



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 12:12 PM BST

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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
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)	:	2.13.1

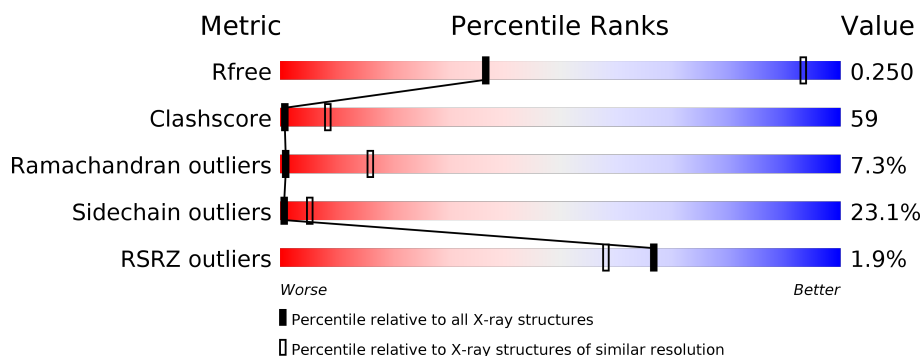
# 1 Overall quality at a glance

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))
$R_{free}$	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1676	<div> <div>2%</div> <div>24% 52% 20%</div> <div>• •</div> </div>
1	C	1676	<div> <div>2%</div> <div>24% 52% 20%</div> <div>• •</div> </div>
2	B	1642	<div> <div>2%</div> <div>23% 38% 13% 25%</div> <div>•</div> </div>
2	D	1642	<div> <div>%</div> <div>23% 38% 13% 25%</div> <div>•</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.

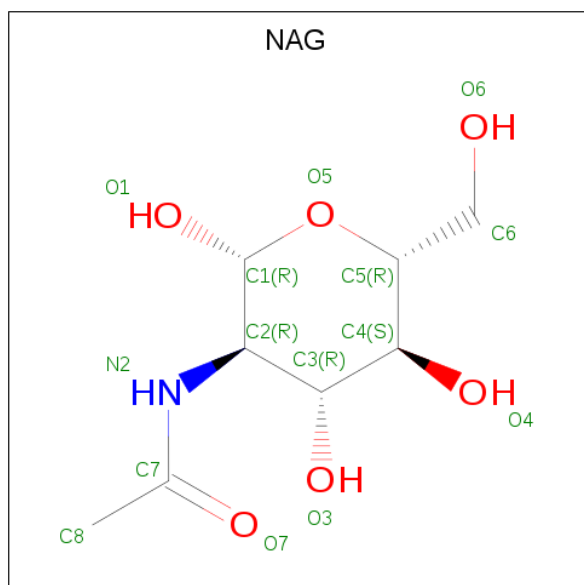
- Molecule 1 is a protein called Complement C5.

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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

