



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:29 AM UTC

PDB ID : 3PVM / pdb\_00003pvm  
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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

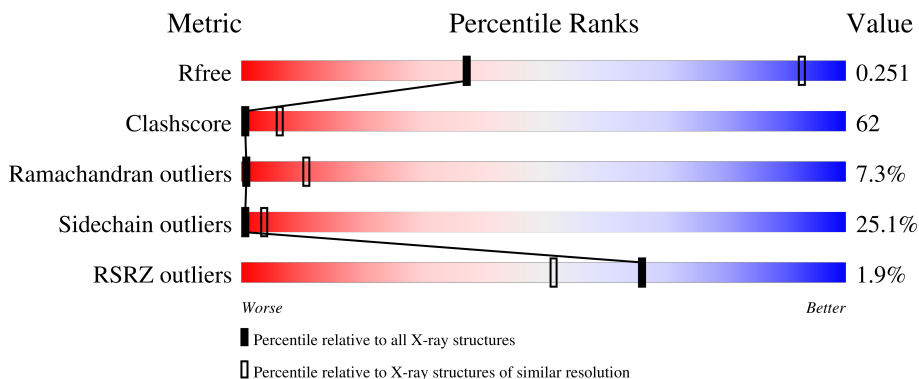
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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  $\geq 3$ , 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	 2% 22% 50% 23% . .
1	C	1676	 3% 22% 50% 23% . .
2	B	1642	 % 21% 37% 15% . 25%
2	D	1642	 % 20% 38% 15% . 25%

## 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.

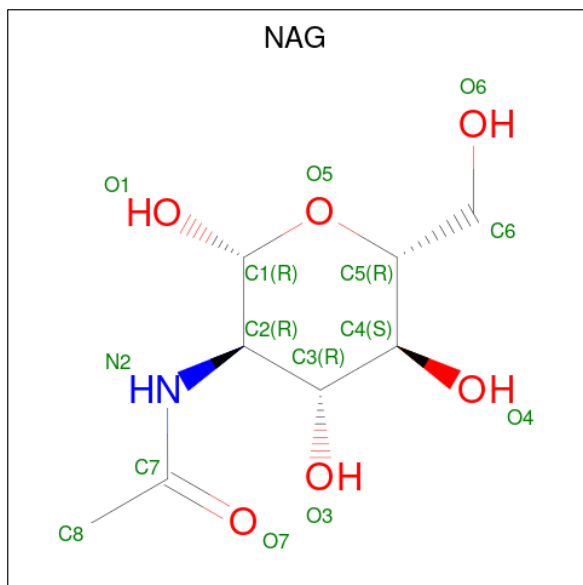
- Molecule 1 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1627	Total 12881	C 8246	N 2114	O 2469	S 52	0	0	0
1	C	1627	Total 12881	C 8246	N 2114	O 2469	S 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	Total 9711	C 6187	N 1633	O 1851	S 40	0	0	0
2	D	1225	Total 9711	C 6187	N 1633	O 1851	S 40	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

