



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:56 am GMT

PDB ID : 4V40
Title : BETA-GALACTOSIDASE
Authors : Jacobson, R.H.; Zhang, X.; Dubose, R.F.; Matthews, B.W.
Deposited on : 1994-07-18
Resolution : 2.50 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
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) : recalc28972

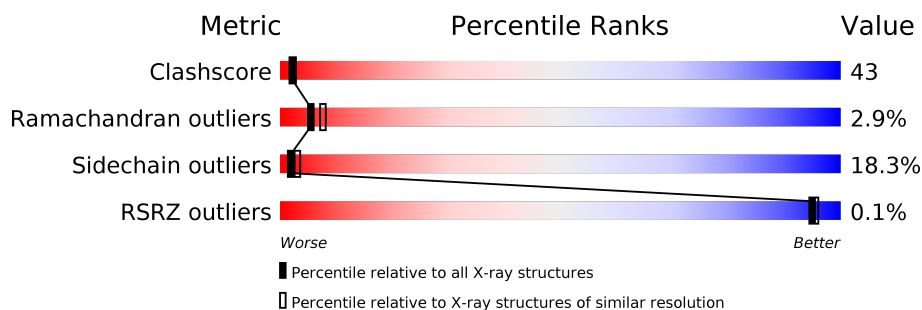
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



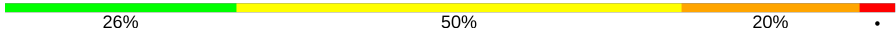

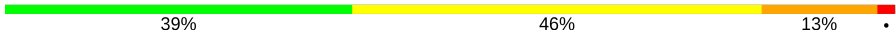
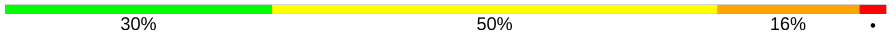


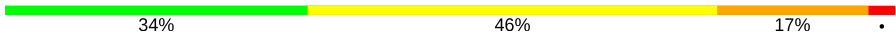
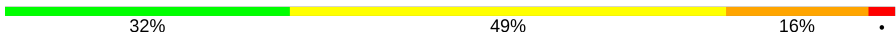
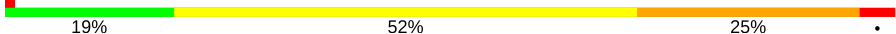
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	1023	
1	B	1023	
1	C	1023	
1	D	1023	
1	E	1023	
1	F	1023	
1	G	1023	

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Mol	Chain	Length	Quality of chain
1	H	1023	
1	I	1023	
1	J	1023	
1	K	1023	
1	L	1023	
1	M	1023	
1	N	1023	
1	O	1023	
1	P	1023	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	1101	-	-	-	X
2	MG	B	1101	-	-	-	X
2	MG	C	1101	-	-	-	X
2	MG	D	1101	-	-	-	X
2	MG	D	1102	-	-	-	X
2	MG	E	1101	-	-	-	X
2	MG	F	1101	-	-	-	X
2	MG	G	1101	-	-	-	X
2	MG	H	1101	-	-	-	X
2	MG	I	1101	-	-	-	X
2	MG	J	1101	-	-	-	X
2	MG	L	1101	-	-	-	X
2	MG	N	1101	-	-	-	X
2	MG	O	1101	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 132654 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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	B	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	C	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	D	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	E	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	F	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	G	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	H	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	I	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	J	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	K	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	L	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	M	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	N	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	O	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			
1	P	1021	Total	C	N	O	S	0	0	0
			8198	5185	1451	1524	38			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total 2	Mg 2	0	0
2	G	2	Total 2	Mg 2	0	0
2	J	2	Total 2	Mg 2	0	0
2	D	2	Total 2	Mg 2	0	0
2	K	2	Total 2	Mg 2	0	0
2	E	2	Total 2	Mg 2	0	0
2	H	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0
2	I	2	Total 2	Mg 2	0	0
2	C	2	Total 2	Mg 2	0	0
2	A	2	Total 2	Mg 2	0	0
2	N	2	Total 2	Mg 2	0	0
2	O	2	Total 2	Mg 2	0	0
2	L	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0
2	M	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total 88	O 88	0	0
3	B	96	Total 96	O 96	0	0
3	C	91	Total 91	O 91	0	0

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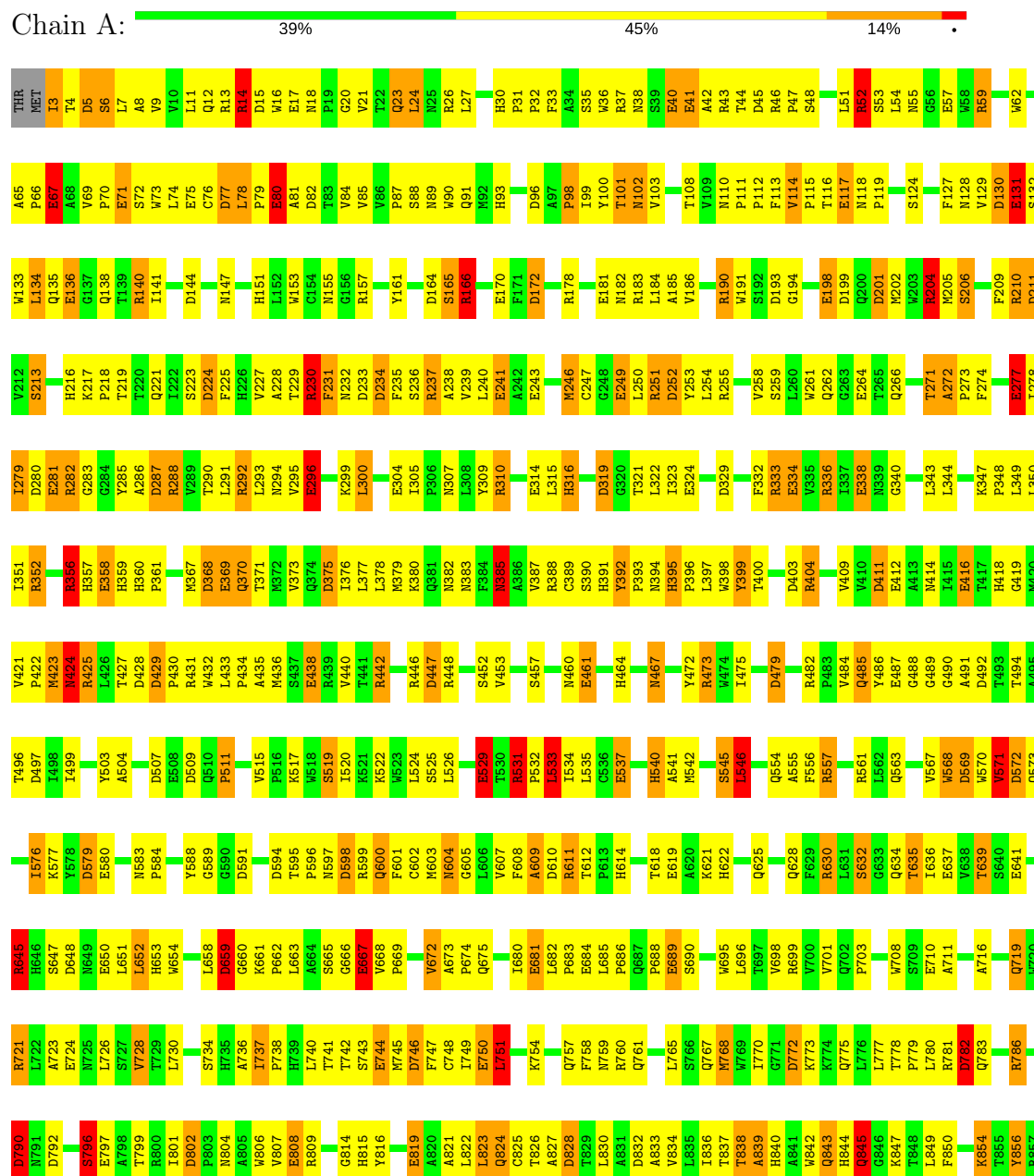
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	97	Total 97	O 97	0	0
3	E	94	Total 94	O 94	0	0
3	F	91	Total 91	O 91	0	0
3	G	95	Total 95	O 95	0	0
3	H	92	Total 92	O 92	0	0
3	I	90	Total 90	O 90	0	0
3	J	97	Total 97	O 97	0	0
3	K	87	Total 87	O 87	0	0
3	L	84	Total 84	O 84	0	0
3	M	79	Total 79	O 79	0	0
3	N	94	Total 94	O 94	0	0
3	O	95	Total 95	O 95	0	0
3	P	85	Total 85	O 85	0	0