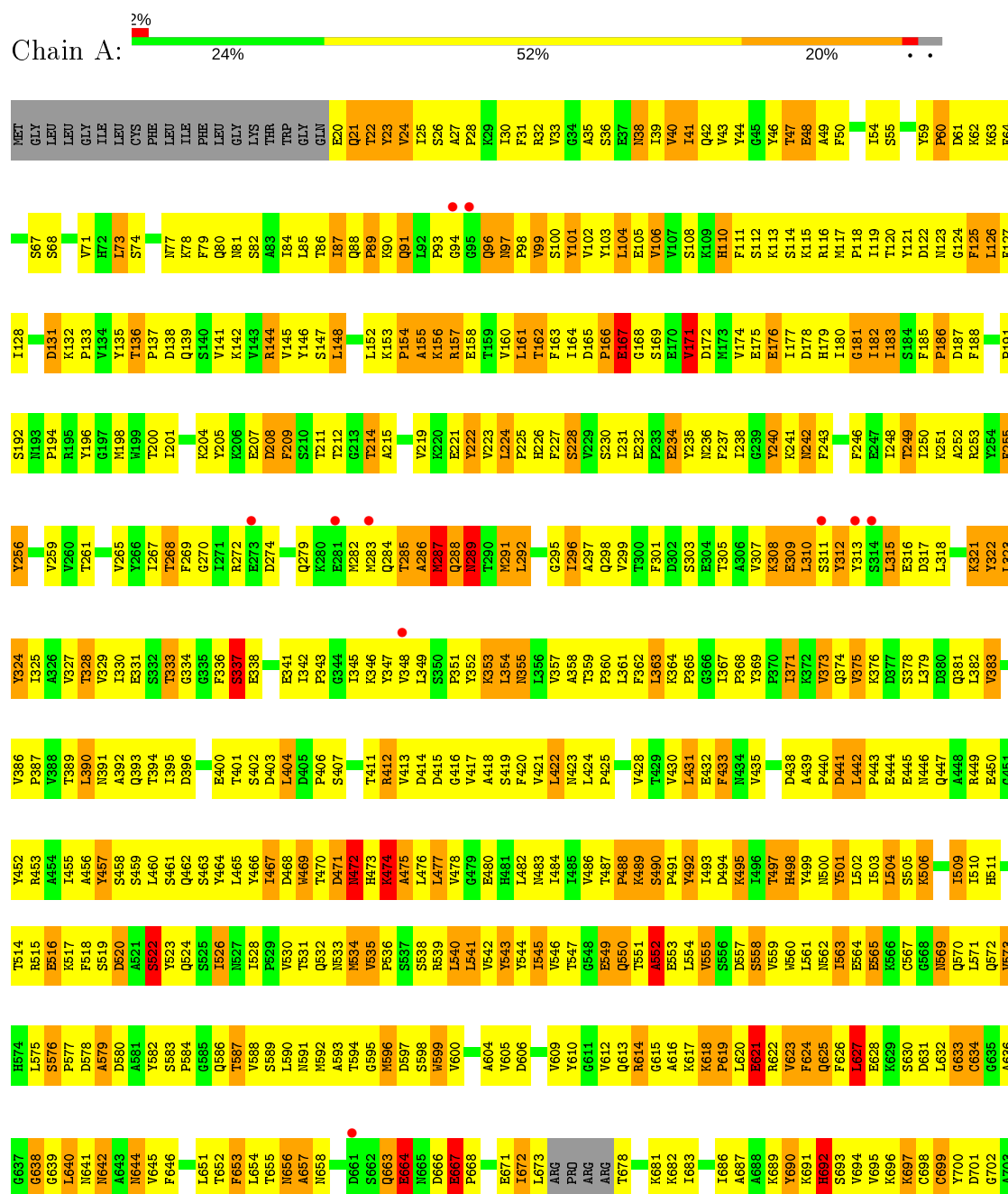


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

### 3 Residue-property plots