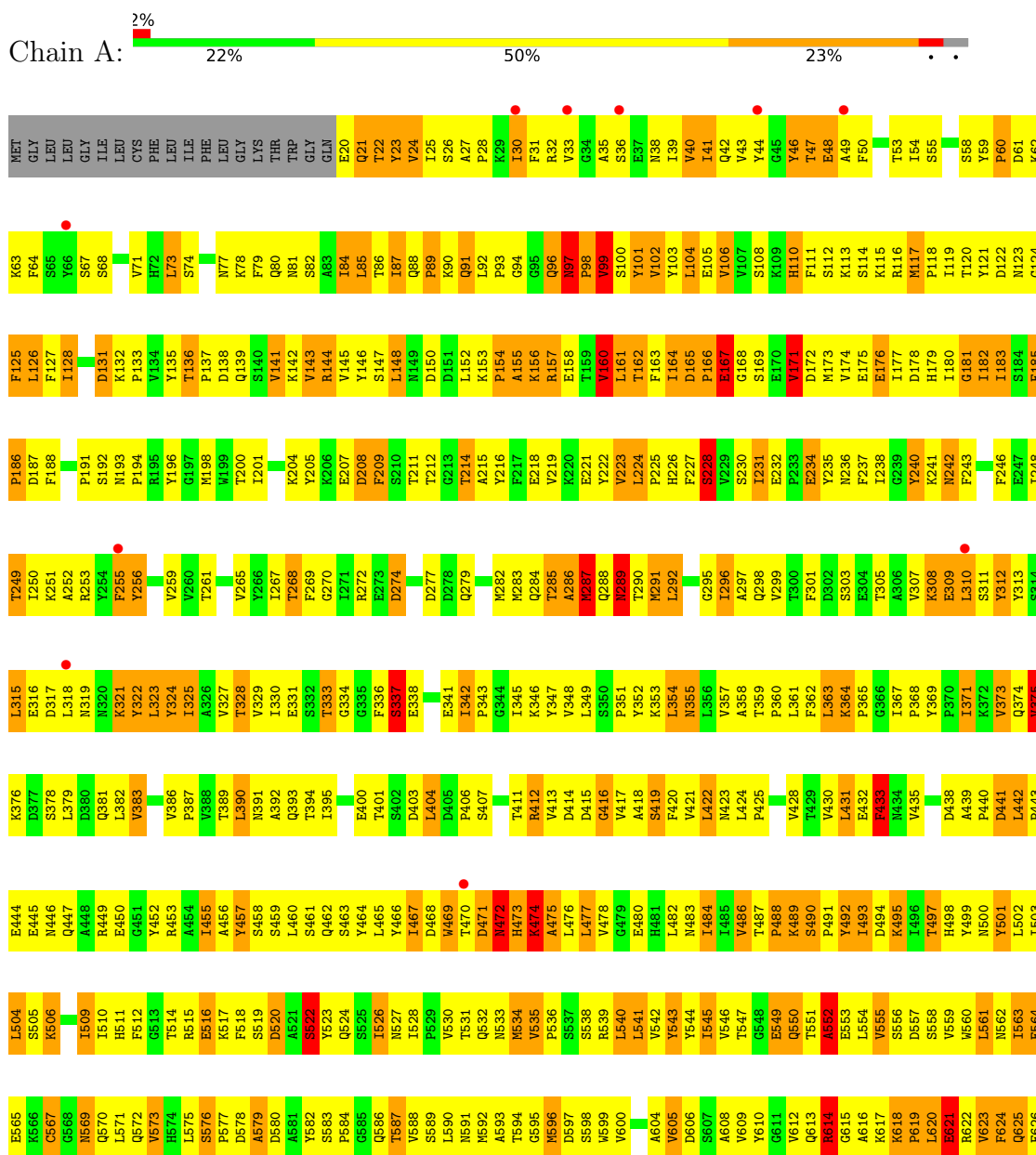


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

### 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



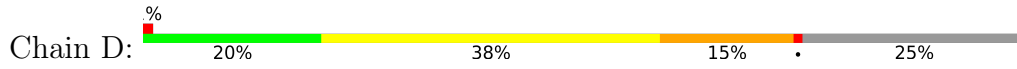
F1477	R1478	F1479	S1480	F1480	Y1408	L1481	L1482	E1483	E1484	V1485	E1413	E1414	S1349	F1350	G1351	F1352	G1353	S1354	L1426	S1427	F1493	T1494	V1495	V1496	E1497	I1498	H1499	R1500	F1501	D1502	K1503	Q1504	C1505	T1506	M1507	F1508	Y1509	S1510	T1511	S1512	M1513	I1514	LYS	ILE	GLN	LYS	VAL	CYS	GLU	GLY	ALA	ALA	HIS	TYR	ARG	GLY	TYR	GLY	ASN	S1397	L1473	C1474	Q1536	M1535	Q1536	E1537	E1538		
V1340	L1341	N1342	N1343	D1344	D1345	L1346	L1347	V1348	S1349	T1350	G1351	F1352	G1353	S1354	L1355	L1356	L1357	T1358	V1359	H1360	V1361	T1362	T1363	V1364	V1365	H1366	T1367	T1368	S1369	T1370	S1371	E1372	E1373	V1374	F1377	Y1378	L1379	K1380	I1381	D1382	T1383	I1386	A1387	ALA	ALA	HIS	TYR	ARG	GLY	TYR	GLY	ASN	S1397	L1461	L1462	Q1463	L1464	M1465	S1466	P1467	P1468	S1469	S1470	D1471	F1472	L1473	C1474	V1475	A1404
E1276	E1277	Q1278	L1279	Y1280	G1281	G1282	G1283	F1284	L1285	S1286	T1287	O1288	D1289	T1290	L1291	I1294	E1295	E1299	Y1300	S1301	L1302	L1303	V1304	K1305	Q1306	L1307	S1308	R1309	S1310	M1311	D1312	D1314	V1315	S1316	Y1317	K1320	G1321	L1322	L1323	H1324	M1325	K1263	M1264	N1265	Y1266	N1268	F1332	F1333	L1334	G1335	R1336	P1337	V1338	E1339															
A1216	L1217	K1218	K1219	G1220	N1221	P1222	F1223	L1224	K1225	R1226	F1227	H1228	K1229	D1230	L1231	L1232	Q1233	H1234	K1235	D1236	S1237	S1238	L1239	P1240	M1241	T1242	L1243	T1244	R1245	M1246	M1247	L1248	E1249	T1250	L1251	L1252	Y1253	A1254	L1255	T1256	T1257	L1258	L1259	M1260	K1261	K1262	I1264	N1265	Y1266	N1268	P1269	L1270	L1271	L1272	W1273	L1274	S1275												
G1087	Q1088	Y1089	M1090	K1091	Y1092	V1093	E1094	L1095	L1096	Y1097	Q1098	F1099	L1100	C1101	M1102	S1103	L1104	L1105	L1106	L1107	Y1108	E1109	Y1110	M1111	Q1112	L1113	D1114	S1117	F1118	K1119	E1120	M1121	L1122	Q1123	Y1089	O1124	M1061	A1062	S1065	Y1066	S1067	M1068	K1070	A1074	S1075	T1076	M1077	L1078	E1109	L1143	L1144	S1120	P1203	Q1204	I1208	Y1143	L1144	S1120	L1145	A1146	F1147	K1121	L1148	V1149	L1214	E1215			
