



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3PRX
Title : Structure of Complement C5 in Complex with CVF and SSL7
Authors : Laursen, N.S.; Andersen, G.R.; Sottrup-Jensen, L.; Andersen, K.R.; Spillner, E.; Braren, I.
Deposited on : 2010-11-30
Resolution : 4.30 Å(reported)

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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

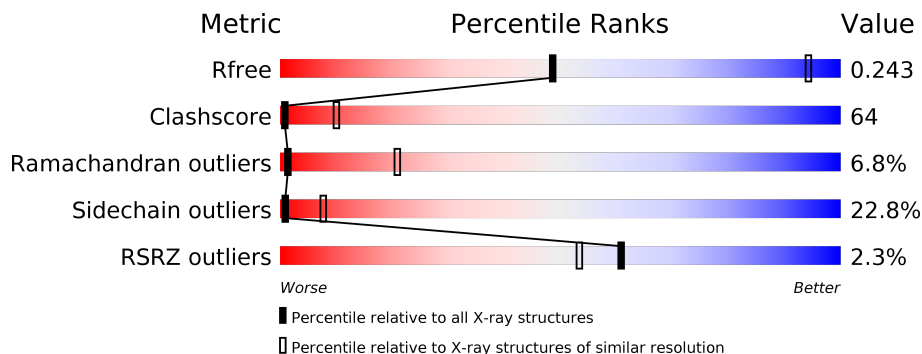
1 Overall quality at a glance

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>24%</div> <div>50%</div> <div>21%</div> <div>• •</div> </div>
1	C	1676	<div> <div>3%</div> <div>23%</div> <div>51%</div> <div>21%</div> <div>• •</div> </div>
2	B	1642	<div> <div>23%</div> <div>38%</div> <div>13%</div> <div>26%</div> </div>
2	D	1642	<div> <div>22%</div> <div>39%</div> <div>12%</div> <div>26%</div> </div>
3	X	231	<div> <div>11%</div> <div>26%</div> <div>44%</div> <div>11%</div> <div>•</div> <div>17%</div> </div>
3	Y	231	<div> <div>6%</div> <div>24%</div> <div>45%</div> <div>13%</div> <div>•</div> <div>17%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48236 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	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			
1	C	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			
2	D	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			

- Molecule 3 is a protein called Superantigen-like protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			
3	Y	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

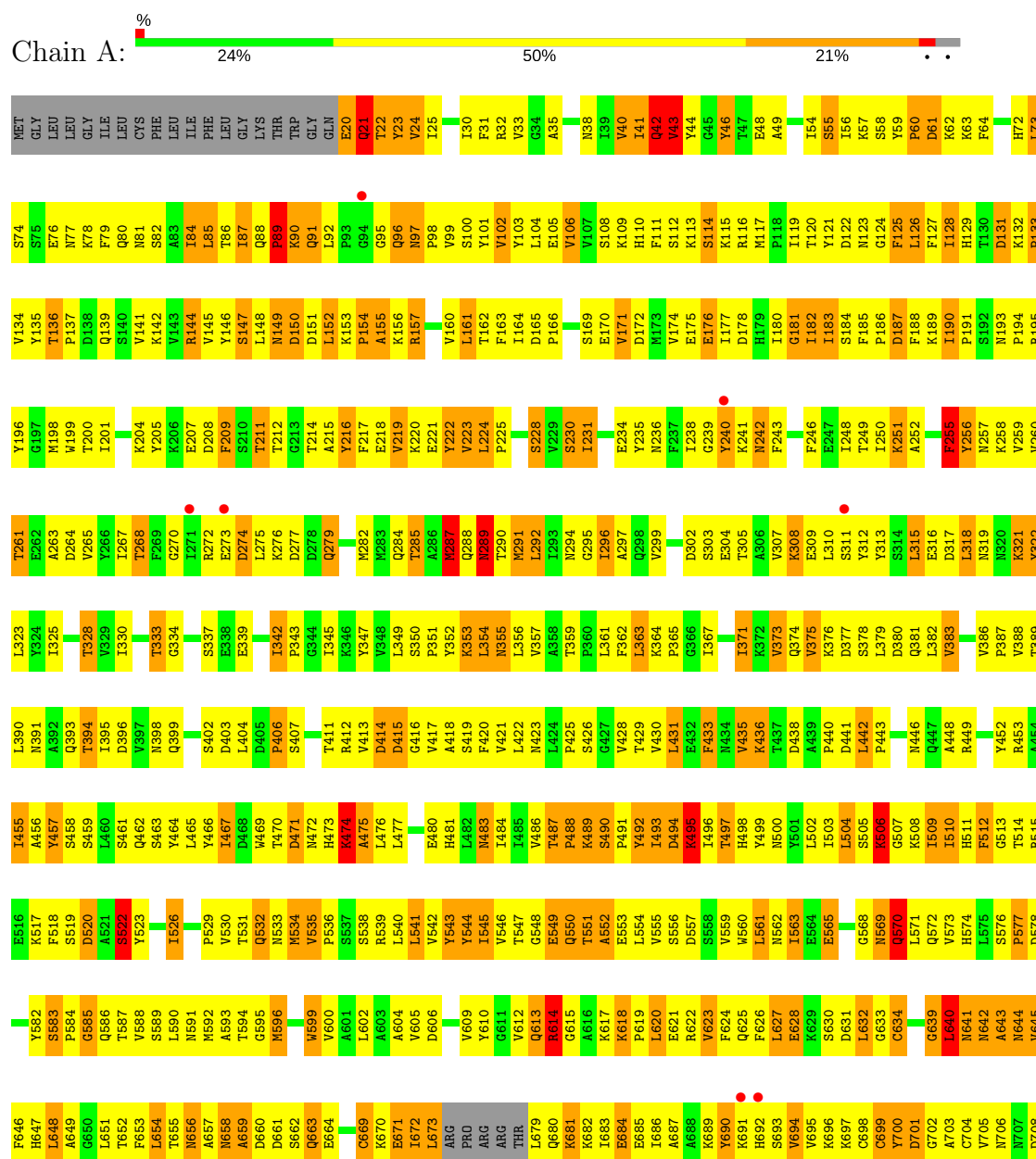
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

