



## wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 06:31 PM EDT

PDB ID : 6DQN  
EMDB ID : EMD-7981  
Title : Class 1 IP3-bound human type 3 1,4,5-inositol trisphosphate receptor  
Authors : Hite, R.K.; Paknejad, N.  
Deposited on : 2018-06-11  
Resolution : 3.33 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

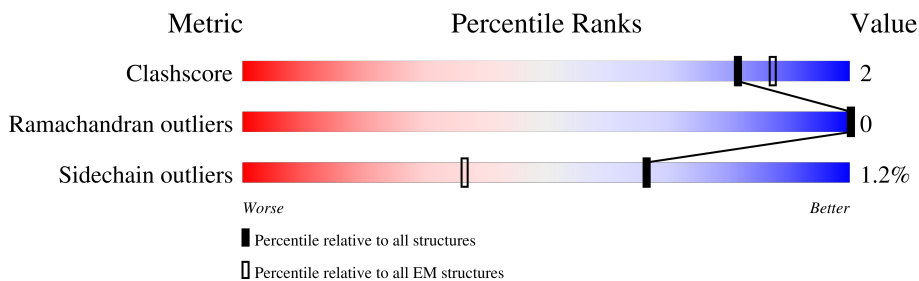
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.33 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2671	
1	B	2671	
1	C	2671	
1	D	2671	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 138912 atoms, of which 69432 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.

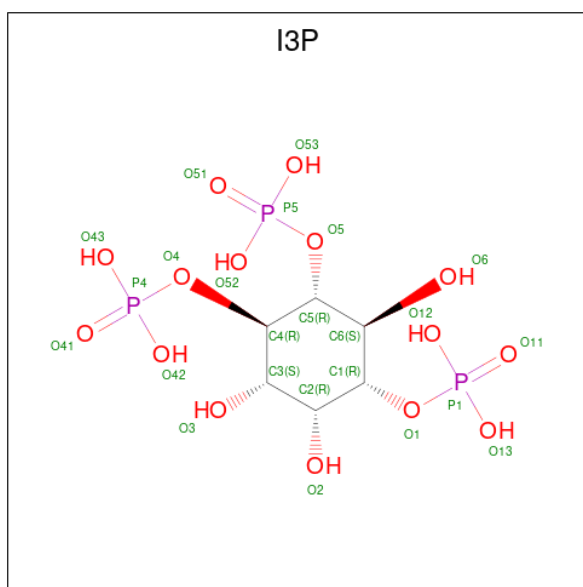
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	2186	34694	11058	17349	2985	3199	103	0	0
1	B	2186	34694	11058	17349	2985	3199	103	0	0
1	C	2186	34694	11058	17349	2985	3199	103	0	0
1	D	2186	34694	11058	17349	2985	3199	103	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:  $C_6H_{15}O_{15}P_3$ ).