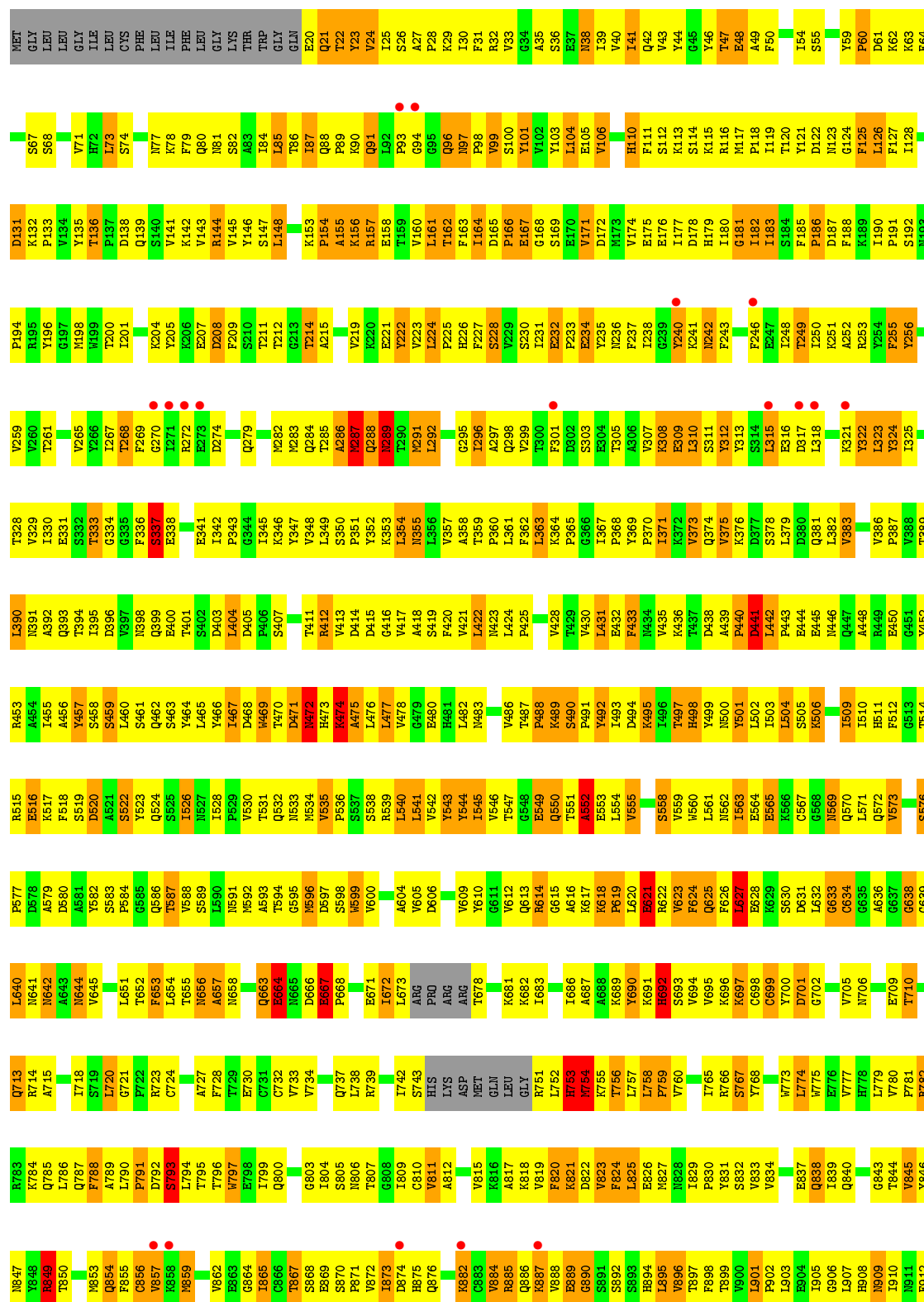
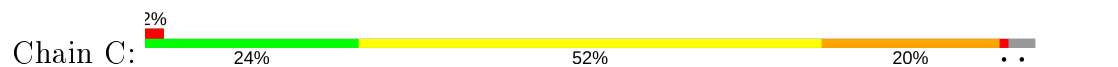
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