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

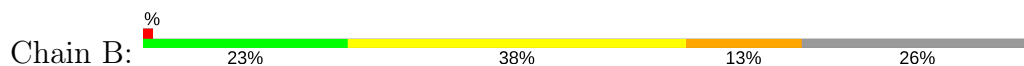


- Molecule 1: Complement C5



L967	M1029	M1088	V1162	D1230	A1293	L1356	H1421	V1485	E1546	C1606	F1672
V968	H1030	S1099	K1163	M1231	A1293	A1357	A1422	G1486	T1547	T1607	L1673
P969	M1031	I1100	I1164	L1232	I1294	T1358	V1423	F1487	R1548	A1609	M1674
K970	M1032	C1101	D1165	K1233	I1294	E1359	E1423	L1488	K1549	E1608	G1675
T971	M1033	M1102	T1166	H1234	G1296	H1360	I1426	S1489	Q1550	E1610	C1676
E972	F1034	S1103	A1167	K1235	L1297	V1361	I1427	P1490	T1551	L1611	
I973	H1035	L1104	L1168	D1236	T1298	T1362	L1428	A1491	A1552	L1612	
K974		L1105		S1237	T1298	T1363	P1429	L1492	C1553	K1613	
R975	E1041	M1106	A1171	S1238	E1299	V1364	T1430	F1493	K1554	G1614	
L976	K1042	L1107	L1175	P1239	S1301	V1365	G1431	T1494	P1555	K1615	
L977		V1108	L1176	P1240	L1302	H1366	I1432	V1496	E1556	Q1616	
S978	K1047	E1109	L1176	M1241	L1303	K1367	S1433	Y1496	I1557	L1617	
W979	K1048	M1110		T1242	V1304	T1368	A1434	A1553	A1558	L1618	
X980	L1049	M1111		G1243	K1305	S1369	M1435	Y1498	Y1559	L1619	
G981	K1050	Y1111		E1249	K1305	T1370	E1436	H1499	A1560	M1620	
L982	K1051	M1112		T1250	Q1306	Q1371		R1500	Y1561	G1621	
L983	M1052	L1113		T1251	L1307	S1371		T1506	K1562	K1622	
V984	G1053	M1121		A1252	R1308	E1372		M1507	V1563	E1623	
G985	L1054	S1122		M1247	L1309	E1373			S1564	A1624	
E986	S1055	Q1123		V1248	I1318				T1565	L1625	
S987	S1056	Y1124		E1249	H1319	S1376	V1443	Q1504	T1566	Q1626	
L988	M1057	Y1125		T1250	K1320	F1377	E1444	C1505	S1567	I1627	
S989	S1058	T1251		T1251	G1321	Y1378	G1445	E1507	I1568	K1628	
A990	M1061	M1121		A1252	S1316	L1379	V1446		T1569	Y1629	
		S1122		Y1253	Y1317	K1380	D1447	S1540	E1570	M1630	
		Q1123		A1254	K1318	E1387	Q1448	T1511	E1571	F1631	
S993		Y1124		L1255	H1319	D1382	L1449	M1512	M1572		
G994	Y1064	P1125		L1256	S1320	T1383	F1450	M1513	V1573	Y1635	
E995	S1065	T1257		T1257	G1321	Q1384	L1451	N1514	F1574	I1636	
G996	Y1066	T1257		S1258	A1194	L1385	D1452	L1514	V1575	Y1637	
S997	S1067	K1128		L1259	L1322	T1386	Y1453	L1514	T1576	P1638	
N998	V1068	L1129		N1260	H1324	E1387	Q1454	T1515	K1576	L1639	
I999	V1069	Q1130		L1261	N1325	ALA	I1455	G1516	Y1577	D1640	
L1000	K1070	G1131		K1262	Y1326	SER	I1456	ALA	K1578	S1641	
T1001	G1071	T1132		D1263	M1327	HIS	D1457	ALA	A1579	L1642	
H1002	G1072	L1133		T1264	M1328	TYR	K1458	GLY	L1581	T1643	
L1003	S1073	P1134		N1265	T1329	ARG	H1459	GLY	L1582	V1644	
P1004	A1074	V1135		Y1266	D1330	GLY	I1460	ALA	D1583	I1645	
K1005	S1075			V1267	K1331	TYR	I1461	ALA	T1584	E1646	
G1006	T1076			N1268	M1332	ASN	Q1462	C1525	Y1585	Y1647	
S1007	W1077			P1269	F1333	GLY	L1464	K1526	K1586	W1648	
A1008	L1078			K1270	L1334	D1398	L1465	C1527	T1587	P1649	
	T1079			I1271	G1335	Y1399	S1466	V1528	G1588	R1650	
E1011	A1080			K1272	P1336	K1400	I1467	E1529	E1589	D1651	
L1012	F1081			W1273	P1337	R1401	P1468	A1530	A1590	T1652	
M1013	A1082			L1274	V1338	I1402	S1469	D1531	V1591	C1654	
S1014	L1083			S1275	E1339	I1403	S1470	C1532	A1592	T1654	
V1015	R1084			E1276	V1340	A1404	D1471	G1533	E1593	L1655	
V1016	V1085			E1277	L1341	C1405	F1472	Q1534	K1594	E1665	
P1017	L1086			Q1278	L1342	C1406	L1473	M1535	D1594	E1666	
V1018	G1087			R1279	M1343	A1407	C1474	Q1536	D1595	F1667	
F1019	Q1088			Y1280	D1344	S1407	V1475	E1537	S1596	L1668	
Y1020	L1152			G1283	D1345	Y1408	R1476	E1538	E1597	M1669	
V1021	R1089			F1284	L1346	K1409		L1541	F1600	K1602	
F1022	M1090			N1221	L1347	P1410		L1542	I1601	A1668	
N1023	A1155			P1222	V1348	S1411		I1543	K1603	E1669	
H1023	F1156			S1285	S1349			S1544	V1604	D1670	
V1024	D1157			T1287	T1350	E1414		A1545	T1605	I1671	
L1025	I1158			Q1288	G1351	S1415					
E1026	Q1095			L1288	F1352	S1416					
T1027	M1096			T1290							
G1028	Q1097										

