



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 07:44 PM EST

PDB ID : 6DQS
EMDB ID : EMD-7983
Title : Class 3 IP3-bound human type 3 1,4,5-inositol trisphosphate receptor
Authors : Hite, R.K.; Paknejad, N.
Deposited on : 2018-06-11
Resolution : 4.12 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

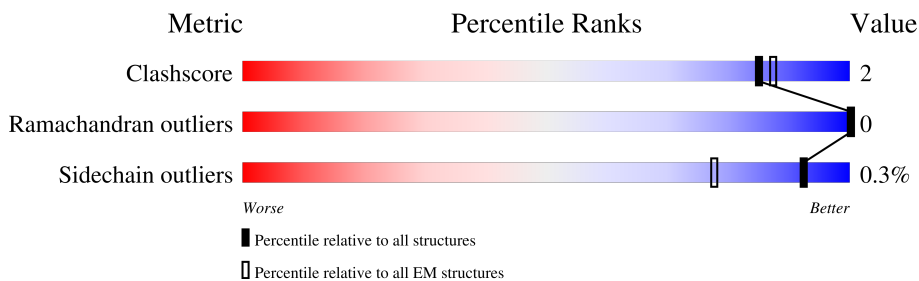
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.12 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2671	43% (Poor fit) 76% (0 outliers) 6% (1 outlier) 18% (Not modelled)
1	B	2671	29% (Poor fit) 77% (0 outliers) 5% (1 outlier) 18% (Not modelled)
1	C	2671	37% (Poor fit) 76% (0 outliers) 6% (1 outlier) 18% (Not modelled)
1	D	2671	52% (Poor fit) 76% (0 outliers) 6% (1 outlier) 18% (Not modelled)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 139350 atoms, of which 69675 are hydrogens and 0 are deuteriums.

In the tables below, 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.

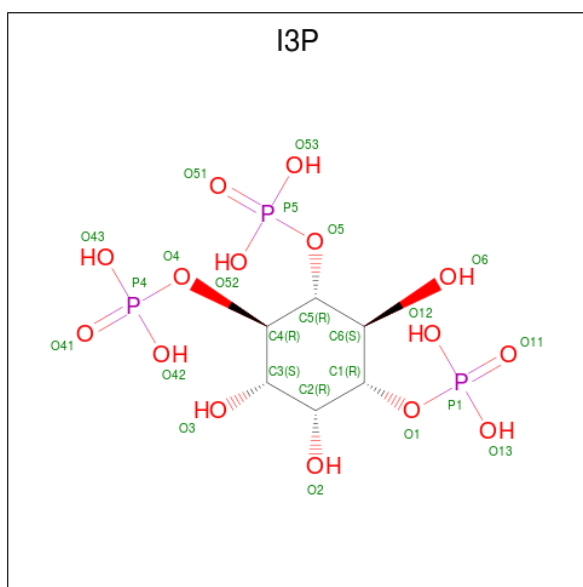
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	2186	34696	11058	17351	2985	3199	103	0	0
1	B	2186	34697	11058	17352	2985	3199	103	0	0
1	C	2186	34694	11058	17349	2985	3199	103	0	0
1	D	2192	35127	11194	17587	3005	3235	106	0	0

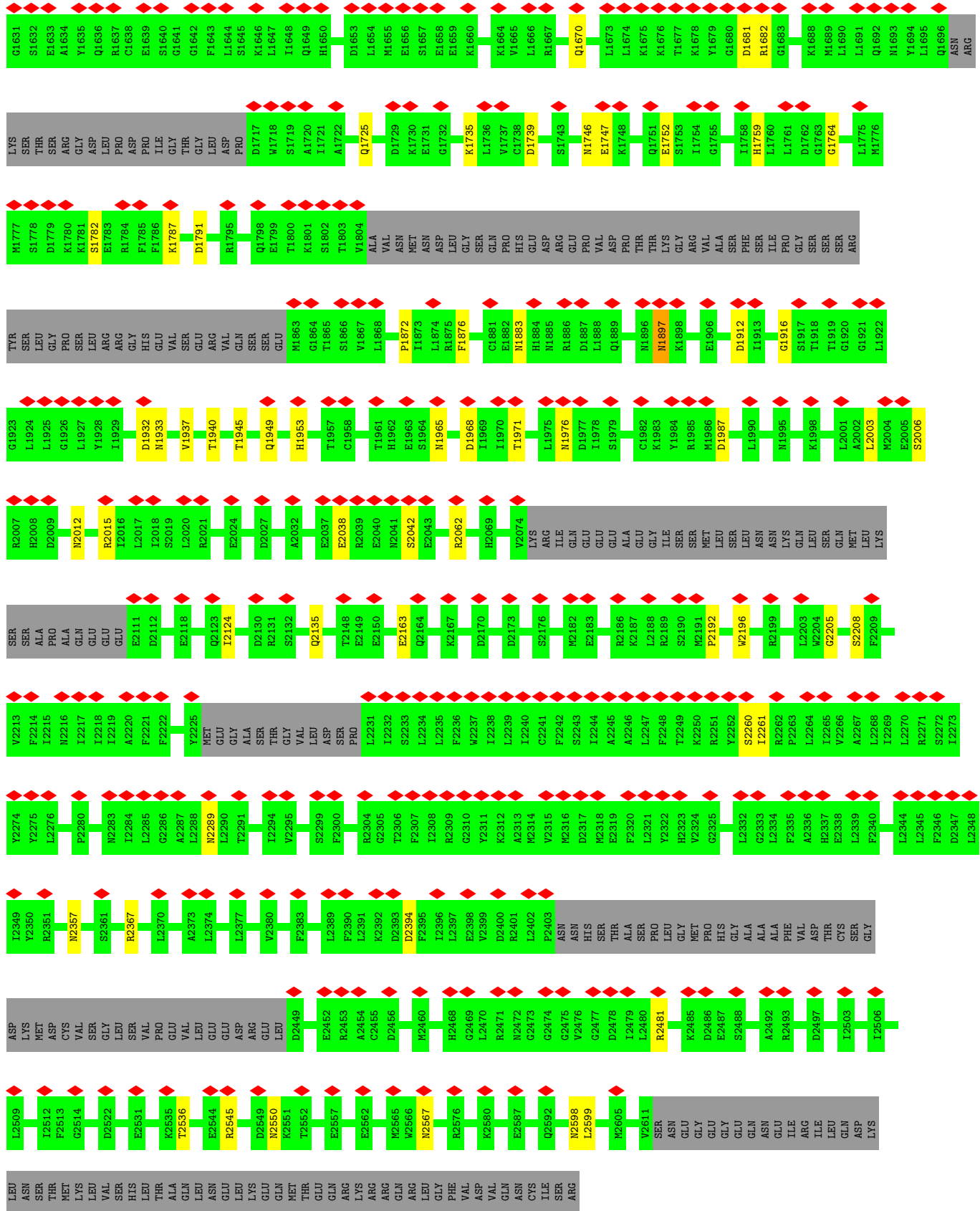
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
2	A	1	1	1	0
2	B	1	1	1	0
2	C	1	1	1	0
2	D	1	1	1	0

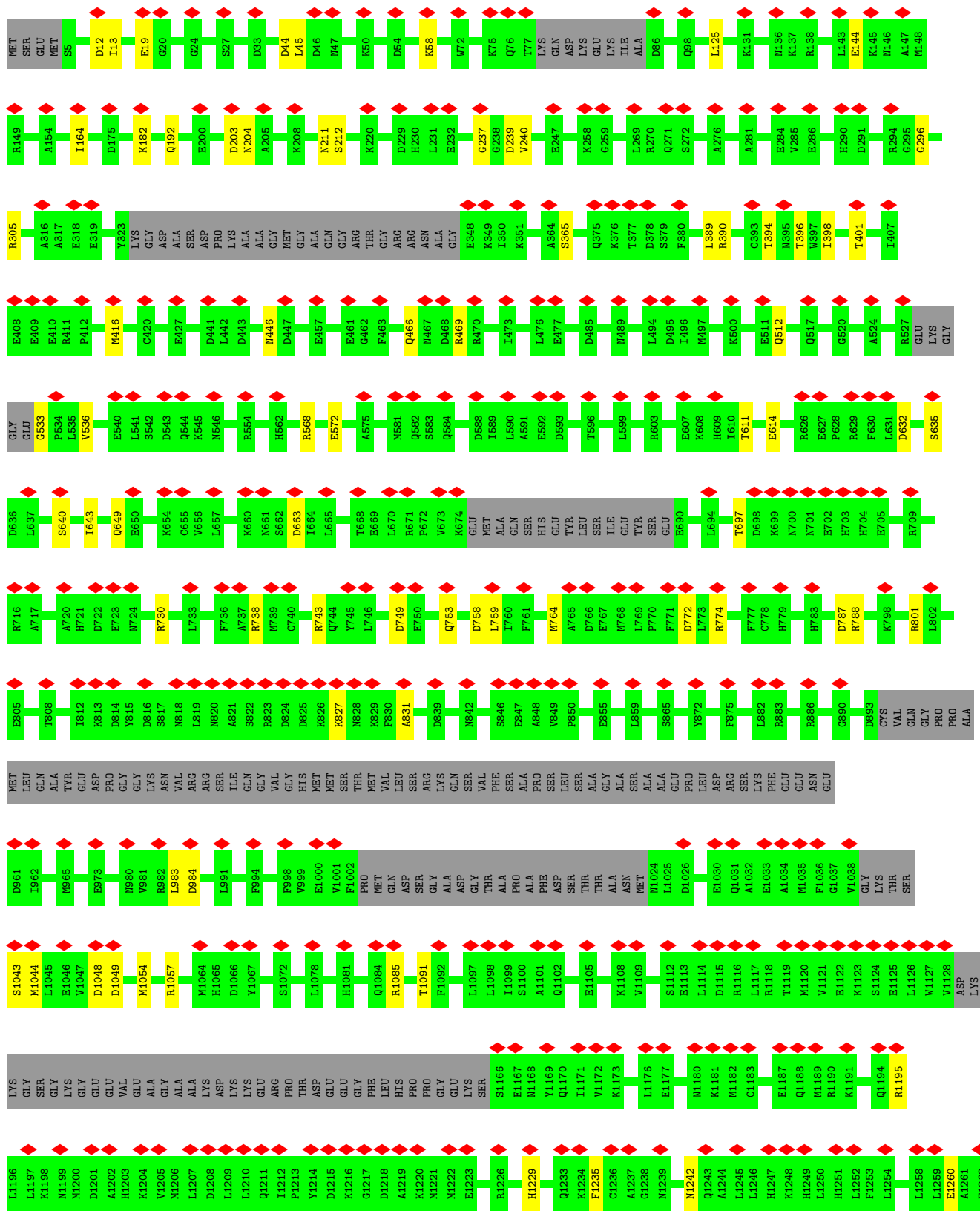
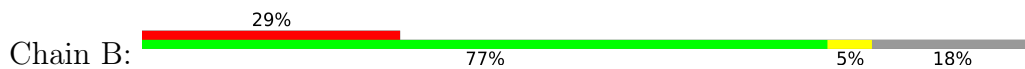
- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).

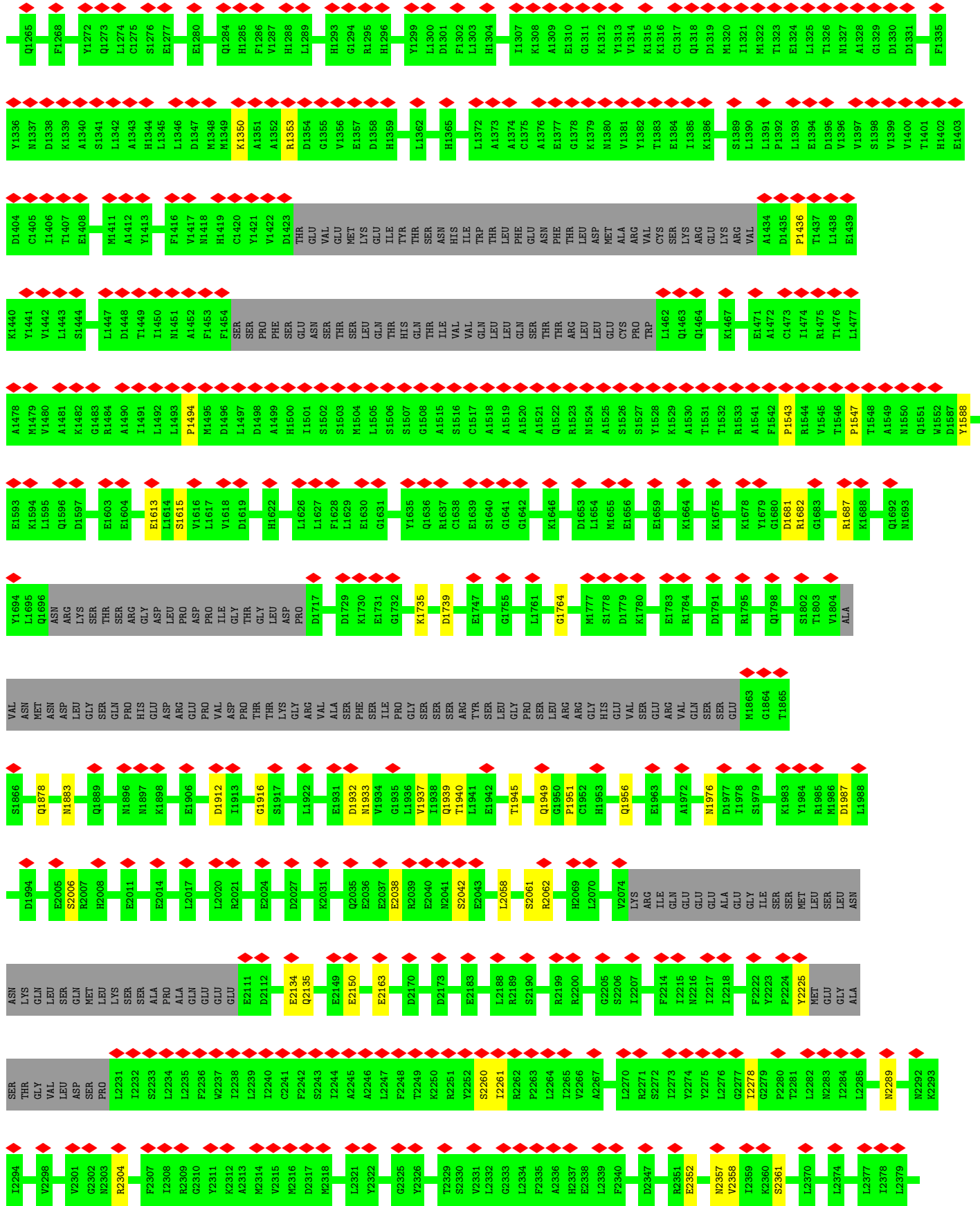


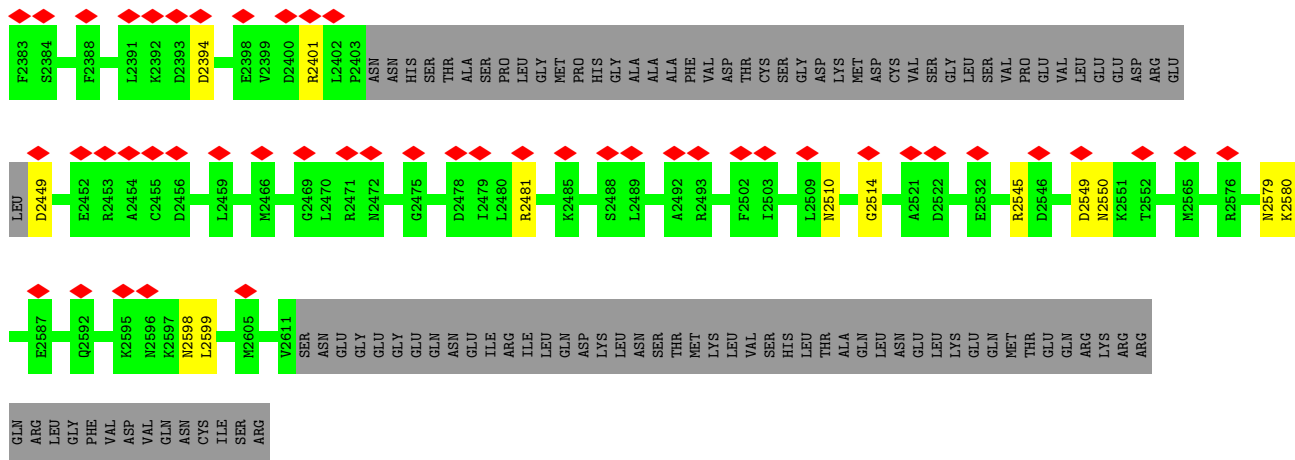
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	



