



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

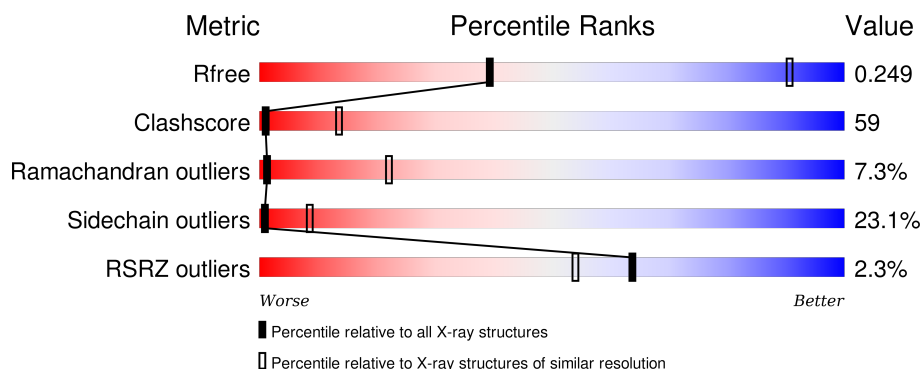
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1676	<div> <div>3%</div> <div>24% 52% 20% . .</div> </div>
1	C	1676	<div> <div>2%</div> <div>24% 52% 20% . .</div> </div>
2	B	1642	<div> <div>2%</div> <div>23% 38% 13% . 25%</div> </div>
2	D	1642	<div> <div>%</div> <div>23% 38% 13% . 25%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

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.

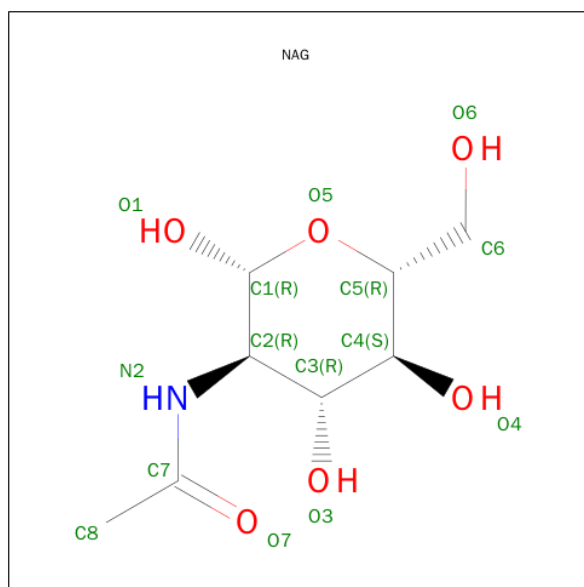
- Molecule 1 is a protein called Complement C5.

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

- Molecule 2 is a protein called Cobra venom factor.