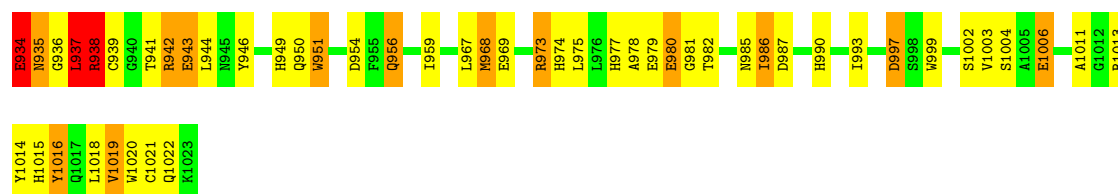
3 Residue-property plots

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: BETA-GALACTOSIDASE

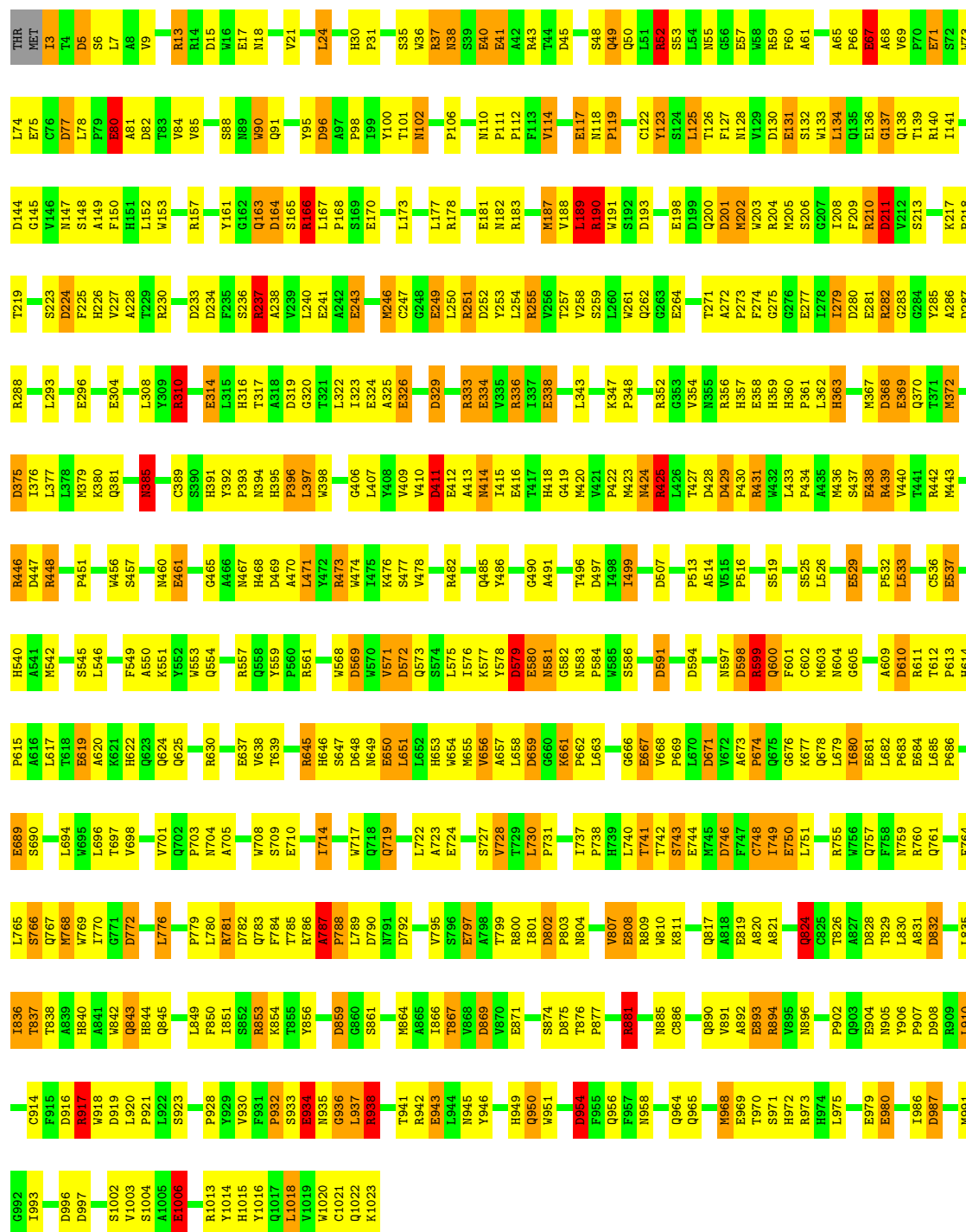


L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	