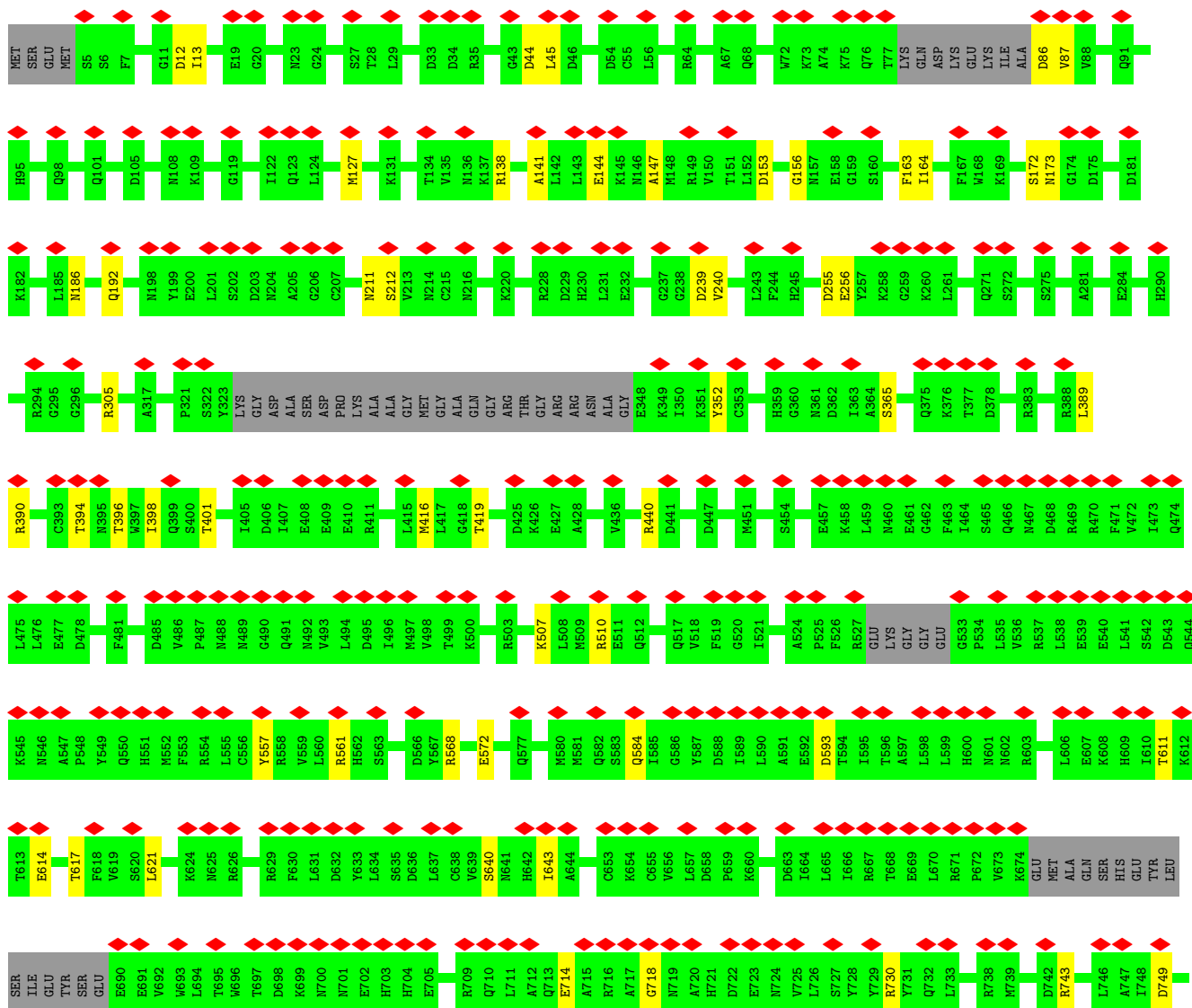
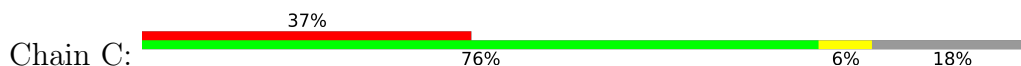
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

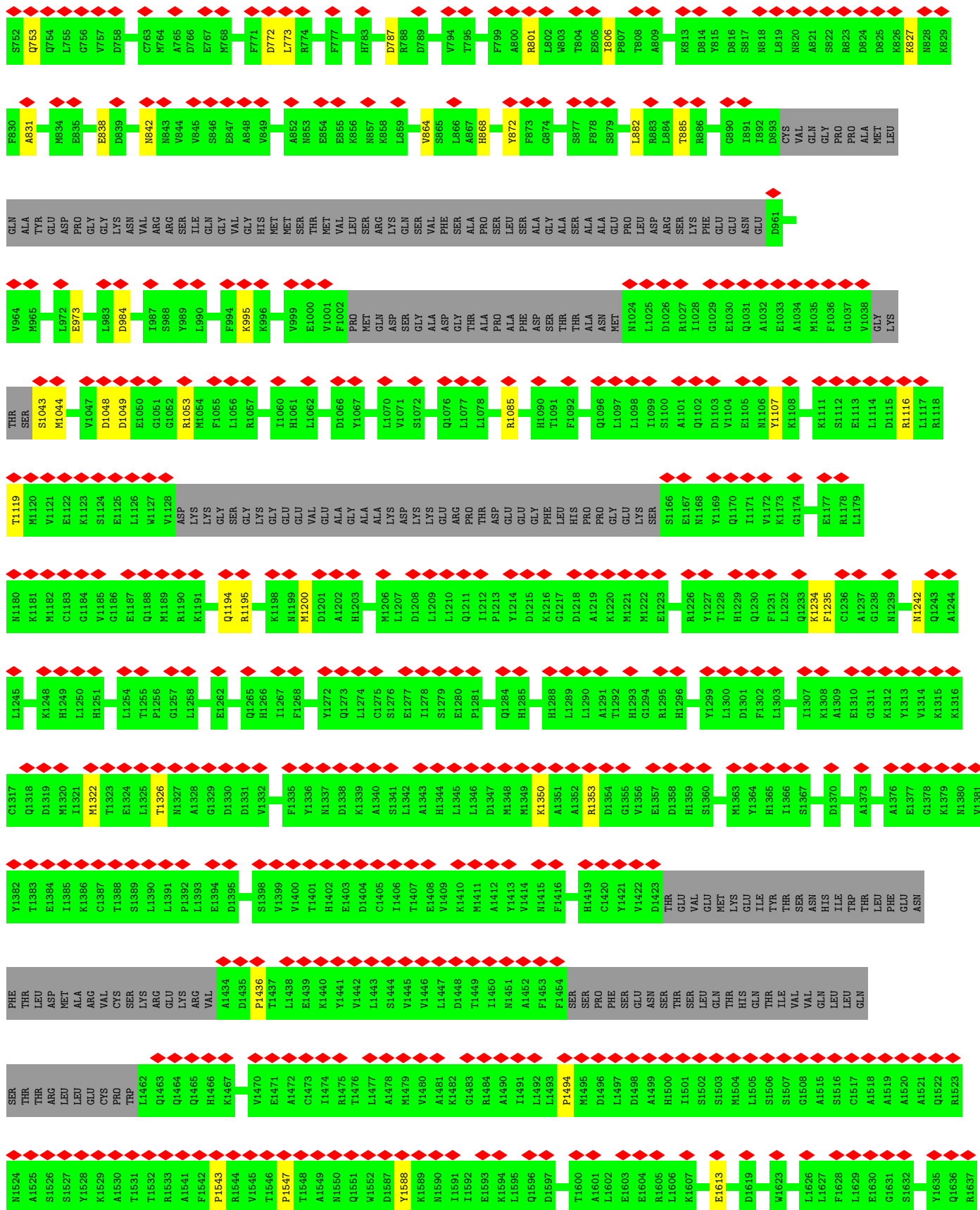


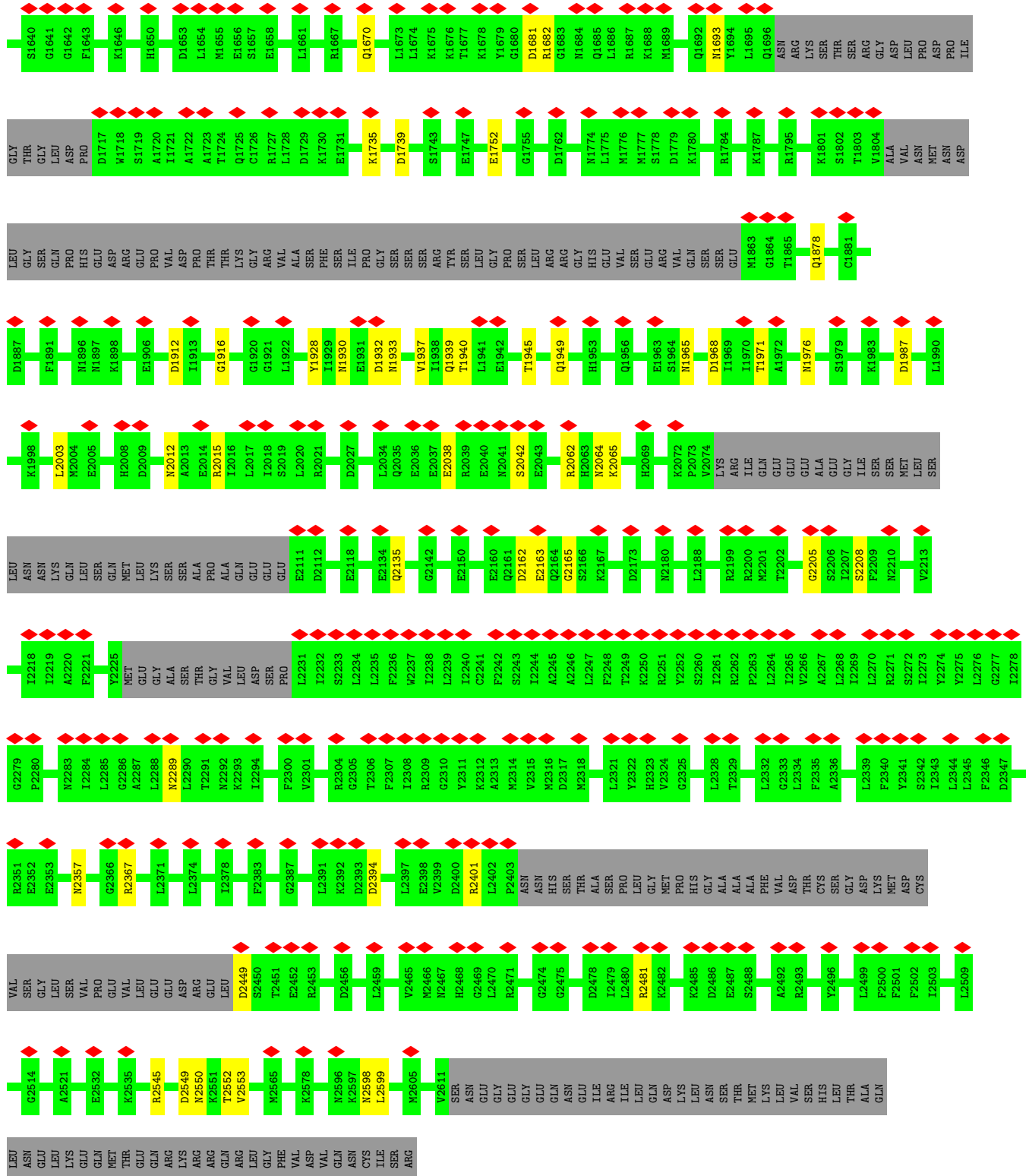




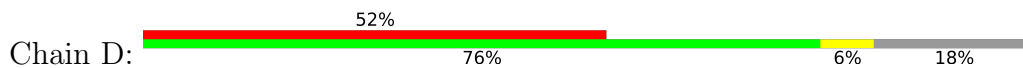
● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