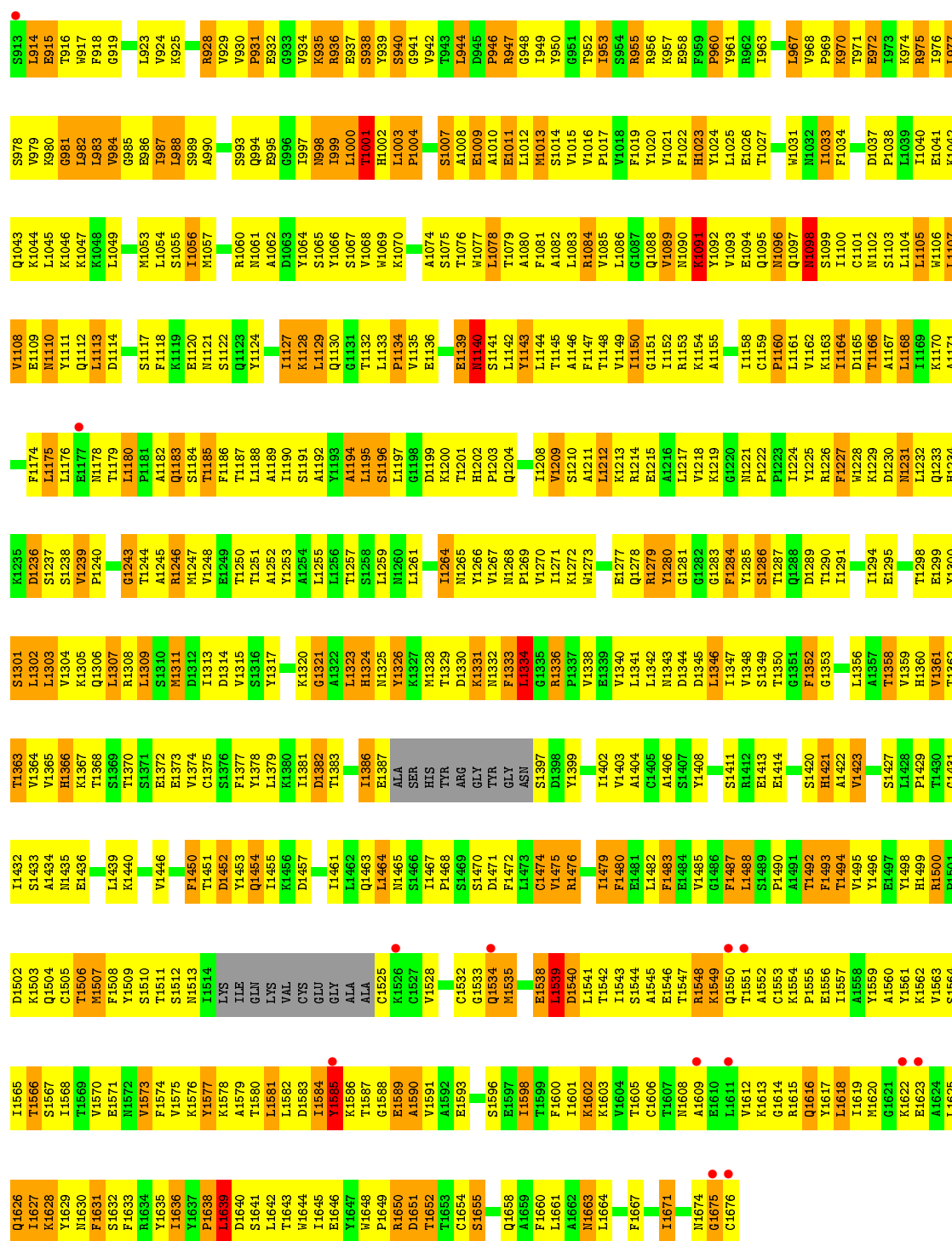


K1628	T1566	Q1504	L1432	T1362	S1301	K1285	F1174	W1106	I1040	R975	H909	G843	L779	C704
Y1629	S1567	C1505	S1433	T1363	L1302	D1286	L1175	L1107	E1041	R976	I910	T844	V780	V705
N1630	I1568	C1506	V1364	V1364	V1303	S1237	L1176	E1108	E1042	L977	N911	V845	R782	M706
F1631	T1569	M1507	V1365	V1365	V1304	S1238	L1177	V1109	Q1043	F912	F912	V846	R783	E710
S1632	V1570	F1508	H1366	H1366	K1305	V1239	E1178	N1110	K1044	V979	S913	N847	K784	T709
F1633	E1571	F1509	K1367	K1367	Q1306	P1240	N1179	Y1111	L1045	K980	L914	K980	K785	E709
R1634	N1572	S1510	K1368	T1368	L1307	P1241	T1178	Q1112	K1046	G981	E915	R843	K786	T710
Y1635	V1446	T1511	S1369	S1369	R1308	G1243	L1180	Q1112	K1047	G982	T916	R843	K787	Q713
S1512	F1574	N1512	T1370	T1370	L1309	T1244	P1181	D1114	L1049	L982	F917	T850	K788	R714
N1513	K1576	N1513	S1371	S1371	M1311	A1245	A1182			L983	F918		K789	
L1514	F1450	L1514	S1372	S1372	K1310	A1246	Q1183			G985		M853	L730	L720
L1515	T1451	L1515	E1373	E1373	D1312	M1247	S1184	S1117	M1053	E986	L923	K854	F788	F788
L1516	V1453	L1516	V1374	V1374	I1313	V1248	F1185	K1119	L1054	F789	V924	K854	L730	L730
L1517	Q1454	L1517	C1375	C1375	D1314	E1249	F1186	E1120	S1055	L988	K925	C856	P722	P722
L1518	T1455	L1518	S1376	S1376	V1315	T1250	T1187	M1121	S1056	S989		V857	D792	D792
L1519	L1456	L1519	S1377	S1377	S1316	T1251	L1188	S1122	M1057	E990		M859	S793	C724
L1520	D1457	L1520	V1378	V1378	Y1317	Y1253	A1189	Q1123	R1060	S993	R928	K858	L794	L794
L1521	G1457	L1521	L1379	L1379	Y1320	Y1254	L1190	Q1124	M1061	V930	V930	K859	K796	K796
L1522	T1461	L1522	K1380	K1380	K1320	A1254	S1191	Y1124	A1062	P931	V930	K863	T729	T729
L1523	L1462	L1523	I1381	I1381	G1321	L1255	A1192	I1127	A1062	E995	V930	K864	E730	E730
L1524	Q1463	L1524	D1382	D1382	A1322	L1256	Y1193	K1128	S1065	G996	E932	K865	C731	C731
L1525	L1464	L1525	T1383	T1383	H1323	T1257	A1194	L1129	S1066	N998	K935	C866	C732	C732
L1526	N1465	L1526	H1324	H1324	S1258	S1258	L1195		S1067	L999	R936	T867	V733	V733
L1527	S1466	L1527	N1325	N1325	L1259	L1259	S1196	T1132	S1067	L1000	E937	S868	V734	V734
L1528	T1467	L1528	Y1326	Y1326	N1280	N1280	L1197	P1133	S1068	T1001	S988	E869	I804	I804
L1529	P1468	L1529	K1327	K1327	L1281	L1281	G1198	P1134	M1069	K987	S988	S870	S805	Q737
L1530	S1469	L1530	M1328	M1328	I1284	I1284	D1199	E1139	A1074	A1008		P871	N806	N806
L1531	S1470	L1531	T1329	T1329	H1285	H1285	K1200	N1140	T1077	E1009		V872	L738	L738
L1532	F1471	L1532	D1330	D1330	N1265	N1265	H1202	S1141	L1078	L944		S940	R739	R739