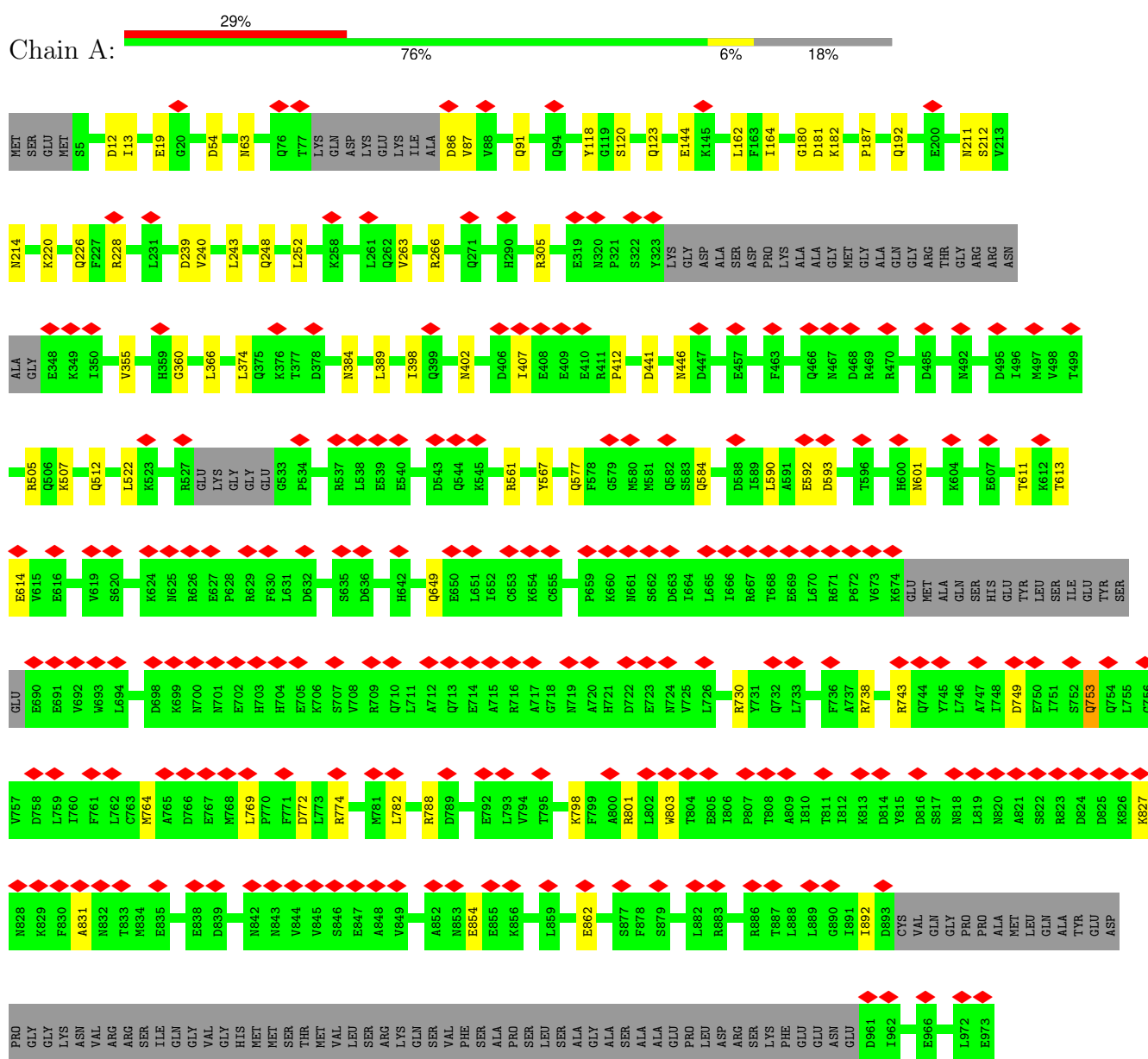


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

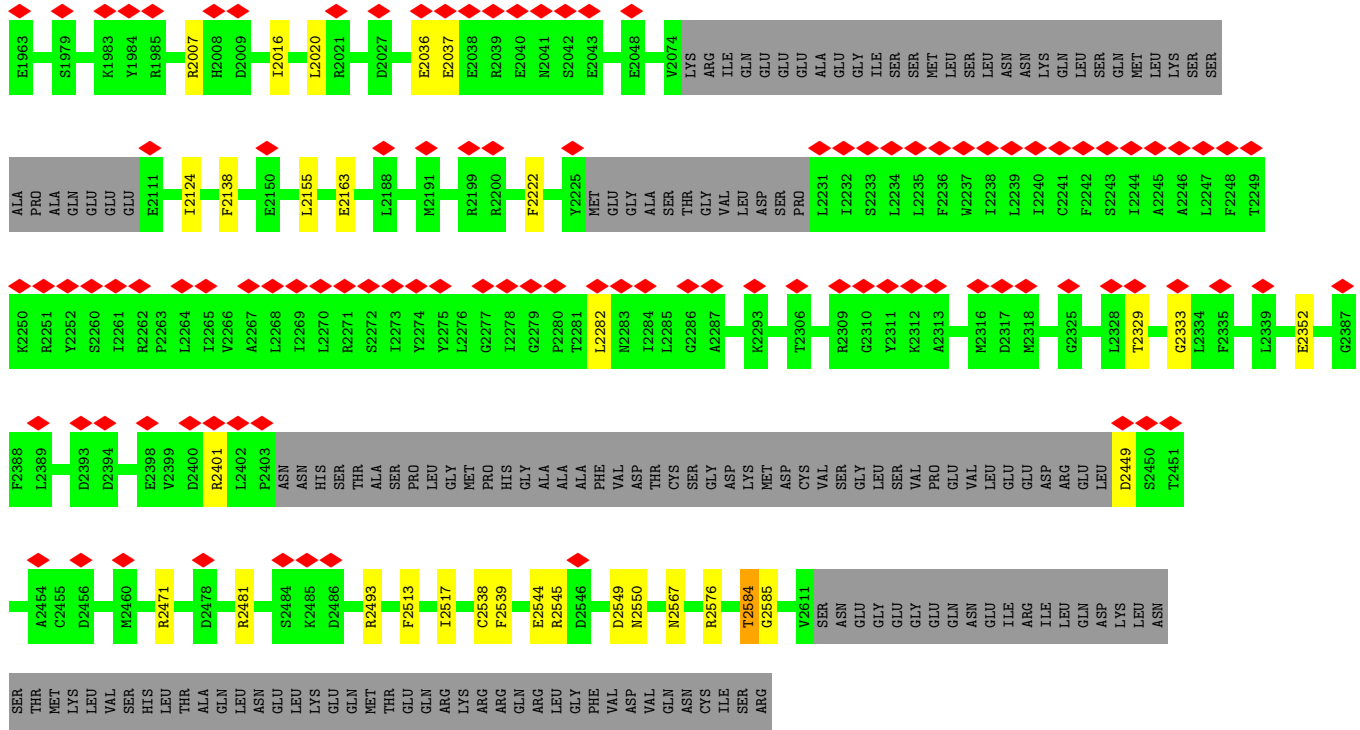
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

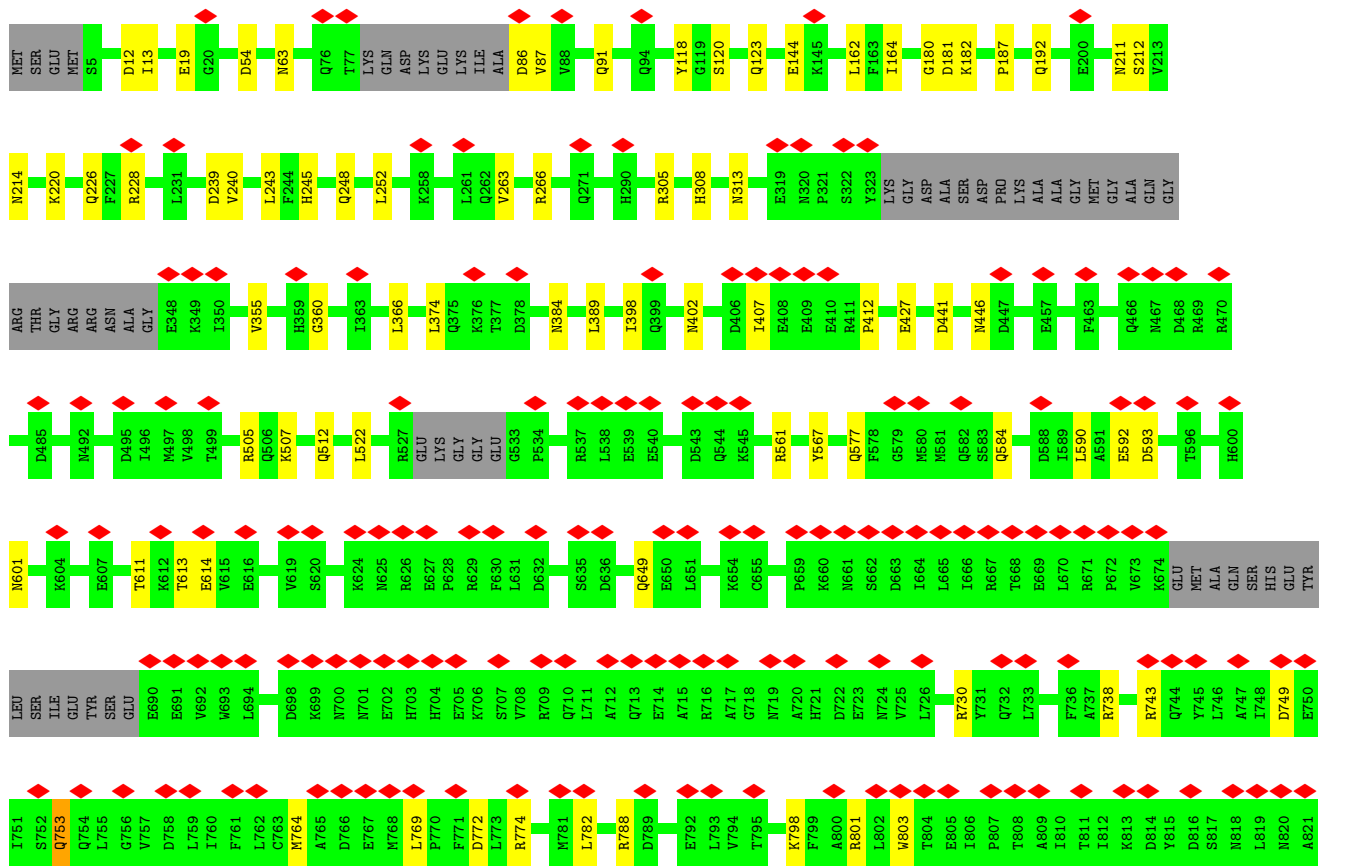
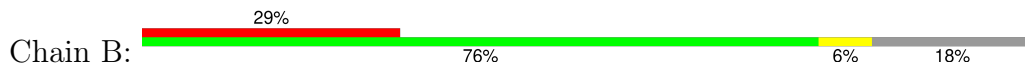
● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