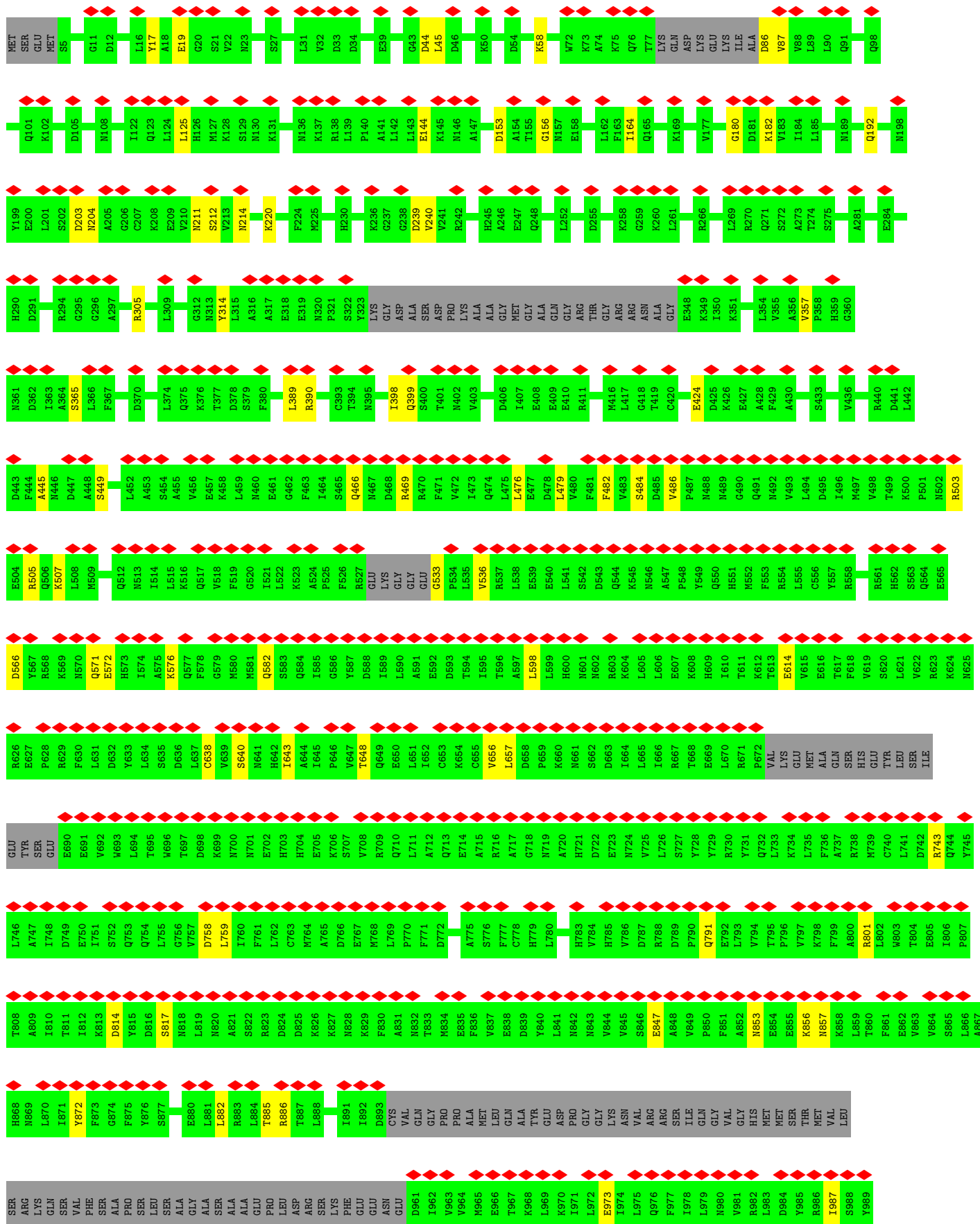






• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





L990	L991	S992	W993	F994	K996	F997	F998	W999	E1000	V1001	F1002	PRO	MET	GLN	ASP	SER	GLY	ALA	ASP	GLY	THR	ALA	PRO	ALA	PHE	ASP	SER	THR	THR	ALA	ASN	M1024	L1025	D1026	R1027	G1029	E1030	Q1031	A1032	E1033	A1034	M1035	F1036	G1037	VAL	GLY	LYS	THR	SER	S1043	M1044	L1045	E1046	V1047	D1048	D1049					
E1050	G1051	G1052	R1053	M1054	F1055	L1056	R1057	V1058	I1059	I1060	H1061	L1062	T1063	M1064	H1065	D1066	Y1067	A1068	V1071	S1072	G1073	A1074	L1075	Q1076	L1077	L1078	F1079	K1080	H1081	F1082	S1083	Q1084	R1085	Q1086	E1087	A1088	M1089	H1090	T1091	F1092	K1093	Q1094	V1095	Q1096	L1097	L1098	I1099	S1100	Q1102	D1103	V1104	E1105	N1106	Y1107	K1108	V1109	L1110				
K1111	S1112	E1113	L1114	D1115	R1116	L1117	R1118	L1119	M1120	V1121	E1122	K1123	S1124	E1125	L1126	Y1127	V1128	D1129	LYS	GLY	SER	GLY	LYS	GLU	VAL	GLU	GLU	ALA	GLY	ALA	ALA	LYS	ASP	LYS	GLU	ARG	PRO	THR	ASP	GLU	GLU	GLY	PHE	LEU	HIS	PRO	GLY	GLY	LYS	SER	S1166	E1167	M1168	Y1169	Q1170						
I1171	V1172	K1173	G1174	I1175	E1177	R1178	L1179	M1180	K1181	M1182	G1183	G1184	V1185	G1186	E1187	Q1188	M1189	R1190	K1191	L1192	Q1193	Q1194	R1195	L1196	L1197	K1198	M1199	M1200	A1201	A1202	H1203	K1204	V1205	M1206	L1207	D1208	L1209	L1210	Q1211	I1212	P1213	Y1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	E1223	I1224	L1225	R1226	Y1227	T1228	H1229	Q1230				
F1231	L1232	Q1233	K1234	F1235	C1236	A1237	G1238	N1239	P1240	G1241	N1242	Q1243	A1244	L1245	L1246	H1247	K1248	H1249	L1250	H1251	L1252	F1253	L1254	T1255	P1256	G1257	L1258	L1259	E1260	A1261	E1262	T1263	M1264	Q1265	H1266	L1267	F1268	L1269	M1270	N1271	Y1272	Q1273	P1274	L1275	C1276	S1277	I1278	S1279	E1280	F1281	V1282	L1283	Q1284	H1285	F1286	V1287	H1288	L1289	L1290		
M1291	T1292	H1293	G1294	L1295	H1296	V1297	Q1298	L1299	L1300	D1301	F1302	L1303	H1304	T1305	V1306	I1307	K1308	A1309	E1310	G1311	K1312	F1313	V1314	K1315	K1316	Q1317	Q1318	D1319	M1320	I1321	M1322	T1323	E1324	L1325	T1326	M1327	A1328	G1329	D1330	D1331	V1332	V1333	V1334	F1335	M1337	D1338	K1339	S1340	S1341	L1342	A1343	H1344	L1345	L1346	D1347	M1348	M1349	K1350			
A1351	A1352	R1353	D1354	G1355	E1357	D1358	H1359	S1360	P1361	L1362	M1363	Y1364	H1365	I1366	S1367	L1368	V1369	D1370	L1371	L1372	A1373	A1374	C1375	A1376	E1377	V1378	K1379	M1380	V1381	Y1382	T1383	L1384	I1385	K1386	C1387	T1388	S1389	R1390	L1391	P1392	L1393	E1394	D1395	V1396	V1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	I1406	L1407	E1408	V1409	K1410			
M1411	A1412	Y1413	V1414	M1415	F1416	V1417	M1418	H1419	C1420	Y1421	V1422	D1423	T1424	E1425	V1426	E1427	M1428	K1429	E1430	I1431	L1432	T1433	S1434	M1435	H1436	I1437	V1438	L1439	T1440	F1441	A1442	M1443	F1444	T1445	L1446	D1447	M1448	A1449	R1450	V1451	C1452	S1453	K1454	L1455	GLU	LYS	ARG	VAL	ALA	PRO	T1463	L1464	E1465	K1466	Y1467	L1468	S1470				
V1471	V1472	L1473	D1474	T1475	I1476	N1477	A1478	F1479	F1480	S1481	S1482	P1483	PHE	SER	GLU	ASN	SER	SER	GLN	THR	HIS	GLN	THR	I1434	VAL	VAL	GLN	LEU	GLN	THR	ARG	LEU	GLU	CYS	PRO	TRP	LEU	GLN	GLN	GLN	HIS	LYS	GLY	SER	VAL	GLU	ALA	CYS	I1455	GLU	LYS	ARG	THR	LEU	A1490						
M1491	V1492	A1493	K1494	G1495	R1496	A1497	I1498	L1499	L1500	P1501	M1502	D1503	L1504	D1505	A1506	H1507	I1508	SER	SER	MET	LEU	SER	GLY	A1515	S1516	C1517	A1518	A1519	A1520	A1521	Q1522	R1523	M1524	A1525	S1526	S1527	Y1528	K1529	A1530	T1531	T1532	M1533	A1541	F1542	P1543	R1544	V1545	T1546	P1547	L1548	A1549	M1550	Q1551	W1552	D1587	V1588	K1589	M1590			
I1591	I1592	E1593	K1594	L1595	Q1596	D1597	I1598	I1599	T1600	A1601	L1602	E1603	E1604	R1605	L1606	K1607	P1608	L1609	E1613	V1616	L1617	V1618	D1619	V1620	L1621	H1622	V1623	P1624	E1625	L1626	L1627	F1628	L1629	E1630	G1631	M1632	E1633	A1634	T1635	Q1636	R1637	C1638	F1639	S1640	G1641	G1642	F1643	K1646	L1647	I1648	Q1649	H1650	V1651	K1652	D1653	L1654					
M1655	E1656	S1657	E1658	E1659	K1660	L1661	C1662	L1663	K1664	R1667	T1668	L1669	Q1670	Q1671	M1672	L1673	L1674	K1675	K1676	T1677	K1678	Y1679	G1680	D1681	M1684	Q1685	K1688	M1689	L1690	L1691	Q1692	M1693	Y1694	L1695	Q1696	ASN	ARG	LYS	SER	THR	SER	ARG	GLY	ASP	LEU	LEU	ASP	PRO	ILE	GLY	THR	GLY	L1646	L1647	I1648	Q1649	H1650	V1651	K1652	D1653	L1654
M1718	S1719	A1720	A1723	C1726	R1727	L1728	D1729	K1730	E1731	G1732	A1733	T1734	K1735	C1738	D1739	T1742	S1743	T1744	K1745	M1746	E1747	I1754	G1755	I1758	L1761	D1762	G1763	G1764	E1767	I1768	Q1769	K1770	S1771	F1772	H1773	M1774	L1775	M1776	M1777	S1778	D1779	K1780	K1781	S1782	E1783	R1784	F1785	F1786	K1787	D1791											

R1795	Q1798	E1799	T1800	K1801	S1802	T1803	V1804	ALA	VAL	ASN	MET	ASN	ASP	LEU	GLY	GLN	HIS	PRO	GLU	ASP	THR	THR	LYS	GLY	ARG	VAL	ALA	SER	PHE	SER	ILE	PRO	GLY	SER	SER	SER	ARG	TVR	SER	GLY	PRO	SER	LEU	ARG	ARG	GLY	HIS	GLU	VAL				
M1950	E1931	D1932	M1933	V1934	G1935	L1936	V1937	T1940	L1941	E1942	T1943	E1946	Q1949	E1954	M1955	Q1956	T1957	C1958	T1961	H1962	E1963	S1964	M1965	L1966	I1967	D1968	T1971	A1972	L1973	I1974	D1977	I1978	S1979	P1980	L1981	C1982	K1983	Y1984	R1985	M1986	D1987	L1988	V1989	L1990	M1995	L2001	A2002	L2003	M2004				
E2005	S2006	R2007	H2008	D2009	S2010	E2011	N2012	A2013	E2014	R2015	I2016	L2017	I2018	S2019	R2021	F2022	Q2023	E2024	D2027	L2034	Q2035	E2036	E2037	E2038	R2039	E2040	N2041	S2042	R2047	H2051	Y2054	L2058	L2060	S2061	R2062	H2063	M2064	K2065	Q2066	L2067	Q2068	H2069	L2070	L2071	F2072	F2073	V2074	LYS	ARG	ILE	GLN		
GLU	GLU	ALA	GLU	ILE	SER	SER	MET	LEU	SER	LEU	ASN	ASN	LYS	GLN	LEU	GLN	MET	LYS	SER	ALA	PRO	ALA	GLN	GLU	GLU	E2111	D2112	A2115	E2118	I2124	E2125	D2130	R2131	S2132	M2133	E2134	G2142	F2146	R2154	E2163	D2170	D2173											
M2182	R2186	K2187	S2190	R2199	R2200	L2201	T2202	G2205	S2206	F2209	F2214	I2215	I2218	I2219	A2220	F2221	Y2225	MET	GLU	GLY	ALA	ALA	THR	GLY	VAL	E2111	D2112	A2115	E2118	I2124	E2125	D2130	R2131	S2132	M2133	E2134	G2142	F2146	R2154	E2163	D2170	D2173											
S2260	I2261	R2262	P2263	L2264	I2265	V2266	A2267	L2268	I2269	L2270	R2271	S2272	I2273	Y2274	Y2275	L2276	G2277	G2279	L2282	N2283	I2284	L2285	G2286	A2287	L2288	N2289	L2290	T2291	I2294	V2295	F2296	V2297	V2298	S2299	F2300	R2304	G2305	T2306	F2307	I2308	R2309	G2310	Y2311	K2312	A2313	M2314	V2315	M2316	D2317	T2318	K2260	R2261	Y2262
V2324	G2325	Y2326	L2327	T2329	L2332	G2333	L2334	F2335	A2336	H2337	F2340	Y2341	L2344	D2347	L2348	R2351	E2352	N2357	K2360	I2369	L2369	A2373	L2377	I2378	L2382	F2383	G2387	F2388	L2389	F2390	L2391	K2392	D2393	D2394	F2395	E2398	V2399	D2400	R2401	L2402	P2403	ASN	ASN	HIS	SER	THR							
I2479	L2480	R2481	K2483	P2483	S2484	K2485	D2486	A2487	A2492	R2493	L2499	F2502	T2507	V2508	L2509	M2510	L2511	I2512	D2518	R2524	E2531	R2545	D2546	D2549	M2550	H2563	M2564	M2565	M2566	M2567	R2576	V2577	K2578	M2579	K2580	T2581	D2582	G2585	K2595	L2470	R2471	M2472	D2478										
SER	ASN	GLU	GLY	GLU	GLU	GLN	ASN	ASN	ILE	ARG	GLU	ILE	LEU	GLN	GLN	LYS	ASP	GLY	ASP	LYS	THR	THR	LEU	LEU	ASN	GLU	GLY	GLU	GLU	GLY	ASP	ARG	GLU	LEU	PHE	VAL	ASP	VAL	GLN	ASN	CYS	ILE	SER	ARG									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	Not provided	
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	19.496	Depositor
Minimum map value	-12.071	Depositor
Average map value	-0.013	Depositor
Map value standard deviation	0.917	Depositor
Recommended contour level	3.93	Depositor
Map size (Å)	417.79202, 417.79202, 417.79202	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.088, 1.088, 1.088	Depositor

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: I3P, ZN

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	0.25	0/17650	0.46	4/23851 (0.0%)
1	B	0.25	0/17650	0.46	4/23851 (0.0%)
1	C	0.25	0/17650	0.46	4/23851 (0.0%)
1	D	0.25	0/17856	0.46	3/24125 (0.0%)
All	All	0.25	0/70806	0.46	15/95678 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1547	PRO	N-CA-CB	5.73	110.18	103.30
1	D	1543	PRO	N-CA-CB	5.71	110.16	103.30
1	D	1547	PRO	N-CA-CB	5.71	110.16	103.30
1	B	1547	PRO	N-CA-CB	5.70	110.14	103.30
1	C	1547	PRO	N-CA-CB	5.69	110.12	103.30
1	A	1494	PRO	N-CA-CB	5.68	110.12	103.30
1	D	1501	PRO	N-CA-CB	5.67	110.11	103.30
1	A	1543	PRO	N-CA-CB	5.64	110.07	103.30
1	C	1494	PRO	N-CA-CB	5.64	110.07	103.30
1	C	1436	PRO	N-CA-CB	5.64	110.06	103.30
1	C	1543	PRO	N-CA-CB	5.58	110.00	103.30
1	B	1543	PRO	N-CA-CB	5.58	110.00	103.30
1	B	1436	PRO	N-CA-CB	5.51	109.92	103.30
1	B	1494	PRO	N-CA-CB	5.51	109.91	103.30
1	A	1436	PRO	N-CA-CB	5.39	109.76	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17345	17351	17180	75	0
1	B	17345	17352	17181	69	0
1	C	17345	17349	17179	77	0
1	D	17540	17587	17485	92	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	0	0
3	B	24	9	9	0	0
3	C	24	9	9	2	0
3	D	24	9	9	1	0
All	All	69675	69675	69061	305	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 2.