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	L172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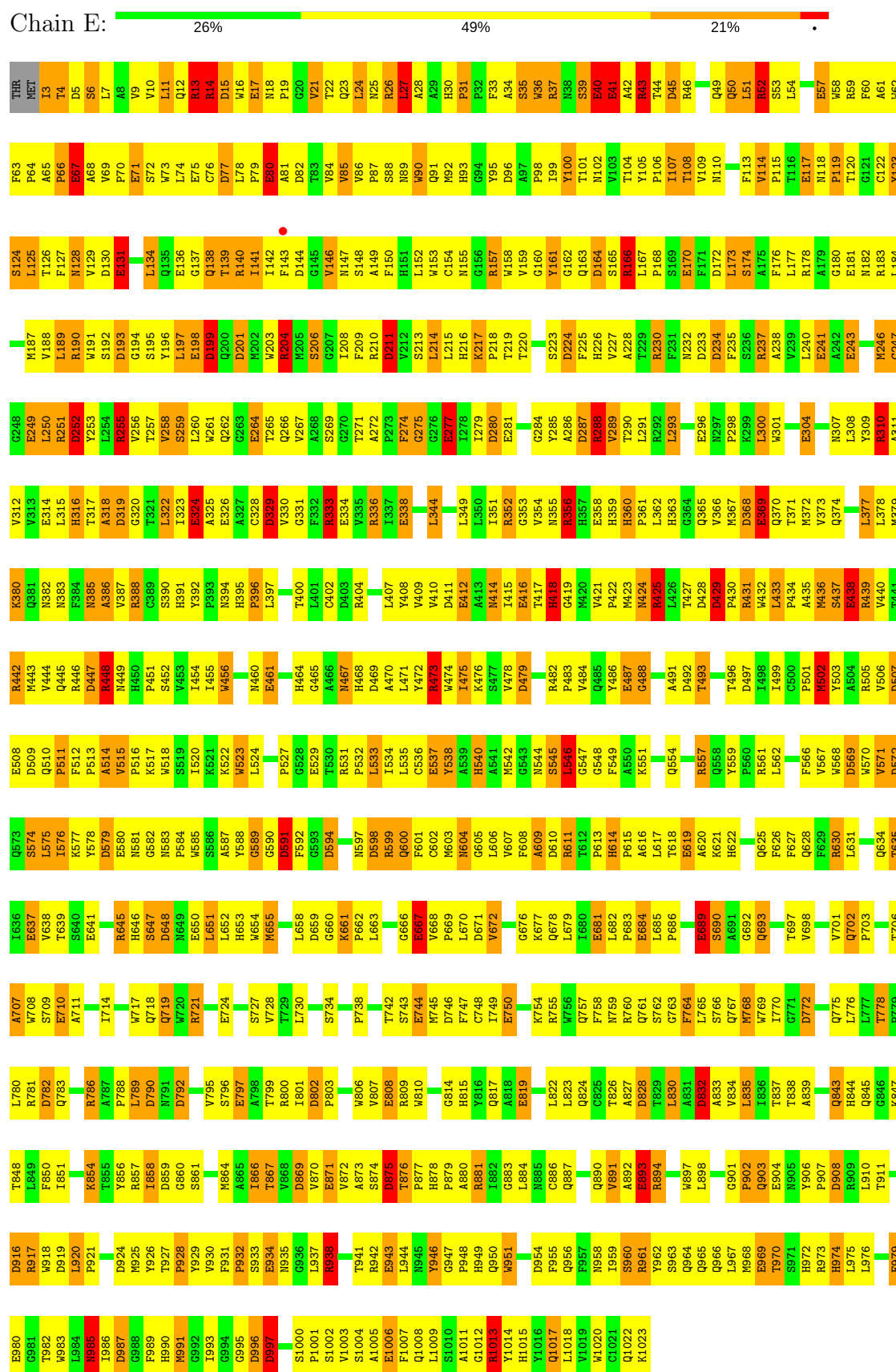
• Molecule 1: BETA-GALACTOSIDASE

Chain C: 44% 41% 12%



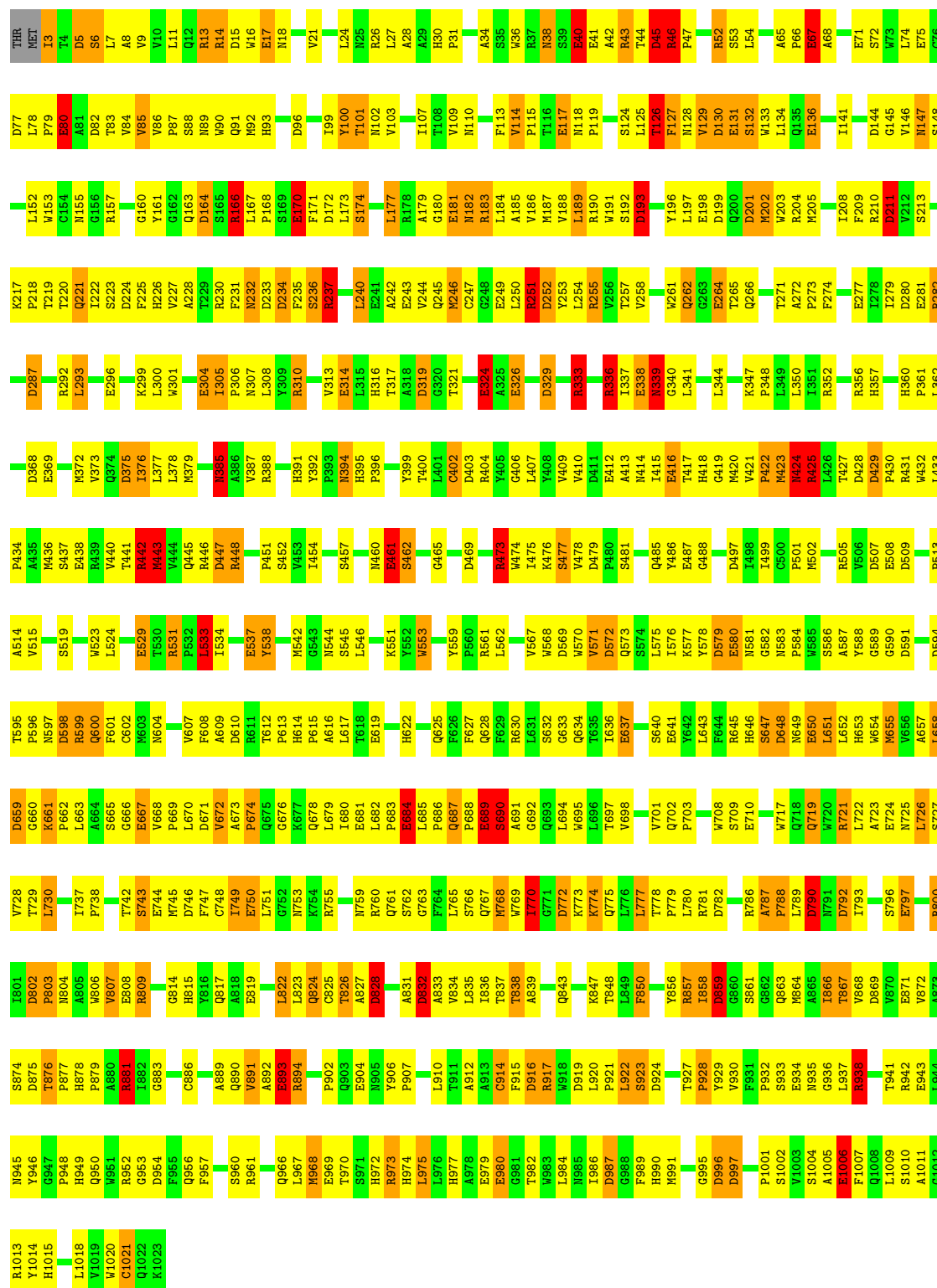
Chain D: 38% 46% 14% .