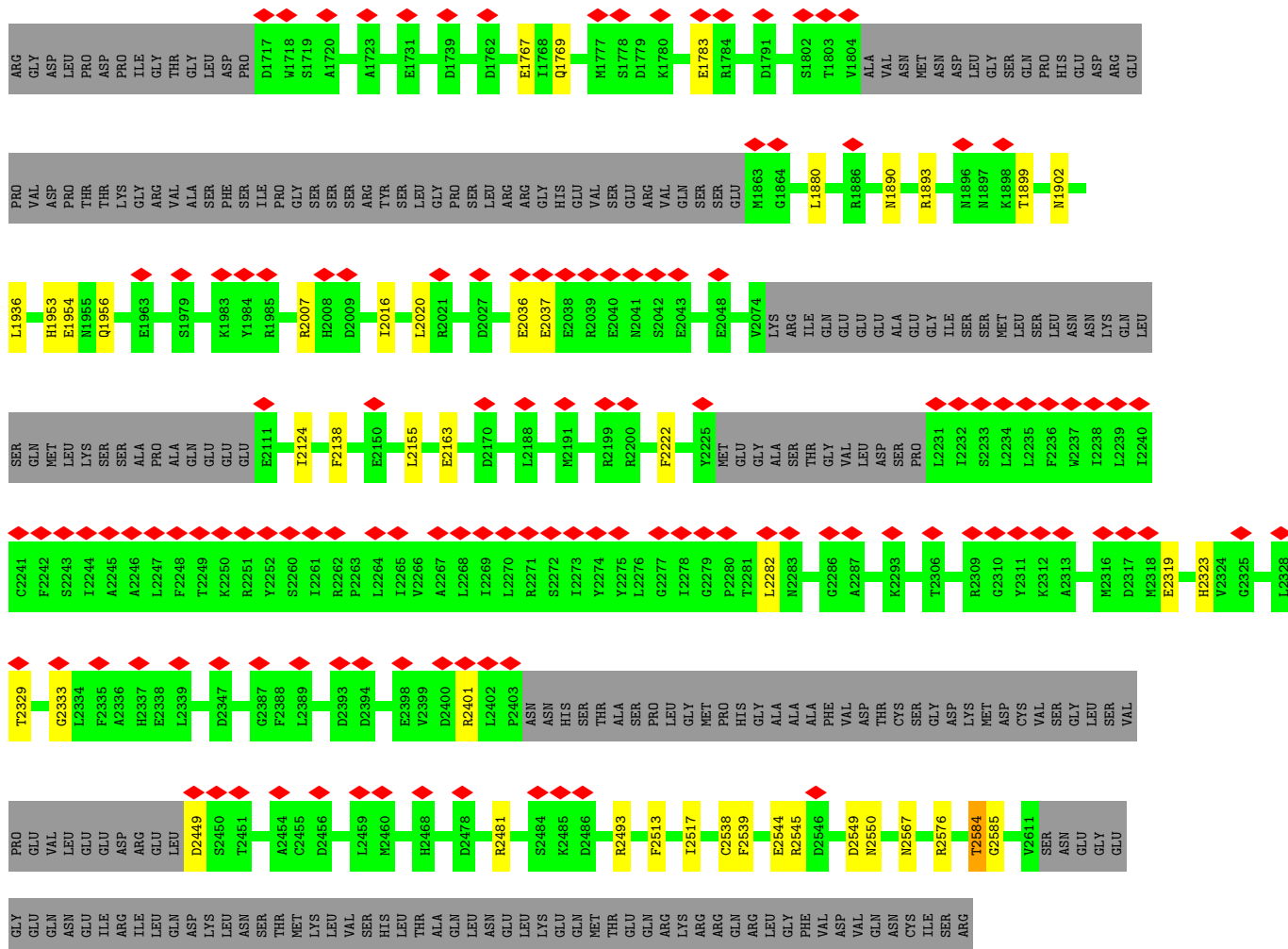


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

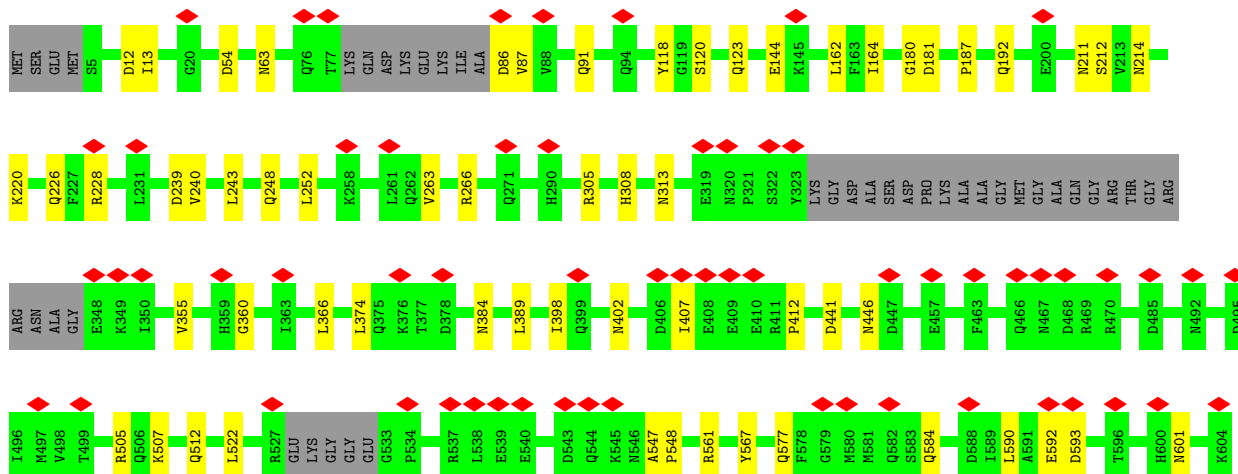
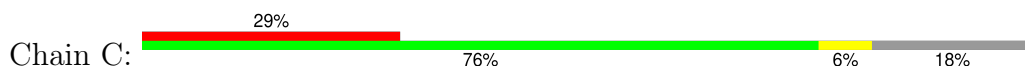