All (305) 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:801:ARG:NH2	1:A:984:ASP:OD1	2.19	0.76
1:B:144:GLU:OE2	1:B:211:ASN:ND2	2.21	0.74
1:A:2545:ARG:NH1	1:D:2163:GLU:O	2.20	0.74
1:C:510:ARG:NH2	3:C:3002:I3P:O52	2.21	0.73
1:B:749:ASP:O	1:B:753:GLN:NE2	2.22	0.73
1:D:144:GLU:OE2	1:D:211:ASN:ND2	2.21	0.73
1:A:1782:SER:OG	1:A:1897:ASN:OD1	2.05	0.73
1:C:144:GLU:OE2	1:C:211:ASN:ND2	2.22	0.73
1:B:192:GLN:O	1:B:212:SER:OG	2.07	0.73
1:C:2163:GLU:O	1:D:2545:ARG:NH1	2.22	0.72
1:A:144:GLU:OE2	1:A:211:ASN:ND2	2.22	0.72
1:A:192:GLN:O	1:A:212:SER:OG	2.08	0.71
1:A:1118:ARG:NH2	1:A:1200:MET:O	2.23	0.71
1:C:127:MET:O	1:C:440:ARG:NH2	2.23	0.71
1:A:749:ASP:O	1:A:753:GLN:NE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLN:O	1:C:212:SER:OG	2.09	0.70
1:A:568:ARG:NH2	1:A:572:GLU:OE2	2.25	0.70
1:B:2163:GLU:O	1:C:2545:ARG:NH1	2.24	0.70
1:A:649:GLN:NE2	1:A:738:ARG:O	2.25	0.70
1:A:2163:GLU:O	1:B:2545:ARG:NH1	2.25	0.70
1:C:2394:ASP:OD1	1:C:2481:ARG:NH2	2.25	0.69
1:A:401:THR:OG1	1:A:416:MET:O	2.10	0.69
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.26	0.69
1:C:568:ARG:NH2	1:C:572:GLU:OE2	2.24	0.69
1:C:2038:GLU:OE2	1:C:2042:SER:OG	2.09	0.69
1:D:1085:ARG:NH1	1:D:1613:GLU:OE2	2.25	0.69
1:B:2006:SER:OG	1:B:2134:GLU:OE1	2.06	0.69
1:D:192:GLN:O	1:D:212:SER:OG	2.09	0.69
1:A:1987:ASP:OD1	1:A:2042:SER:OG	2.07	0.69
1:C:1987:ASP:OD1	1:C:2042:SER:OG	2.07	0.69
1:C:749:ASP:O	1:C:753:GLN:NE2	2.26	0.69
1:D:533:GLY:N	1:D:536:VAL:O	2.26	0.69
1:B:1937:VAL:O	1:B:1940:THR:OG1	2.10	0.68
1:A:1735:LYS:NZ	1:A:1739:ASP:OD2	2.20	0.68
1:A:533:GLY:N	1:A:536:VAL:O	2.27	0.68
1:B:533:GLY:N	1:B:536:VAL:O	2.27	0.68
1:D:305:ARG:NH2	1:D:365:SER:O	2.25	0.68
1:B:1235:PHE:O	1:B:1242:ASN:ND2	2.26	0.68
1:C:827:LYS:O	1:C:831:ALA:N	2.27	0.68
1:A:1085:ARG:NH1	1:A:1613:GLU:OE2	2.26	0.67
1:B:446:ASN:ND2	1:B:512:GLN:OE1	2.27	0.67
1:B:611:THR:OG1	1:B:614:GLU:OE1	2.11	0.66
1:D:1956:GLN:NE2	1:D:2002:ALA:O	2.28	0.66
1:C:401:THR:OG1	1:C:416:MET:O	2.13	0.66
1:C:1968:ASP:O	1:C:1971:THR:OG1	2.13	0.66
1:D:572:GLU:O	1:D:576:LYS:NZ	2.28	0.66
1:D:1053:ARG:NH1	1:D:1694:TYR:O	2.29	0.66
1:C:1085:ARG:NH1	1:C:1613:GLU:OE2	2.29	0.66
1:C:2003:LEU:O	1:C:2012:ASN:ND2	2.30	0.65
1:C:561:ARG:NH1	1:C:593:ASP:O	2.30	0.65
1:C:2401:ARG:NE	1:C:2449:ASP:OD2	2.29	0.65
1:C:352:TYR:O	1:C:419:THR:OG1	2.13	0.64
1:D:305:ARG:NH2	1:D:365:SER:OG	2.30	0.64
1:B:389:LEU:HB2	1:B:398:ILE:HD12	1.80	0.63
1:A:2038:GLU:OE2	1:A:2042:SER:OG	2.15	0.63
1:A:838:GLU:O	1:A:842:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:LEU:HB2	1:D:398:ILE:HD12	1.79	0.62
1:B:2401:ARG:NE	1:B:2449:ASP:OD2	2.32	0.62
1:D:1214:TYR:OH	1:D:1222:MET:SD	2.50	0.62
1:B:743:ARG:NH1	1:B:787:ASP:O	2.32	0.62
1:B:1987:ASP:OD1	1:B:2042:SER:OG	2.10	0.62
1:A:1725:GLN:NE2	1:A:1759:HIS:O	2.33	0.62
1:A:352:TYR:O	1:A:419:THR:OG1	2.13	0.62
1:B:401:THR:OG1	1:B:416:MET:O	2.18	0.61
1:B:568:ARG:NH2	1:B:572:GLU:OE2	2.33	0.61
1:C:1235:PHE:O	1:C:1242:ASN:ND2	2.33	0.61
1:B:1945:THR:O	1:B:1949:GLN:N	2.33	0.61
1:C:557:TYR:OH	1:C:584:GLN:OE1	2.17	0.61
1:C:2062:ARG:NH1	1:C:2135:GLN:OE1	2.34	0.60
1:A:1945:THR:O	1:A:1949:GLN:N	2.34	0.60
1:C:138:ARG:NH1	1:D:1425:GLU:O	2.34	0.60
1:C:389:LEU:HB2	1:C:398:ILE:HD12	1.84	0.60
1:C:1878:GLN:OE1	1:C:1939:GLN:NE2	2.35	0.59
1:C:1945:THR:O	1:C:1949:GLN:N	2.35	0.59
1:A:75:LYS:NZ	1:A:489:ASN:O	2.36	0.59
1:D:466:GLN:OE1	1:D:469:ARG:NH2	2.36	0.59
1:D:2394:ASP:OD1	1:D:2481:ARG:NH2	2.36	0.59
1:B:649:GLN:NE2	1:B:738:ARG:O	2.36	0.58
1:D:814:ASP:O	1:D:817:SER:OG	2.14	0.58
1:A:611:THR:OG1	1:A:614:GLU:OE1	2.11	0.58
1:B:632:ASP:O	1:B:635:SER:OG	2.16	0.58
1:B:2394:ASP:OD1	1:B:2481:ARG:NH2	2.37	0.58
1:B:1735:LYS:NZ	1:B:1739:ASP:OD2	2.32	0.58
1:D:153:ASP:OD2	1:D:156:GLY:N	2.36	0.58
1:B:1085:ARG:NH1	1:B:1613:GLU:OE2	2.37	0.58
1:C:1937:VAL:O	1:C:1940:THR:OG1	2.13	0.58
1:D:1391:LEU:O	1:D:1421:TYR:OH	2.21	0.58
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.37	0.57
1:B:2038:GLU:OE2	1:B:2042:SER:OG	2.21	0.57
1:A:1937:VAL:O	1:A:1940:THR:OG1	2.15	0.57
1:C:611:THR:OG1	1:C:614:GLU:OE1	2.14	0.56
1:D:1054:MET:SD	1:D:1057:ARG:NH2	2.78	0.56
1:D:1937:VAL:O	1:D:1940:THR:OG1	2.16	0.56
1:D:1890:ASN:OD1	1:D:1893:ARG:NH2	2.37	0.56
1:D:2125:GLU:OE1	1:D:2563:HIS:NE2	2.38	0.56
1:D:2369:ILE:HG23	1:D:2512:ILE:HG23	1.87	0.56
1:A:389:LEU:HB2	1:A:398:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1951:PRO:O	1:B:1956:GLN:NE2	2.38	0.56
1:C:1928:TYR:O	1:C:1933:ASN:ND2	2.39	0.56
1:A:1912:ASP:O	1:A:1916:GLY:N	2.38	0.56
1:A:561:ARG:NH1	1:A:593:ASP:O	2.39	0.56
1:C:806:ILE:O	1:C:995:LYS:NZ	2.25	0.56
1:C:1116:ARG:O	1:C:1119:THR:OG1	2.16	0.56
1:A:2205:GLY:O	1:A:2208:SER:OG	2.24	0.55
1:B:19:GLU:OE1	1:B:182:LYS:NZ	2.26	0.55
1:A:2003:LEU:O	1:A:2012:ASN:ND2	2.39	0.55
1:A:482:PHE:O	1:A:505:ARG:NH1	2.40	0.55
1:A:663:ASP:OD1	1:A:697:THR:OG1	2.22	0.55
1:A:2192:PRO:O	1:A:2196:TRP:N	2.40	0.55
1:D:2047:ARG:O	1:D:2051:HIS:ND1	2.40	0.54
1:B:2062:ARG:NH1	1:B:2135:GLN:OE1	2.40	0.54
1:D:1968:ASP:O	1:D:1971:THR:OG1	2.17	0.54
1:D:1603:GLU:O	1:D:1607:LYS:N	2.41	0.53
1:D:2010:SER:O	1:D:2014:GLU:N	2.41	0.53
1:D:17:TYR:O	1:D:220:LYS:N	2.39	0.53
1:C:1194:GLN:NE2	1:C:1234:LYS:O	2.42	0.53
1:C:1053:ARG:NE	1:C:1693:ASN:O	2.43	0.52
1:A:58:LYS:N	1:A:125:LEU:O	2.42	0.52
1:D:656:VAL:HG13	1:D:657:LEU:HD22	1.90	0.52
1:B:827:LYS:O	1:B:831:ALA:N	2.43	0.52
1:D:399:GLN:NE2	1:D:424:GLU:OE2	2.43	0.52
1:D:2329:THR:O	1:D:2333:GLY:N	2.44	0.51
1:B:305:ARG:NH2	1:B:365:SER:O	2.43	0.51
1:A:1385:ILE:O	1:A:1388:THR:OG1	2.15	0.51
1:B:1615:SER:OG	1:B:1687:ARG:NE	2.43	0.51
1:C:153:ASP:OD2	1:C:156:GLY:N	2.42	0.51
1:B:1764:GLY:O	1:B:1883:ASN:ND2	2.44	0.51
1:C:1322:MET:O	1:C:1326:THR:OG1	2.17	0.51
1:D:2507:ILE:O	1:D:2511:LEU:N	2.43	0.51
1:A:1670:GLN:NE2	1:A:1752:GLU:OE1	2.42	0.51
1:C:12:ASP:OD1	1:C:13:ILE:N	2.44	0.50
1:C:730:ARG:NH2	1:C:772:ASP:OD2	2.44	0.50
1:D:1385:ILE:O	1:D:1388:THR:OG1	2.29	0.50
1:A:1787:LYS:NZ	1:A:1791:ASP:OD2	2.44	0.50
1:B:640:SER:O	1:B:643:ILE:N	2.42	0.50
1:B:764:MET:O	1:B:774:ARG:NH2	2.44	0.50
1:B:2150:GLU:OE2	1:B:2304:ARG:NH2	2.44	0.50
1:D:482:PHE:O	1:D:505:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1033:GLU:OE2	1:D:1085:ARG:NH2	2.42	0.50
1:D:1337:ASN:OD1	1:D:1338:ASP:N	2.45	0.50
1:C:2205:GLY:O	1:C:2208:SER:OG	2.25	0.50
1:A:1953:HIS:NE2	1:A:2006:SER:O	2.45	0.50
1:A:2062:ARG:NH1	1:A:2135:GLN:OE1	2.46	0.49
1:C:864:VAL:O	1:C:868:HIS:N	2.46	0.49
1:C:163:PHE:N	1:C:186:ASN:O	2.45	0.49
1:D:1895:GLN:O	1:D:1900:ASN:ND2	2.45	0.49
1:C:1965:ASN:OD1	1:C:2015:ARG:NH2	2.44	0.49
1:B:237:GLY:N	1:B:296:GLY:O	2.46	0.49
1:C:1670:GLN:NE2	1:C:1752:GLU:OE1	2.44	0.49
1:B:663:ASP:OD1	1:B:697:THR:OG1	2.15	0.49
1:A:632:ASP:O	1:A:635:SER:OG	2.23	0.48