L1533	F1472	L1533	K1331	K1331	K1331	K1331	P1203	E1142	L1078	D945		L804	I742	I742
L1534	GLY	L1534	N1332	N1332	L1271	L1271	Q1204	I1143	S1075	S1007		K816	S743	S743
L1535	GLY	L1535	L1333	L1333	I1272	I1272	T1209	Y1143	T1079	L944		K817	H15	H15
L1536	ASN	L1536	F1334	F1334	K1335	K1335	V1208	E1143	L1078	L944		K818	ASP	ASP
L1537	GLY	L1537	L1335	L1335	I1271	I1271	S1210	Y1144	A1080	P946		K819	GLN	GLN
L1538	GLY	L1538	L1336	L1336	K1336	K1336	S1211	L1144	F1081	R947		K820	LEU	LEU
L1539	ASN	L1539	V1337	V1337	V1338	V1338	A1211	L1145	F1082	L949		K821	GLY	GLY
L1540	T1479	L1540	E1339	E1339	L1274	L1274	L1212	F1147	L1083	V950		K822	R751	R751
L1541	L1480	L1541	V1340	V1340			K1213	I1148	R1084	G951		K823	R752	R752
L1542	L1482	L1542	L1341	L1341	E1277	E1277	R1214	V1149	V1085	T952		K824	R753	R753
L1543	E1481	L1543	L1342	L1342	Q1278	Q1278	E1215	I1150	L1086	P1017		K825	R754	R754
L1544	F1483	L1544	N1343	N1343	R1279	R1279	A1216	G1151	G1087	S954		K826	K755	K755
L1545	E1484	L1545	D1344	D1344	Y1280	Y1280	L1217	I1152	Q1088	F1019		K827	T756	T756
L1546	V1485	L1546	D1345	D1345	G1281	G1281	V1218	R1153	V1089	R956		K828	L757	L757
L1547	G1486	L1547	L1346	L1346	E1282	E1282	K1219	K1154	M1090	V1021		K829	L758	L758
L1548	F1487	L1548	L1347	L1347	F1283	F1283	G1220		R1091	F1022		K830	P759	P759
L1549	L1488	L1549	V1348	V1348	F1284	F1284	N1221	I1158	Y1092	H1023		K831	V760	V760
L1550	S1489	L1550	E1413	E1413	T1285	T1285	P1222	C1159	P980	L895		K832	L759	L759
L1551	P1490	L1551	S1349	S1349	S1286	S1286	P1223	P1160	E1094	T961		K833	V760	V760
L1552	A1491	L1552	T1350	T1350	T1287	T1287	L1224	L1161	Q1095	R962		K834		
L1553	T1492	L1553	G1351	G1351	Q1287	Q1287	Y1225	V1162	M1096	L963		K835	I765	I765
L1554	F1493	L1554	F1352	F1352	D1288	D1288	R1226	K1163	Q1097			K836	R766	R766
L1555	T1494	L1555	G1353	G1353	T1290	T1290	F1227	I1164	N1098	F1023		K837	S767	S767
L1556	V1495	L1556	E1354	E1354	I1291	I1291	M1228	L1165	S1099	L901		K838	Y768	Y768
L1557	Y1496	L1557	G1355	G1355	T1294	T1294	K1229	T1166	L1003	V968		K839	V773	V773
L1558	E1497	L1558	L1356	L1356	E1295	E1295	Y1225	V1162	C1101	L903		K840	I774	I774
L1559	Y1498	L1559	A1357	A1357	T1294	T1294	N1231	L1168	M1102	T971		K841	W775	W775
L1560	H1499	L1560	T1358	T1358	E1295	E1295	L1232	L1169	S1103	E972		K842	E776	E776
L1561	H1499	L1561	V1359	V1359	E1299	E1299	L1233	L1170	P1038	K974		K843	W777	W777
L1562	L1428	L1562	T1430	T1430	E1299	E1299	H1234	A1171	L1105			K844	H778	H778
L1563	P1429	L1563	G1431	G1431	Y1300	Y1300						K845		