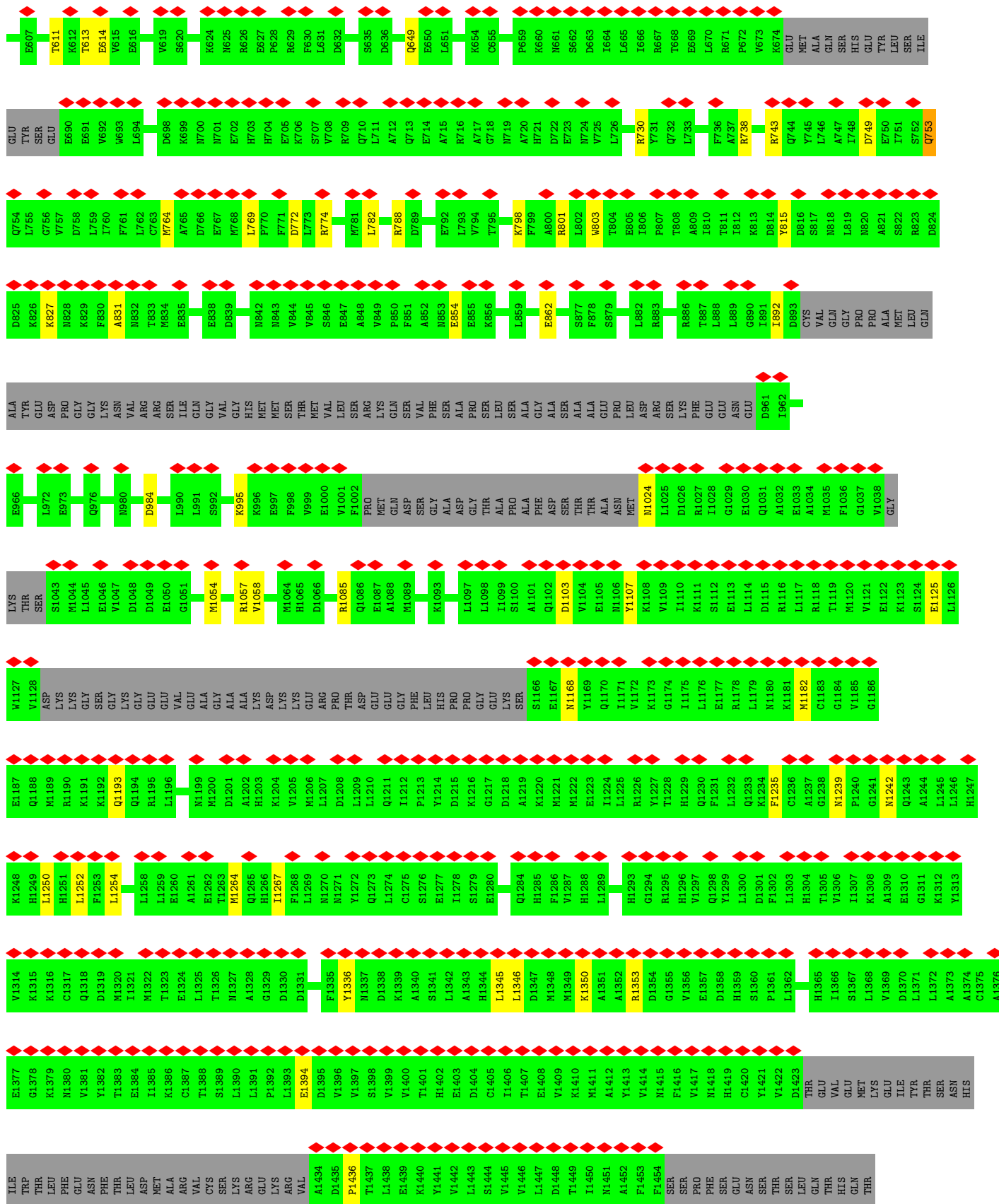
L1617	V1618	D1619	V1620	W1623	L1626	A1519	F1628	L1629	E1630	G1631	S1632	E1633	A1634	Y1635	Q1636	R1637	C1638	E1639	S1640	G1641	G1642	K1646	D1653	L1654	M1655	E1656	S1657	E1658	E1659	K1675	K1676	T1677	K1678	Y1679	G1680	D1681	R1682	G1683	M1684	Q1685	K1688	M1689	Q1692	M1693	Q1696	ASN	ARG	LYS	SER	THR	SER												
S1507	G1508	A1515	S1516	C1517	A1518	A1519	A1520	A1521	Q1522	R1523	N1524	A1525	S1526	S1527	Y1528	K1529	A1530	T1531	T1532	R1533	G1541	G1542	P1543	R1544	V1545	T1546	P1547	T1548	A1549	N1550	Q1551	W1552	D1557	Y1558	K1559	N1590	G1591	I1592	E1593	K1594	L1595	Q1596	I1597	I1598	I1599	T1600	A1601	L1602	M1603	E1604	R1605	L1606	L1609	E1613	L1614	S1615	V1616						
HIS	GLN	THR	VAL	VAL	GLN	LEU	LEU	LEU	SER	THR	THR	ARG	MET	ALA	ARG	VAL	CYS	PRO	TRP	L1462	Q1463	Q1464	Q1465	H1466	K1467	G1468	S1469	V1470	E1471	A1472	C1473	I1474	R1475	T1476	L1477	A1478	M1479	V1480	A1481	K1482	G1483	R1484	A1490	I1491	L1492	L1493	P1494	M1495	D1496	L1497	D1498	A1499	H1500	T1501	S1502	S1503	M1504	L1505	S1506				
SER	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	LEU	ASP	MET	ALA	ARG	CYS	SER	LYS	ARG	GLU	LYS	ARG	VAL	A1434	D1435	P1436	T1437	L1438	E1439	K1440	Y1441	V1442	L1443	S1444	V1445	V1446	L1447	D1448	T1449	I1450	M1451	A1452	F1453	F1454	SER	SER	PRO	PHE	SER	GLU	ASN	SER	THR	SER	GLN	THR						
L1245	L1246	H1247	K1248	H1249	L1250	H1251	L1252	F1253	L1254	L1258	L1259	E1260	A1261	E1262	M1264	Q1265	H1266	I1267	F1268	L1269	N1271	Y1272	Q1273	L1274	C1275	S1276	E1277	I1278	S1279	E1280	Q1284	H1285	F1286	Y1287	H1288	L1289	H1293	G1294	R1295	H1296	V1297	Q1298	Y1299	L1300	D1301	F1302	L1303	H1304	T1305	V1306	I1307	K1308	A1309	E1310									
G1184	V1185	G1186	E1187	Q1188	M1189	M1190	K1191	K1192	Q1193	Q1194	R1195	L1196	M1199	M1200	D1201	A1202	H1203	K1204	V1205	L1206	L1207	D1208	L1209	L1210	Q1211	G1212	P1213	L1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	L1224	L1225	R1226	Y1227	L1228	H1229	Q1230	F1231	L1232	Q1233	K1234	F1235	G1236	A1237	G1238	M1239	F1240	G1241	M1242	Q1243	A1244					
L1124	E1125	L1126	W1127	V1128	ASP	LYS	LYS	GLY	SER	GLY	GLY	GLU	GLU	VAL	ALA	ALA	ASP	LYS	LYS	LYS	GLU	ARG	PRO	THR	ASP	GLU	Q1211	G1212	P1213	L1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	L1224	L1225	R1226	Y1227	L1228	H1229	Q1230	F1231	L1232	Q1233	K1234	F1235	G1236	A1237	G1238	M1239	F1240	G1241	M1242	Q1243	A1244			
S1124	E1125	L1126	W1127	V1128	ASP	LYS	LYS	GLY	SER	GLY	GLY	GLU	GLU	VAL	ALA	ALA	ASP	LYS	LYS	LYS	GLU	ARG	PRO	THR	ASP	GLU	Q1211	G1212	P1213	L1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	L1224	L1225	R1226	Y1227	L1228	H1229	Q1230	F1231	L1232	Q1233	K1234	F1235	G1236	A1237	G1238	M1239	F1240	G1241	M1242	Q1243	A1244			
G1037	V1038	GLY	LYS	THR	SER	S1043	M1044	L1045	E1046	W1047	D1048	D1049	E1050	G1051	M1054	R1057	V1058	M1064	H1065	D1066	R1085	Q1086	A1087	E1088	H1089	K1093	L1097	L1098	I1099	S1100	A1101	Q1102	D1103	V1104	E1105	M1106	Y1107	K1108	V1109	I1110	K1111	S1112	G1112	E1113	L1114	D1115	R1116	L1117	R1118	T1119	M1120	V1121	E1122	K1123									
D961	I962	E966	L972	E973	Q976	W980	D984	L990	L991	S992	K996	K996	E997	F998	V999	E1000	V1001	F1002	PRO	MET	GLN	SER	ASP	GLY	ALA	ASP	PRO	THR	ALA	PRO	PRO	ALA	PHE	ASP	SER	SER	THR	THR	ALA	ASN	LEU	ASP	ARG	SER	LYS	PHE	GLU	GLU	ASN	GLU	M1024	L1025	D1026	R1027	I1028	G1029	E1030	Q1031	A1032	A1033	A1034	M1035	F1036
LEU	GLN	ALA	TYR	GLU	ASP	PRO	GLY	GLY	LYS	ASN	VAL	ARG	ARG	ARG	THR	ILE	GLN	GLY	VAL	HIS	MET	SER	THR	VAL	LEU	LEU	ARG	ARG	LYS	GLN	GLN	SER	VAL	PHE	ASP	THR	GLY	ALA	ALA	PRO	LEU	ASP	ARG	SER	LYS	PHE	GLU	GLU	ASN	GLU	M1024	L1025	D1026	R1027	I1028	G1029	E1030	Q1031	A1032	A1033	A1034	M1035	F1036
S822	R823	D824	D825	K826	K827	N828	K829	F830	A831	N832	T833	M834	E835	E838	D839	N842	N843	V844	V845	S846	E847	A848	V849	P850	V851	A852	N853	E854	E855	K856	L859	E862	S877	F878	S879	L882	R883	R886	T887	L888	L889	G890	I891	I892	D893	CYS	VAL	GLN	GLY	PRO	PRO	ALA											