1:D:58:LYS:N	1:D:125:LEU:O	2.44	0.48
1:C:1350:LYS:O	1:C:1353:ARG:NH1	2.47	0.48
1:D:1985:ARG:NH2	1:D:1987:ASP:OD2	2.46	0.48
1:D:1932:ASP:OD1	1:D:1933:ASN:N	2.47	0.48
1:B:2549:ASP:OD1	1:B:2550:ASN:N	2.47	0.48
1:D:1103:ASP:O	1:D:1107:TYR:N	2.46	0.48
1:B:1350:LYS:O	1:B:1353:ARG:NH1	2.46	0.48
1:D:743:ARG:NH2	1:D:791:GLN:O	2.47	0.48
1:C:141:ALA:N	1:C:147:ALA:O	2.44	0.47
1:B:466:GLN:OE1	1:B:469:ARG:NH2	2.46	0.47
1:D:847:GLU:OE1	1:D:856:LYS:NZ	2.45	0.47
1:D:582:GLN:NE2	1:D:614:GLU:OE2	2.46	0.47
1:D:872:TYR:OH	1:D:973:GLU:O	2.30	0.47
1:A:394:THR:CB	1:A:396:THR:HG1	2.25	0.47
1:A:2536:THR:O	1:A:2545:ARG:N	2.47	0.47
1:D:314:TYR:N	1:D:357:VAL:O	2.45	0.47
1:A:314:TYR:N	1:A:357:VAL:O	2.46	0.47
1:A:2394:ASP:OD1	1:A:2481:ARG:NH2	2.45	0.47
1:B:1229:HIS:NE2	1:B:1260:GLU:OE2	2.48	0.47
1:B:1932:ASP:OD1	1:B:1933:ASN:N	2.48	0.47
1:B:2358:VAL:O	1:B:2361:SER:OG	2.16	0.47
1:D:1490:ALA:O	1:D:1494:LYS:N	2.48	0.47
1:B:1048:ASP:OD1	1:B:1049:ASP:N	2.48	0.47
1:C:882:LEU:O	1:C:885:THR:OG1	2.26	0.47
1:D:1893:ARG:NH1	1:D:1955:ASN:OD1	2.48	0.46
1:D:2187:LYS:O	1:D:2190:SER:OG	2.20	0.46
1:D:1891:PHE:O	1:D:1895:GLN:NE2	2.48	0.46
1:A:2124:ILE:HD11	1:A:2567:ASN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASP:OD1	1:B:240:VAL:N	2.47	0.46
1:C:394:THR:CB	1:C:396:THR:HG1	2.28	0.46
1:A:305:ARG:NH2	1:A:365:SER:OG	2.48	0.46
1:B:730:ARG:NH2	1:B:772:ASP:OD2	2.49	0.46
1:B:2058:LEU:O	1:B:2061:SER:OG	2.27	0.46
1:C:507:LYS:NZ	3:C:3002:I3P:O53	2.46	0.46
1:D:180:GLY:O	1:D:220:LYS:NZ	2.49	0.46
1:B:983:LEU:HD21	1:B:1091:THR:HG21	1.98	0.46
1:C:2549:ASP:OD1	1:C:2550:ASN:N	2.47	0.46
1:D:44:ASP:OD1	1:D:45:LEU:N	2.49	0.46
1:D:503:ARG:NH2	1:D:566:ASP:O	2.49	0.46
1:A:1932:ASP:OD1	1:A:1933:ASN:N	2.49	0.46
1:D:239:ASP:OD1	1:D:240:VAL:N	2.49	0.46
1:D:1223:GLU:OE1	1:D:1226:ARG:NH2	2.49	0.46
1:D:1965:ASN:OD1	1:D:2015:ARG:NH2	2.49	0.46
1:D:758:ASP:OD1	1:D:759:LEU:N	2.49	0.46
1:A:1280:GLU:OE2	1:A:1284:GLN:NE2	2.49	0.46
1:B:1681:ASP:OD1	1:B:1682:ARG:N	2.49	0.46
1:D:476:LEU:HD23	1:D:479:LEU:HD12	1.98	0.46
1:A:758:ASP:OD1	1:A:759:LEU:N	2.49	0.45
1:D:1048:ASP:OD1	1:D:1049:ASP:N	2.49	0.45
1:A:1965:ASN:OD1	1:A:2015:ARG:NH2	2.49	0.45
1:C:838:GLU:O	1:C:842:ASN:OD1	2.34	0.45
1:C:872:TYR:OH	1:C:973:GLU:O	2.32	0.45
1:A:1178:ARG:O	1:A:1182:MET:N	2.50	0.45
1:B:12:ASP:OD1	1:B:13:ILE:N	2.50	0.45
1:B:758:ASP:OD1	1:B:759:LEU:N	2.50	0.45
1:A:1681:ASP:OD1	1:A:1682:ARG:N	2.50	0.45
1:C:714:GLU:O	1:C:718:GLY:N	2.48	0.45
1:B:164:ILE:HG23	1:B:164:ILE:O	2.17	0.45
1:D:164:ILE:HG23	1:D:164:ILE:O	2.17	0.45
1:D:638:CYS:HA	1:D:648:THR:HG21	1.97	0.45
1:D:2124:ILE:HD11	1:D:2567:ASN:O	2.17	0.45
1:A:1043:SER:OG	1:A:1044:MET:N	2.50	0.45
1:D:1735:LYS:NZ	1:D:1739:ASP:OD2	2.50	0.45
1:D:1930:ASN:N	1:D:1933:ASN:OD1	2.48	0.45
1:D:2319:GLU:O	1:D:2323:HIS:ND1	2.48	0.45
1:B:1195:ARG:NH2	1:B:1588:TYR:OH	2.50	0.45
1:A:314:TYR:O	1:A:357:VAL:N	2.50	0.45
1:B:2225:TYR:CE1	1:B:2278:ILE:HG21	2.52	0.45
1:C:164:ILE:HG23	1:C:164:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:SER:O	1:D:486:VAL:HG23	2.18	0.44
1:C:305:ARG:NH2	1:C:365:SER:O	2.51	0.44
1:C:1912:ASP:O	1:C:1916:GLY:N	2.50	0.44
1:C:1932:ASP:OD1	1:C:1933:ASN:N	2.50	0.44
1:D:203:ASP:OD1	1:D:204:ASN:N	2.51	0.44
1:A:239:ASP:OD1	1:A:240:VAL:N	2.50	0.44
1:C:1930:ASN:N	1:C:1933:ASN:OD1	2.45	0.44
1:A:1764:GLY:O	1:A:1883:ASN:ND2	2.51	0.44
1:A:2550:ASN:ND2	1:D:2604:ARG:O	2.48	0.44
1:D:1889:GLN:NE2	1:D:1946:GLU:O	2.50	0.44
1:C:1048:ASP:OD1	1:C:1049:ASP:N	2.51	0.44
1:D:1930:ASN:OD1	1:D:1931:GLU:N	2.50	0.44
1:A:86:ASP:OD1	1:A:87:VAL:N	2.50	0.43
1:A:165:GLN:O	1:A:184:ILE:N	2.46	0.43
1:A:1365:HIS:CD2	1:A:1413:TYR:HH	2.36	0.43
1:C:2162:ASP:OD1	1:C:2165:GLY:N	2.51	0.43
1:D:886:ARG:NH1	1:D:1047:VAL:O	2.51	0.43
1:C:2598:ASN:OD1	1:C:2599:LEU:N	2.52	0.43
1:A:164:ILE:O	1:A:164:ILE:HG23	2.18	0.43
1:A:563:SER:O	1:A:570:ASN:ND2	2.52	0.43
1:D:86:ASP:OD1	1:D:87:VAL:N	2.52	0.43
1:D:2549:ASP:OD1	1:D:2550:ASN:N	2.48	0.43
1:B:44:ASP:OD1	1:B:45:LEU:N	2.52	0.43
1:D:445:ALA:O	1:D:449:SER:N	2.49	0.43
1:A:255:ASP:OD1	1:A:256:GLU:N	2.51	0.43
1:C:86:ASP:OD1	1:C:87:VAL:N	2.51	0.43
1:C:640:SER:O	1:C:643:ILE:N	2.50	0.43
1:D:192:GLN:NE2	1:D:214:ASN:OD1	2.50	0.43
1:A:466:GLN:OE1	1:A:469:ARG:NH2	2.47	0.42
1:B:2510:ASN:O	1:B:2514:GLY:N	2.52	0.42
1:C:239:ASP:OD1	1:C:240:VAL:N	2.52	0.42
1:D:853:ASN:O	1:D:857:ASN:ND2	2.52	0.42
1:A:1968:ASP:O	1:A:1971:THR:OG1	2.30	0.42
1:C:255:ASP:OD1	1:C:256:GLU:N	2.53	0.42
1:C:772:ASP:OD1	1:C:773:LEU:N	2.52	0.42
1:C:1195:ARG:NH2	1:C:1588:TYR:OH	2.52	0.42
1:D:1987:ASP:OD1	1:D:1988:LEU:N	2.53	0.42
1:D:640:SER:O	1:D:643:ILE:N	2.48	0.42
1:A:772:ASP:OD1	1:A:773:LEU:N	2.52	0.42
1:B:1878:GLN:OE1	1:B:1939:GLN:NE2	2.47	0.42
1:D:2579:ASN:OD1	1:D:2580:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:LYS:O	1:A:831:ALA:N	2.52	0.42
1:B:58:LYS:N	1:B:125:LEU:O	2.48	0.42
1:C:743:ARG:NH1	1:C:787:ASP:O	2.53	0.42
1:D:507:LYS:NZ	3:D:3002:I3P:O53	2.51	0.42
1:B:743:ARG:NH1	1:B:788:ARG:O	2.51	0.42
1:C:44:ASP:OD1	1:C:45:LEU:N	2.52	0.42
1:C:172:SER:OG	1:C:173:ASN:N	2.53	0.41
1:C:1735:LYS:NZ	1:C:1739:ASP:OD2	2.45	0.41
1:C:2552:THR:HG23	1:C:2553:VAL:HG13	2.01	0.41
1:D:19:GLU:OE1	1:D:182:LYS:NZ	2.29	0.41
1:D:314:TYR:O	1:D:357:VAL:N	2.53	0.41
1:A:2367:ARG:NE	1:B:2352:GLU:OE2	2.54	0.41
1:C:1043:SER:OG	1:C:1044:MET:N	2.52	0.41
1:C:2064:ASN:OD1	1:C:2065:LYS:N	2.53	0.41
1:A:2260:SER:OG	1:A:2261:ILE:N	2.54	0.41
1:A:1746:ASN:OD1	1:A:1747:GLU:N	2.53	0.41
1:A:2598:ASN:OD1	1:A:2599:LEU:N	2.52	0.41
1:B:305:ARG:NH2	1:B:365:SER:OG	2.54	0.41
1:B:1912:ASP:O	1:B:1916:GLY:N	2.53	0.41
1:A:1024:ASN:OD1	1:A:1025:LEU:N	2.53	0.41
1:B:1043:SER:OG	1:B:1044:MET:N	2.52	0.41
1:D:2215:ILE:HD12	1:D:2341:TYR:CD2	2.54	0.41
1:A:1350:LYS:O	1:A:1353:ARG:NH1	2.54	0.41
1:B:1054:MET:SD	1:B:1057:ARG:NH2	2.91	0.41
1:A:44:ASP:OD1	1:A:45:LEU:N	2.54	0.41
1:A:1872:PRO:O	1:A:1876:PHE:N	2.47	0.41
1:B:2579:ASN:OD1	1:B:2580:LYS:N	2.54	0.41
1:C:1681:ASP:OD1	1:C:1682:ARG:N	2.54	0.41
1:A:1054:MET:SD	1:A:1057:ARG:NH2	2.94	0.41
1:B:2260:SER:OG	1:B:2261:ILE:N	2.53	0.41
1:B:2598:ASN:OD1	1:B:2599:LEU:N	2.54	0.41
1:D:571:GLN:NE2	1:D:598:LEU:O	2.53	0.41
1:C:2367:ARG:NH2	1:D:2352:GLU:OE2	2.54	0.40
1:A:1411:MET:O	1:A:1415:ASN:ND2	2.54	0.40
1:D:882:LEU:O	1:D:885:THR:OG1	2.29	0.40
1:D:1115:ASP:OD1	1:D:1116:ARG:N	2.54	0.40
1:D:1448:MET:SD	1:D:1469:LEU:HD22	2.62	0.40
1:B:203:ASP:OD1	1:B:204:ASN:N	2.54	0.40
1:C:1107:TYR:OH	1:C:1200:MET:SD	2.61	0.40
1:D:1787:LYS:NZ	1:D:1791:ASP:OD2	2.54	0.40
1:D:1934:VAL:HA	1:D:1937:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:THR:CB	1:B:396:THR:HG1	2.32	0.40
1:C:617:THR:O	1:C:621:LEU:N	2.51	0.40
1:D:801:ARG:NH1	1:D:987:ILE:HG21	2.36	0.40