• Molecule 2: Cobra venom factor

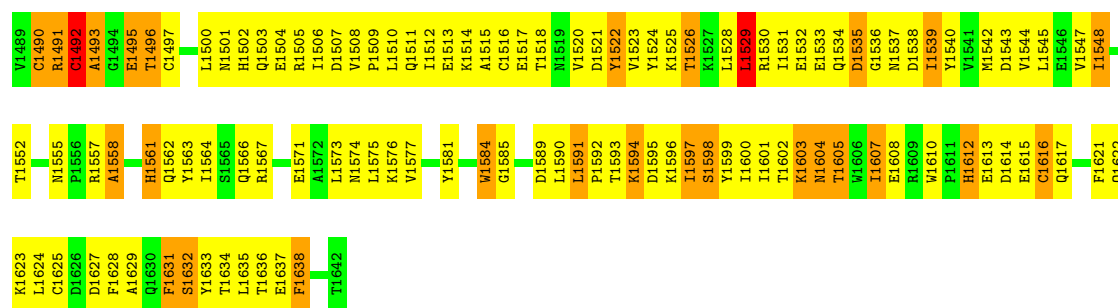


MET	R63	E39	P51	F1660	K52	Q53	L54	D55	L56	F57	V58	H59	P61	P62
GLU	K64	Q40	K41	L1661	A1662	M1663	D1664	E1665	E1666	F1667	V1668	S1669	S1670	I1671
ARG	Q65	L41	L42	M1662	M1663	L1664	L1665	E1666	F1667	V1668	S1669	S1670	I1671	
MET		L42	V43	L1663	L1664	L1665	E1666	F1667	V1668	S1669	S1670	I1671		
ALA		E44	E45	L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
LEU		A45	H46	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	S1670	I1671
TYR		G47	D48	L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
LEU				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
VAL				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
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R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R77				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R73				L1660	L1661	L1662	L1663	L1664	L1665	E1666	F1667	V1668	S1669	I1671
R72				L1660	L1661	L1662</								