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

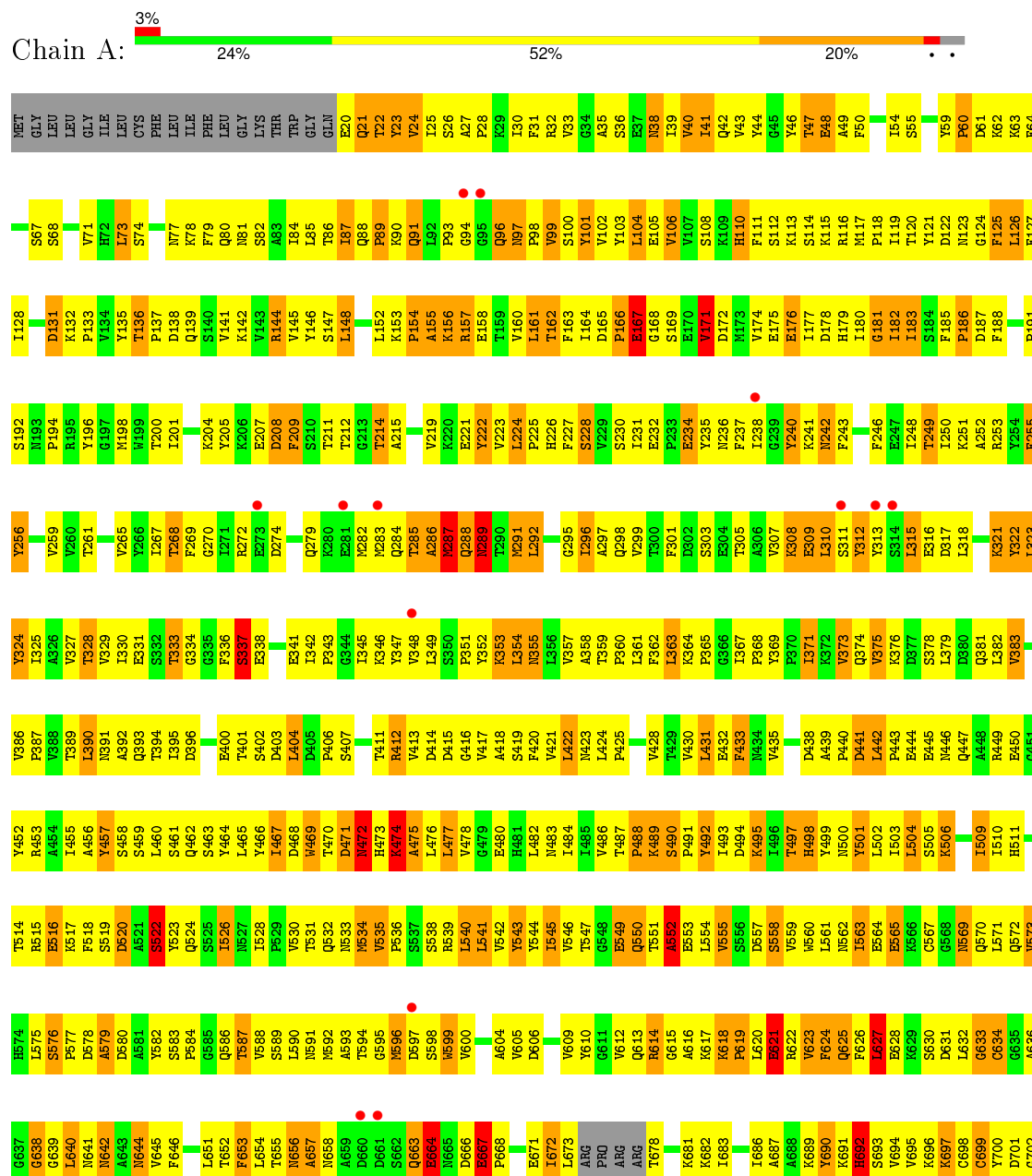


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

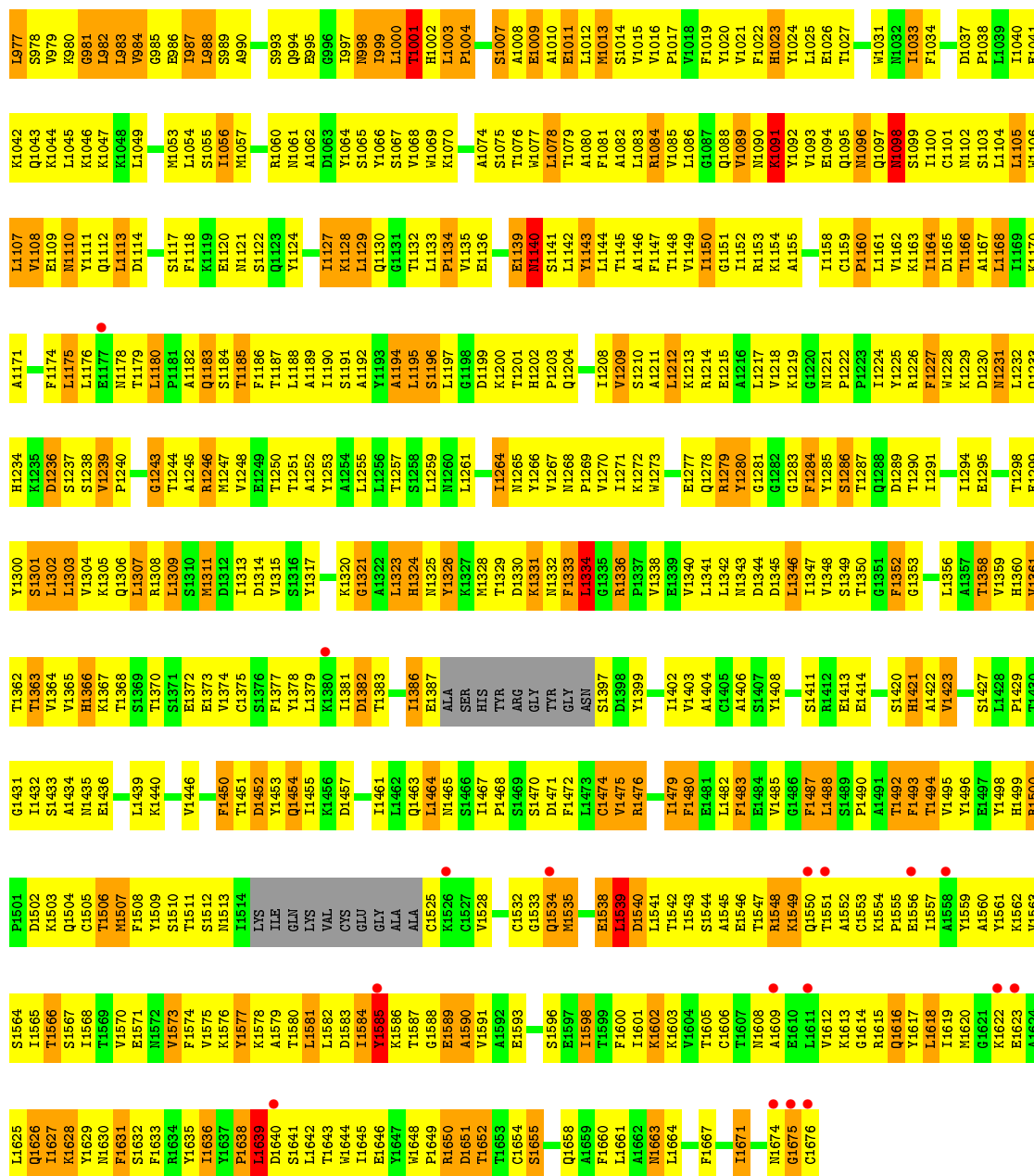
• Molecule 1: Complement C5



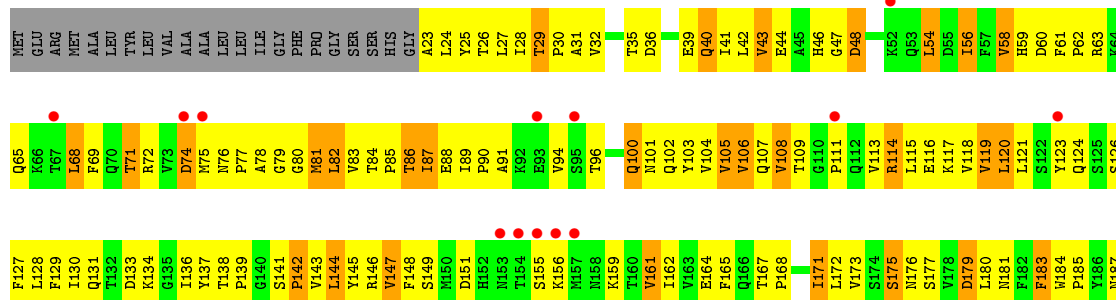
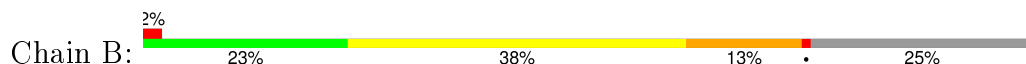
L1625	V1563	P1429	V1359	L1232	L1169	S1103	D1037	E972	H908	H778	A703
Q1626	S1564	T1430	H1360	Q1233	K1170	L1104	P1038	I973	H909	L779	C704
L1627	I1565	G1431	V1361	H1234	A1171	L1105	L1039	K974	I910	L780	C705
K1628	T1566	L1432	T1362	K1235	F1174	W1106	T1040	K975	I911	P781	N706
L1629	S1567	S1433	T1363	D1236	L1175	V1107	E1041	L976	F912	R782	E709
N1630	T1568	L1434	L1364	S1237	L1176	V1108	K1042	L977	S913	K784	T710
F1631	M1507	L1439	V1365	S1238	L1177	E1109	Q1043	S978	L914	R785	E709
S1632	F1508	L1440	H1366	P1239	L1178	M1110	K1044	V979	E915	Q713	Q713
F1633	L1509	K1440	K1367	Q1240	L1179	Q1112	L1045	K980	P917	W787	R714
L1634	S1510	V1446	T1368	G1243	L1180	L1113	K1046	K981	F918	F788	Q713
L1635	T1511	F1450	L1369	T1244	L1181	D1114	K1048	L983	G919	K789	L720