• Molecule 1: BETA-GALACTOSIDASE

Chain F: 37% 46% 13%

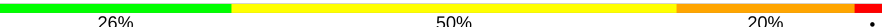


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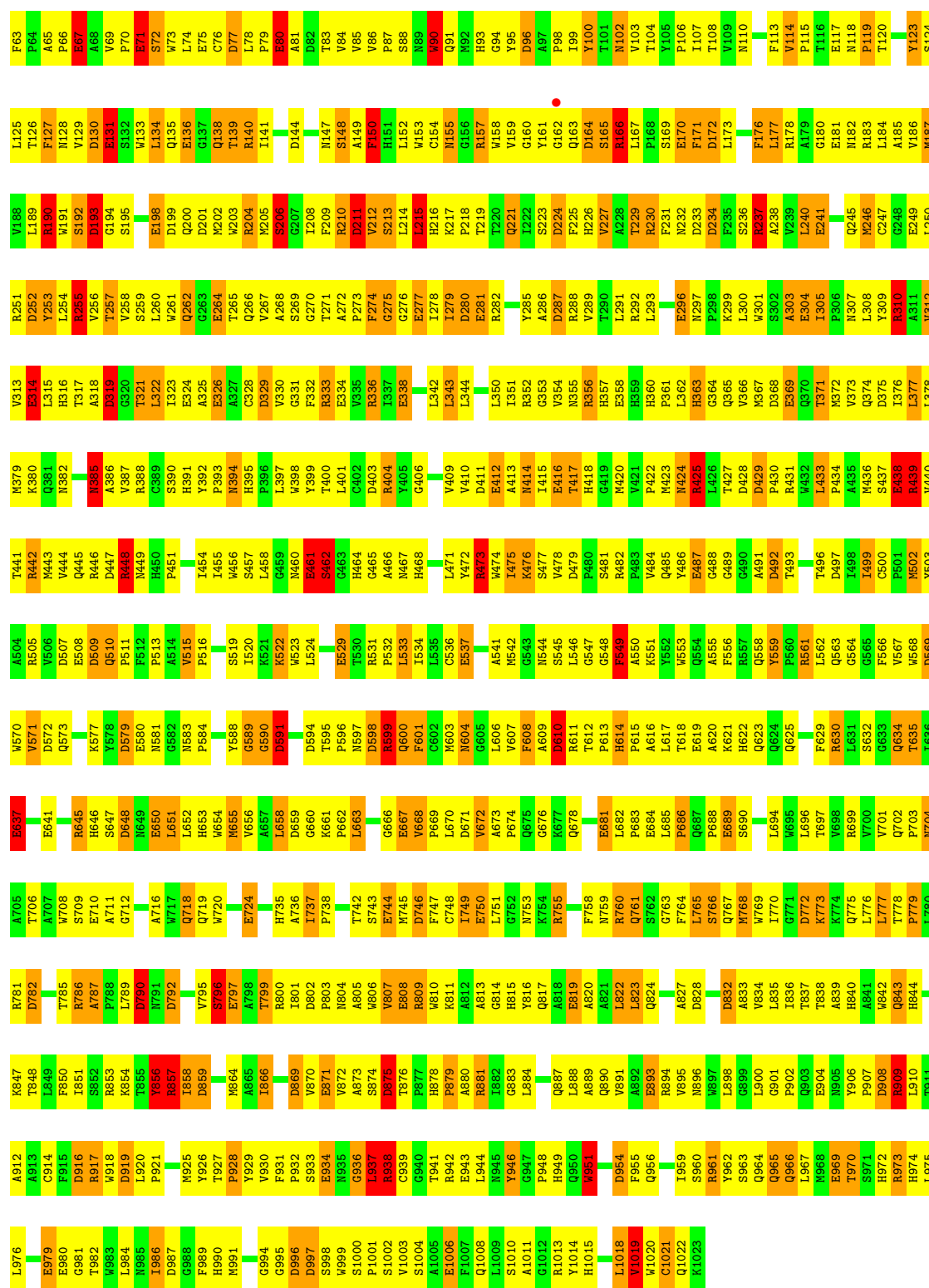
Chain G: 35% 44% 18%

THR	W73	Q138	P209	G276	L350	H418	D492	L562	R630	T897	G771	H844	A913	D987
MET	L74	T139	R210	E277	I351	H418	T493	Q563	L631	V698	D772	Q845	C914	
I3	E76	R140	D211	I278	R352	V421	T496	F566	S632	R699	L777	G846	F915	H990
T4	G75		T212	I279	G353	P422	D497	F567	G633	V700	L778	K847	D916	H991
D5	D77	G145	S213	D281	V354	N424	T498	V668	G634	W701	P778	T848	R917	G992
S6	L78	V146		E281	N424	N424	T499	V669	T635	Q702	P779	L849	W918	I993
L7	P79	N147	K217	R282	R356	R425	C500	D569	L636	P703	L780	F850	D919	G994
	E80	S148	T218	G283	H357	L426		W570	E637	T706	W781	R853	L920	G995
R13	A81	H151	T219	G284	E358	T427	P501	V571	V638	W707	D782	K854	D924	D996
R14	D82	L152		Y285	H359	D428	R505	Q573	S640	W708	F784	R855		D997
D15	T83	W153	D224	A286	R361	P430	V506	Q572	E641	S709	L789	R856	T927	S1002
W16	V84	C154	P225	D287	L362	R431	D507		F644	W710	D790	R857	P928	R1003
E17	V85	N155	V227	R288	H363	W432	E508		R645	A711	D791	I858	Y929	S1004
N18	V86	G156	A228	V289	G364	L433	D509		H646	A716	F792	D859	Y930	E1005
	P87	L157	A229	T290	Q365	P434	Q510		D647		S796	Q863	F931	F1007
	S88	W158	R230	L291	V366	M436	P511		N648	Q719	S796	M864	P932	Q1008
T22	H89	W159	R231	L292	D367	S437	F512		E650	W720	E797	A865	S933	Q1009
Q23	W90	G160	F231	L293	D368	E438	P513		L651	R721	R800	I866	F934	L1009
L24	Q91	Y161	D232	L294	E369	R439	A514		L652	L722	R801	T867	G936	S1010
W25	H92		D233	E296	M372		W518		L653	L723	D802	V868	G937	G1012
	H93		D234	N297	V373	R442	W519		L654	E724	P803	V869	L937	R1013
L27	D96	S165	F235	W301	D374	M443	S519		W655		N804	W871	C939	Y1014
H30	A97	R166	R237	E304	D375	V444	I520		V656	L730	R805	V872	R942	H1015
P31	P98	L167		I305	L376	Q445	W522		A657	P731	A805		E943	Y1016
S35	Y100	S169	L240	P306	L377	R446	W523		L658	I737	E808	D875		Q1017
N37	N102	F171	E242	P307	L378	D447	W524		D659	P738	R809	D876	Y946	L1018
N38	F172	D172	E243	L308	M379	R448	S525		V660	H739	P877	H878		W1019
S39	L173	L173	M246	Y309	K390	N449	L526		K661	L740	G814	H879	Q949	C1021
E40	I107		C247	R310	Q381	H450	L533		P682	D746	H815	P879	Q950	Q1022
E41	V109	F176	G248	E314	N382	P451	E529		L663	T741	T816	A880	W950	K1023
A42	N110	L177	E249	L315	N383	S452	T530		D660	W742	W817	R881	W951	
R43	P111		R251	H316	F384	I454	R531		G665	S743	A818	R882	G952	S35
T44	P112	G180	L250	T317	N385		P532		G666	W744	E819	L884	D954	W36
D45	F113	E181	D252	A318	A386	L458	L534		E667	D745	A820		F955	R37
R46	V114	N182	Y253	D319	R388	G459	L534		V668	W747	A821	Q887	Q956	N38
	P115	L183	L254	G320	C389	E461			P669	C748	L822	L888	F957	S39
E117	N118	A185	R255	L322	S390	E461			L670	I749	L823	A889	F958	E40
P119		V186	T257	L323	H391	H464			D671	W750	Q824	Q890	I959	A42
		M187	V258	E324	Y392	G465			V672	L751	C825	V891	S960	R43
R52	L54	V188	S259	A325	N394	A466				W752	T826	A892	R961	T44
N55		L189	L260	E326	H395	N467				W753	A827	E893		D45
G56		R190	W261			H468				K754	D826	R894	L967	R46
E57		D193	Q262	D329	D402	L471				W755	T829	V895	W968	P47
R59		G194	E264	R333	D403	R473				W756	L830	N896	E969	S48
F63		E198	T265	E334	R404	W474				N759	A831	W897	T970	Q50
P64		D199	Q266	Y335	B404	I475				R760	R832	L900	R973	L51
A65		Q200	V267	V336	L407	W476				Q761	V834		H974	R52
P66		D201	A268	I337	Y408	K476				S762	L835	Q903	L975	S53
E67		M202	S269	E338	Y409	S477				S763	T818	E904		L54
		W203	G270	E338	V409	S477				F764	E819	N905	E979	E57
A68		L134	T271	L343	V410	V478				W765	T838	Y906	E980	W58
V69		Q135	A272		D411					S766	R839	P907	G981	R59
F70		E136	A273			E487				Q767	R840	D908		W62
E71		L208	P274		N414	G490				W768	A841	R909	L984	F60
S72			G275		T417	A491				I770	Q843	L910	N985	A61