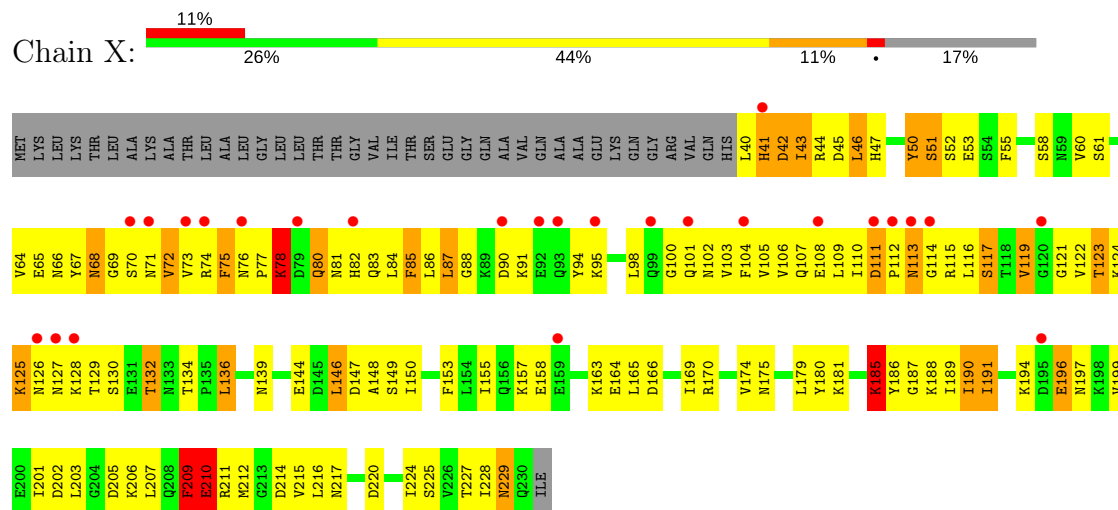




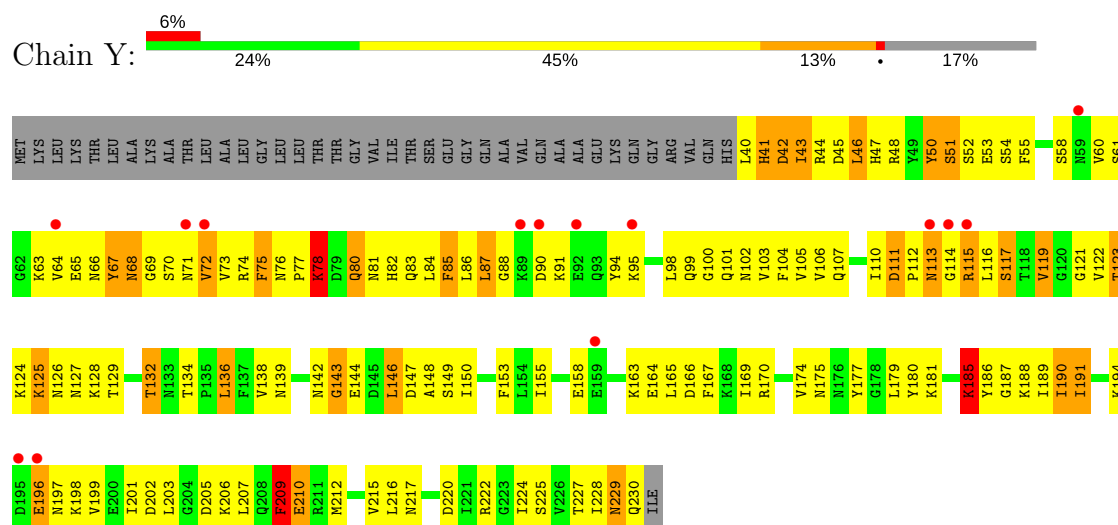
K4422	V1349	V1286	LYS	LEU	ALA	ASP	LEU	ILE	I924	T861	I800	G608	V538	K4713
V1423	E1360	P1287	PHE	GLN	PRO	HIS	GLN	ILE	V925	K862	C801	C609	V538	K4713
I1424	E1351	I1288	ASP	ARG	VAL	SER	ARG	ILE	I926	K863	V802	T610	K541	S472
I1425	I1352	I1289	GLN	PRO	LEU	TYR	LEU	THR	I927	Q864	A803	A611	K541	Q475
Y1426	H1353	Y1290	THR	SER	GLY	ALA	SER	PRO	V928	R865	R805	R612	T543	L476
L1427	L1354	L1291	GLY	THR	GLY	ALA	SER	GLY	K929	R866	E804	S613	C544	K477
N1428	ASN	I1292	PRO	THR	THR	PHE	GLY	GLY	L930	R867	Y806	G614	M646	Y478
K1429	ALA	M1293	ILE	THR	THR	THR	CYS	CYS	D931	Q868	E907	Q615	G546	F479
V1430	MET	Y1294	VAL	LEU	GLN	ASN	GLY	GLU	P932	Q869	I808	N616	T547	T480
S1431	GLY	E1295	ARG	THR	GLY	ARG	GLY	GLN	R933	F871	R809	N617	L548	Y481
H1432	ALA	M1296	TRP	ALA	GLY	ALA	ALA	GLN	Q933	P870	R809	M710	V549	L482
K1433	K1360	A1297	THR	ILE	ILE	SER	SER	ASN	V937	Q873	M811	G619	V550	L483
E1434	THR	L1298	LEU	ALA	GLN	SER	SER	MET	G938	K874	K812	T620	K551	L484
L1363	ASP	L1299	ASP	GLY	GLY	SER	SER	ILE	G939	A874	V813	F621	G552	L488
E1436	GLN	A1300	GLN	ALA	ALA	TRP	TRP	ARG	T940	L875	F814	E622	N553	K489
M1364	ASN	R1301	ASN	ALA	GLU	LEU	LEU	MET	Q941	S876	F815	A626	N554	L489
K1365	THR	T1302	PHE	ALA	GLU	THR	THR	ALA	L942	S877	I816	L626	L555	F490
K1366	THR	V1303	THR	GLY	GLU	ALA	ALA	ALA	E943	R878	D817	T628	I566	K491