L1636	S1512	F1451	S1370	T1245	A1182	S1117	L1049	L984	K920	L790	G721
N1637	M1513	E1452	E1371	K1246	Q1183	F1118	M1053	K985	F921	P791	P722
P1638	K1514	D1452	E1372	V1248	S1184	K1119	L1054	E986	W922	S792	P722
D1640	L1515	Y1453	V1374	L1249	T1185	L1120	L1055	K987	Y924	S793	R723
S1641	G1516	Q1454	C1375	E1249	F1186	E1120	S1055	L988	K925	K938	C724
L1642	T1580	L1455	S1376	T1250	T1187	N1121	T1056	S989	Y926	L794	A727
T1643	L1581	K1456	F1377	L1251	L1188	S1122	M1057	A990	R928	W796	F728
L1644	C1582	D1457	Y1378	L1252	A1189	Q1123	M1057	H1001	Y929	W797	T729
L1645	D1583	L1457	L1379	Y1253	L1190	Y1124	R1060	S993	V930	E798	E730
E1646	I1584	L1461	K1380	L1254	S1191	K1127	M1061	K994	P931	I799	C731
Y1647	Y1585	L1462	T1381	L1255	A1192	L1128	A1062	E995	E932	Q800	C732
W1648	K1586	Q1463	D1382	L1256	Y1193	K1128	S1065	G996	G933	T867	V733
P1649	T1587	L1464	L1383	T1257	A1194	L1129	Y1066	I997	Y934	S868	W734
R1650	G1588	N1465	H1384	S1258	L1195	L1132	S1067	N998	K935	E869	Q737
D1651	E1589	S1466	N1325	L1259	L1196	L1133	S1068	I999	R936	S870	N805