F1019	Y1020	F1021	F1022	H1023	Y1024	L1025	E1026	T1027	W1031	Q1038	F1039	I1040	K1041	L1042	D1037	P1038	L1039	I1040	K1041	Q1043	K1044	L1045	K1046	K1047	K1048	L1049	M1053	L1054	S1055	M1057	L1058	Y1059	O1123	M1061	A1062	S1065	Y1066	S1067	M1068	K1070	A1074	S1075	T1076	M1077	L1078	E1109	L1143	L1144	S1120	P1203	Q1204	I1208	Y1143	L1144	S1120	L1145	A1146	F1147	K1121	L1148	V1149	L1214	E1215						
L895	V896	R897	F898	Y899	V900	L901	P902	L903	E904	I905	G906	L907	H908	N909	T910	L911	N912	Y913	Y914	W915	F916	F918	E921	L922	L923	Y924	K925	M1053	L1054	S1055	M1057	L1058	Y1059	O1123	M1061	A1062	S1065	Y1066	S1067	M1068	K1070	A1074	S1075	T1076	M1077	L1078	E1109	L1143	L1144	S1120	P1203	Q1204	I1208	Y1143	L1144	S1120	L1145	A1146	F1147	K1121	L1148	V1149	L1214	E1215					
M827	R828	L829	P830	Y831	S832	L833	V834	E837	Q838	I839	Q840	G843	T844	L845	Y846	N847	R848	R849	T850	M853	F788	Y789	F855	C856	V857	R858	S793	L794	T795	T796	E863	G864	L865	C866	T867	S868	E869	S870	P871	V872	L873	G808	D874	H875	Q876	K882	C883	V884	Q885	R886	L887	V888	F820	K821	E889	G890	S891	S892	S893	F824	L825	H894							
V760	I765	S766	T767	Y768	F769	W773	E774	Q775	G776	Y777	H778	L779	V780	T781	Y782	R783	K784	Q785	L786	M853	F788	Y789	F855	C856	V857	R858	S793	L794	T795	T796	E863	G864	L865	C866	T867	S868	E869	S870	P871	V872	L873	G808	D874	H875	Q876	K882	C883	V884	Q885	R886	L887	V888	F820	K821	E889	G890	S891	S892	S893	F824	L825	H894							
V694	V695	R696	K697	D631	C698	C699	W700	D701	G702	L774	E703	G704	W705	N706	L707	M641	N642	A643	N644	V645	F646	L651	T652	F653	L654	T655	M656	A657	N658	P661	S662	Q663	D664	M665	D666	E667	P668	E671	L672	L673	ARG	PRO	ARG	ARG	T678	K681	K682	L683	T686	A687	H763	M764	K689	Y690	K691	L692	L757	L758	P759										