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 PDB entries followed by that with respect to all EM entries.

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	2144/2671 (80%)	2055 (96%)	89 (4%)	0	100	100
1	B	2144/2671 (80%)	2062 (96%)	82 (4%)	0	100	100
1	C	2144/2671 (80%)	2059 (96%)	85 (4%)	0	100	100
1	D	2152/2671 (81%)	2069 (96%)	83 (4%)	0	100	100
All	All	8584/10684 (80%)	8245 (96%)	339 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	1879/2385 (79%)	1874 (100%)	5 (0%)	92	95
1	B	1879/2385 (79%)	1875 (100%)	4 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1879/2385 (79%)	1875 (100%)	4 (0%)	93	96
1	D	1927/2385 (81%)	1921 (100%)	6 (0%)	92	95
All	All	7564/9540 (79%)	7545 (100%)	19 (0%)	92	95

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	ARG
1	A	1897	ASN
1	A	1976	ASN
1	A	2289	ASN
1	A	2357	ASN
1	B	390	ARG
1	B	1976	ASN
1	B	2289	ASN
1	B	2357	ASN
1	C	390	ARG
1	C	1976	ASN
1	C	2289	ASN
1	C	2357	ASN
1	D	390	ARG
1	D	1693	ASN
1	D	1902	ASN
1	D	2064	ASN
1	D	2289	ASN
1	D	2357	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	I3P	C	3002	1	24,24,24	1.29	3 (12%)	36,39,39	0.59	0
3	I3P	A	3002	-	24,24,24	1.29	3 (12%)	36,39,39	0.68	1 (2%)
3	I3P	B	3002	-	24,24,24	1.29	3 (12%)	36,39,39	0.59	0
3	I3P	D	3002	-	24,24,24	1.29	3 (12%)	36,39,39	0.70	1 (2%)

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	I3P	C	3002	1	-	1/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	4/15/39/39	0/1/1/1
3	I3P	D	3002	-	-	4/15/39/39	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	I3P	P4-O4	3.25	1.65	1.59
3	D	3002	I3P	P1-O1	3.19	1.65	1.59
3	A	3002	I3P	P4-O4	3.17	1.65	1.59
3	B	3002	I3P	P4-O4	3.16	1.65	1.59
3	D	3002	I3P	P4-O4	3.13	1.65	1.59
3	A	3002	I3P	P1-O1	3.10	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	I3P	P1-O1	3.09	1.65	1.59
3	B	3002	I3P	P1-O1	3.08	1.65	1.59
3	A	3002	I3P	P5-O5	3.05	1.65	1.59
3	D	3002	I3P	P5-O5	3.02	1.65	1.59
3	B	3002	I3P	P5-O5	3.01	1.65	1.59
3	C	3002	I3P	P5-O5	2.95	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3002	I3P	C5-C6-C1	2.14	113.40	108.96
3	A	3002	I3P	C5-C6-C1	2.01	113.14	108.96

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	3002	I3P	C5-O5-P5-O51
3	B	3002	I3P	C4-O4-P4-O42
3	B	3002	I3P	C5-O5-P5-O53
3	D	3002	I3P	C5-O5-P5-O53
3	D	3002	I3P	C6-C1-O1-P1
3	A	3002	I3P	C6-C1-O1-P1
3	A	3002	I3P	C4-O4-P4-O43
3	B	3002	I3P	C4-O4-P4-O43
3	C	3002	I3P	C3-C4-O4-P4
3	D	3002	I3P	C4-O4-P4-O43
3	D	3002	I3P	C5-O5-P5-O52

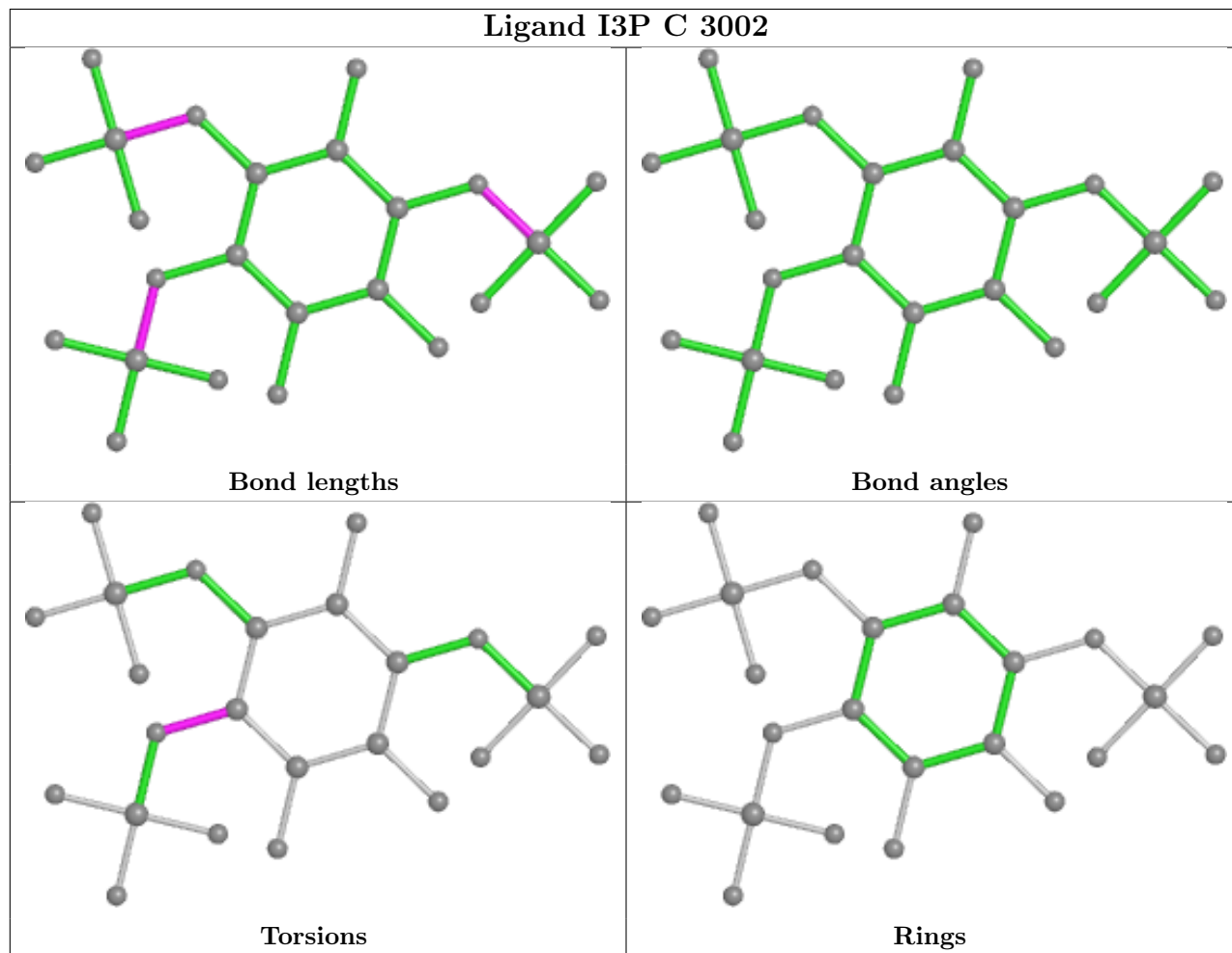
There are no ring outliers.

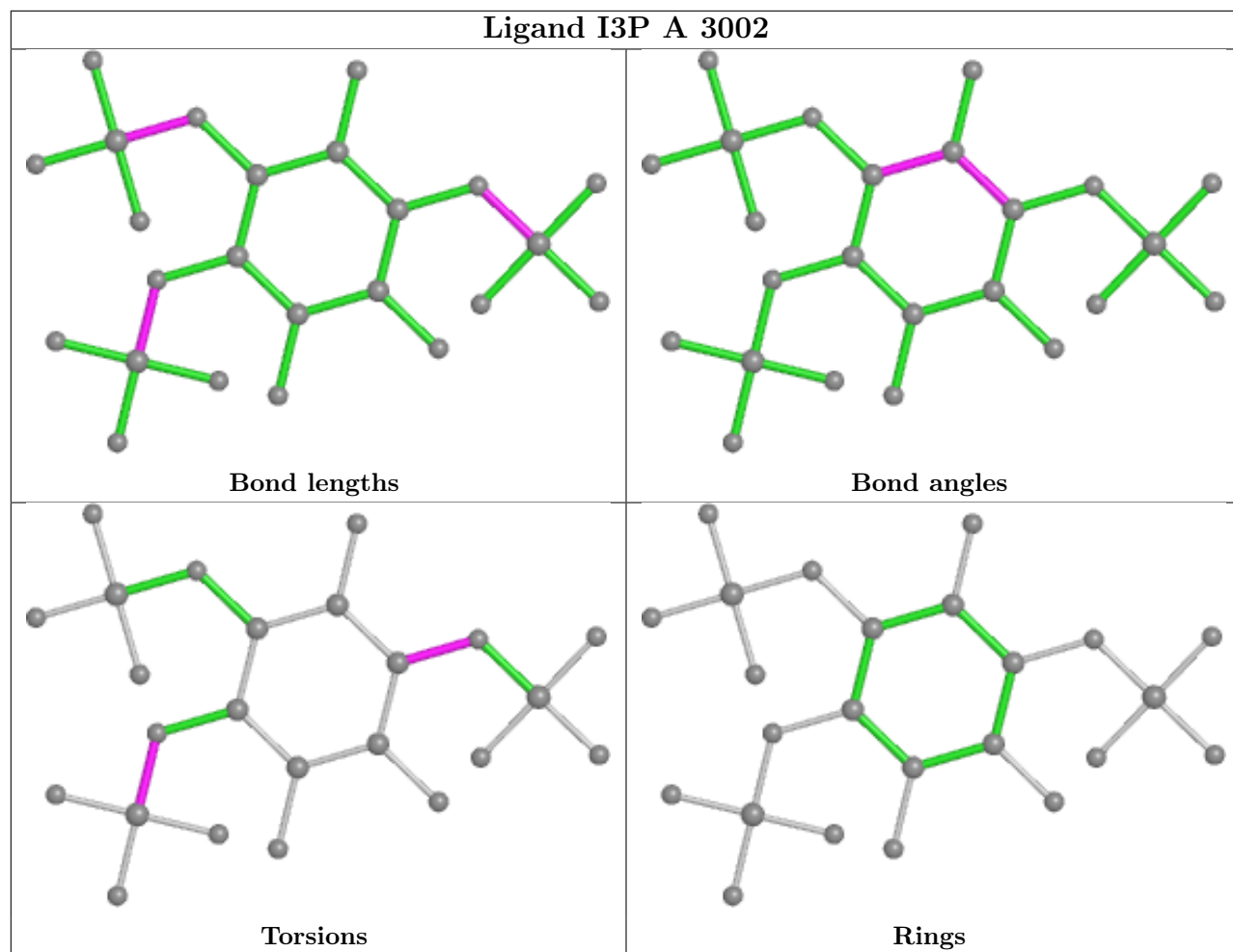
2 monomers are involved in 3 short contacts:

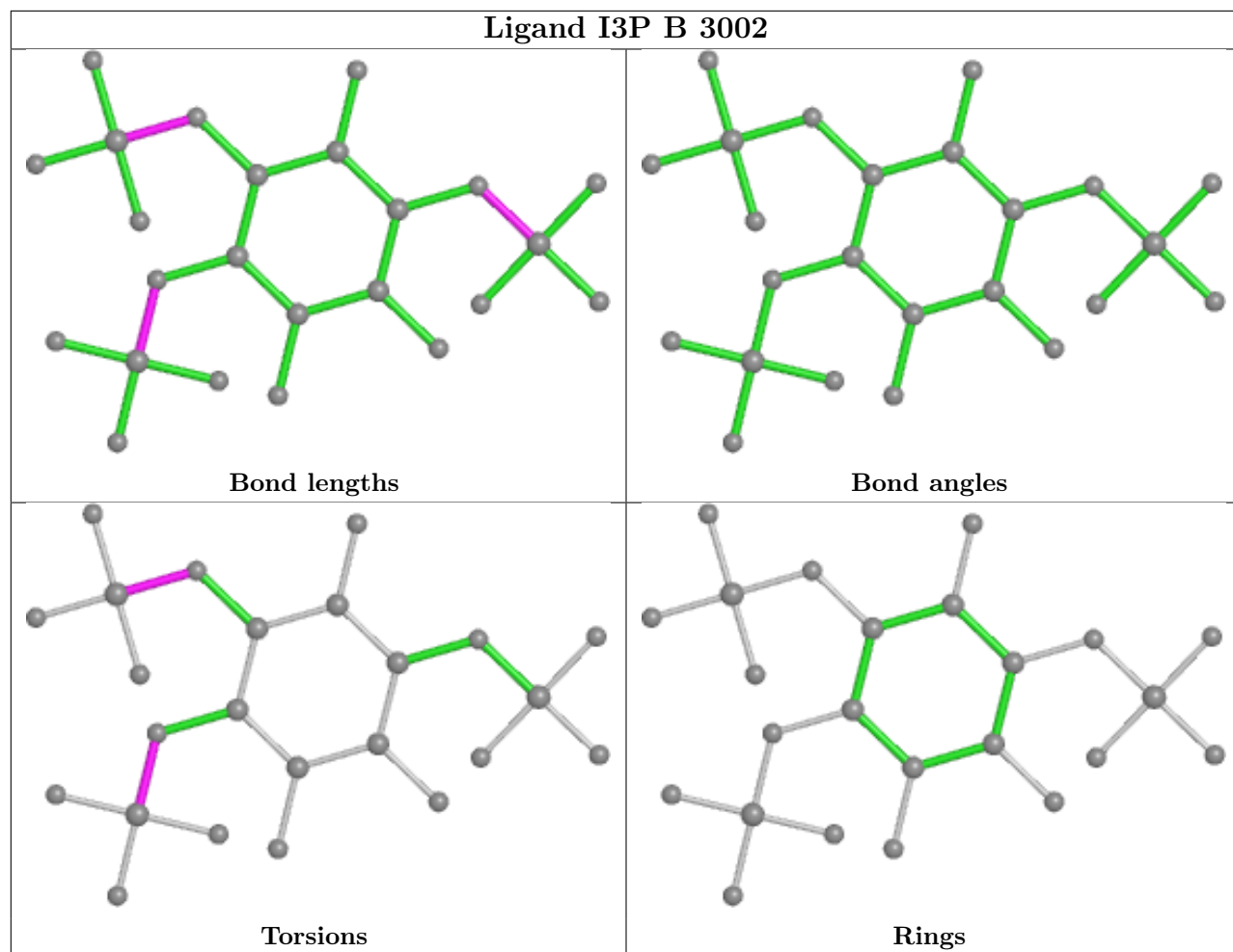
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3002	I3P	2	0
3	D	3002	I3P	1	0