● Molecule 1: BETA-GALACTOSIDASE

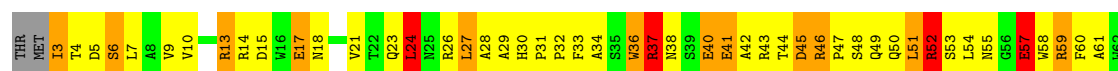
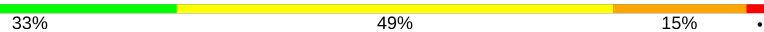
Chain H: 

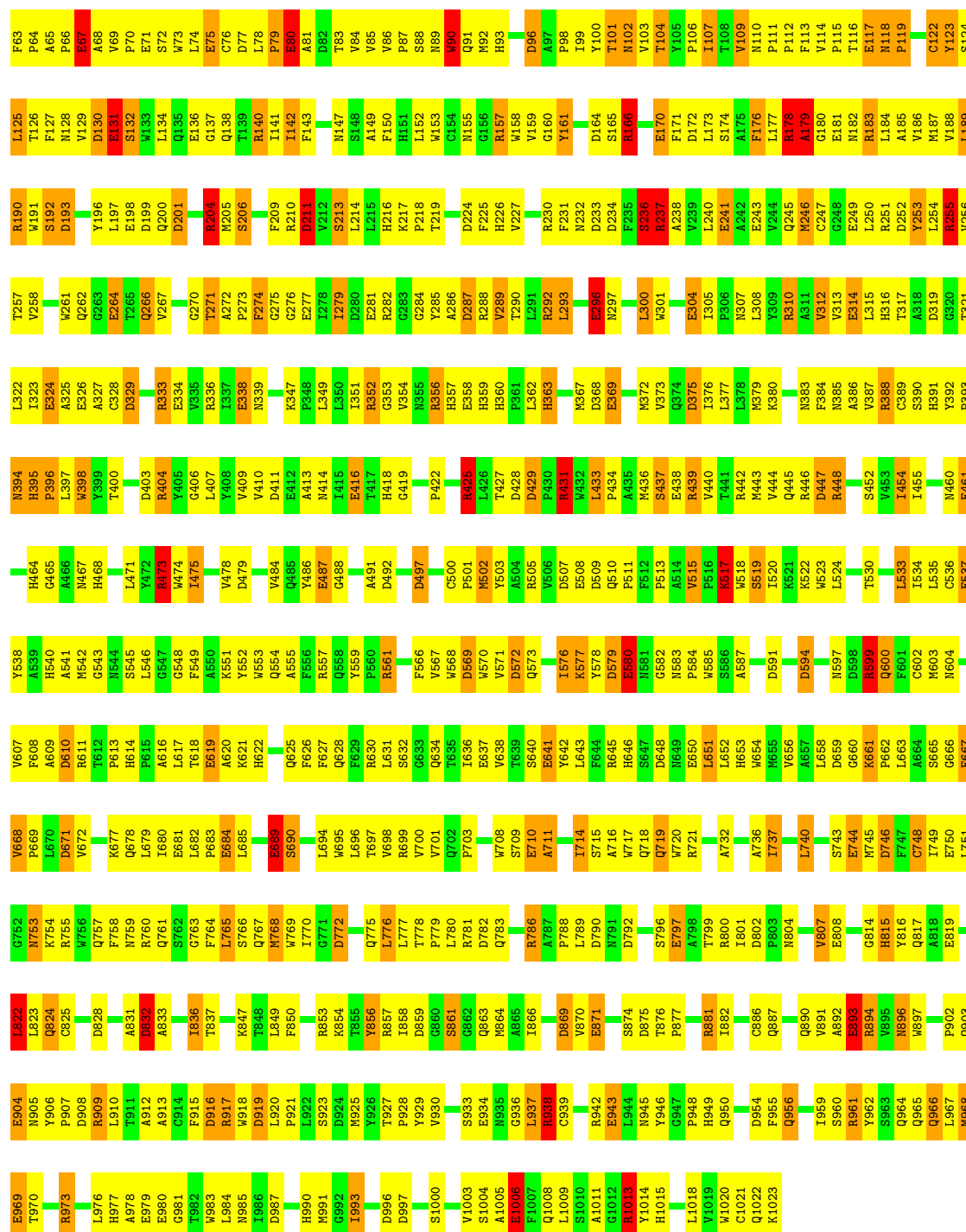
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• Molecule 1: BETA-GALACTOSIDASE

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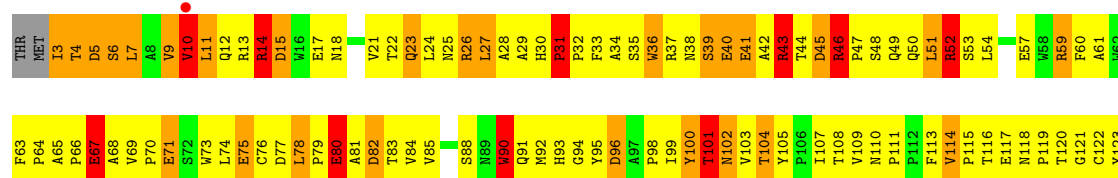






