



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:53 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

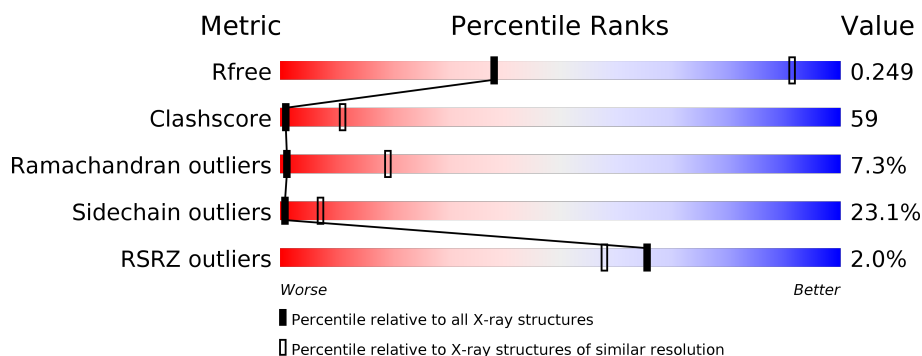
1 Overall quality at a glance

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}	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

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>2%</div> <div> <div></div> <div>24%</div> <div>52%</div> <div>20%</div> <div>• •</div> </div> </div>
1	C	1676	<div> <div>2%</div> <div> <div></div> <div>24%</div> <div>52%</div> <div>20%</div> <div>• •</div> </div> </div>
2	B	1642	<div> <div>%</div> <div> <div></div> <div>23%</div> <div>38%</div> <div>13%</div> <div>•</div> <div>25%</div> </div> </div>
2	D	1642	<div> <div>%</div> <div> <div></div> <div>23%</div> <div>38%</div> <div>13%</div> <div>•</div> <div>25%</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.

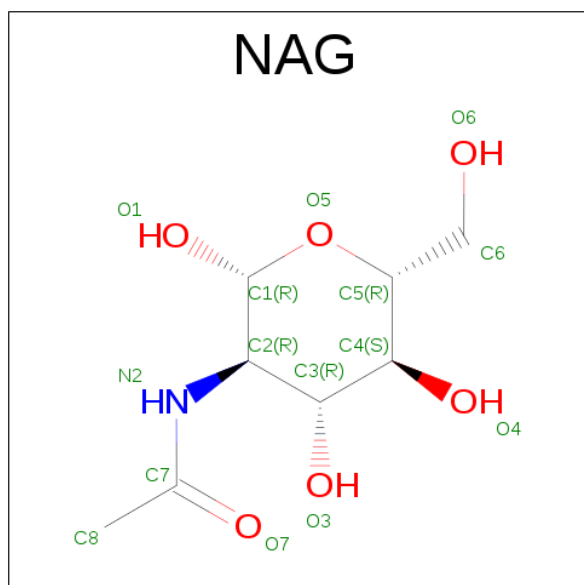
- Molecule 1 is a protein called Complement C5.