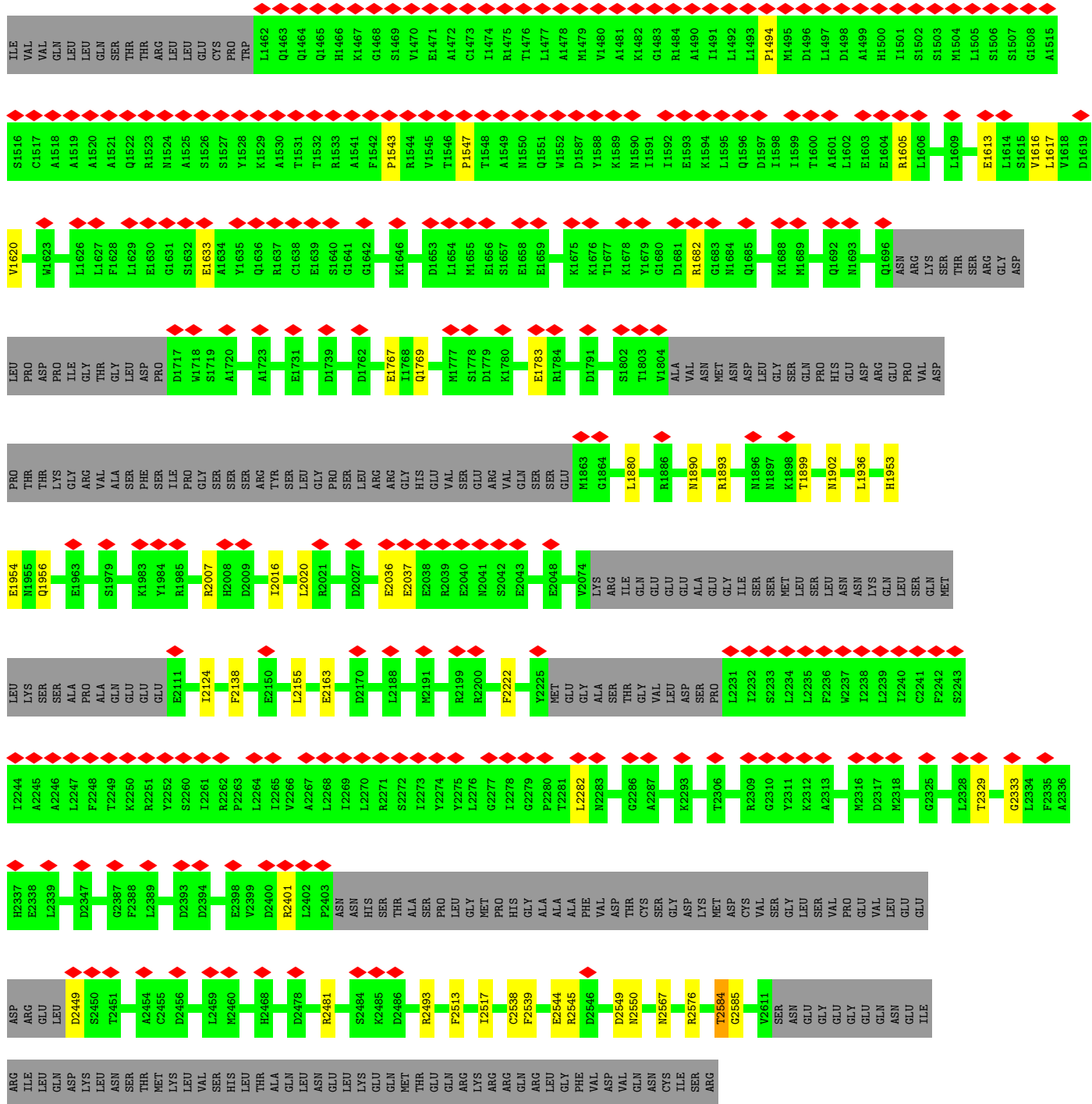




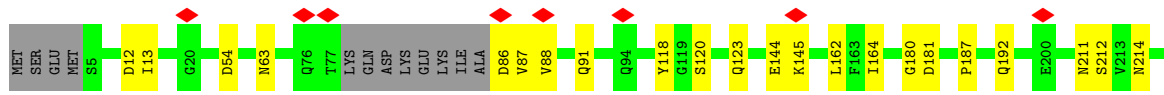
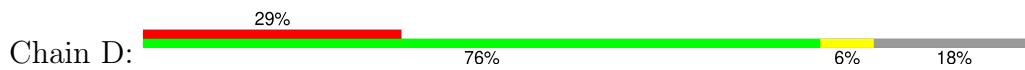
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