T1652	C1527	L1467	Y1326	L1261	L1197	P1134	W1069	L1000	E937	P871	L738
L1653	V1528	P1468	K1327	L1264	G1198	E1135	K1070	H1002	S938	W872	T807
C1654	G1532	S1469	M1328	I1264	D1199	L1136	L1074	L1003	Y939	G808	G808
S1655	Q1533	S1470	T1329	N1265	K1200	E1139	A1074	P1004	S940	I873	I809
C1656	Q1534	D1471	T1330	N1266	T1201	E1140	S1075	P1007	G941	C810	S743
Q1658	M1535	F1472	K1331	Y1266	H1202	S1141	T1076	A1008	Y942	W811	H15
A1659	E1537	C1473	F1333	V1267	P1203	L1142	T1077	E1009	I944	A812	LYS
F1660	T1599	L1475	T1334	P1269	Q1204	L1143	L1078	D945	P946	W815	ASP
L1661	E1538	W1476	GLY	G1335	V1270	Y1143	T1079	K884	R947	K816	GLN
A1662	L1539	S1397	ASN	R1336	I1271	L1144	A1080	R885	I947	A817	LEU
L1663	D1540	T1402	S1397	P1337	K1272	L1145	F1081	Q886	G948	K818	GLY
T1664	T1542	V1403	V1338	V1338	W1273	A1146	A1082	K887	I949	W819	R751
T1665	S1543	A1404	E1339	L1274	L1212	F1147	L1083	V888	Y950	F820	L752
L1666	S1544	F1483	C1405	E1277	R1214	T1148	R1084	E889	G951	K821	L753
L1667	A1545	A1406	C1407	Q1278	E1215	V1149	V1085	E890	T952	D822	A754