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

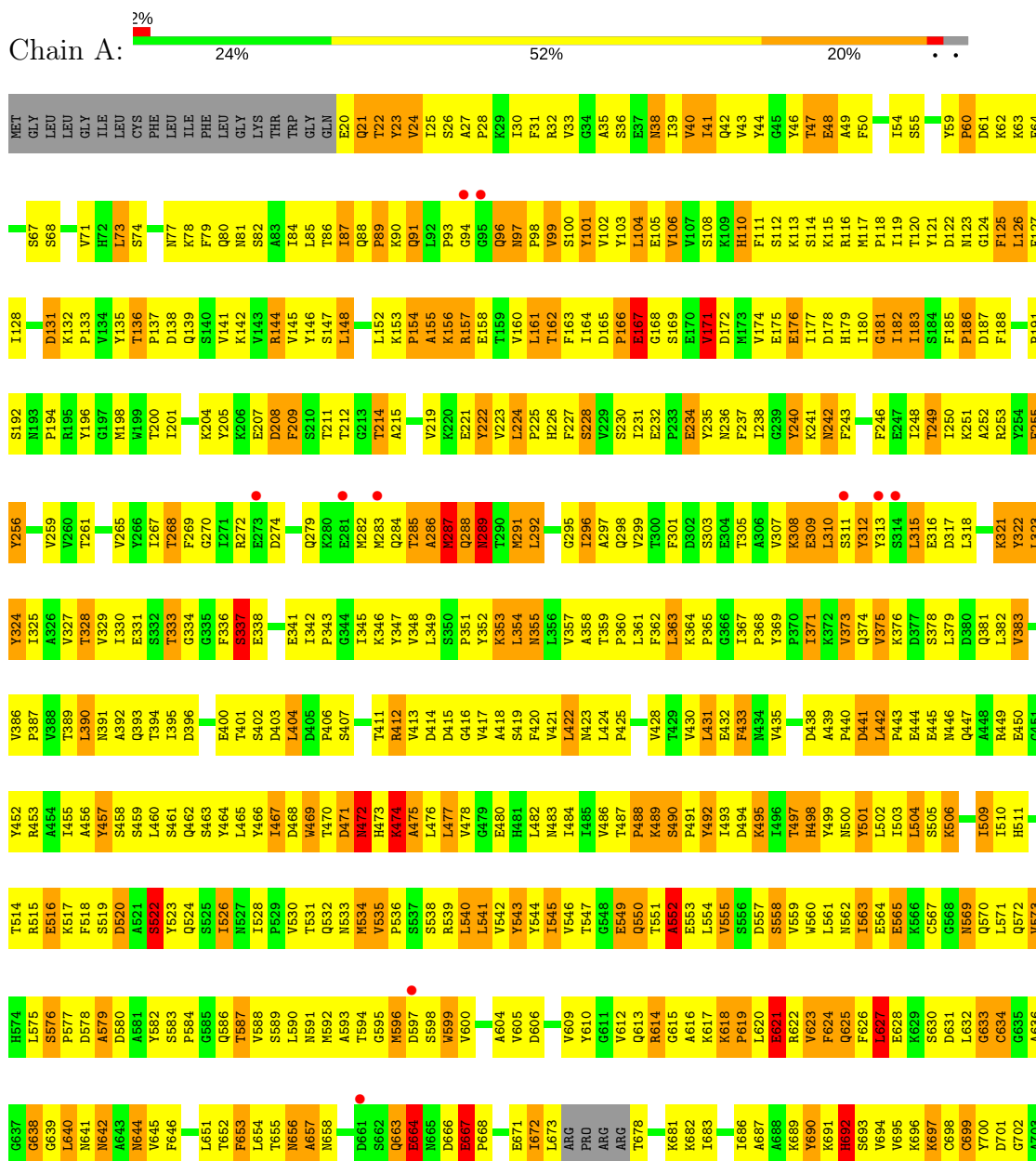


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

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 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

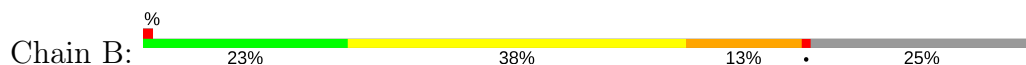


- Molecule 1: Complement C5



Q1043	Q1044	Q1045	Q1046	Q1047	Q1048	Q1049	Q1050	Q1051	Q1052	Q1053	Q1054	Q1055	Q1056	Q1057	Q1058	Q1059	Q1060	Q1061	Q1062	Q1063	Q1064	Q1065	Q1066	Q1067	Q1068	Q1069	Q1070	Q1071	Q1072	Q1073	Q1074	Q1075	Q1076	Q1077	Q1078	Q1079	Q1080	Q1081	Q1082	Q1083	Q1084	Q1085	Q1086	Q1087	Q1088	Q1089	Q1090	Q1091	Q1092	Q1093	Q1094	Q1095	Q1096	Q1097	Q1098	Q1099	Q1100	Q1101	Q1102	Q1103	Q1104	Q1105	Q1106	Q1107					
V1108	E1109	M1110	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						
F1174	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									
K1235	D1236	S1237	H1238	K1239	P1240	G1241	L1242	A1243	M1244	L1245	M1246	M1247	V1248	E1249	L1250	L1251	A1252	L1253	A1254	L1255	L1256	L1257	L1258	L1259	M1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	E1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	G1282	L1283	L1284	L1285	L1286	L1287	G1288	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								
T1363	V1364	L1365	H1366	K1367	L1368	S1369	L1370	L1371	E1372	E1373	V1374	L1375	E1376	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
D1502	K1503	Q1504	C1505	T1506	M1507	F1508	L1509	S1510	L1511	S1512	M1513	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	S1567	L1568	L1569	L1570	E1571	L1572	L1573	F1574	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										
Q1625	L1626	K1627	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										