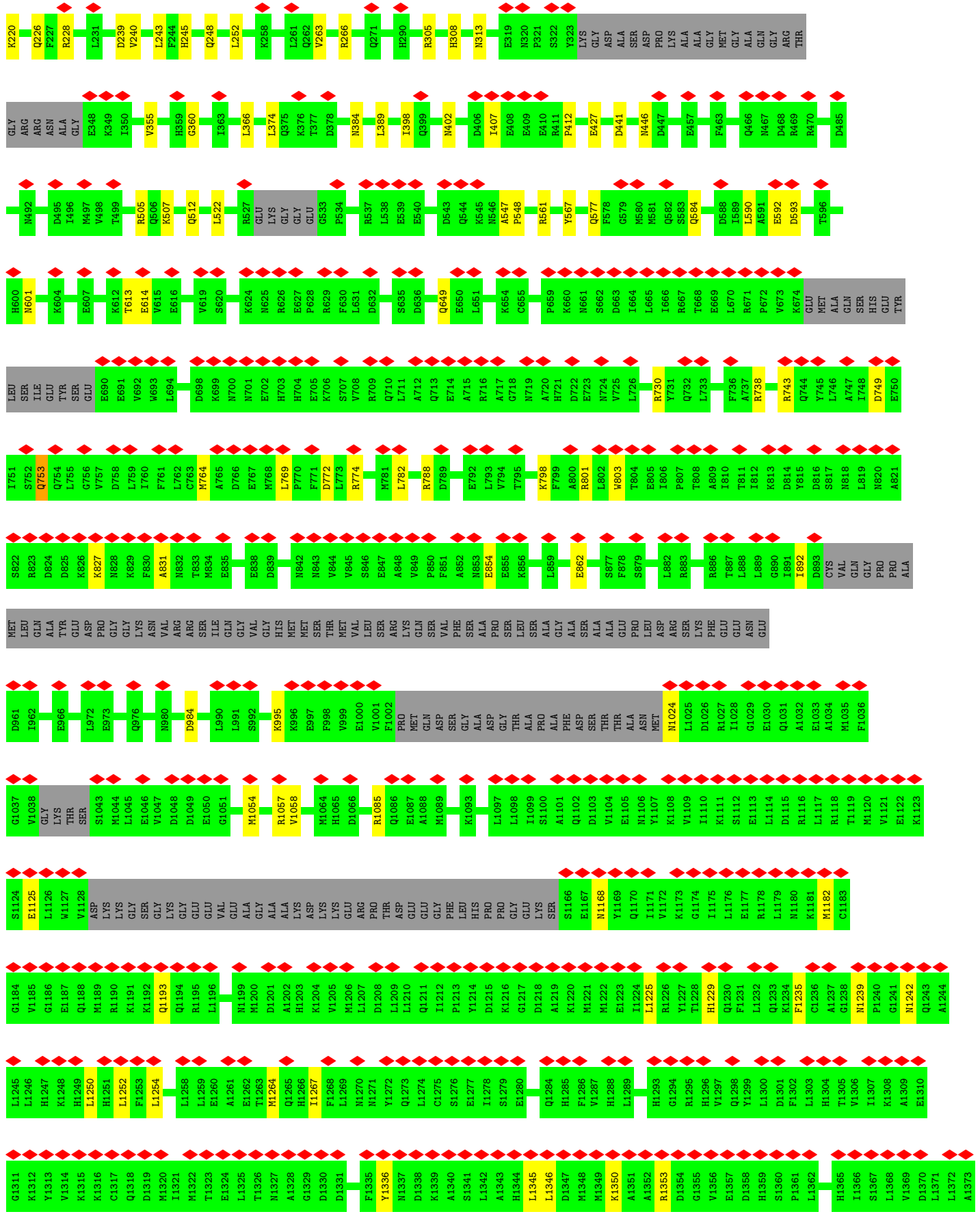






● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





GLU	GLN	ASN	GLY	VAL	LEU	LEU	GLU	GLY	ASP	D2449	D2450	T2451	A2454	C2455	D2456	L2459	M2460	H2468	D2478	R2481	S2484	K2485	D2486	R2493	F2513	I2517	C2538	F2539	E2544	R2545	D2546	N2549	N2550	M2567	R2576	T2584	C2585	V2611	ASN	ASN	GLU	GLY	GLU	VAL	PRO																
L2384	F2385	A2386	H2387	E2388	L2389	D2393	D2394	E2388	V2389	D2400	R2401	L2402	P2403	ASN	ASN	HIS	SER	THR	ALA	ALA	PRO	GLY	PRO	HIS	GLY	ALA	ALA	PHE	VAL	ASP	THR	CYS	GLY	ASP	LYS	MET	ASP	CYS	VAL	GLY	ASN	GLU	GLY	VAL	PRO																
C2241	F2242	S2243	I2244	A2245	A2246	L2247	F2248	T2249	K2250	R2251	Y2252	S2260	I2261	R2262	P2263	L2264	I2265	V2266	A2267	L2268	I2269	R2271	S2272	I2273	Y2274	Y2275	L2276	G2277	G2278	P2280	L2281	L2282	N2283	G2286	A2287	K2293	T2306	R2309	G2310	Y2311	K2312	A2313	M2316	D2317	M2318	G2325	L2328	T2329	G2333												
C2291	F2292	S2293	I2294	A2295	A2296	L2297	F2298	T2299	K2300	R2301	Y2302	S2310	I2311	R2312	P2313	L2314	I2315	V2316	A2317	L2318	I2319	R2321	S2322	I2323	Y2324	Y2325	L2326	G2327	G2328	P2330	L2331	L2332	N2333	G2336	A2337	K2338	T2339	R2340	G2341	Y2342	K2343	A2344	M2345	D2346	L2347	L2348	L2349														
L1936	H1953	E1954	N1955	Q1956	E1963	S1979	K1983	Y1984	R1985	R2007	H2008	D2009	I2016	L2020	R2021	D2027	E2036	E2037	E2038	R2039	E2040	N2041	S2042	E2043	E2048	Y2074	LYS	ILE	GLN	GLU	GLU	ALA	ALA	GLY	ILE	SER	SER	MET	LEU	SER	LEU	ASN	ASN	GLN	GLN	LEU															
PRO	VAL	ASP	PRO	THR	THR	LYS	GLY	ARG	GLY	VAL	VAL	ALA	ALA	SER	PHE	SER	ILE	PRO	GLY	SER	TYR	ARG	LEU	PRO	SER	LEU	ARG	M1863	G1864	L1880	R1886	M1890	R1893	M1896	N1897	K1898	T1899	M1902	PRO	VAL	ASP	PRO	THR	GLY	VAL	LEU	ASP	PRO	L2231	I2232	S2233	G2234	L2235	F2236	W2237	L2238	L2239	I2240			
ARG	GLY	ASP	PRO	PRO	ILE	ARG	GLY	THR	GLY	D1717	W1718	S1719	A1720	A1723	E1731	D1739	S1640	G1641	G1642	K1646	D1653	L1654	M1655	E1656	S1657	E1658	E1659	K1675	K1676	T1677	K1678	Y1679	G1680	D1681	R1682	G1683	M1684	Q1685	K1688	M1689	Q1692	M1693	Q1696	ASN	ARG	LYS	SER	THR	SER												
L1617	V1618	D1619	V1620	W1623	L1626	L1627	F1628	L1629	E1630	G1631	S1632	E1633	A1634	Y1635	Q1636	R1637	C1638	E1639	S1640	G1641	G1642	K1646	D1653	L1654	M1655	E1656	S1657	E1658	E1659	K1675	K1676	T1677	K1678	Y1679	G1680	D1681	R1682	G1683	M1684	Q1685	K1688	M1689	Q1692	M1693	Q1696	ASN	ARG	LYS	SER	THR	SER										
S1507	G1508	A1515	S1516	C1517	A1518	A1519	A1520	A1521	Q1522	R1523	N1524	A1525	S1526	S1527	Y1528	K1529	A1530	T1531	T1532	R1533	A1541	F1542	P1543	V1544	T1546	P1547	T1548	A1549	N1550	Q1551	W1552	D1557	Y1558	K1559	N1590	I1591	I1592	E1593	K1594	L1595	Q1596	D1597	I1598	I1599	T1600	A1601	L1602	E1603	E1604	R1605	L1606	L1609	E1613	L1614	S1615	V1616					
HIS	GLN	THR	ILE	VAL	VAL	GLN	LEU	GLN	SER	THR	THR	ARG	LEU	ALA	GLY	CYS	PRO	SER	L1462	Q1463	Q1464	Q1465	H1466	K1467	G1468	S1469	V1470	E1471	A1472	C1473	I1474	R1475	L1476	L1477	A1478	M1479	V1480	A1481	G1482	N1484	A1490	I1491	L1492	L1493	P1494	M1495	D1496	L1497	D1498	A1499	H1500	I1501	S1502	S1503	M1504	L1505	S1506				
SER	ASN	HIS	ILE	TRP	THR	PHE	GLU	ASN	THR	THR	LEU	ASP	MET	ALA	ARG	CYS	SER	SER	L1434	D1435	V1436	T1437	L1438	E1439	K1440	Y1441	L1442	L1443	S1444	V1445	I1446	T1447	D1448	T1449	I1450	N1451	A1452	F1453	F1454	SER	PRO	PHE	SER	SER	GLU	ASN	SER	THR	SER	LEU	GLN	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TVR	THR
GLU	VAL	LEU	LEU	GLU	GLU	LEU	GLU	ASN	THR	THR	LEU	ASP	MET	ALA	ARG	CYS	SER	SER	L1434	D1435	V1436	T1437	L1438	E1439	K1440	Y1441	L1442	L1443	S1444	V1445	I1446	T1447	D1448	T1449	I1450	N1451	A1452	F1453	F1454	SER	PRO	PHE	SER	SER	GLU	ASN	SER	THR	SER	LEU	GLN	THR	GLU	VAL	GLU	MET	LYS	GLU	ILE	TVR	THR

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	38777	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	40.044	Depositor
Minimum map value	-27.584	Depositor
Average map value	-0.009	Depositor
Map value standard deviation	1.073	Depositor
Recommended contour level	5.13	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: ZN, I3P

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	0.44	4/23851 (0.0%)
1	B	0.25	0/17650	0.44	4/23851 (0.0%)
1	C	0.25	0/17650	0.44	4/23851 (0.0%)
1	D	0.25	0/17650	0.44	4/23851 (0.0%)
All	All	0.25	0/70600	0.44	16/95404 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1543	PRO	N-CA-CB	5.65	110.08	103.30
1	B	1543	PRO	N-CA-CB	5.65	110.08	103.30
1	C	1543	PRO	N-CA-CB	5.65	110.08	103.30
1	D	1543	PRO	N-CA-CB	5.65	110.08	103.30
1	A	1547	PRO	N-CA-CB	5.65	110.08	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	17349	17180	83	0
1	B	17345	17349	17180	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	17345	17349	17180	83	0
1	D	17345	17349	17180	86	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	2	0
3	B	24	9	9	2	0
3	C	24	9	9	2	0
3	D	24	9	9	2	0
All	All	69480	69432	68756	329	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.