T1667	E1546	S1407	S1407	R1279	L1216	G1151	L1086	S891	I953	W823	K755
L1668	T1547	V1485	D1344	Y1280	L1217	R1152	G1087	V1018	E954	F824	K756
A1609	R1548	G1486	D1345	G1281	V1218	R1153	V1089	F1019	R955	E826	L758
V1612	K1549	F1487	Y1408	G1282	K1219	K1154	Q1088	V1021	K957	L827	P759
K1613	Q1550	S1411	L1347	G1283	G1220	I1158	K1081	F1022	E958	W828	V760
G1614	T1551	R1412	T1348	F1284	N1221	C1159	V1092	H1023	F959	I829	L765
L1615	A1552	E1413	V1348	Y1285	P1222	P1160	V1093	Y1024	P960	P830	I765
Q1616	C1553	E1414	T1349	S1286	P1223	E1094	E1094	L1025	Y961	R831	R766
L1617	K1554	S1420	G1351	T1287	L1124	L1161	Q1095	E1026	R962	S832	S767
L1618	E1556	H1421	F1352	Q1288	Y1225	V1162	M1096	T1027	V900	S833	V768
L1619	L1557	V1495	G1353	T1289	R1226	K1163	Q1097	L1031	L901	W834	
M1620	A1558	V1423	S1354	T1290	F1227	I1164	N1098	W1031	P902		
G1621	Y1559	E1497	G1355	I1291	W1228	D1165	S1099	M1032	I903		
K1622	Y1498	Y1498	L1356	L1294	W1229	I1100	I1033	E904	E937		
L1623	Y1561	S1427	A1357	L1230	D1230	A1167	C1101	W1033	Q838		
A1624	K1562	L1428	T1358	E1295	N1231	L1168	N1102	F1034	Q840		