• Molecule 2: Cobra venom factor



L188	P189	D190	L191	V192	S193	L194	G195	L196	L197	R198	L199	V200	K201	K202	K203	E204											P207	E208	E209	E210	E211	E212	E213	E214	E215	E216	E217	E218	E219	E220	E221	E222	E223	E224	E225	E226	E227	E228	E229	E230	E231	E232	E233	E234	E235	E236	E237	E238	E239	E240	E241	E242	E243	E244	E245	E246	E247	T248																					
F127	L128	F129	L130	Q131	T132	D133	K134	G135	L136	V137	T138	P139	G140	S141	P142	V143	L144	V145	L146	L147	F148	S149	M150	H151	H152	H153	H154	H155	H156	H157	H158	H159	H160	H161	H162	H163	H164	H165	H166	H167	H168											H171	H172	H173	H174	H175	H176	H177	H178	H179	H180	H181	F182	H183	H184	H185	H186	H187																					
Q65	K66	L67	L68	F69	Q70	T71	R72	V73	D74	M75	N76	P77	A78	G79	G80	M81	L82	R83	T84	P85	I86	T87	E88	E89	E90	E91	E92	E93	E94	E95	E96	E97	E98	E99	E100	E101	E102	E103	E104	E105	E106	E107	E108	E109	E110	E111	E112	E113	E114	E115	E116	E117	E118	E119	E120	E121	E122	E123	E124	E125	E126																												
MET	GLU	ARG	ARG	ALA	ALA	LEU	TYR	VAL	VAL	ALA	ALA	LEU	LEU	ILE	GLY	PHE	PRO	GLY	GLY	SER	SER	HIS	HIS	GLY	A23	L24	E25	L26	L27	I28	T29	P30	A31	V32											T35	D36											E39	Q40	I41	L42	V43	E44	A45	H46	G47	D48											K52	Q53	L54	D55	I56	F57	V58	H59	D60	F61	P62	R63	E64