L627	E628	K629	S630	D631	L632	G633	C634	G635	A636	G637	N706	N707	G638	G639	L640	N641	N642	N643	N644	N645	L651	T652	F653	L654	T655	N656	A657	N658	D661	S662	Q663	E664	N665	D666	E667	P668	E671	L672	L673	ARG	ARG	PRO	ARG	ARG	T678	K681	K682	I683	T686	A687	A688	K689	Y690	K691	H692	S693	V694																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
V695	K696	R697	C698	C699	Y700	D701	G702	W773	L774	W775	W706	N707	W777	H778	E709	Y710	N642	Y711	Q713	Y714	Y715	L718	S719	F720	G721	F722	R723	C724	A727	F728	W729	E730	C731	C732	W733	Y734	Q737	L738	R739	ARG	ARG	ARG	ASP	MET	GLN	LEU	GLY	R751	L752	H753	A688	K821	F755	T756	L757	F758	S693	V694																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
L765	R766	S767	Y768	F769	D770	W773	L774	W775	W776	W777	W778	L779	W780	P781	R782	Y783	K784	Q785	L786	Q787	W788	Y789	F790	G791	P791	D792	S793	L794	W795	T796	W797	E798	Y799	Q800	Q801	Q802	Q803	L804	S805	N806	T807	R808	P811	Y812	Y813	Y814	Y815	Y816	Y817	Y818	Y819	Y820	Y821	Y822	Y823	Y824	Y825	Y826	Y827	Y828	Y829	Y830	Y831	Y832	Y833	Y834	Y835	Y836	Y837	Y838	Y839	Y840	Y841	Y842	Y843	Y844	Y845	Y846	Y847	Y848	Y849	Y850	Y851	Y852	Y853	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	Y870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980	L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L20







