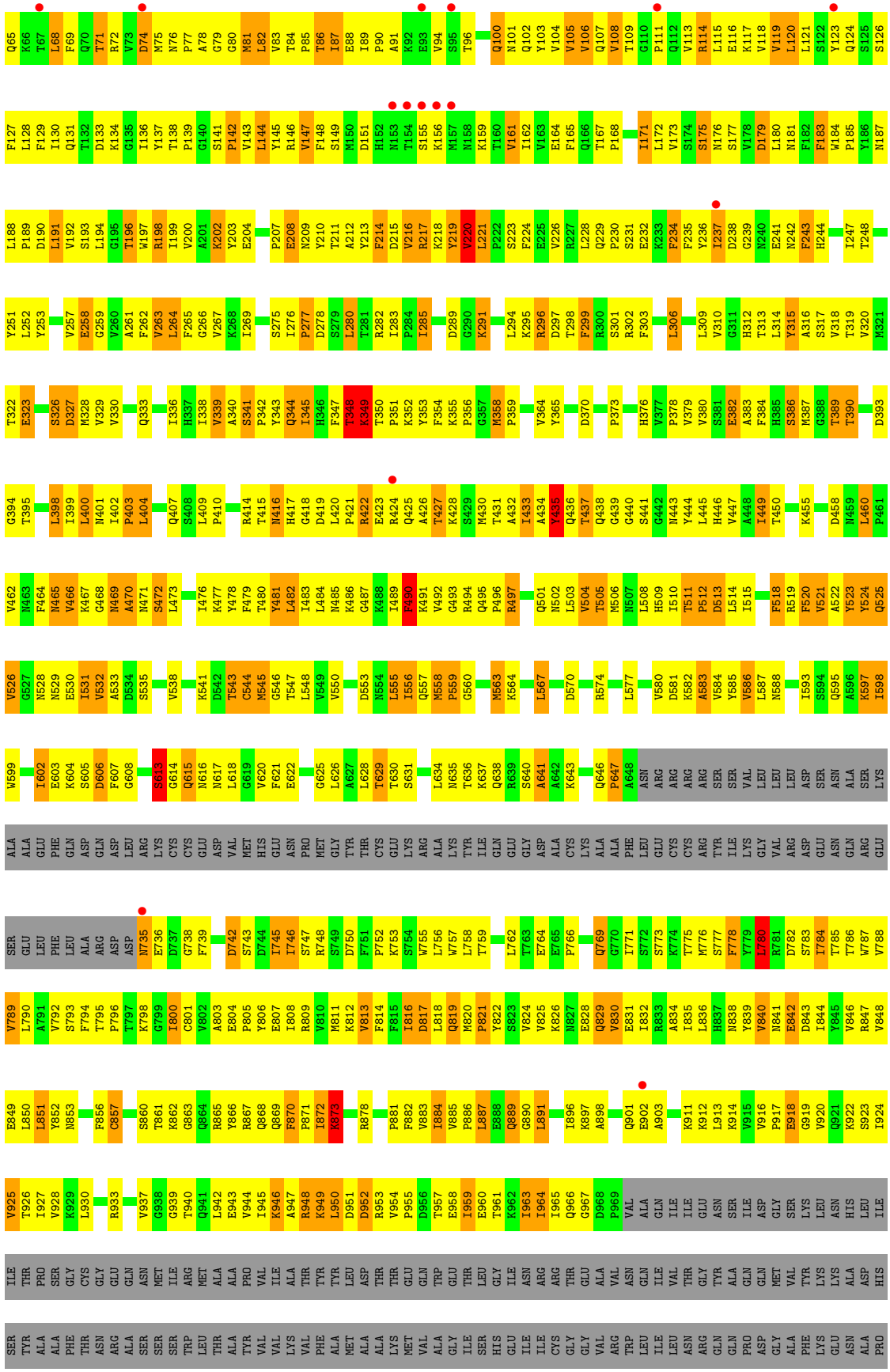
Chain C:

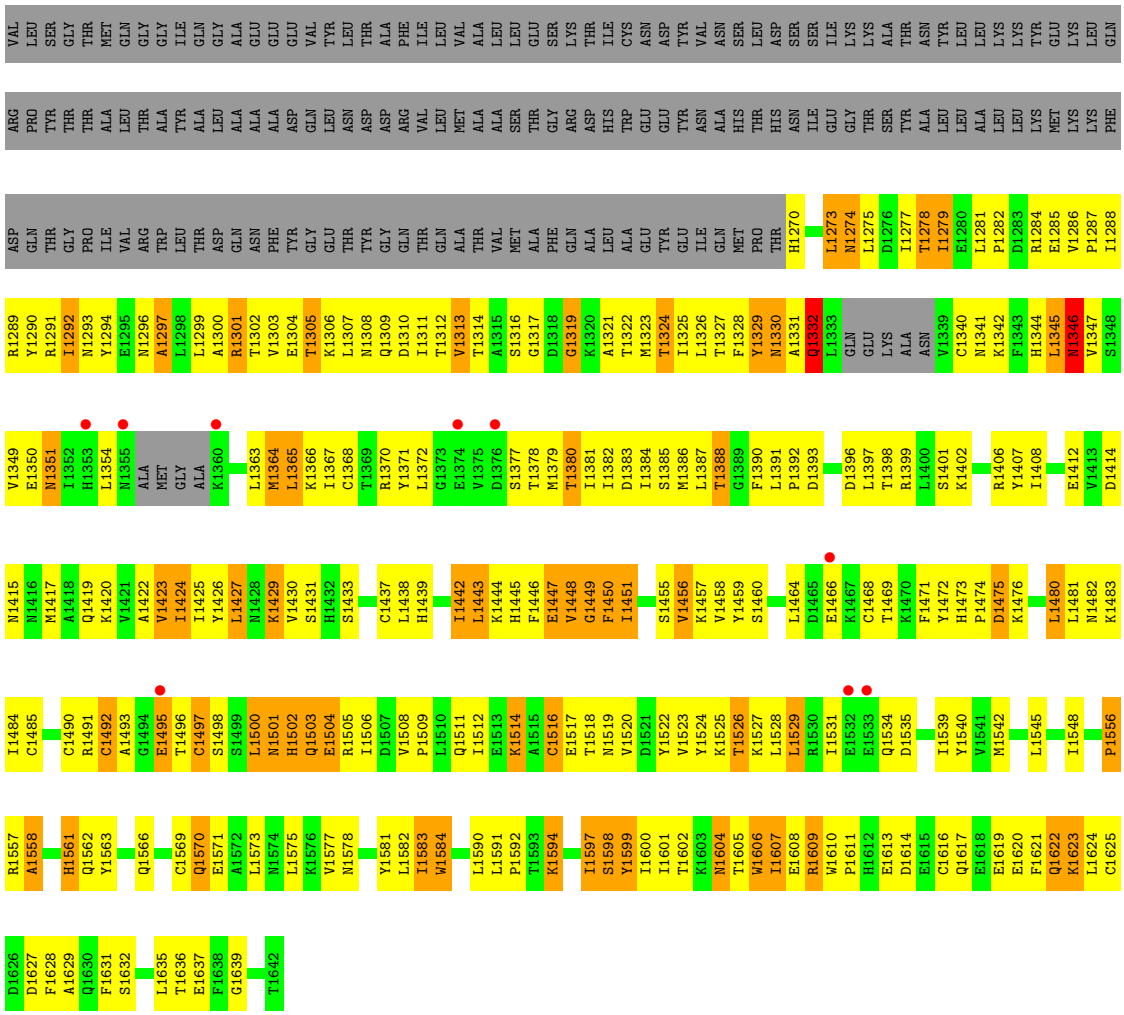




• Molecule 2: Cobra venom factor

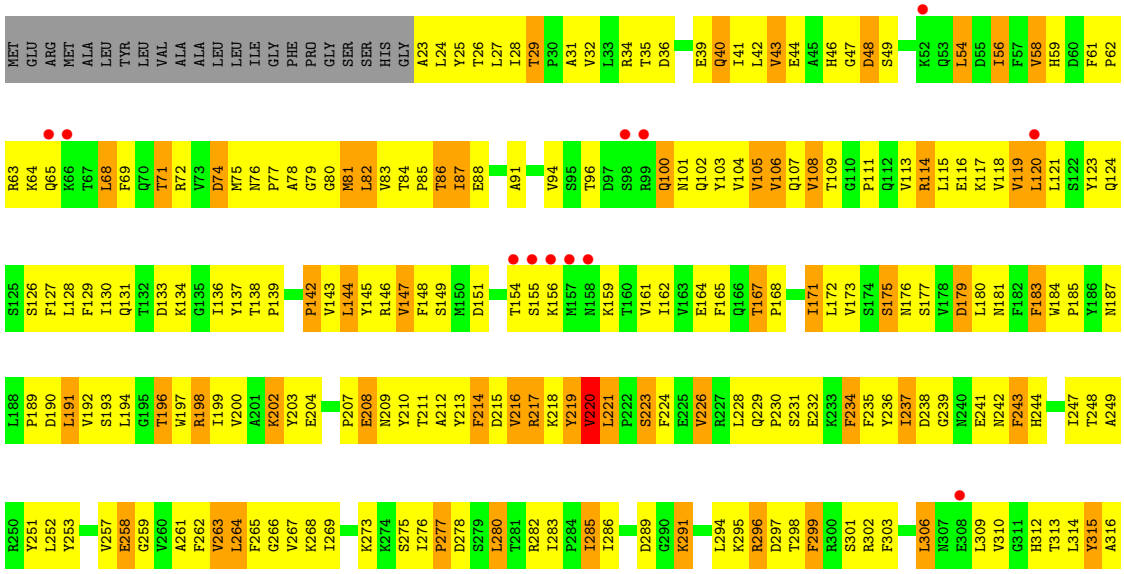
Chain B:

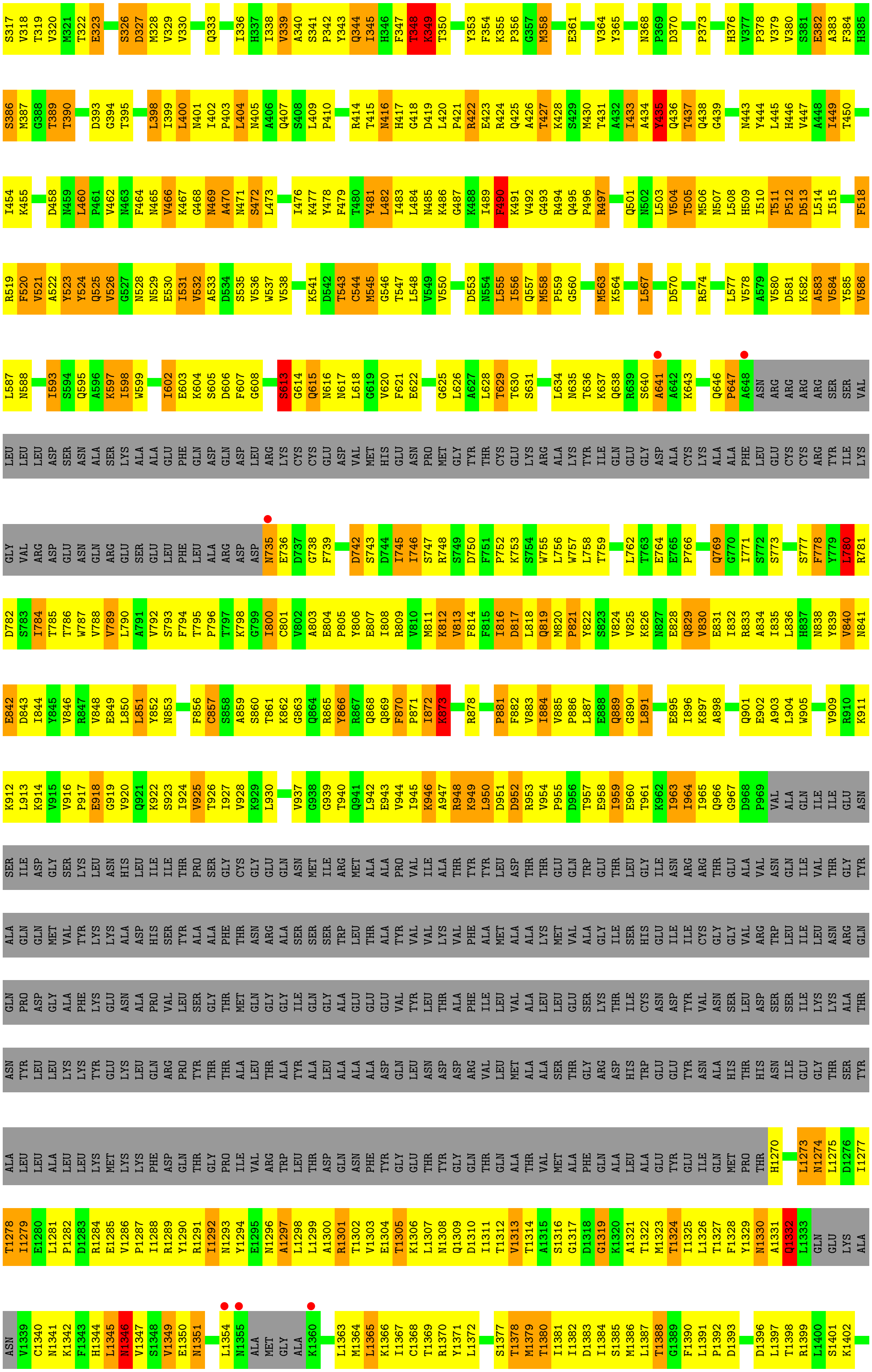




- Molecule 2: Cobra venom factor

Chain D:

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S386 M387 G388 T389 T390 D393 G394 T395 L398 I399 L400 N401 I402 P403 L404 N405 A406 Q407 S408 L409 P410 R414 T415 N416 H417 G418 D419 L420 P421 R422 E423 R424 Q425 A426 T427 K428 S429 M430 T431 A432 I433 A434 Y435 Q436 T437 Q438 G439 N443 Y444 L445 H446 V447 A448 I449 T450
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GLY VAL ARG ASP GLU ASN GLN ARG GLU SER GLU LEU PHE LEU ALA ARG ASP N735 E736 D737 G738 F739 D742 S743 D744 I745 I746 S747 R748 S749 D750 F751 P752 K753 S754 W755 L756 W757 L758 T759 L762 T763 E764 E765 P766 Q769 G770 I771 S772 S773 S777 F778 Y779 L780 R781
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ALA GLN GLN MET VAL TYR LYS LYS ALA ASP HIS SER TYR ALA ALA PHE THR ASN ARG ALA SER SER TRP LEU THR ALA TYR VAL VAL LYS VAL PHE ALA MET ALA ALA LYS MET VAL ALA GLY ILE SER HIS GLU ILE ILE CYS GLY GLY VAL ARG TRP LEU ILE LEU ASN ARG GLN