• Molecule 1: Complement C5

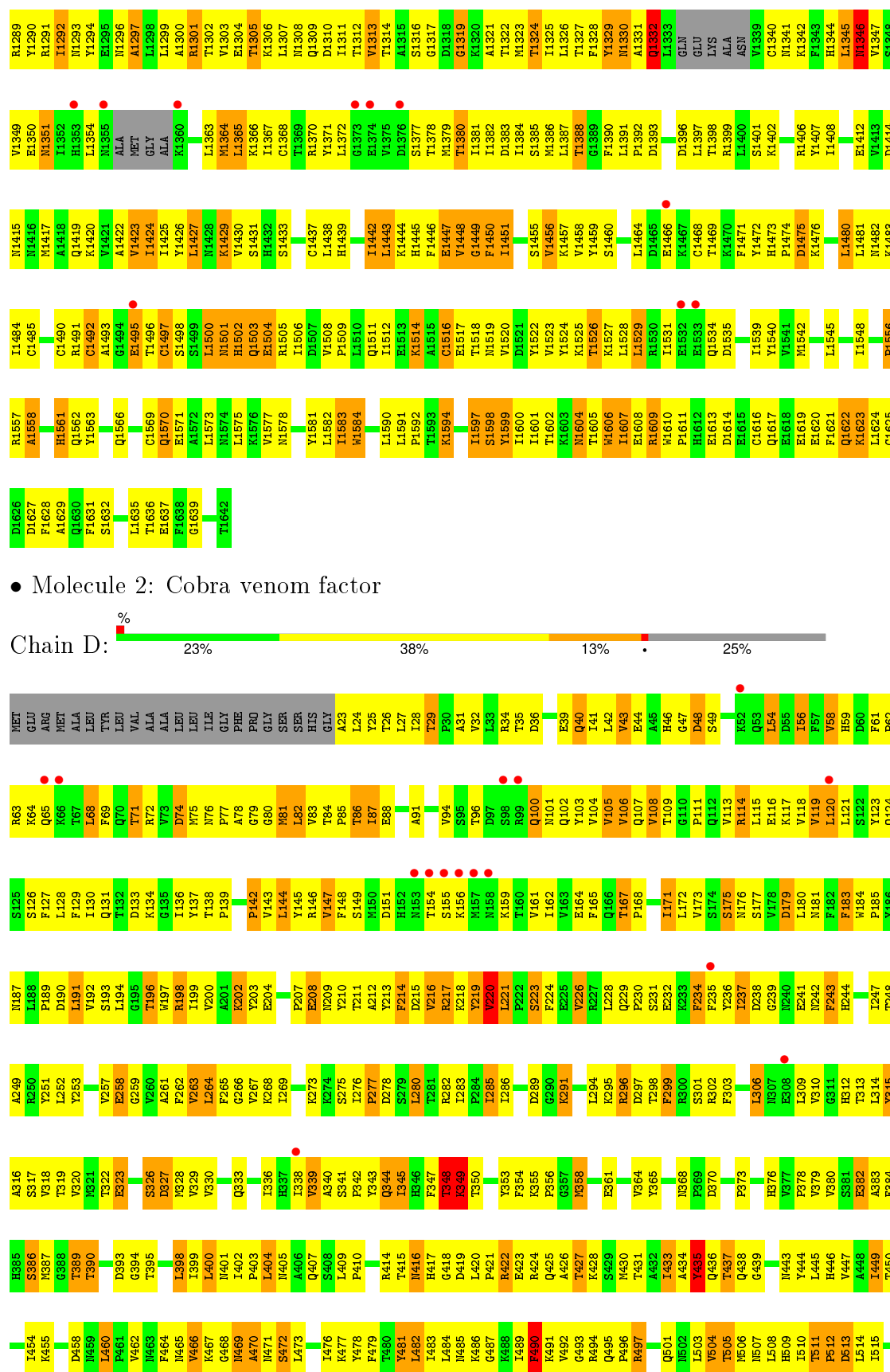




● Molecule 2: Cobra venom factor









Q1622	K1623	L1624	C1625	D1626	D1627	F1628	A1629	Q1630	F1631	S1632	L1635	T1636	E1637	T1642
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4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.233 , 0.262 0.221 , 0.249	Depositor DCC
R_{free} test set	1732 reflections (2.17%)	DCC
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 , 173.2	EDS
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 79835 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(°)	Ideal(°)
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(°)	Ideal(°)
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