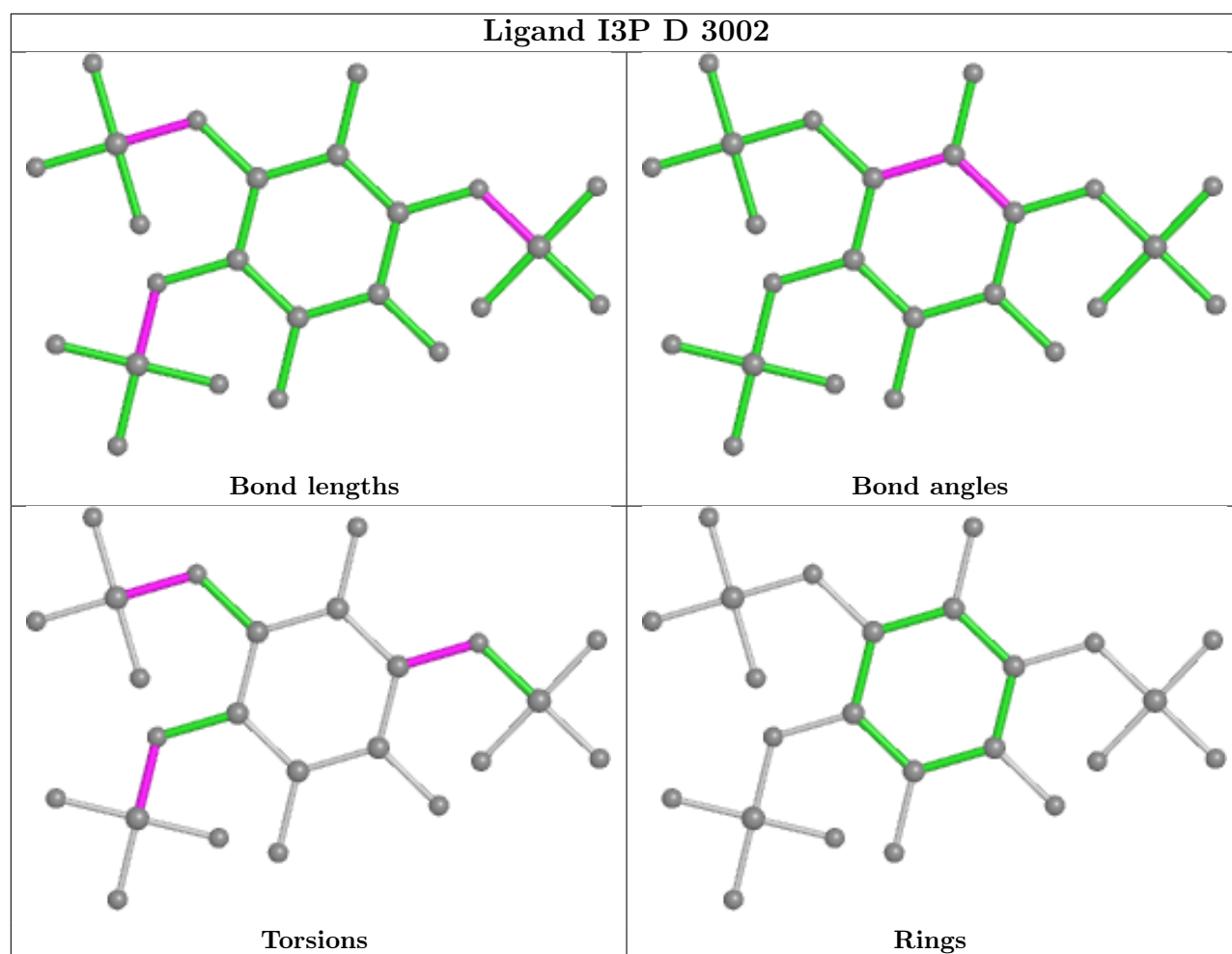
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	5
1	A	5
1	B	5
1	D	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1552:TRP	C	1587:ASP	N	51.54

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1552:TRP	C	1587:ASP	N	49.80
1	A	1552:TRP	C	1587:ASP	N	49.30
1	B	1552:TRP	C	1587:ASP	N	48.40
1	D	1533:ARG	C	1541:ALA	N	15.42
1	A	1484:ARG	C	1490:ALA	N	15.30
1	C	1484:ARG	C	1490:ALA	N	15.09
1	B	1484:ARG	C	1490:ALA	N	15.07
1	C	1533:ARG	C	1541:ALA	N	14.93
1	A	1533:ARG	C	1541:ALA	N	14.58
1	B	1533:ARG	C	1541:ALA	N	14.30
1	C	1508:GLY	C	1515:ALA	N	8.45
1	A	1508:GLY	C	1515:ALA	N	8.18
1	B	1508:GLY	C	1515:ALA	N	7.81
1	D	2252:TYR	C	2260:SER	N	6.71
1	A	2252:TYR	C	2260:SER	N	6.67
1	C	2252:TYR	C	2260:SER	N	6.25
1	B	2252:TYR	C	2260:SER	N	6.18

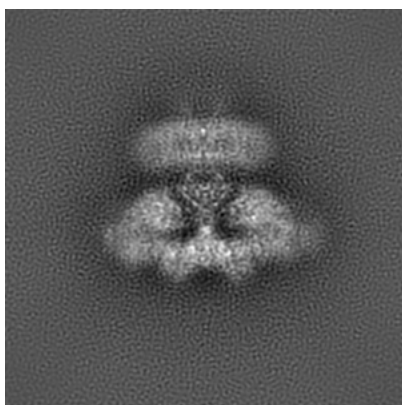
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7983. These allow visual inspection of the internal detail of the map and identification of artifacts.

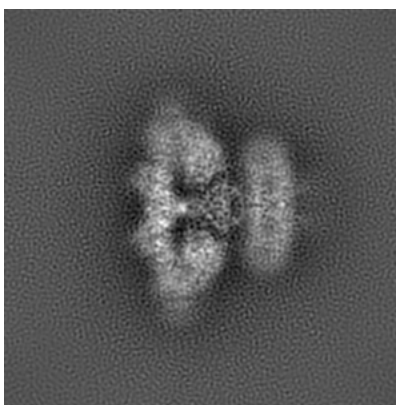
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

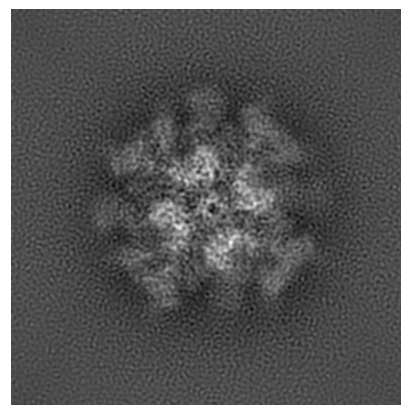
6.1.1 Primary map



X



Y

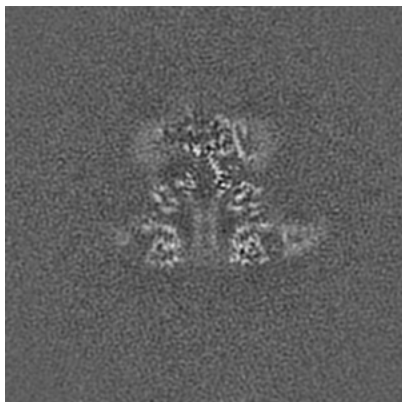


Z

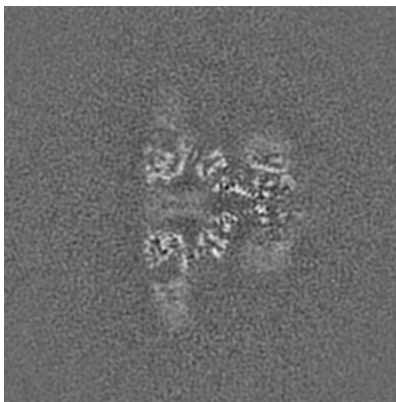
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192

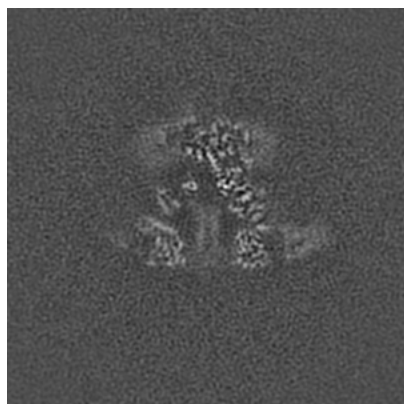


Z Index: 192

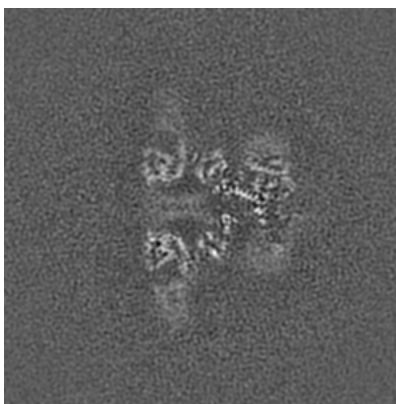
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

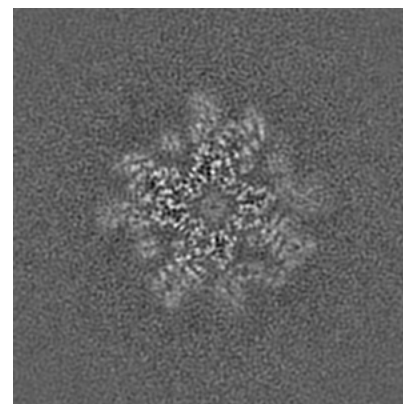
6.3.1 Primary map



X Index: 190



Y Index: 193

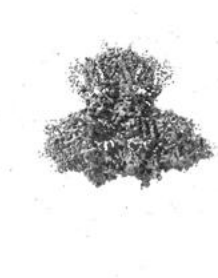


Z Index: 153

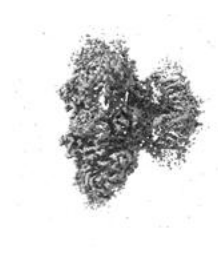
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.93. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

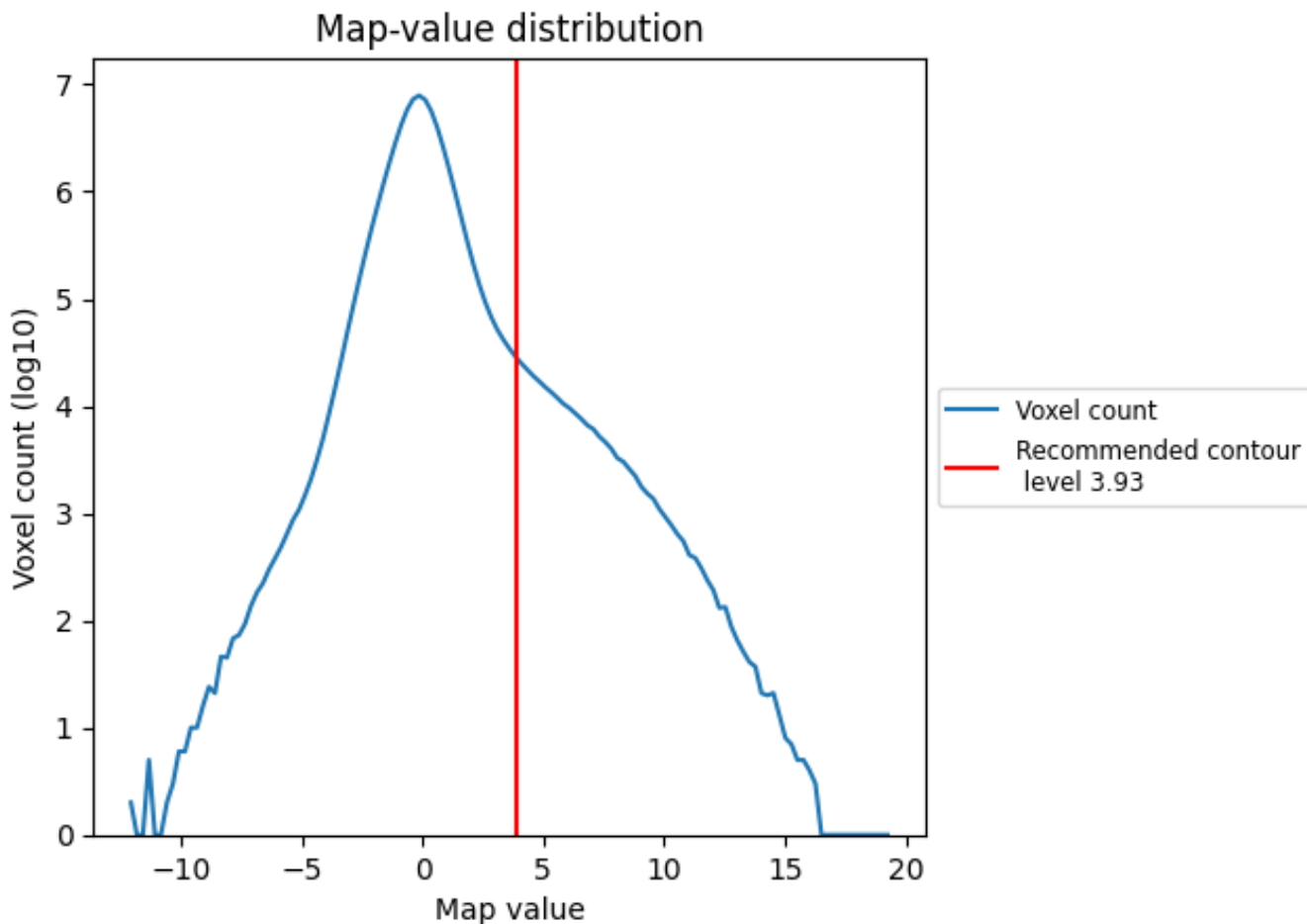
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

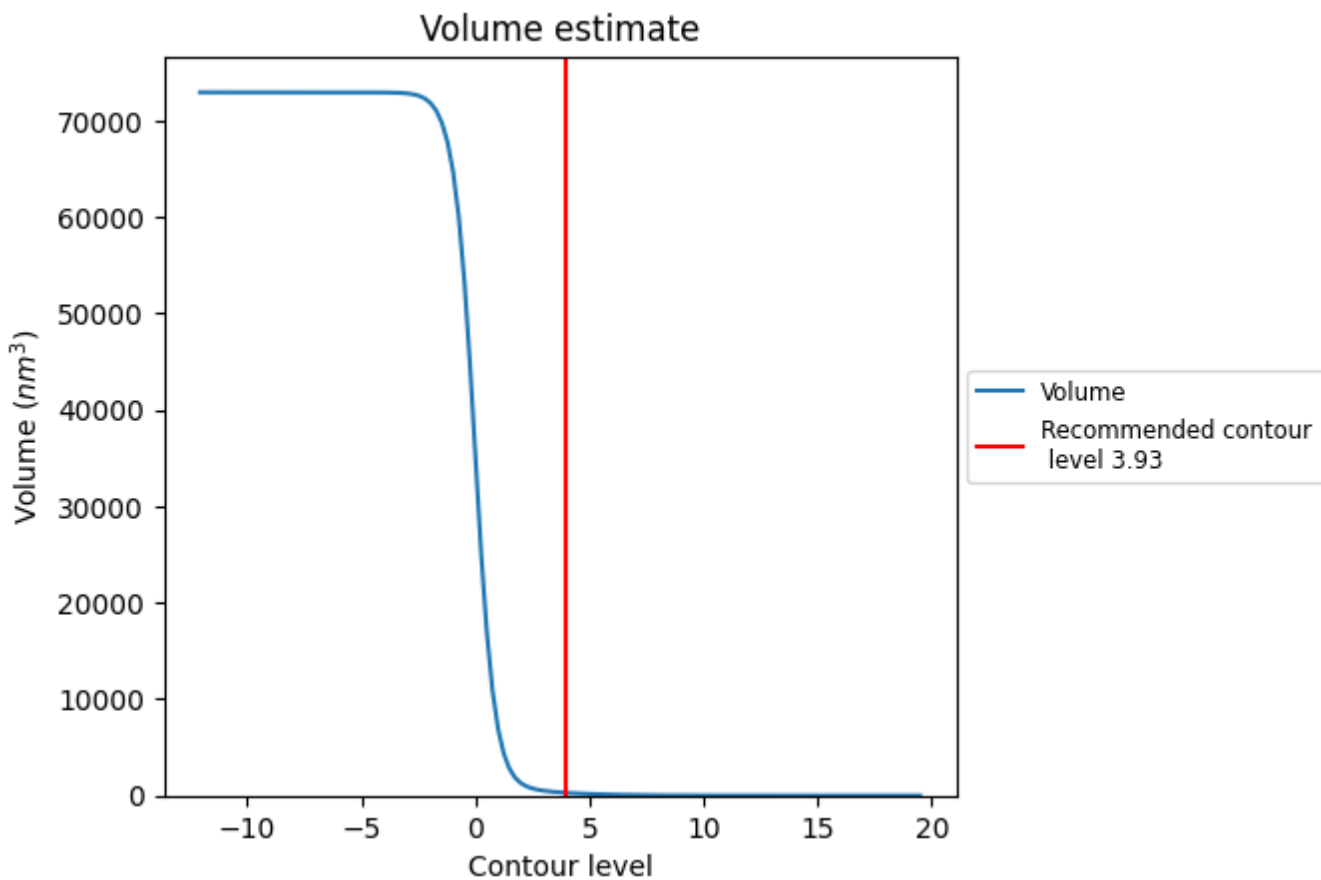
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