Percentage	Color
30%	Green
50%	Yellow
16%	Orange
4%	Red





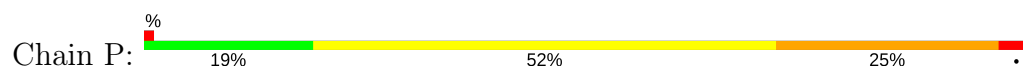


Category	Percentage
Very bad	34%
Bad	46%
Good	17%



F955	Q887	E819	I749	E681	R611	L546	I475	D411	G340	Q262	Q200	S132
Q956	L888	A820	E750	L682	T612	G547	K476	E412	L341	G263	D201	W133
F957	A889	A821	L751	L683	T613	G548	S477	E413	L342	G264	M202	L134
N958	B890	L822	G752	E684	H614	F549	V478	M414	L343	T265	Q203	Q135
F959	B891	L823	N753	L685	T615	A550	D479	I415	G341	Q266	M204	Q136
S960	A892	Q824	K754	P686	L617	K551		E416	T351		M205	G137
R961	B893		R755	Q687	L618	W552	V484	L417	R352	S269	S206	L138
Y962	B894	D828	F758	P688	E619	W553	Q485	H418	G353	G270		T139
Q963	B895	T829	N759	E689	A620	Q554	V486	G419	N354	T271	F209	R140
Q964	W897	L830	R759	S690	K621	A555	E487	M420	V355	A772	R210	I441
L967		A831	K760	P686	L617	F556	G488	V421	R356	P273	D211	I442
N968	L900	B832	Q761	Q693	Q624	R557	G489	P422	H357	F274	V212	F443
F969	G901	A833	S762	L694	Q625	Q558		M423	E358		S213	D144
E970	P902	W834	K763	W695	Q628	F560	D492	M424	R359	E277	L214	G145
T970	Q903	L835	F764	L696	Q628	P560		R425	H360	L215	L215	V146
S971	Q903	L836	L765	T697	S632	R561	D496	L426	P361	I279	H216	N147
R972		T837	S766	P698	G633	L562	D497	T427	L362	K217	K217	N148
R973	Y906	T838	Q767	R699	E633		I498	D428	H363	E281	P218	A149
H974	P907	A839	W768	W701	Q634	F566	I499	R429	G364	R282	T219	F150
L975	R908	H840	W769	Q702	T635	W567	P501					
L976	R909	A841	I770	P703	V638		Q510	P430	Q366	T220		H151
		R842	G771				P511	R439	Q374	L293		
E979	A912	Q843	D772	W704	E641	W570	W506	P434	E368	R289	D224	N155
Q980		Q844	K773	A705		W571	D507	P435	Q370	T290	F225	G156
G981	F915	Q845	K774	T706	R645	F579	E508	M436	T371	L291	H226	R157
D987	D916	A846	Q775	A707	R646	Q573	E509	S437	K372	R292	V227	W158
G988	W918	L848	L776	S709	S647	Q510	P511	E438	Q373	L293	A228	
F989	R919	L849	T778	E710	D648			R439	Q374			
H990	L920	F850	W779	A711	N649	W576		R446	K380	Y309		Q163
	P921	L851	L780	G712	E650	K577	S519	D447	R381		T299	
T993	L922	T852	R781	H713	L651	D578	E520	L441	D375	E296	R230	D164
G994	S923	R853	D782	Q718	H653	E580		R442	L376	T297	F231	S165
G995	D924	K854		Q718	H653		W518	M449	L377	P298	N232	R166
D996		T855	R786	Q719	W654	N583	S519	H450	L378	K299	D233	L167
N997	Y929	T856	A787	R721	A657	P584	E521	M449	N379	D234	F235	P168
Q998	V930	R857	F789	L722	L658	S586	K522	H450	K381		S236	E170
W999	F932	L1858	D790	D659	D659	A587	N523	P451	N382	V312	R237	F171
	S933	H664	N791	L726	G660	W588	L524	S452	N383	E314	V239	D172
L1003	E934	A665	D792	Q661	G661		S525		N385		E241	F176
A1005	N935	T866	I793	W728	P662	D591		W453	V387	A318		A179
	G936	T867		L729	A663	F592	G528	I454	R388	D319	E242	L179
F1007	L937	W868	S796	L730	L664	G593	E529	I455		L322	E243	G180
L1008	R938	D869	E797	P731	D594	D594	T530	W456	H391	L323	Q245	E181
L1009	Q939	W870	A798	G666	S666	T595	R531		N392	E324	Q246	R182
	G940	E871	T799	E667	G667	P596	P532		P393	R325	C247	L184
	T941	R872	R800	W785	P668	N597	L533	M460	N394	E326	G248	
	R942	A873	L801	A736	P669	D598	L534	E461	H395	A327	E249	M187
Y1014	E943	S874	D802	T737	L670	E599	L535	G463	P396	R328	L250	L188
H1015	L944	D875	P803	P738	D671	Q600	C536	H464	L397	D329	R251	L189
Q1017	N945	T876		H739	P672	F601	E537	G465			D252	R190
L1018	Y946	R877	W807	L740	A673	C502	Y538	A466	L401	F332	V253	W191
V1019		H878	E808	P674	P674	M603	A539	M467	G402	R333	L254	S192
W1020	H949	P879		S743	Q675	M604	H940	H468	P403	V335	R255	G194
G1021	Q950	A880	G814	E744	Q676			L471	L407	R336	V258	L197
Q1022	R952	R881	H815	W745	K677	P608	G543	V472	V408	I337	S259	E198
K1023			H816	D746	Q678	A609	N544	R473	V409	E338	L260	D199
			Q817	F747	L679		S545	R472	V410	N239		
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F1007	R942	R881	H815	N753	L685	Q623	Y559	G490	P430	D368	N307	Q345	A185	G122
Q1008	E943	L884	Y816	K754	P666	Q624	P560	A491	R631	E369	L308	M246	V186	Y123
S1010	N945	N885	Q817	R755	Q688	F626	R561	T492	W432	Q370	Y309	C247	M187	
	Y946	C886	A818		P688		L562	T493	L433		R310	G248	V188	T126
R1013	G947	Q887	E819	F758	S890	F629	Q663	T494	P434	Q373	A311	E249	L189	F127
Y1014	P943	L883	L822	R760	L694	L630	F566	T496	A435	Q374	N312	L250	R190	N128
H1015	Q890	Q890	L823	Q761	W895	L631	P567	D498	M436	D375	V313	R351	V191	N129
Y1016	D828		Q824		L696	S632	W568	T498	S437	L376	E314	D262	S192	D130
Q1017	T829	E892	L825	F764	T697	Q633	W569	L499	A438	L377	L316	L254	G194	E131
L1018	R952	N891	Q824		L696	Q634	W570	C500	R439	L378	H316	R255	S195	S133
V1019	G953	E893	T829	S766	T698	T635	W571	M501	V440	M379	T317	R255	S195	S133
H1020	R894	R894	L830	Q767	R899	L636	M502	M502	T441	K380	A318	V256	V196	L134
C1021	F955	V895	L831	Q767	R899	L636	D572	R442	R442	Q381	D319	T257	L197	Q135
Q1022	Q956	N896	A831	N763	V700	E637	Q573	Y503	W443	N382	Q320	V258	E198	E136
K1023	F957	N897	D832	W769	V701	W638	S574	A504	V444	N383	T321	S259	D199	G137
	Q966	W897	A833	W770	Q702	T639	L575	A505	Q445	F384	L322	L260	Q200	Q138
N958	N958	L898	W834	W778	P703	Q641	S576	V506	R446	N385	I323	Q261	D201	T139
N959	N959	L899	L835	D772	N704	E641	K577	D507	D447	A386	E324	Q262	N202	R140
S960	S960	L900	L836	K773	A705	W642	Y578	E508	R448	Q387	A325	G263	W203	I141
R961	R961	Q901	T837	K774	T706	L643	D579	D509	W449	R388	E326	E264	R204	I142
Y962	Y962	P902	T838	Q775	A707	F644	E580		H450	C389	A327	T265	M205	F143
	Q965	Q903	A839	L776	W708	R645	N583	V515	P451	S390	C328	Q266	S206	D144
	Q966	E904	H840	L777	S709	H646	P584	W518	S452	H391	D329	V267	G207	G145
L967	L967	N905	W842	T778	E710	S647	W585	S519	V453	Y392	V330	A268	I208	V146
N968	N968	Y906	W842	P779	A711	D648	W586	I520	I454	P393	G331	S269	F209	N147
	Q969	P907	Q843	L780	G712	R649	S587	K521	W456	N394	F332	C270	R210	S148
	T970	N908	H844	R781	H713	E650	A587	K522	S457	H395	R333	T271	D211	A149
	S971	R909	Q845	D782	W714	L651	G590	G528	G463	P396	E334	A272	F150	
H972	H972	L910	K846	Q783	S715	L652	D591	W524	L458	N397	V335	P273	S213	H151
R973	R973	T911	K847	F784	A716	H653	N591	L524	G459	W398	R336	F274	L214	L152
H974	H974	A912	T848	T785	W717	W654	F592	S525	W460	Y399	I337	G275	L215	W153
	L975	A913	L849	R786	W717	W655	G593	L526	E461	T400	E338	G276	H216	G154
L976	L976	C914	F850	A787	L722	W656	D594	P527	S462	L401		I278	K217	N156
	E980	D916	R853	R788	A723	A657	S595	G528	G463	C402	L342	I279	F218	G157
G981	G981	R917	K854	L789	E724	L658	P596	T530	H464	D403	L343	D280	T219	V158
T982	T982	Q918	T855	D790	N726	D659	N597	R531	G465	R404	L344	E281	T220	V159
	N985	L920	W856	D792	S727	K681	R599	P532	M467	L407	N345	R382	T222	G160
N986	N986	P921	R857	I793	V728	P682	Q600	L533	H468	Y408	G346	G283	S223	Y161
D987	D987	L922	L858	G794	T729	L683	F601	T534	D469	V409	K347	G284	D224	G162
		S923	D859	W795	L730	A664	C602	L535	A470	V410	P348	Y285	F225	Q163
		D924	G860	S796	L730	S665	M603	C536	L471	D411	L349	A286	H226	D164
	H990	N925	S861	E797	H735	G666	N604	E537	Y472	E412	L350	D287	V227	S165
N991	N991	Y926	G667	A798	A736	E667	G605	Y538	R473	A413	L353	R288	A228	R166
G992	G992	T927	E668	T799	I737	W688	L606	A539	W474	N414	R352	V289	T229	
I993	I993	P928	M864	R800	P738	P689	V607	H540	T475	I415	G353	L293	R230	E170
G994	G994	Y929	A865	I801	H739	L670	F608	A541	K476	E416	V354	N294	F231	F171
G995	G995	V930	T866	D802	L740	D671	A609	N542	S477	T417	N355	V295	N232	D172
D996	D996	F931	T867	P803	T741	W672	D610	G543	V478	R418	R356	E296	D234	L173
D997	D997	P932	W668	N804	T742	A673	R611	N544	D479	G419	H357	N297	F235	S174
	S998	S933	D869	A805	S743	P674	T612	S545	P480	M420	E358	N297	F235	A175
	Y999	E934	W870	W806	E744		P613	L546	R481	V421	H599	K299	S236	F176
S1000	S1000	N935	E871	W807	M745	K677	A616	G547	R482	P422	H360	K299	R237	L177
G996	G996	L937	S874	E808	D746	Q678	L617	G548	P483	M423	P361	L300	A238	R178
S1002	S1002	P1001	D875	R809	F747	L679	V549	F549	V484	N424	L362	W301	V239	A179
V1003	V1003	R938	T876	W810	C748	L680	T618	Q485	V486	R425	H363	S302	L240	G180
S1004	S1004	C939	T876	R811	I749	E681	E619	K551	Y486	L426	G364	A363	E241	E181
A1005	A1005	G940	P877	A812	E750	L682	A620	W552	E487	T427	Q365	E304	A242	N182
E1006	E1006	T941	H877	G814	L751	P683	K621	W553	G488	D428	V366	I305	E243	R183
					G752	E684	H622		G489	D429	N367	P306	V244	L184