C1368	GLY	E1304	GLY	VAL	VAL	TYR	TYR	PRO	V944	A879	L818	T629	Q557	Y492
T1369	LEU	T1305	GLY	THR	TYR	VAL	VAL	VAL	I945	V880	Q819	T630	M558	G493
R1370	ASN	M1308	THR	LEU	VAL	VAL	VAL	ILE	K946	P881	P820	G560	P559	R494
Y1371	ASP	Q1309	ASP	THR	ALA	LYS	ALA	ALA	A947	V882	Y822	ARG	A561	R497
L1372	GLN	D1310	ARG	PHE	ALA	PHE	ALA	TYR	K949	V884	S823	ALA	A562	R498
S1377	THR	I1311	VAL	ILE	ILE	ALA	ALA	TYR	L950	V885	V824	LYS	M563	L502
T1378	GLN	T1312	LEU	LEU	LEU	MET	LEU	LEU	D951	P886	V825	TYR	K564	L503
M1379	THR	V1313	MET	VAL	VAL	ALA	ASP	ASP	D952	L887	R826	ILE	I566	L504
T1380	ALA	T1314	ALA	ALA	ALA	ALA	THR	THR	R953	E888	N827	GLN	K566	V504
V1381	VAL	A1315	VAL	ALA	LEU	LYS	THR	THR	V954	Q889	Q828	GLY	L567	V504
I1382	MET	I1318	MET	SER	LEU	MET	GLY	GLY	P955	Q890	V830	ASP	E568	T505
D1383	ALA	G1319	ALA	THR	GLY	VAL	VAL	GLN	D956	L891	V831	ASP	G569	N506
I1384	PHE	G1319	PHE	SER	SER	ALA	ALA	TRP	P957	E895	E831	ALA	D570	N507
S1385	GLN	T1322	GLN	LYS	LYS	GLY	GLY	GLU	E958	E896	I832	CYS	A573	L508
S1386	ALA	M1323	ALA	THR	THR	ILE	ILE	THR	P959	K896	R833	LYS	R574	L509
L1387	ALA	T1324	ALA	TRP	CYS	HIS	HIS	GLY	E960	K897	I835	ALA	V575	L510
F1390	GLY	I1325	GLY	GLY	ASN	GLY	GLY	ILE	K962	A898	L836	ALA	P612	T511
L1391	TYR	L1326	TYR	GLY	ASP	ILE	ASN	ASN	I963	Q901	H837	PRO	V880	P512
P1392	GLY	T1327	GLY	THR	THR	ILE	ILE	ARG	I964	E902	N838	ALA	D551	D513
F1328	ILE	F1328	ILE	ASN	VAL	CYS	ARG	ARG	P965	A903	Y839	ARG	K552	D514