The worst 5 of 329 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:B:1054:MET:SD	1:B:1057:ARG:NH2	2.65	0.70
1:D:1182:MET:O	1:D:1193:GLN:NE2	2.25	0.70
1:A:1054:MET:SD	1:A:1057:ARG:NH2	2.65	0.69
1:C:1054:MET:SD	1:C:1057:ARG:NH2	2.65	0.69
1:C:1182:MET:O	1:C:1193:GLN:NE2	2.25	0.69

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%)	2070 (96%)	74 (4%)	0	100	100
1	B	2144/2671 (80%)	2070 (96%)	74 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	2144/2671 (80%)	2070 (96%)	74 (4%)	0	100	100
1	D	2144/2671 (80%)	2070 (96%)	74 (4%)	0	100	100
All	All	8576/10684 (80%)	8280 (96%)	296 (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%)	1856 (99%)	23 (1%)	67	80
1	B	1879/2385 (79%)	1856 (99%)	23 (1%)	67	80
1	C	1879/2385 (79%)	1856 (99%)	23 (1%)	67	80
1	D	1879/2385 (79%)	1856 (99%)	23 (1%)	67	80
All	All	7516/9540 (79%)	7424 (99%)	92 (1%)	66	80

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1024	ASN
1	D	355	VAL
1	C	1250	LEU
1	C	2222	PHE
1	D	590	LEU

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 oligosaccharides 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	B	3002	-	24,24,24	1.34	3 (12%)	39,39,39	0.84	1 (2%)
3	I3P	A	3002	-	24,24,24	1.33	3 (12%)	39,39,39	0.84	1 (2%)
3	I3P	C	3002	-	24,24,24	1.34	3 (12%)	39,39,39	0.84	1 (2%)
3	I3P	D	3002	-	24,24,24	1.34	3 (12%)	39,39,39	0.84	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	B	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	C	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	D	3002	-	-	2/15/39/39	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	I3P	P4-O4	3.28	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3002	I3P	P4-O4	3.25	1.65	1.59
3	C	3002	I3P	P4-O4	3.25	1.65	1.59
3	D	3002	I3P	P4-O4	3.25	1.65	1.59
3	B	3002	I3P	P1-O1	3.24	1.65	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3002	I3P	C5-C6-C1	2.28	113.72	109.11
3	C	3002	I3P	C5-C6-C1	2.28	113.72	109.11
3	A	3002	I3P	C5-C6-C1	2.27	113.70	109.11
3	D	3002	I3P	C5-C6-C1	2.25	113.67	109.11

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3002	I3P	C5-O5-P5-O51
3	B	3002	I3P	C5-O5-P5-O51
3	C	3002	I3P	C5-O5-P5-O51
3	D	3002	I3P	C5-O5-P5-O51
3	A	3002	I3P	C4-O4-P4-O43

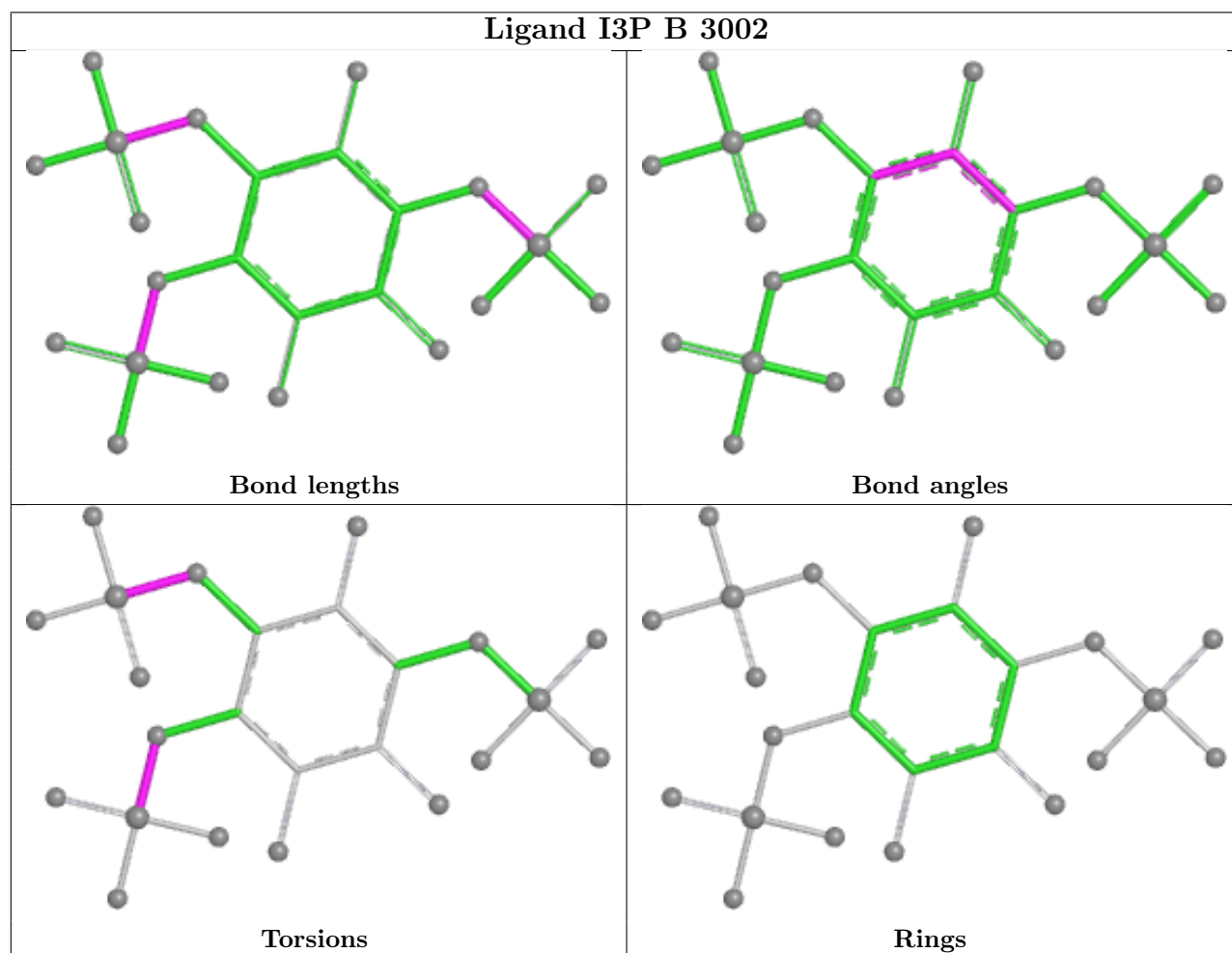
There are no ring outliers.