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ASN TYR LEU LEU LYS LYS TYR GLU LYS LEU GLN ARG PRO TYR THR THR ALA LEU THR ALA TYR ALA LEU ALA ALA ALA ASP GLN LEU ASN ASP ASP ARG VAL LEU MET ALA ALA SER THR GLY ARG ASP HIS TRP GLU GLU TYR ASN ALA HIS THR HIS ASN ILE GLU GLY THR SER TYR
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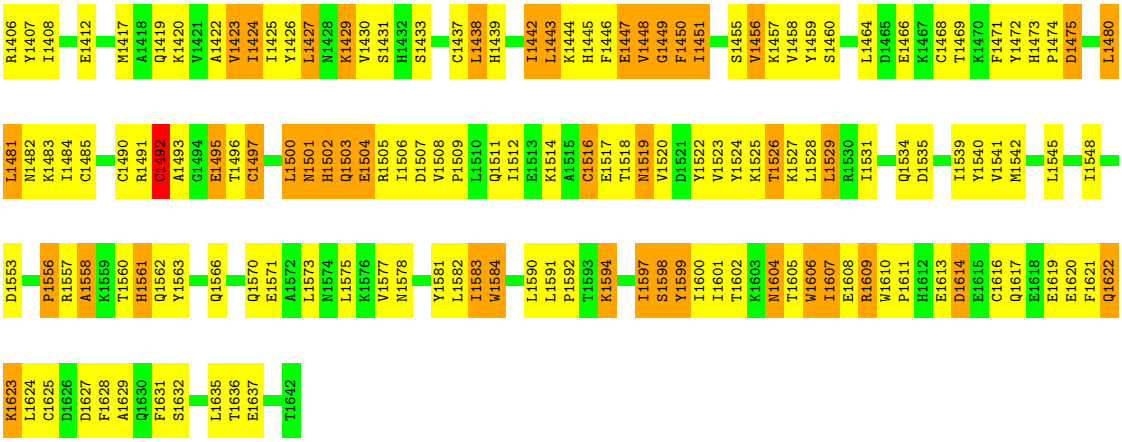
ASN V1339 C1340 N1341 K1342 F1343 H1344 L1345 N1346 V1347 S1348 V1349 E1350 N1351 L1354 N1355 ALA MET GLY ALA K1360 L1363 M1364 L1365 K1366 I1367 C1368 T1369 R1370 Y1371 L1372 S1377 T1378 M1379 T1380 I1381 I1382 D1383 I1384 S1385 M1386 L1387 T1388 G1389 F1390 L1391 P1392 D1393 D1396 L1397 T1398 R1399 L1400 S1401 K1402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T1526
K1527
L1528
L1529
R1530
I1531
Q1534
D1535
I1539
Y1540
V1541
M1542
L1545
I1548
D1553
P1556
R1557
A1558
K1559
T1560
H1561
Q1562
Y1563
Q1566
Q1570
E1571
A1572
L1573
H1574
L1575
K1576
V1577
N1578
Y1581
L1582
I1583
W1584
L1590
L1591
P1592
T1593
K1594
I1597
S1598
Y1599
I1600
I1601
T1602
K1603
N1604
T1605
W1606
I1607
E1608
R1609
W1610
P1611
H1612
E1613
D1614
E1615
C1616
Q1617
E1618
E1619
E1620
F1621
Q1622
K1623
L1624
C1625
D1626
D1627
F1628
A1629
Q1630
F1631
S1632
L1635
T1636
E1637
T1642