MET	GLU	ARG	MET	ALA	LEU	TYR	LEU	VAL	ALA	ALA	LEU	LEU	ILE	GLY	PHE	GLY	PRO	GLY	SER	HIS	GLY	A23	L24	Y25	T26	L27	L28	T29	F30	A31	V32	L33	R34	T35	D36	E39	Q40	I41	L42	V43	E44	A45	H46	G47	D48	S49	T50	L54	D55	L56	F57	V58	H59	P60	F61	P62	F127	L128				
K64	Q65	L68	F69	Q70	T71	R72	V73	D74	M75	N76	P77	A78	G79	M81	R82	V83	T84	M85	H86	I87	E88	Y89	T96	Q100	M101	Q102	E103	Y104	V105	V106	Q107	I108	T109	L110	G111	P111	E112	V113	H114	S115	L116	D117	L118	V119	L120	L121	S122	F123	H124	I247	V125	M126	L127	L128								
F129	I130	Q131	T132	K133	D134	G135	I136	Y137	T138	P139	P140	V141	L142	L143	L144	Y145	M146	V147	F148	S149	M150	D151	I87	T154	S155	K156	M157	K158	K159	T160	V161	I162	V163	E164	F165	T166	Q167	P168	I171	L172	V173	G174	S175	M176	S177	V178	D179	L180	M181	V182	F183	M184	P185	V186	H187	L188	P189	D190	F191	L191		
V192	S193	L194	G195	T196	W197	R198	I199	V200	K201	K202	Y203	E204	H205	S206	P207	E208	N209	L82	F147	F148	T211	A212	Y213	D214	D215	R216	R217	K218	Y219	L220	L221	P222	S223	F224	E225	V226	R227	L228	Q229	P230	S231	E232	K233	F234	F235	Y236	I237	D238	G239	M240	E241	N242	F243	H244	I247	A316	A317	A249	R250	F251	L252	
Y253	V257	E258	G259	V260	A261	V262	V263	L264	F265	G266	V267	K268	L269	D270	K273	K274	S275	I276	P277	L280	T281	R282	L283	P284	L285	I286	D289	G290	K291	L294	K295	R296	D297	F298	F299	R300	S301	R302	F303	L306	V307	P308	L309	V310	G311	H312	T313	L314	Y315	F316	A316	S317	V318	R319	V320							
K321	T322	E323	S326	D327	M328	V329	V330	V331	Q333	Q334	I336	H337	V339	V339	A340	S341	P342	Q344	I345	H346	F347	T348	K349	T350	P351	K352	Y353	I286	K355	P356	G357	M358	E361	V364	Y365	V366	D370	P373	H376	E382	A383	F384	H385	S386	M387	T388	V389															
T390	L391	D392	D393	G394	T395	L396	I399	L400	N401	L402	L404	M405	A406	Q407	S408	L409	P410	R414	T415	M416	H417	G418	D419	L420	P421	R422	N423	E424	Q425	A426	T427	K428	S429	M430	T431	A432	I433	A434	Y435	Q436	T437	Q438	G439	M506	S441	G442	M443	Y444	L445	H446	V447	A448	L449	T450	S451							
L454	K455	D456	H459	L460	P461	V462	H463	N464	M465	V466	K467	G468	M469	A470	S471	N472	L473	I476	K477	Y478	F479	T480	I481	L482	L483	L484	N485	V486	G487	K488	L489	F490	T491	K492	V493	G493	R494	P495	A496	R497	Q501	H502	L503	V504	T505	M506	N507	L508	H509	L510	T511	A383	H446	V447	H385	L449	M581	H582	S451	F518		
R519	F520	V521	A522	Y523	Y524	O525	V526	G527	N528	N529	E530	F531	V532	A533	D534	G535	S536	N472	L473	K541	D542	T543	C544	H545	G546	T547	L548	V549	V550	D553	N554	L555	A556	O557	M558	P559	O560	M563	K564	L565	K566	L567	E568	G569	A641	D570	A642	K643	L574	L577	V578	A648	V580	D581	H582	A583	V584					
V585	V586	L587	N588	I593	S594	Q595	A596	N597	I598	M599	D600	T601	L602	E603	K604	S605	D606	F607	G608	S613	G614	O615	N616	L617	L618	G619	G620	F621	E622	G625	N626	L627	A627	L628	T629	T630	S631	L634	N635	T636	K637	Q638	R639	S640	A641	A642	K643	Q646	V578	A648	ASN	ARG	ARG	ARG	ARG	ARG						
SER	SER	VAL	LEU	LEU	LEU	ASP	SER	ASN	ALA	SER	LYS	ALA	ALA	GLU	PHE	GLN	ASP	GLN	ASP	LEU	ARG	ARG	LYS	CYS	CYS	GLU	ASP	VAL	VAL	GLY	THR	THR	CYS	GLU	LYS	ALA	LYS	TYR	ILE	GLN	GLU	GLY	GLY	ASP	ALA	CYS	LYS	ALA	ALA	ALA	PHE	LEU	GLU	CYS	ARG	ARG	ARG	ARG	ARG			
TYR	ILE	GLY	VAL	ARG	ASP	GLU	ASN	GLN	ARG	LEU	LEU	PHE	LEU	ALA	LEU	ALA	ARG	ASP	ASP	ASP	ASP	ASP	E736	D737	G738	F739	D742	S743	E744	I745	T746	S747	M811	K812	V813	F814	F815	D816	L817	L818	Q819	M820	P821	Y822	S823	V824	R825	K826	E827	Q829	E830	R831	L832	R833	A834	L835	L836	H837				
F778	T779	L780	R781	D782	S783	I784	T785	V786	F787	W788	L789	V790	A791	V792	S793	F794	T795	C857	S858	K798	G799	L800	C801	H802	A803	E804	P805	Y806	Q807	R808	R809	H810	M811	K812	V813	F814	F815	D816	L817	L818	Q819	M820	P821	Y822	S823	V824	R825	K826	E827	Q829	E830	R831	L832	R833	A834	L835	L836	H837				
N838	L839	Y840	N841	E842	D843	L844	T845	V846	R847	W848	V849	L850	L851	H852	N853	F856	C857	S858	K859	H859	V895	T896	I897	G898	G899	H864	R865	H866	R867	Q868	G869	H870	P871	L872	E843	K873	S876	S877	R878	A879	V880	P881	L950	D951	F952	R953	V954	P955	L956	V957	F958	O959	L891	E961	E962	L963	L964	L965	Q966	S967	V900	Q901
E902	A903	L904	Y905	V909	R910	K911	K912	L913	R914	W915	V916	P917	E918	G919	Y920	Q921	K922	S923	I924	V925	T926	I927	V928	G929	L930	V937	G938	G939	T940	Q941	L942	E943	Y944	L945	K946	A947	R948	K949	L950	D951	F952	R953	V954	P955	L956	V957	F958	O959	L891	E961	E962	L963	L964	L965	Q966	S967	V900	Q901				