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 207.50Å 509.90Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 92.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 39.3 (92.62-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.00Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.174 , (Not available) 0.169 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 89.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	132654	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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: MG

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	1.16	51/8440 (0.6%)	1.52	139/11516 (1.2%)
1	B	1.17	54/8440 (0.6%)	1.51	130/11516 (1.1%)
1	C	1.18	56/8440 (0.7%)	1.50	132/11516 (1.1%)
1	D	1.16	55/8440 (0.7%)	1.52	148/11516 (1.3%)
1	E	1.16	55/8440 (0.7%)	1.56	145/11516 (1.3%)
1	F	1.18	45/8440 (0.5%)	1.53	144/11516 (1.3%)
1	G	1.16	58/8440 (0.7%)	1.51	151/11516 (1.3%)
1	H	1.16	56/8440 (0.7%)	1.57	150/11516 (1.3%)
1	I	1.13	53/8440 (0.6%)	1.52	140/11516 (1.2%)
1	J	1.12	48/8440 (0.6%)	1.48	134/11516 (1.2%)
1	K	1.09	53/8440 (0.6%)	1.45	115/11516 (1.0%)
1	L	1.13	53/8440 (0.6%)	1.54	134/11516 (1.2%)
1	M	1.16	55/8440 (0.7%)	1.58	142/11516 (1.2%)
1	N	1.14	51/8440 (0.6%)	1.49	127/11516 (1.1%)
1	O	1.11	54/8440 (0.6%)	1.49	141/11516 (1.2%)
1	P	1.17	57/8440 (0.7%)	1.60	151/11516 (1.3%)
All	All	1.15	854/135040 (0.6%)	1.52	2223/184256 (1.2%)

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	1	0
1	B	1	0
1	D	2	1
1	E	1	0
1	F	2	0
1	G	2	0
1	H	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	1	0
1	J	1	0
1	L	1	0
1	M	2	0
1	P	2	0
All	All	17	1

The worst 5 of 854 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	358	GLU	CD-OE2	11.52	1.38	1.25
1	F	75	GLU	CD-OE1	10.30	1.36	1.25
1	K	358	GLU	CD-OE2	9.34	1.35	1.25
1	B	650	GLU	CD-OE1	9.31	1.35	1.25
1	F	326	GLU	CD-OE2	9.01	1.35	1.25

The worst 5 of 2223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	ARG	NE-CZ-NH2	-14.45	113.08	120.30
1	B	166	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	N	561	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	L	425	ARG	NE-CZ-NH2	13.74	127.17	120.30
1	L	997	ASP	CB-CG-OD2	-13.64	106.02	118.30

5 of 17 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	90	TRP	CA
1	B	718	GLN	CA
1	D	95	TYR	CA
1	D	914	CYS	CA
1	E	118	ASN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	473	ARG	Sidechain

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	8198	0	7796	540	0
1	B	8198	0	7796	546	0
1	C	8198	0	7796	446	0
1	D	8198	0	7796	551	0
1	E	8198	0	7795	892	0
1	F	8198	0	7796	579	0
1	G	8198	0	7796	641	0
1	H	8198	0	7796	882	0
1	I	8198	0	7796	618	0
1	J	8198	0	7795	507	0
1	K	8198	0	7796	781	0
1	L	8198	0	7796	792	0
1	M	8198	0	7796	1078	0
1	N	8198	0	7795	630	0
1	O	8198	0	7796	659	0
1	P	8198	0	7796	1151	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	88	0	0	7	0
3	B	96	0	0	14	0
3	C	91	0	0	9	0
3	D	97	0	0	13	0
3	E	94	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	91	0	0	9	0
3	G	95	0	0	13	0
3	H	92	0	0	18	0
3	I	90	0	0	15	0
3	J	97	0	0	9	0
3	K	87	0	0	9	0
3	L	84	0	0	12	0
3	M	79	0	0	17	0
3	N	94	0	0	19	0
3	O	95	0	0	12	0
3	P	85	0	0	21	0
All	All	132654	0	124733	11096	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 43.