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	176.52Å 179.20Å 389.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 4.30 49.47 – 4.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.47-4.30) 94.3 (49.47-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.233 , 0.262 0.225 , 0.250	Depositor DCC
R_{free} test set	1734 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å^2)	135.2	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 172.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	45268	wwPDB-VP
Average B, all atoms (Å^2)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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

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	0.57	1/13158 (0.0%)	0.77	6/17851 (0.0%)
1	C	0.58	0/13158	0.76	5/17851 (0.0%)
2	B	0.55	0/9912	0.74	1/13454 (0.0%)
2	D	0.55	0/9912	0.74	2/13454 (0.0%)
All	All	0.57	1/46140 (0.0%)	0.75	14/62610 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
2	B	0	1
2	D	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	CYS	CB-SG	-5.27	1.73	1.81

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1539	LEU	CA-CB-CG	6.88	131.12	115.30
1	A	1539	LEU	CA-CB-CG	6.87	131.10	115.30
1	A	1195	LEU	CA-CB-CG	-6.42	100.53	115.30
1	C	1195	LEU	CA-CB-CG	-6.27	100.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1346	ASN	CA-CB-CG	5.54	125.58	113.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472	ASN	Peptide
1	A	552	ALA	Peptide
1	A	667	GLU	Peptide
2	B	1351	ASN	Peptide
1	C	472	ASN	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	12881	0	12821	1676	0
1	C	12881	0	12821	1666	0
2	B	9711	0	9702	1046	0
2	D	9711	0	9702	1061	0
3	A	14	0	13	2	0
3	B	28	0	26	1	0
3	C	14	0	13	2	0
3	D	28	0	26	1	0
All	All	45268	0	45124	5374	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 59.