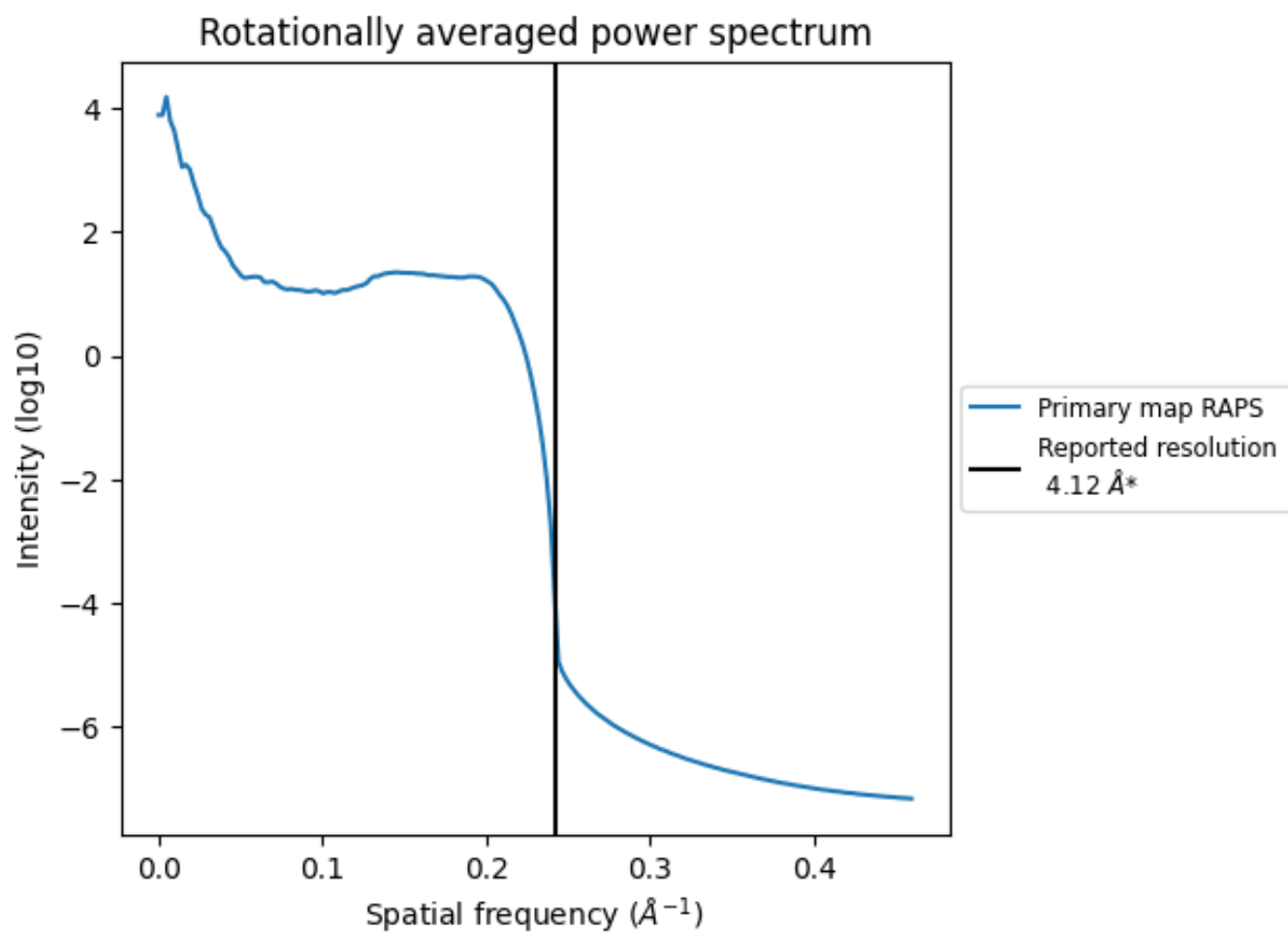
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 291 nm³; this corresponds to an approximate mass of 263 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.243\AA^{-1}

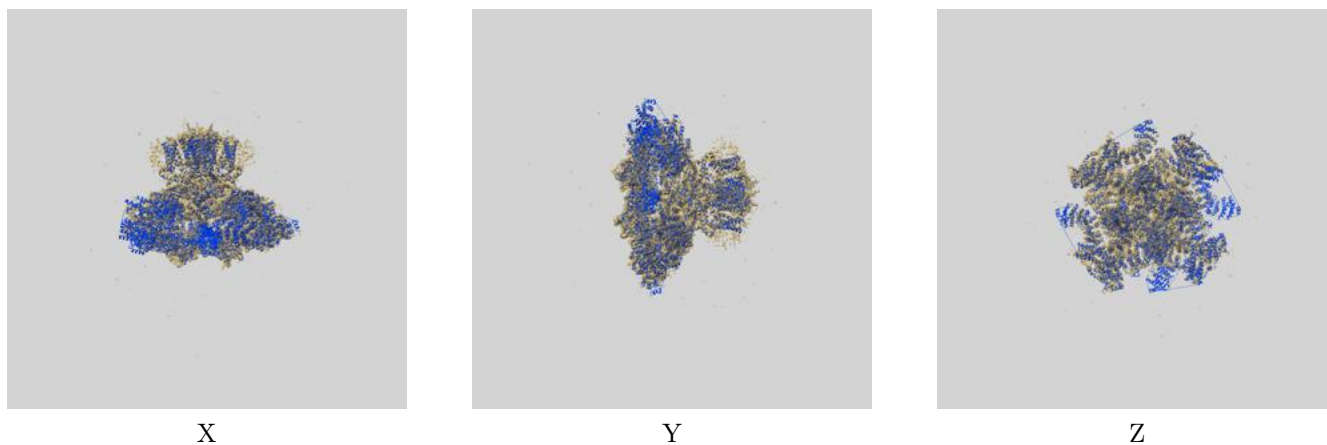
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

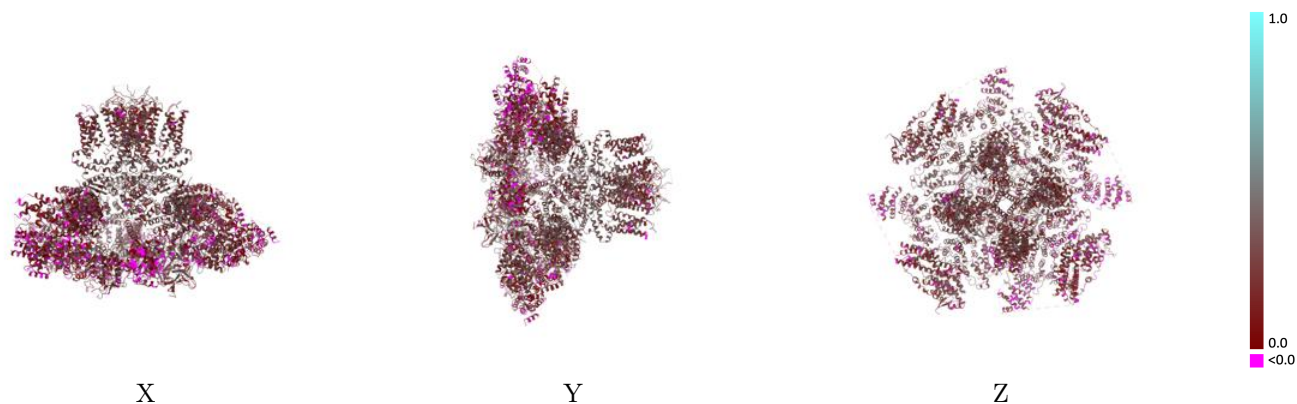
This section contains information regarding the fit between EMDB map EMD-7983 and PDB model 6DQS. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



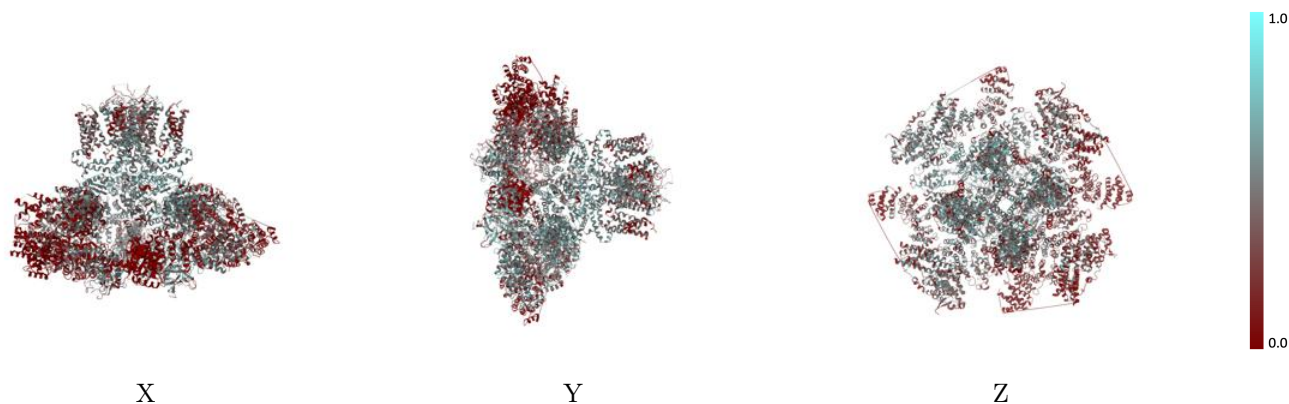
The images above show the 3D surface view of the map at the recommended contour level 3.93 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



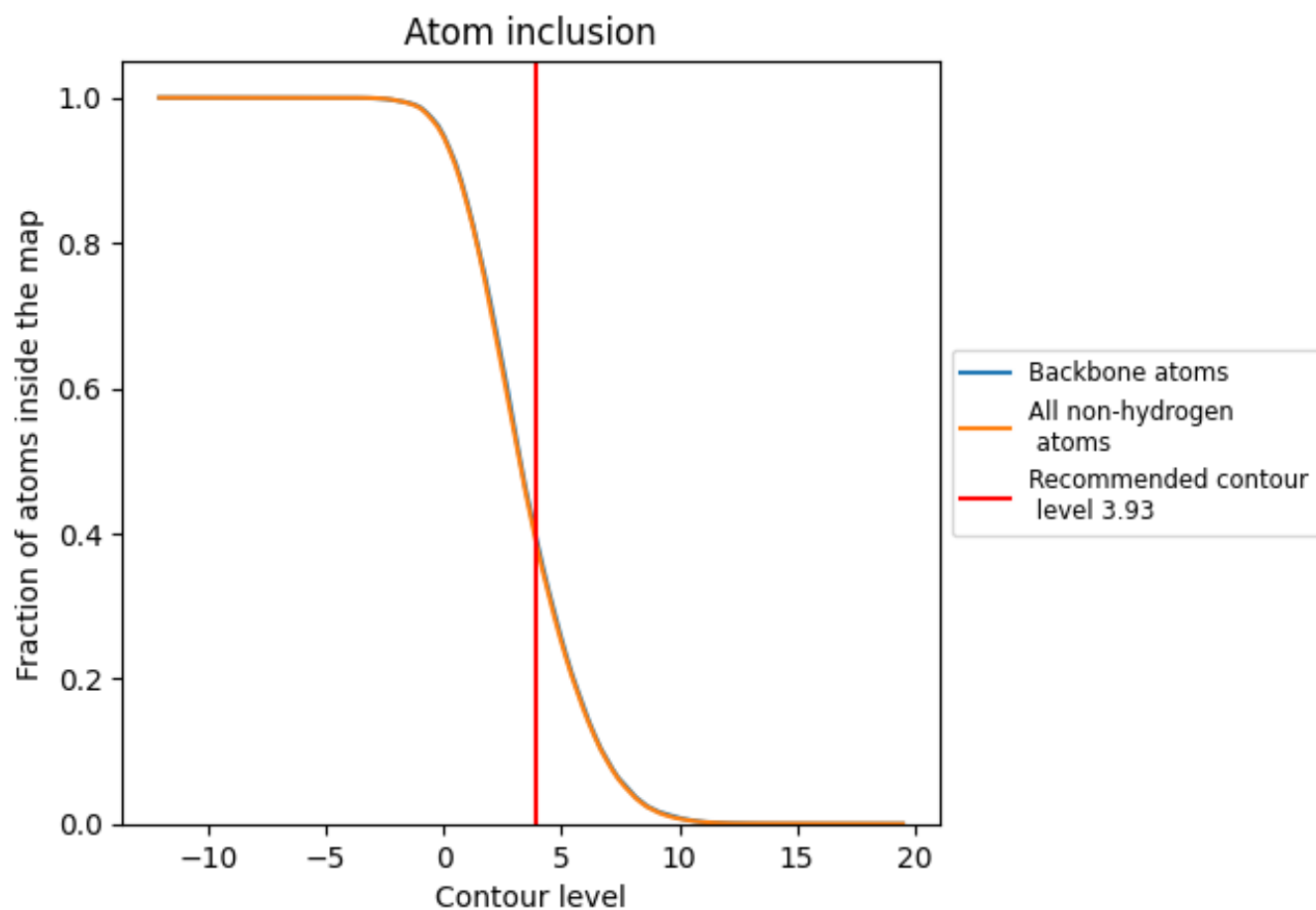
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.93).











9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 39% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (3.93) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3864	 0.2360
A	 0.3656	 0.2260
B	 0.4829	 0.2670
C	 0.4196	 0.2460
D	 0.3004	 0.2050