R1289	ASP	ARG	VAL	SER	ILE	V925	E849	V789	SER	ALA	W599	V526	V462	G394	T322	V251
Y1290	GLN	PRO	LEU	THR	THR	T926	L850	L790	GLU	ALA	T602	G527	N463	T395	E323	L252
R1291	THR	THR	SER	ALA	PRO	Y927	L851	A791	LEU	GLU	E603	N528	F464			Y253
N1292	GLY	THR	GLY	ALA	SER	V928	T852	T792	PHE	PHE	E604	N529	N465	L398	S326	
N1293	PRO	THR	THR	THR	GLY	K929	N853	S793	LEU	GLN	K604	E530	V466	L399	M327	E257
Y1294	ILE	ALA	MET	THR	CYS	L930		T794	ALA	ASP	S605	I531	K467	L400	M328	
E1295	VAL	LEU	GLN	ASN	GLY		F856	T795	ASN	GLN	D606	V532	G468	N401	V329	G259
N1296	ARG	THR	GLY	ARG	GLY	R933	C857	T796	ASP	ASP	F607	A533	N469	I402	V330	V260
A1297	TRP	ALA	GLN	ALA	GLN			T797	ASP	LEU	G608	D534	A470	F403	A261	
L1298	LEU	THR	ILE	SER	ASN	V937	S860	K798	N735	LYS	S613	S535	N471	F404	V262	
L1299	THR	ALA	GLN	SER	ILE	G938	T861	G799	F737	CYS	G614		S472	L404	V263	
A1300	GLY	LEU	GLY	SER	ARG	G939	K862	I800	N736	CYS	G615	V538	L473	Q407	L264	
R1301	ALA	ALA	ALA	TRP	ARG	T940	C863	C801	G738	CYS	G616		L476	S408	L265	
T1302	ASN	ALA	GLU	LEU	MET	Q941	S864	V602	F739	GLU	N616	K541	I477	L409	G266	
V1303	PHE	ALA	GLU	THR	ALA	L942	R865	A903	D742	ASP	N617	D542	K477	P410	V267	
V1304	ASP	ALA	GLU	ALA	ALA	E943	T866	E804	T543	VAL	L618	C544	F478	A340	K268	
T1305	GLY	GLN	VAL	THR	PRO	V944	R867	P805	S743	MET	G619	C544	F479	S341	T269	
K1306	GLU	LEU	THR	VAL	VAL	I945	Q868	T806	D744	HIS	V620	N545	T480	R414	T415	
L1307	THR	ASN	LEU	VAL	ILE	K946	O869	T807	I745	GLU	F621	G546	T481	N416	Y343	
N1308	THR	ASP	THR	LYS	ALA	A947	F870	T808	I746	ASN	E622	T547	L482	H417	Q344	
Q1309	GLY	ASP	ALA	VAL	THR	R948	P871	R809	S747	PRO		L548	L483	G418	T277	
D1310	GLN	ARG	PHE	PHE	THR	K949	T872	V810	R748	MET	G625	V549	L484	D419	H346	D278
I1311	THR	VAL	ILE	ALA	THR	L950	K873	N811	S749	GLY	L626	V550	N485	L420	S279	
T1312	GLN	LEU	LEU	MET	ASP	D951		K812	T750	THR	A627		K486	P421	T348	
V1313	ALA	MET	VAL	ALA	ASP	D952	B878	V813	F751	THR	L628	D553	G487	B422	T281	
T1314	THR	ALA	ALA	ALA	THR	R953		F814	P752	CYS	T629	N554	K488	E423	R282	
A1315	VAL	ALA	LEU	LYS	THR	V954	P881	F815	K753	GLU	T630	I556	L489	R424	P351	
S1316	MET	SER	LEU	MET	GLU	P955	F882	T816	S754	LYS	S631	I556	P490	Q425	K352	P284
D1317	ALA	THR	GLY	VAL	GLN	T956	N883	D817	T755	ARG	K491	Q557	F492	A426	Y353	T285
G1318	PHE	GLY	SER	ALA	TRP	T957	T894	L818	L756	ALA	L634	N558	V492	T427	F354	
G1319	GLN	ARG	LYS	GLY	GLU	K958	V885	Q819	T757	LYS	N635	P559	G493	K428	K355	D289
K1320	ALA	ASP	THR	ILE	THR	I959	P886	N820	L758	THR	T636	G560	R494	S429	P356	G290
A1321	LEU	HIS	ILE	SER	LEU	E960	L887	P821	T759	ILE	K637		Q495	N430	G357	K291
T1322	ALA	TRP	CYS	HIS	GLY	T961	S888	Y822		GLU	P638	M563	P496	T431	M358	
M1323	GLU	GLU	ASN	GLU	ILE	K962	Q889	S823	L762	GLU	R639	K564	R497	A432	P359	
T1324	TYR	ASP	ASP	ASN	ASN	I963	G890	V824	E763	ASP	S640		I433	I433		L294
I1325	GLU	TYR	TYR	ILE	ARG	T964	L891	V825	E764	ASP	A641	L567	Q501	A434	V364	K295
L1326	ILE	ASN	VAL	CYS	ARG	I965		K826	F765	ALA	A642		N502	K435	Y365	K296
T1327	GLN	ALA	ASN	GLY	THR	Q966	T896	E828	P766	CYS	K643	D570	L503	Q436	D297	T298
F1328	PRO	HIS	SER	VAL	GLU	G967	K897	Q829	Q769	ALA	Q646	R574	V504	Q437	D370	F299
N1330	THR	HIS	ASP	ARG	VAL	D968	A898	V830	G770	ALA	P647		M506	Q439	P373	S301
A1331		ASN	SER	TRP	ASN	VAL	Q901	E831	I771	PHE	A648	L577	N507	G440	H376	R302
Q1332	H1270	ILE	LEU	LEU	GLN	ALA	E902	T832	S772	LEU	ASN		L508	S441	V377	F303
L1333	L1273	GLY	ILE	ILE	ILE	GLN	A903	R833	S773	GLU	ARG	V580	H509	G442	G377	L306
L1274	GLN	THR	LYS	LEU	VAL	ILE		A834	K774	CYS	ARG	D581	T510	N443	P378	
D1275	THR	LYS	LYS	ASN	THR	ILE	K911	T835	T775	CYS	ARG	K582	T511	Y444	V379	L309
D1276	SER	ALA	ARG	GLY	GLY	GLU	K912	L836	M776	ARG	ARG	A583	P612	L445	V380	
I1277	TYR	THR	THR	ASN	THR	ASN	L913	H837	S777	TYR	SER	V584	D513	H446	S381	V310
T1278	ALA	ALA	ASN	GLN	ALA	SER	K914	N838	F778	ILE	SER	Y585	L514	V447	E382	G311
I1279	LEU	LEU	TYR	GLN	GLN	ILE	V915	Y839	T779	LYS	VAL	V586	L515	A448	A383	H312
E1280	LEU	LEU	ASP	ASP	GLN	ASP	P916	N840	L780	GLY	LEU	L587	F518	T449	F394	T313
L1281	ALA	ALA	GLY	GLY	MET	GLY	P917	N841	R781	VAL	LEU	N588	T450		L314	L309
P1282	LEU	LEU	SER	ALA	VAL	SER	E918	E842	D782	ARG	LEU		R519		S386	V315
D1283	LYS	LYS	LYS	THR	THR	LYS	G919	D843	S783	ASP	GLU	I593	F520	K455	M37	A316
H1344	LEU	LYS	LYS	LYS	LYS	LEU	V920	T844	I784	GLY	SER	S594	V501		G388	S317
L1345	MET	MET	ASN	ASN	LYS	ASN	Q921	V845	T785	ASN	ASN	Q595	A522	D458	T389	V318
E1285	LYS	LYS	HIS	ASN	ALA	HIS	R922	V846	T786	GLN	ALA	A596	Y523	N459	T390	T319
R1346	P1287	LYS	LEU	ALA	ASP	LYS	S923	R847	W787	ARG	SER	K597	Y524	L460	V320	V320
S1348	I1288	PHE	GLN	PRO	HIS	ILE	T924	V848	V788	GLU	LYS	I598	Q525	P461	D393	X321