The worst 5 of 5374 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:B:380:VAL:HG12	2:B:387:MET:HB3	1.24	1.15
2:D:380:VAL:HG12	2:D:387:MET:HB3	1.26	1.15
2:D:1609:ARG:HG2	2:D:1609:ARG:HH11	1.12	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:VAL:H	1:A:411:THR:HG22	1.02	1.12
1:C:386:VAL:H	1:C:411:THR:HG22	1.00	1.11

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	1617/1676 (96%)	1173 (72%)	292 (18%)	152 (9%)	0	12
1	C	1617/1676 (96%)	1179 (73%)	288 (18%)	150 (9%)	0	12
2	B	1215/1642 (74%)	998 (82%)	161 (13%)	56 (5%)	2	24
2	D	1215/1642 (74%)	995 (82%)	162 (13%)	58 (5%)	2	23
All	All	5664/6636 (85%)	4345 (77%)	903 (16%)	416 (7%)	1	16

5 of 416 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	60	PRO
1	A	89	PRO
1	A	96	GLN
1	A	97	ASN

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	1446/1484 (97%)	1108 (77%)	338 (23%)	1 5
1	C	1446/1484 (97%)	1109 (77%)	337 (23%)	1 5
2	B	1093/1435 (76%)	845 (77%)	248 (23%)	1 6
2	D	1093/1435 (76%)	845 (77%)	248 (23%)	1 6
All	All	5078/5838 (87%)	3907 (77%)	1171 (23%)	1 5

5 of 1171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	54	LEU
2	D	1497	CYS
2	D	191	LEU
2	D	43	VAL
2	D	588	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	344	GLN
2	D	528	ASN
2	D	1330	ASN
2	B	469	ASN
2	B	417	HIS

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)

6 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	NAG	B	2002	2	14,14,15	0.92	0	17,19,21	1.16	1 (5%)
3	NAG	B	2001	2	14,14,15	0.81	1 (7%)	17,19,21	2.07	3 (17%)
3	NAG	C	2003	1	14,14,15	0.58	0	17,19,21	2.21	4 (23%)
3	NAG	A	2003	1	14,14,15	0.60	0	17,19,21	2.19	4 (23%)
3	NAG	D	2002	2	14,14,15	0.92	0	17,19,21	1.16	1 (5%)
3	NAG	D	2001	2	14,14,15	0.74	0	17,19,21	2.16	4 (23%)

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	NAG	B	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	B	2001	2	-	2/6/23/26	0/1/1/1
3	NAG	C	2003	1	-	3/6/23/26	0/1/1/1
3	NAG	A	2003	1	-	3/6/23/26	0/1/1/1
3	NAG	D	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	D	2001	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	NAG	C1-C2	2.16	1.55	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2001	NAG	C1-O5-C5	6.57	121.10	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2001	NAG	C1-O5-C5	6.17	120.56	112.19
3	A	2003	NAG	C1-O5-C5	5.70	119.91	112.19
3	C	2003	NAG	C1-O5-C5	5.67	119.87	112.19
3	C	2003	NAG	C4-C3-C2	4.36	117.41	111.02

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2003	NAG	C3-C2-N2-C7
3	A	2003	NAG	C8-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
3	B	2001	NAG	C8-C7-N2-C2
3	B	2001	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	NAG	1	0
3	C	2003	NAG	2	0
3	A	2003	NAG	2	0
3	D	2001	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1627/1676 (97%)	0.03	37 (2%)	60	51	90, 187, 312, 465	0
1	C	1627/1676 (97%)	0.01	31 (1%)	66	58	97, 186, 299, 486	0
2	B	1225/1642 (74%)	-0.01	25 (2%)	65	56	107, 174, 261, 395	0
2	D	1225/1642 (74%)	-0.01	18 (1%)	73	64	114, 181, 263, 371	0
All	All	5704/6636 (85%)	0.01	111 (1%)	66	58	90, 183, 291, 486	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1355	ASN	5.3
1	A	1650	ARG	5.2
1	A	1622	LYS	4.9
2	B	155	SER	4.8
1	C	1676	CYS	4.8

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)

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(Å^2)	Q<0.9
3	NAG	B	2002	14/15	0.45	0.44	321,327,336,339	0
3	NAG	A	2003	14/15	0.64	0.38	284,286,289,289	0
3	NAG	C	2003	14/15	0.72	0.34	260,272,284,287	0
3	NAG	D	2002	14/15	0.74	0.47	289,293,305,308	0
3	NAG	B	2001	14/15	0.78	0.26	275,285,305,313	0
3	NAG	D	2001	14/15	0.80	0.31	285,296,309,310	0

6.5 Other polymers (i)

There are no such residues in this entry.