## 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) 94.2 (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)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.233 , 0.262 0.228 , 0.251	Depositor DCC
$R_{free}$ test set	1734 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	135.2	Xtrriage
Anisotropy	0.503	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 193.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.026 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	45268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	192.0	wwPDB-VP

Xtrriage'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 [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	0.74	0/13158	1.13	75/17851 (0.4%)
1	C	0.74	2/13158 (0.0%)	1.13	80/17851 (0.4%)
2	B	0.71	1/9912 (0.0%)	1.12	57/13454 (0.4%)
2	D	0.71	1/9912 (0.0%)	1.12	59/13454 (0.4%)
All	All	0.73	4/46140 (0.0%)	1.12	271/62610 (0.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1563	VAL	CA-CB	-6.26	1.51	1.55
2	B	584	VAL	C-O	5.80	1.30	1.24
2	D	584	VAL	C-O	5.67	1.30	1.24
1	C	686	ILE	CA-CB	5.07	1.60	1.54

The worst 5 of 271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1346	ASN	CA-CB-CG	12.98	125.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1346	ASN	CA-CB-CG	12.96	125.56	112.60
1	C	930	VAL	CA-C-N	11.60	134.34	119.84
1	C	930	VAL	C-N-CA	11.60	134.34	119.84
1	A	930	VAL	CA-C-N	11.25	133.90	119.84

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	1762	0
1	C	12881	0	12821	1740	0
2	B	9711	0	9702	1104	0
2	D	9711	0	9702	1112	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	5642	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 62.