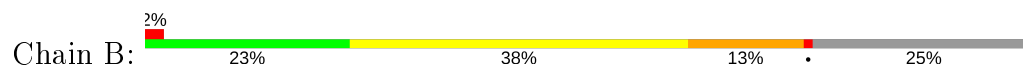
## ● Molecule 1: Complement C5







- Molecule 2: Cobra venom factor



SER	TYR	ALA	ALA	THR	ILE	V925	E849	V789	SER	ALA	W599	V526	V462	G394	T322	Y251	L188	F127	Q65
THR	ALA	GLU	GLU	THR	THR	T926	L250	L790	GLU	ALA	I602	G827	M463	T395	E323	L252	P189	L128	A66
ALA	ALA	LEU	PHE	GLU	GLU	I927	I851	A791	LEU	PHE	I602	M829	M464	L398	S326	Y253	D190	F129	T67
PHE	GLY	LEU	LEU	GLN	GLN	V928	V928	V792	LEU	GLN	E603	M829	M465	I399	S326	Y253	L191	I130	L68
THR	GLY	LEU	ALA	ASP	ASP	N853	N853	V793	LEU	GLN	K604	E530	K467	I399	S326	Y253	V192	Q131	G70
ASN	GLY	ASP	ASP	GLN	GLN	K929	K929	F794	ASP	GLN	S605	I531	K467	I400	N328	E258	S193	F69	F70
ARG	GLU	ASP	ASP	ASP	ASP	L330	L330	T795	ASP	ASP	D606	V832	G468	M401	V329	G259	L194	D133	T71
ALA	GLN	ASP	ASP	LEU	LEU	R933	C857	T796	LEU	LEU	F607	A533	M469	I402	V330	A261	G195	K134	A72
SER	ASN	SER	SER	GLY	GLY	V937	S860	K798	ASP	ARG	S613	S535	M471	L404	Q333	T196	G196	G135	V73
SER	SER	SER	SER	ILE	ILE	G938	T861	G799	ASP	CYS	G614	V638	L473	Q407	H336	F262	I197	I136	D74
TRP	ARG	TRP	ARG	ARG	ARG	T940	K862	I800	GLU	CYS	Q615	V638	L473	L409	H337	F263	K198	T136	M75
LEU	MET	LEU	LEU	MET	MET	Q941	Q864	V802	GLU	GLU	Q616	V638	L473	P410	I338	F265	T137	T138	M76
THR	ALA	ALA	ALA	ALA	ALA	L942	R865	A803	ASP	ASP	M617	K641	I476	L409	I338	L264	I199	T139	M77
ALA	ALA	ALA	ALA	ALA	ALA	E943	R866	E804	VAL	VAL	M618	K641	I476	P410	V339	L264	V200	P77	A78
TYR	PRO	TYR	PRO	PRO	PRO	V944	R867	P805	VAL	VAL	G619	K641	I476	P410	V339	L264	K202	S141	G79
VAL	VAL	VAL	VAL	VAL	VAL	I945	Q868	Y806	GLY	HIS	V620	M545	T480	R414	S341	G268	K202	S141	G80
VAL	VAL	VAL	VAL	VAL	VAL	K946	Q869	E807	GLU	GLU	F621	G546	Y481	R415	S341	G268	K202	S141	G81
LYS	ALA	ALA	ALA	ALA	ALA	A947	F870	R808	ASN	ASN	E822	T547	L482	T415	S341	G268	K202	S141	G82
VAL	THR	VAL	THR	THR	THR	R948	P871	R809	PRO	PRO	E822	L548	L482	T415	S341	G268	K202	S141	G83
PHE	PHE	PHE	PHE	PHE	PHE	K949	I872	V810	MET	MET	G625	L548	L482	T415	S341	G268	K202	S141	G84
ALA	ALA	ALA	ALA	ALA	ALA	L950	K873	M811	GLY	GLY	L626	V550	L482	T415	S341	G268	K202	S141	G85
MET	MET	MET	MET	MET	MET	D951	R878	K812	TYR	TYR	A627	V550	L482	T415	S341	G268	K202	S141	G86
ALA	ALA	ALA	ALA	ALA	ALA	D952	R878	V813	THR	THR	L628	V550	L482	T415	S341	G268	K202	S141	G87
ALA	ALA	ALA	ALA	ALA	ALA	R853	F814	F814	CYS	CYS	T629	V550	L482	T415	S341	G268	K202	S141	G88
LYS	LYS	LYS	LYS	LYS	LYS	V954	F881	F815	GLU	GLU	I555	V550	L482	T415	S341	G268	K202	S141	G89
MET	MET	MET	MET	MET	MET	P955	F882	I816	LYS	LYS	I555	V550	L482	T415	S341	G268	K202	S141	G90
VAL	VAL	VAL	VAL	VAL	VAL	D956	D956	D817	ARG	ARG	S631	V550	L482	T415	S341	G268	K202	S141	G91