Y1329	GLN	Y1329	GLN	ALA	ASN	GLY	THR	THR	Q966	L904	V840	ARG	A583	L515
M1330	MET	N1330	MET	HIS	SER	GLY	GLY	GLY	G967	W905	N841	ARG	V584	F518
A1331	PRO	A1331	PRO	THR	LEU	VAL	VAL	ALA	D968	S906	E842	SER	Y585	R519
Q1332	THR	Q1332	THR	THR	ASP	ARG	ASP	VAL	P969	D907	D843	ILE	F520	F520
L1333	HIS	L1333	HIS	ASN	SER	TRP	TRP	ASN	VAL	G968	I844	VAL	N588	V521
GLN	K1271	GLN	K1271	ILE	SER	LEU	TRP	GLN	ALA	V909	Y845	GLY	A522	A522
LYS	D1272	LYS	D1272	ILE	SER	LEU	ILE	ILE	GLN	V910	V846	VAL	I593	Y523
ALA	N1274	ALA	N1274	LYS	ILE	ILE	ILE	VAL	ILE	K911	R847	ARG	S594	Y524
ASN	L1275	ASN	L1275	THR	LYS	ASN	ASN	THR	ILE	K912	T786	ASP	Q595	Q525
V1339	D1276	V1339	D1276	THR	ALA	ARG	ARG	GLY	GLY	L913	L850	SER	V526	V526
C1340	T1277	C1340	T1277	THR	THR	GLN	GLN	TYR	VAL	K914	L851	ASN	I598	G527
M1341	ALA	M1341	ALA	ASN	ALA	GLN	GLN	ALA	SER	V915	N852	ALA	M599	N528
K1342	LEU	K1342	LEU	TYR	TYR	PRO	PRO	ILE	ILE	V916	N853	ARG	D600	N529
E1280	LEU	E1280	LEU	LEU	LEU	ASP	GLN	GLN	ASP	P917	P854	LYS	T601	E530
F1343	ALA	F1343	ALA	LEU	LYS	GLY	GLY	MET	GLY	E918	A855	SER	I602	T531
H1344	LEU	H1344	LEU	LYS	LYS	ALA	ALA	VAL	SER	G919	F856	ALA	E603	V532
L1345	LEU	L1345	LEU	LYS	LYS	PHE	PHE	TYR	LYS	V920	C857	LEU	K604	A533
M1346	LYS	M1346	LYS	TYR	TYR	LYS	LYS	LYS	LEU	Q921	S958	PHE	S605	D534
V1347	MET	V1347	MET	GLU	GLU	GLY	GLY	LYS	ASN	K922	A859	GLN	D606	S535
E1285	LYS	E1285	LYS	LYS	LYS	ASN	ASN	ALA	HIS	S923	S860	ASP	F607	F607