The worst 5 of 5642 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

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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:D:1609:ARG:HG2	2:D:1609:ARG:HH11	1.12	1.13
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	8
1	C	1617/1676 (96%)	1179 (73%)	288 (18%)	150 (9%)	0	8
2	B	1215/1642 (74%)	998 (82%)	161 (13%)	56 (5%)	2	17
2	D	1215/1642 (74%)	995 (82%)	162 (13%)	58 (5%)	2	16
All	All	5664/6636 (85%)	4345 (77%)	903 (16%)	416 (7%)	1	11

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%)	1068 (74%)	378 (26%)	0	3
1	C	1446/1484 (97%)	1069 (74%)	377 (26%)	0	3
2	B	1093/1435 (76%)	834 (76%)	259 (24%)	1	5
2	D	1093/1435 (76%)	830 (76%)	263 (24%)	1	4
All	All	5078/5838 (87%)	3801 (75%)	1277 (25%)	0	4

5 of 1277 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1301	SER
2	D	742	ASP
1	C	1381	ILE
1	C	1294	ILE
2	D	162	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 166 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1234	HIS
2	D	525	GLN
1	C	1319	HIS
2	D	124	GLN
2	D	869	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 oligosaccharides 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	0.85	1 (7%)	17,19,21	2.08	3 (17%)
3	NAG	D	2002	2	14,14,15	0.94	0	17,19,21	1.18	1 (5%)
3	NAG	C	2003	1	14,14,15	0.59	0	17,19,21	2.24	4 (23%)
3	NAG	B	2002	2	14,14,15	0.94	0	17,19,21	1.19	1 (5%)
3	NAG	D	2001	2	14,14,15	0.78	1 (7%)	17,19,21	2.17	3 (17%)
3	NAG	A	2003	1	14,14,15	0.61	0	17,19,21	2.22	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	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	B	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	D	2001	2	-	2/6/23/26	0/1/1/1
3	NAG	A	2003	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	NAG	C1-C2	2.36	1.55	1.52
3	D	2001	NAG	C1-C2	2.08	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2001	NAG	C1-O5-C5	6.65	121.10	112.19
3	B	2001	NAG	C1-O5-C5	6.25	120.56	112.19
3	A	2003	NAG	C1-O5-C5	5.76	119.91	112.19
3	C	2003	NAG	C1-O5-C5	5.74	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	D	2001	NAG	1	0
3	A	2003	NAG	2	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%)	0.23	28 (1%) 69 54	90, 187, 312, 465	0
1	C	1627/1676 (97%)	0.27	47 (2%) 53 41	97, 186, 299, 486	0
2	B	1225/1642 (74%)	0.14	14 (1%) 78 62	107, 174, 261, 395	0
2	D	1225/1642 (74%)	0.17	20 (1%) 70 55	114, 181, 263, 371	0
All	All	5704/6636 (85%)	0.21	109 (1%) 66 51	90, 183, 291, 486	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	490	SER	4.4
2	D	642	ALA	3.8
1	A	1449	LEU	3.8
1	C	997	ILE	3.7
2	B	111	PRO	3.6

### 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, 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	2001	14/15	0.61	0.14	275,285,305,313	0
3	NAG	A	2003	14/15	0.62	0.21	284,286,289,289	0
3	NAG	B	2002	14/15	0.65	0.27	321,327,336,339	0
3	NAG	D	2002	14/15	0.66	0.19	289,293,305,308	0
3	NAG	D	2001	14/15	0.74	0.14	285,296,309,310	0
3	NAG	C	2003	14/15	0.81	0.19	260,272,284,287	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.