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:D:380:VAL:HG12	2:D:387:MET:HB3	1.26	1.15
2:B:380:VAL:HG12	2:B:387:MET:HB3	1.24	1.15
2:D:1609:ARG:HH11	2:D:1609:ARG:HG2	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%)	1	16
1	C	1617/1676 (96%)	1179 (73%)	288 (18%)	150 (9%)	1	16
2	B	1215/1642 (74%)	998 (82%)	161 (13%)	56 (5%)	3	33
2	D	1215/1642 (74%)	995 (82%)	162 (13%)	58 (5%)	3	32
All	All	5664/6636 (85%)	4345 (77%)	903 (16%)	416 (7%)	1	22

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	8
1	C	1446/1484 (97%)	1109 (77%)	337 (23%)	1	8
2	B	1093/1435 (76%)	845 (77%)	248 (23%)	1	9
2	D	1093/1435 (76%)	845 (77%)	248 (23%)	1	9
All	All	5078/5838 (87%)	3907 (77%)	1171 (23%)	1	8

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

Mol	Chain	Res	Type
2	B	1364	MET
1	C	333	THR
2	D	918	GLU
2	B	1437	CYS
1	C	47	THR

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

Mol	Chain	Res	Type
2	B	1341	ASN
1	C	391	ASN
2	D	901	GLN
2	B	1473	HIS
1	C	80	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 carbohydrates in this entry.

5.6 Ligand geometry

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	A	2003	1	14,14,15	0.57	0	15,19,21	2.17	3 (20%)
3	NAG	B	2001	2	14,14,15	0.81	1 (7%)	15,19,21	2.04	2 (13%)
3	NAG	B	2002	2	14,14,15	0.91	0	15,19,21	0.78	0
3	NAG	C	2003	1	14,14,15	0.55	0	15,19,21	2.18	3 (20%)
3	NAG	D	2001	2	14,14,15	0.74	0	15,19,21	2.16	2 (13%)
3	NAG	D	2002	2	14,14,15	0.91	0	15,19,21	0.78	0

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	A	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2001	2	-	0/6/23/26	0/1/1/1
3	NAG	B	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	D	2001	2	-	0/6/23/26	0/1/1/1
3	NAG	D	2002	2	-	0/6/23/26	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	2.24	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2001	NAG	C2-N2-C7	-2.95	119.24	123.04
3	B	2001	NAG	C2-N2-C7	-2.74	119.52	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2003	NAG	C3-C4-C5	3.04	115.50	110.20
3	A	2003	NAG	C3-C4-C5	3.08	115.56	110.20
3	A	2003	NAG	C4-C3-C2	3.86	117.23	111.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2003	NAG	C8-C7-N2-C2
3	A	2003	NAG	C8-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
3	C	2003	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	A	2003	NAG	2	0
3	B	2001	NAG	1	0
3	C	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%)	0.08	44 (2%) 58 48	90, 187, 312, 465	0
1	C	1627/1676 (97%)	0.06	40 (2%) 61 50	97, 186, 299, 486	0
2	B	1225/1642 (74%)	0.04	27 (2%) 65 56	107, 174, 261, 395	0
2	D	1225/1642 (74%)	0.04	21 (1%) 73 63	114, 181, 263, 371	0
All	All	5704/6636 (85%)	0.06	132 (2%) 64 54	90, 183, 291, 486	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1585	TYR	5.5
2	D	1355	ASN	5.4
2	B	155	SER	5.2
1	A	1622	LYS	5.0
1	A	1650	ARG	5.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	2002	14/15	0.45	0.43	2.53	321,327,336,339	0
3	NAG	D	2002	14/15	0.73	0.47	1.42	289,293,305,308	0
3	NAG	C	2003	14/15	0.73	0.35	-	260,272,284,287	0
3	NAG	A	2003	14/15	0.64	0.37	-	284,286,289,289	0
3	NAG	D	2001	14/15	0.80	0.30	-	285,296,309,310	0
3	NAG	B	2001	14/15	0.78	0.26	-	275,285,305,313	0

6.5 Other polymers [i](#)

There are no such residues in this entry.