• Molecule 3: Superantigen-like protein 7



• Molecule 3: Superantigen-like protein 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	163.65Å 181.96Å 392.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 4.30 49.21 – 4.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.21-4.30) 96.9 (49.21-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.208 , 0.261 0.191 , 0.243	Depositor DCC
R_{free} test set	1815 reflections (2.33%)	DCC
Wilson B-factor (Å ²)	116.2	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 160.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	48236	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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

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	0.60	1/13151 (0.0%)	0.80	3/17841 (0.0%)
1	C	0.60	0/13151	0.80	5/17841 (0.0%)
2	B	0.53	1/9833 (0.0%)	0.73	2/13345 (0.0%)
2	D	0.54	0/9833	0.74	3/13345 (0.0%)
3	X	0.47	1/1560 (0.1%)	0.67	1/2096 (0.0%)
3	Y	0.49	0/1560	0.69	1/2096 (0.0%)
All	All	0.57	3/49088 (0.0%)	0.77	15/66564 (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	2
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	210	GLU	C-N	5.35	1.46	1.34
2	B	347	PHE	CB-CG	-5.29	1.42	1.51
1	A	42	GLN	CB-CG	5.16	1.66	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	PHE	CB-CA-C	-7.26	95.88	110.40
2	D	347	PHE	CB-CA-C	-6.90	96.60	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	640	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	871	PRO	CA-N-CD	-6.16	102.87	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1504	GLN	Peptide
1	A	98	PRO	Peptide
1	C	1504	GLN	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	12874	0	12814	1855	0
1	C	12874	0	12814	1901	0
2	B	9635	0	9630	1082	0
2	D	9635	0	9630	1079	0
3	X	1539	0	1530	166	0
3	Y	1539	0	1530	194	0
4	A	14	0	13	1	0
4	C	14	0	13	2	0
5	B	56	0	50	6	0
5	D	56	0	50	7	0
All	All	48236	0	48074	6152	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 64.

The worst 5 of 6152 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)
1:A:1525:CYS:O	1:A:1528:VAL:HG22	1.34	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:207:LEU:O	3:X:207:LEU:HD12	1.32	1.24
3:Y:207:LEU:HD12	3:Y:207:LEU:O	1.32	1.23
1:C:386:VAL:H	1:C:411:THR:HG22	1.03	1.17
1:A:500:ASN:HB2	1:A:543:TYR:CE1	1.79	1.17

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1616/1676 (96%)	1165 (72%)	300 (19%)	151 (9%)	1	14
1	C	1616/1676 (96%)	1179 (73%)	290 (18%)	147 (9%)	1	15
2	B	1203/1642 (73%)	981 (82%)	176 (15%)	46 (4%)	4	34
2	D	1203/1642 (73%)	982 (82%)	177 (15%)	44 (4%)	4	35
3	X	189/231 (82%)	148 (78%)	31 (16%)	10 (5%)	2	27
3	Y	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	2	25
All	All	6016/7098 (85%)	4605 (76%)	1002 (17%)	409 (7%)	1	21

5 of 409 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	60	PRO
1	A	89	PRO
1	A	96	GLN
1	A	150	ASP

5.3.2 Protein sidechains ⓘ

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	1445/1484 (97%)	1090 (75%)	355 (25%)	1	6
1	C	1445/1484 (97%)	1098 (76%)	347 (24%)	1	6
2	B	1084/1435 (76%)	849 (78%)	235 (22%)	1	8
2	D	1084/1435 (76%)	855 (79%)	229 (21%)	1	9
3	X	175/205 (85%)	143 (82%)	32 (18%)	2	14
3	Y	175/205 (85%)	142 (81%)	33 (19%)	2	13
All	All	5408/6248 (87%)	4177 (77%)	1231 (23%)	1	8

5 of 1231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1480	LEU
1	C	435	VAL
2	D	1480	LEU
2	B	1539	ILE
1	C	161	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	77	ASN
1	C	658	ASN
3	X	113	ASN
1	C	97	ASN
1	C	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

8 carbohydrates 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$
5	NAG	B	2001	2,5	14,14,15	0.99	1 (7%)	15,19,21	2.11	5 (33%)
5	NAG	B	2002	5	14,14,15	1.02	1 (7%)	15,19,21	2.45	4 (26%)
5	NAG	B	2003	2,5	14,14,15	2.07	7 (50%)	15,19,21	3.37	7 (46%)
5	NAG	B	2004	5	14,14,15	1.70	1 (7%)	15,19,21	2.11	5 (33%)
5	NAG	D	2001	2,5	14,14,15	0.90	1 (7%)	15,19,21	2.09	6 (40%)
5	NAG	D	2002	5	14,14,15	1.08	1 (7%)	15,19,21	1.76	4 (26%)
5	NAG	D	2003	2,5	14,14,15	2.00	6 (42%)	15,19,21	3.55	7 (46%)
5	NAG	D	2004	5	14,14,15	1.59	1 (7%)	15,19,21	2.25	5 (33%)