ALA	ALA	ALA	ALA	ALA	ALA	T957	I884	L818	ALA	ALA	L634	M557	Y492	T427	F354	R217	T211	S149	G92
GLY	GLY	GLY	GLY	GLY	GLY	E958	R885	Q819	LYS	LYS	M635	P559	G493	K428	F354	R217	T211	S149	G93
ILE	ILE	ILE	ILE	ILE	ILE	I959	P886	M820	TYR	TYR	T636	G560	G494	R494	F354	R217	T211	S149	G94
SER	SER	SER	SER	SER	SER	E960	L887	P821	ILE	ILE	K637	G560	G494	R494	F354	R217	T211	S149	G95
HIS	HIS	HIS	HIS	HIS	HIS	T961	E888	S823	GLN	GLN	Q638	G560	G494	R494	F354	R217	T211	S149	G96
ILE	ILE	ILE	ILE	ILE	ILE	I963	Q889	V824	GLY	GLY	S640	G560	G494	R494	F354	R217	T211	S149	G97
ILE	ILE	ILE	ILE	ILE	ILE	I964	L931	V825	ASP	ASP	A641	G560	G494	R494	F354	R217	T211	S149	G98
CYS	CYS	CYS	CYS	CYS	CYS	I965	I896	K826	ALA	ALA	A642	G560	G494	R494	F354	R217	T211	S149	G99
GLY	GLY	GLY	GLY	GLY	GLY	G967	K897	E828	CYS	CYS	K643	G560	G494	R494	F354	R217	T211	S149	G100
VAL	VAL	VAL	VAL	VAL	VAL	D968	A898	Q829	LYS	LYS	V646	G560	G494	R494	F354	R217	T211	S149	G101
ARG	ARG	ARG	ARG	ARG	ARG	P969	Q901	V830	ALA	ALA	Q646	G560	G494	R494	F354	R217	T211	S149	G102
TRP	TRP	TRP	TRP	TRP	TRP	ALA	E802	E831	PHE	PHE	A648	G560	G494	R494	F354	R217	T211	S149	G103
LEU	LEU	LEU	LEU	LEU	LEU	GLN	A903	I832	LEU	LEU	ASN	G560	G494	R494	F354	R217	T211	S149	G104
ILE	ILE	ILE	ILE	ILE	ILE	ILE	GLN	I833	GLU	GLU	ASN	G560	G494	R494	F354	R217	T211	S149	G105
LEU	LEU	LEU	LEU	LEU	LEU	ILE	ILE	A834	CYS	CYS	ARG	G560	G494	R494	F354	R217	T211	S149	G106
ASN	ASN	ASN	ASN	ASN	ASN	ILE	K911	I835	CYS	CYS	ARG	G560	G494	R494	F354	R217	T211	S149	G107
ARG	ARG	ARG	ARG	ARG	ARG	GLU	K912	L836	TYR	TYR	P812	G560	G494	R494	F354	R217	T211	S149	G108
GLN	GLN	GLN	GLN	GLN	GLN	ASN	L913	H837	TYR	TYR	A883	G560	G494	R494	F354	R217	T211	S149	G109
GLN	GLN	GLN	GLN	GLN	GLN	SER	K914	N838	ILE	ILE	SER	G560	G494	R494	F354	R217	T211	S149	G110
PRO	PRO	PRO	PRO	PRO	PRO	ILE	V915	Y839	LYS	LYS	VAL	G560	G494	R494	F354	R217	T211	S149	G111
ASP	ASP	ASP	ASP	ASP	ASP	ASP	V916	V840	GLY	GLY	LEU	G560	G494	R494	F354	R217	T211	S149	G112
GLY	GLY	GLY	GLY	GLY	GLY	GLY	P917	N841	VAL	VAL	LEU	G560	G494	R494	F354	R217	T211	S149	G113
ALA	ALA	ALA	ALA	ALA	ALA	SER	E918	E842	ARG	ARG	LEU	G560	G494	R494	F354	R217	T211	S149	G114
PHE	PHE	PHE	PHE	PHE	PHE	LYS	G919	D843	ASP	ASP	LEU	G560	G494	R494	F354	R217	T211	S149	G115
LYS	LYS	LYS	LYS	LYS	LYS	LEU	V920	I844	GLU	GLU	ASP	G560	G494	R494	F354	R217	T211	S149	G116
GLU	GLU	GLU	GLU	GLU	GLU	ASN	Q921	Y845	ASN	ASN	SER	G560	G494	R494	F354	R217	T211	S149	G117
ASN	ASN	ASN	ASN	ASN	ASN	HIS	K922	R846	ALA	ALA	ASN	G560	G494	R494	F354	R217	T211	S149	G118
ALA	ALA	ALA	ALA	ALA	ALA	LEU	S923	R847	GLN	GLN	ALA	G560	G494	R494	F354	R217	T211	S149	G119
PRO	PRO	PRO	PRO	PRO	PRO	ILE	I924	V848	GLU	GLU	LYS	G560	G494	R494	F354	R217	T211	S149	G120