The worst 5 of 11096 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:E:7:LEU:HD13	1:E:74:LEU:HD11	1.23	1.17
1:C:427:THR:HA	1:C:436:MET:HE1	1.21	1.16
1:D:572:ASP:HB3	1:D:603:MET:HG2	1.25	1.16
1:A:770:ILE:HD11	1:A:1022:GLN:HG2	1.18	1.15
1:I:316:HIS:HA	1:I:323:ILE:HD13	1.24	1.13

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	1019/1023 (100%)	909 (89%)	92 (9%)	18 (2%)	10 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1019/1023 (100%)	914 (90%)	85 (8%)	20 (2%)	9	14
1	C	1019/1023 (100%)	919 (90%)	81 (8%)	19 (2%)	9	15
1	D	1019/1023 (100%)	910 (89%)	98 (10%)	11 (1%)	17	29
1	E	1019/1023 (100%)	842 (83%)	135 (13%)	42 (4%)	3	4
1	F	1019/1023 (100%)	892 (88%)	101 (10%)	26 (3%)	6	9
1	G	1019/1023 (100%)	893 (88%)	101 (10%)	25 (2%)	6	10
1	H	1019/1023 (100%)	845 (83%)	140 (14%)	34 (3%)	4	6
1	I	1019/1023 (100%)	884 (87%)	111 (11%)	24 (2%)	7	11
1	J	1019/1023 (100%)	887 (87%)	118 (12%)	14 (1%)	13	23
1	K	1019/1023 (100%)	855 (84%)	131 (13%)	33 (3%)	5	6
1	L	1019/1023 (100%)	838 (82%)	146 (14%)	35 (3%)	4	5
1	M	1019/1023 (100%)	836 (82%)	127 (12%)	56 (6%)	2	2
1	N	1019/1023 (100%)	875 (86%)	117 (12%)	27 (3%)	6	9
1	O	1019/1023 (100%)	889 (87%)	102 (10%)	28 (3%)	6	9
1	P	1019/1023 (100%)	797 (78%)	164 (16%)	58 (6%)	2	2
All	All	16304/16368 (100%)	13985 (86%)	1849 (11%)	470 (3%)	5	7

5 of 470 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	277	GLU
1	A	389	CYS
1	A	541	ALA
1	A	659	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	873/875 (100%)	723 (83%)	150 (17%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	873/875 (100%)	709 (81%)	164 (19%)	2	3
1	C	873/875 (100%)	754 (86%)	119 (14%)	4	8
1	D	873/875 (100%)	729 (84%)	144 (16%)	2	4
1	E	873/875 (100%)	686 (79%)	187 (21%)	1	2
1	F	873/875 (100%)	735 (84%)	138 (16%)	3	5
1	G	873/875 (100%)	717 (82%)	156 (18%)	2	3
1	H	873/875 (100%)	693 (79%)	180 (21%)	1	2
1	I	873/875 (100%)	716 (82%)	157 (18%)	2	3
1	J	873/875 (100%)	755 (86%)	118 (14%)	4	8
1	K	873/875 (100%)	722 (83%)	151 (17%)	2	4
1	L	873/875 (100%)	704 (81%)	169 (19%)	1	3
1	M	873/875 (100%)	677 (78%)	196 (22%)	1	1
1	N	873/875 (100%)	717 (82%)	156 (18%)	2	3
1	O	873/875 (100%)	715 (82%)	158 (18%)	2	3
1	P	873/875 (100%)	665 (76%)	208 (24%)	1	1
All	All	13968/14000 (100%)	11417 (82%)	2551 (18%)	2	3

5 of 2551 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	523	TRP
1	J	277	GLU
1	P	71	GLU
1	H	724	GLU
1	I	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 370 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	262	GLN
1	I	950	GLN
1	O	1008	GLN
1	H	460	ASN
1	I	38	ASN

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 [i](#)

Of 31 ligands modelled in this entry, 31 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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	1021/1023 (99%)	-1.08	0 100 100	2, 24, 54, 79	0
1	B	1021/1023 (99%)	-1.10	0 100 100	2, 23, 54, 81	0
1	C	1021/1023 (99%)	-1.06	0 100 100	4, 21, 52, 80	0
1	D	1021/1023 (99%)	-1.10	0 100 100	4, 25, 56, 81	0
1	E	1021/1023 (99%)	-0.94	1 (0%) 95 95	8, 34, 61, 86	0
1	F	1021/1023 (99%)	-1.03	0 100 100	2, 23, 55, 78	0
1	G	1021/1023 (99%)	-1.07	0 100 100	3, 27, 58, 82	0
1	H	1021/1023 (99%)	-0.92	1 (0%) 95 95	6, 33, 61, 89	0
1	I	1021/1023 (99%)	-1.02	0 100 100	4, 30, 59, 80	0
1	J	1021/1023 (99%)	-1.02	0 100 100	8, 28, 56, 85	0
1	K	1021/1023 (99%)	-0.89	1 (0%) 95 95	10, 35, 64, 92	0
1	L	1021/1023 (99%)	-0.86	1 (0%) 95 95	6, 35, 63, 84	0
1	M	1021/1023 (99%)	-0.80	2 (0%) 94 95	12, 39, 65, 80	0
1	N	1021/1023 (99%)	-0.97	0 100 100	9, 30, 59, 89	0
1	O	1021/1023 (99%)	-1.00	0 100 100	11, 31, 60, 81	0
1	P	1021/1023 (99%)	-0.47	15 (1%) 74 75	14, 43, 69, 89	0
All	All	16336/16368 (99%)	-0.96	21 (0%) 95 95	2, 30, 60, 92	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	81	ALA	4.1
1	P	313	VAL	3.4
1	P	143	PHE	3.3
1	P	70	PRO	3.1
1	P	141	ILE	3.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	A	1101	1/1	0.98	0.15	13.18	37,37,37,37	0
2	MG	F	1101	1/1	0.78	0.19	12.48	35,35,35,35	0
2	MG	C	1101	1/1	0.97	0.18	11.03	23,23,23,23	0
2	MG	G	1101	1/1	0.91	0.17	9.44	32,32,32,32	0
2	MG	B	1101	1/1	0.96	0.15	6.04	25,25,25,25	0
2	MG	I	1101	1/1	0.99	0.13	5.76	33,33,33,33	0
2	MG	N	1101	1/1	0.97	0.14	4.50	32,32,32,32	0
2	MG	H	1101	1/1	0.96	0.15	3.80	27,27,27,27	0
2	MG	J	1101	1/1	0.94	0.14	3.71	34,34,34,34	0
2	MG	D	1102	1/1	0.95	0.13	3.38	42,42,42,42	0
2	MG	E	1101	1/1	0.96	0.15	3.33	39,39,39,39	0
2	MG	O	1101	1/1	0.92	0.12	2.59	40,40,40,40	0
2	MG	D	1101	1/1	0.97	0.12	2.34	28,28,28,28	0
2	MG	L	1101	1/1	0.98	0.14	2.33	31,31,31,31	0
2	MG	M	1101	1/1	0.94	0.14	1.54	56,56,56,56	0
2	MG	N	1102	1/1	0.98	0.11	0.18	26,26,26,26	0
2	MG	C	1102	1/1	0.93	0.08	-0.01	28,28,28,28	0
2	MG	P	1101	1/1	0.93	0.12	-0.29	49,49,49,49	0
2	MG	I	1102	1/1	0.98	0.08	-0.45	33,33,33,33	0
2	MG	E	1102	1/1	0.95	0.08	-0.52	32,32,32,32	0
2	MG	A	1102	1/1	0.95	0.08	-0.56	37,37,37,37	0
2	MG	K	1101	1/1	0.89	0.08	-0.70	34,34,34,34	0
2	MG	O	1102	1/1	0.99	0.09	-0.82	15,15,15,15	0
2	MG	H	1102	1/1	0.99	0.06	-1.23	22,22,22,22	0
2	MG	L	1102	1/1	0.95	0.04	-1.70	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	K	1102	1/1	0.98	0.05	-1.78	25,25,25,25	0
2	MG	F	1102	1/1	0.99	0.07	-1.93	26,26,26,26	0
2	MG	J	1102	1/1	0.96	0.05	-2.47	29,29,29,29	0
2	MG	B	1102	1/1	0.99	0.05	-2.56	23,23,23,23	0
2	MG	P	1102	1/1	0.99	0.05	-2.62	26,26,26,26	0
2	MG	G	1102	1/1	0.99	0.03	-5.22	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.