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
5	NAG	B	2001	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2002	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2004	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2001	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2002	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2004	5	-	0/6/23/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2003	NAG	C3-C2	2.11	1.57	1.52
5	B	2003	NAG	C2-N2	2.12	1.50	1.46
5	B	2002	NAG	C3-C2	2.22	1.57	1.52
5	D	2003	NAG	C3-C2	2.35	1.57	1.52
5	D	2003	NAG	C4-C5	2.44	1.58	1.53

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2004	NAG	O5-C1-C2	-3.35	106.82	111.47
5	D	2004	NAG	O5-C1-C2	-3.23	106.97	111.47
5	D	2001	NAG	O3-C3-C2	-2.70	103.61	109.39
5	D	2004	NAG	O7-C7-C8	-2.50	117.50	122.06
5	B	2004	NAG	O7-C7-C8	-2.28	117.91	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	NAG	3	0
5	B	2002	NAG	3	0
5	B	2003	NAG	3	0
5	D	2001	NAG	4	0
5	D	2002	NAG	4	0
5	D	2003	NAG	3	0

5.6 Ligand geometry

2 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
4	NAG	A	2003	1	14,14,15	1.86	5 (35%)	15,19,21	3.49	12 (80%)
4	NAG	C	2003	1	14,14,15	2.06	4 (28%)	15,19,21	2.60	9 (60%)

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
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	0/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2003	NAG	O5-C5	2.05	1.47	1.43
4	A	2003	NAG	C4-C5	2.16	1.57	1.53
4	A	2003	NAG	C4-C3	2.22	1.58	1.52
4	C	2003	NAG	O4-C4	2.22	1.48	1.43
4	A	2003	NAG	O4-C4	2.49	1.48	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	NAG	O7-C7-C8	-5.21	112.57	122.06
4	C	2003	NAG	O7-C7-C8	-3.61	115.49	122.06
4	A	2003	NAG	C3-C4-C5	-3.54	103.97	110.22
4	A	2003	NAG	O3-C3-C4	-3.36	103.06	110.36
4	C	2003	NAG	C1-C2-N2	-2.77	105.75	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2003	NAG	1	0
4	C	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, 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	1626/1676 (97%)	-0.04	19 (1%) 79 72	72, 150, 260, 469	0
1	C	1626/1676 (97%)	0.03	43 (2%) 56 47	60, 153, 277, 515	0
2	B	1215/1642 (73%)	0.02	22 (1%) 69 61	73, 160, 235, 335	0
2	D	1215/1642 (73%)	-0.03	16 (1%) 77 69	85, 155, 241, 362	0
3	X	191/231 (82%)	0.68	26 (13%) 3 5	99, 230, 333, 437	0
3	Y	191/231 (82%)	0.41	14 (7%) 16 13	95, 195, 300, 385	0
All	All	6064/7098 (85%)	0.03	140 (2%) 61 53	60, 157, 264, 515	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	112	PRO	11.7
3	Y	114	GLY	6.7
1	C	1651	ASP	5.6
3	X	113	ASN	5.6
3	X	114	GLY	5.5

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](#)

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
5	NAG	B	2002	14/15	0.72	0.69	-	228,239,253,257	0
5	NAG	D	2001	14/15	0.88	0.41	-	228,253,282,288	0
5	NAG	D	2002	14/15	0.66	0.60	-	228,239,251,252	0
5	NAG	B	2001	14/15	0.74	0.55	-	278,305,319,322	0
5	NAG	D	2004	14/15	0.72	0.84	-	271,274,277,278	0
5	NAG	D	2003	14/15	0.54	0.53	-	246,253,258,265	0
5	NAG	B	2003	14/15	0.24	0.77	-	225,233,240,245	0
5	NAG	B	2004	14/15	0.56	0.77	-	297,301,307,310	0

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
4	NAG	C	2003	14/15	0.74	0.39	0.84	177,180,183,183	0
4	NAG	A	2003	14/15	0.78	0.29	0.34	166,169,171,172	0

6.5 Other polymers [i](#)

There are no such residues in this entry.