[illegible]



K1623	L1624	C1625	D1626	D1627	F1628	A1629	Q1630	F1631	S1632	L1635	T1636	E1637	T1642	D1553	P1556	D1557	A1558	K1559	T1560	H1561	Q1562	Y1563	Q1566	Q1570	E1571	A1572	L1573	N1574	L1575	K1576	Y1577	N1578	Y1581	L1582	T1583	W1584	L1590	L1591	P1592	T1593	K1594	I1597	S1598	Y1599	I1600	I1601	T1602	N1604	T1605	W1606	I1607	E1608	R1609	W1610	P1611	H1612	E1613	D1614	E1615	C1616	Q1617	E1618	E1619	E1620	F1621	Q1622	L1481	M1482	K1483	I1484	C1485	G1490	R1491	C1492	A1493	G1494	E1495	T1496	C1497	L1500	M1501	H1502	Q1503	E1504	R1505	I1506	D1507	V1508	P1509	L1510	Q1511	I1512	E1513	K1514	A1515	C1516	E1517	T1518	M1519	V1520	D1521	Y1522	V1523	Y1524	K1525	T1526	K1527	L1528	L1529	R1530	I1531	Q1534	D1535	I1539	Y1540	V1541	M1542	L1545	I1548	L1486	Y1487	I1488	E1412	M1417	A1418	Q1419	K1420	V1421	A1422	V1423	I1424	I1425	Y1426	L1427	N1428	K1429	V1430	S1431	H1432	S1433	C1437	L1438	H1439	I1442	L1443	K1444	H1445	F1446	E1447	V1448	G1449	F1450	I1451	S1455	V1456	K1457	V1458	Y1459	S1460	L1464	D1465	E1466	K1467	C1468	T1469	K1470	F1471	Y1472	H1473	P1474	D1475	L1480
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	135.2	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 172.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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%)	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	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 [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

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	2001	2	14,14,15	0.81	1 (7%)	17,19,21	2.07	3 (17%)
3	NAG	D	2002	2	14,14,15	0.92	0	17,19,21	1.16	1 (5%)
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	2001	2	14,14,15	0.74	0	17,19,21	2.16	4 (23%)
3	NAG	B	2002	2	14,14,15	0.92	0	17,19,21	1.16	1 (5%)

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	2001	2	-	2/6/23/26	0/1/1/1
3	NAG	D	2002	2	-	0/6/23/26	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	2001	2	-	2/6/23/26	0/1/1/1
3	NAG	B	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	2.16	1.55	1.52

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	B	2001	NAG	C8-C7-N2-C2
3	B	2001	NAG	O7-C7-N2-C2
3	C	2003	NAG	C3-C2-N2-C7
3	C	2003	NAG	C8-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	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, 95<sup>th</sup> 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 <sup>2</sup> )	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, 95<sup>th</sup> 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
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.