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 , 172.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 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, 0.333 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(°)	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	14
1	C	1617/1676 (96%)	1179 (73%)	288 (18%)	150 (9%)	1	14
2	B	1215/1642 (74%)	998 (82%)	161 (13%)	56 (5%)	3	30
2	D	1215/1642 (74%)	995 (82%)	162 (13%)	58 (5%)	2	29
All	All	5664/6636 (85%)	4345 (77%)	903 (16%)	416 (7%)	1	19

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	7
1	C	1446/1484 (97%)	1109 (77%)	337 (23%)	1	7
2	B	1093/1435 (76%)	845 (77%)	248 (23%)	1	8
2	D	1093/1435 (76%)	845 (77%)	248 (23%)	1	8
All	All	5078/5838 (87%)	3907 (77%)	1171 (23%)	1	7

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 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	0.59	0	15,19,21	2.30	4 (26%)
3	NAG	B	2001	2	14,14,15	0.82	1 (7%)	15,19,21	2.17	3 (20%)
3	NAG	B	2002	2	14,14,15	0.91	0	15,19,21	1.35	1 (6%)
3	NAG	C	2003	1	14,14,15	0.57	0	15,19,21	2.32	4 (26%)
3	NAG	D	2001	2	14,14,15	0.75	0	15,19,21	2.23	3 (20%)
3	NAG	D	2002	2	14,14,15	0.91	0	15,19,21	1.34	1 (6%)

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	2.26	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	NAG	O5-C1-C2	-4.33	105.45	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2002	NAG	O5-C1-C2	-4.31	105.48	111.47
3	C	2003	NAG	C1-C2-N2	-3.17	105.07	110.49
3	A	2003	NAG	C1-C2-N2	-3.07	105.25	110.49
3	D	2001	NAG	C2-N2-C7	-2.54	119.24	122.94

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%)	0.03	38 (2%) 61 53	90, 187, 312, 465	0
1	C	1627/1676 (97%)	0.02	33 (2%) 65 58	97, 186, 299, 486	0
2	B	1225/1642 (74%)	-0.00	24 (1%) 65 58	107, 174, 261, 395	0
2	D	1225/1642 (74%)	-0.00	18 (1%) 74 66	114, 181, 263, 371	0
All	All	5704/6636 (85%)	0.01	113 (1%) 65 58	90, 183, 291, 486	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1355	ASN	5.2
1	A	1585	TYR	5.0
2	B	155	SER	5.0
1	A	1622	LYS	5.0
2	B	156	LYS	4.9

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	2.56	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	0.72	0.35	-	260,272,284,287	0
3	NAG	A	2003	14/15	0.64	0.38	-	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.