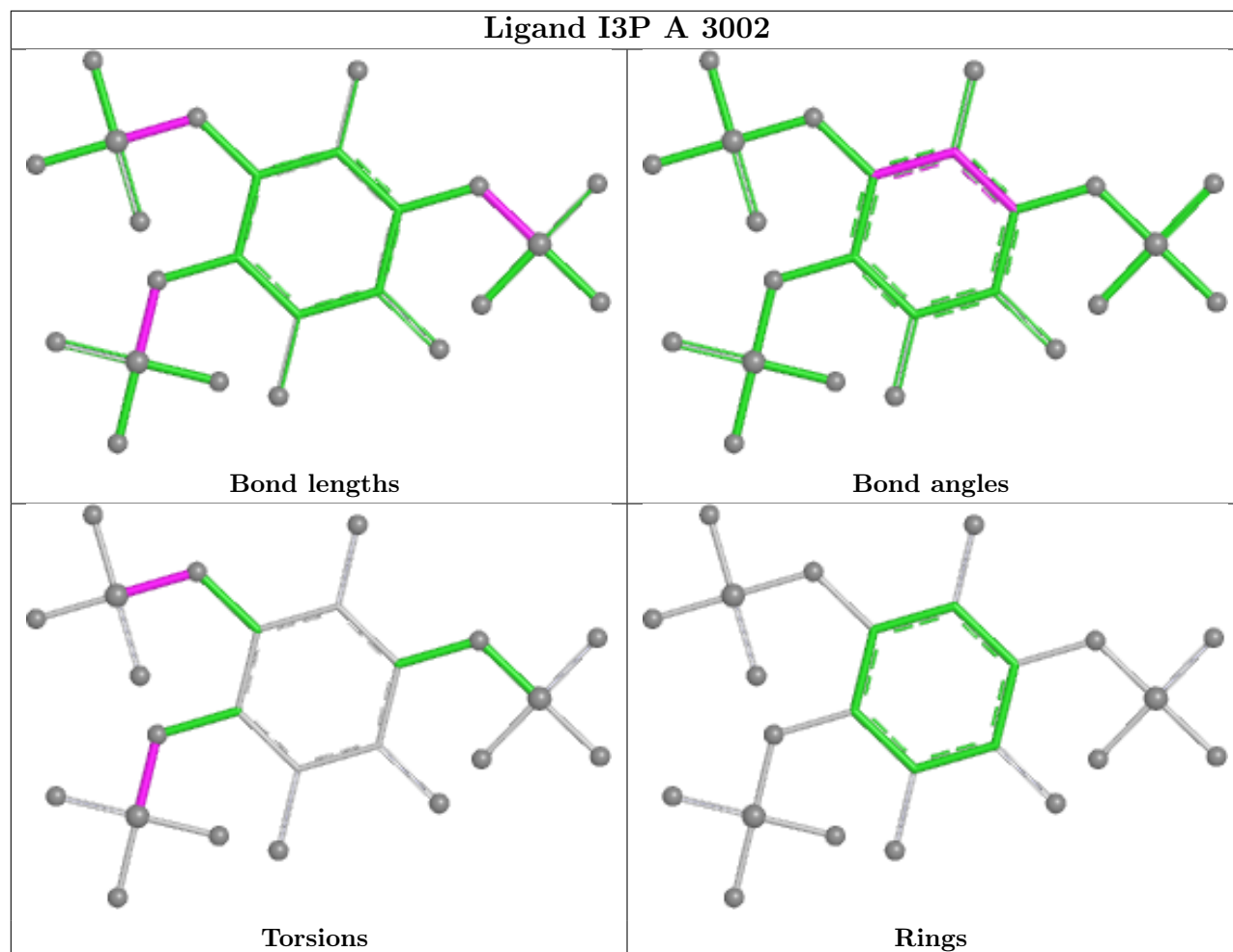
4 monomers are involved in 8 short contacts:

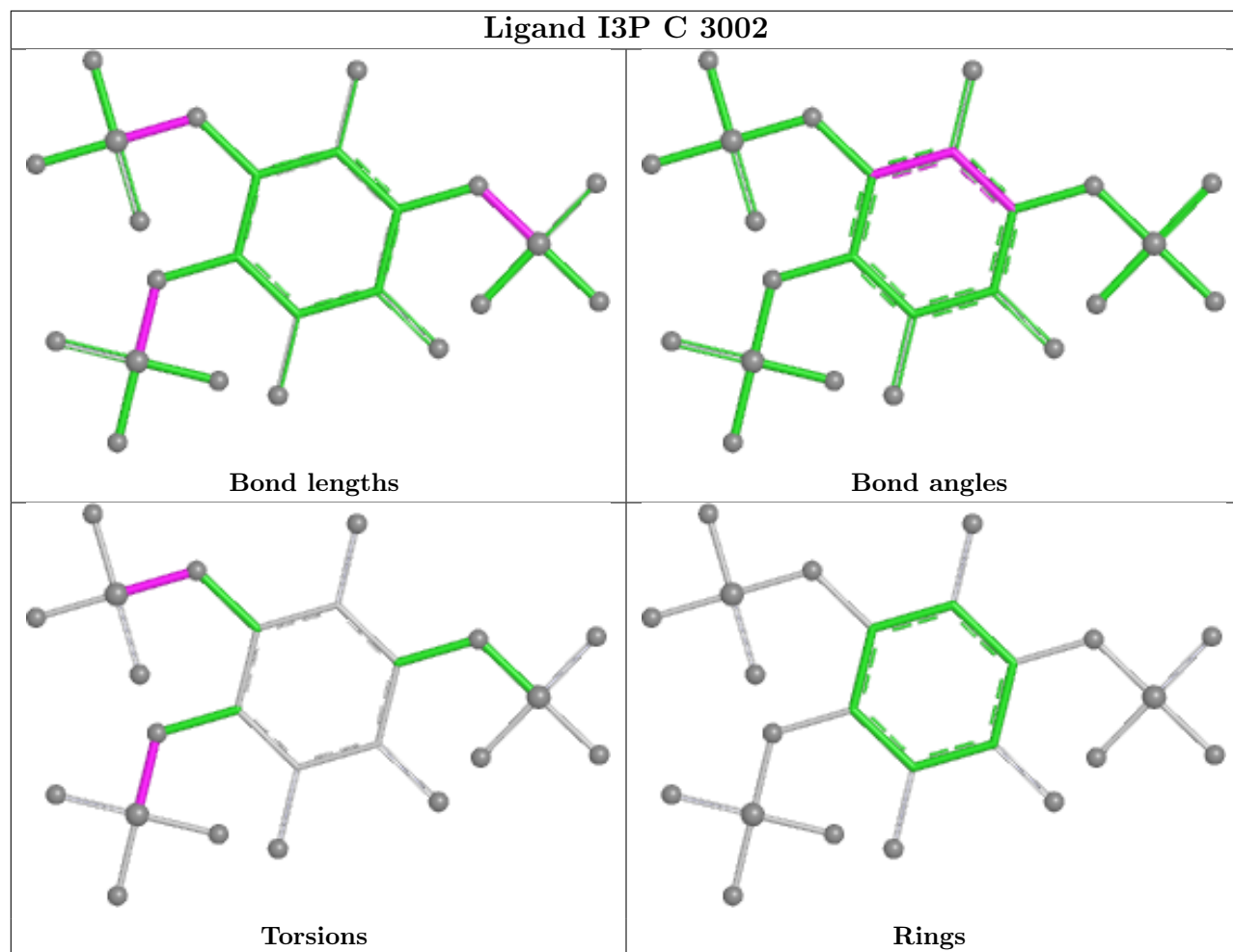
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3002	I3P	2	0
3	A	3002	I3P	2	0
3	C	3002	I3P	2	0
3	D	3002	I3P	2	0

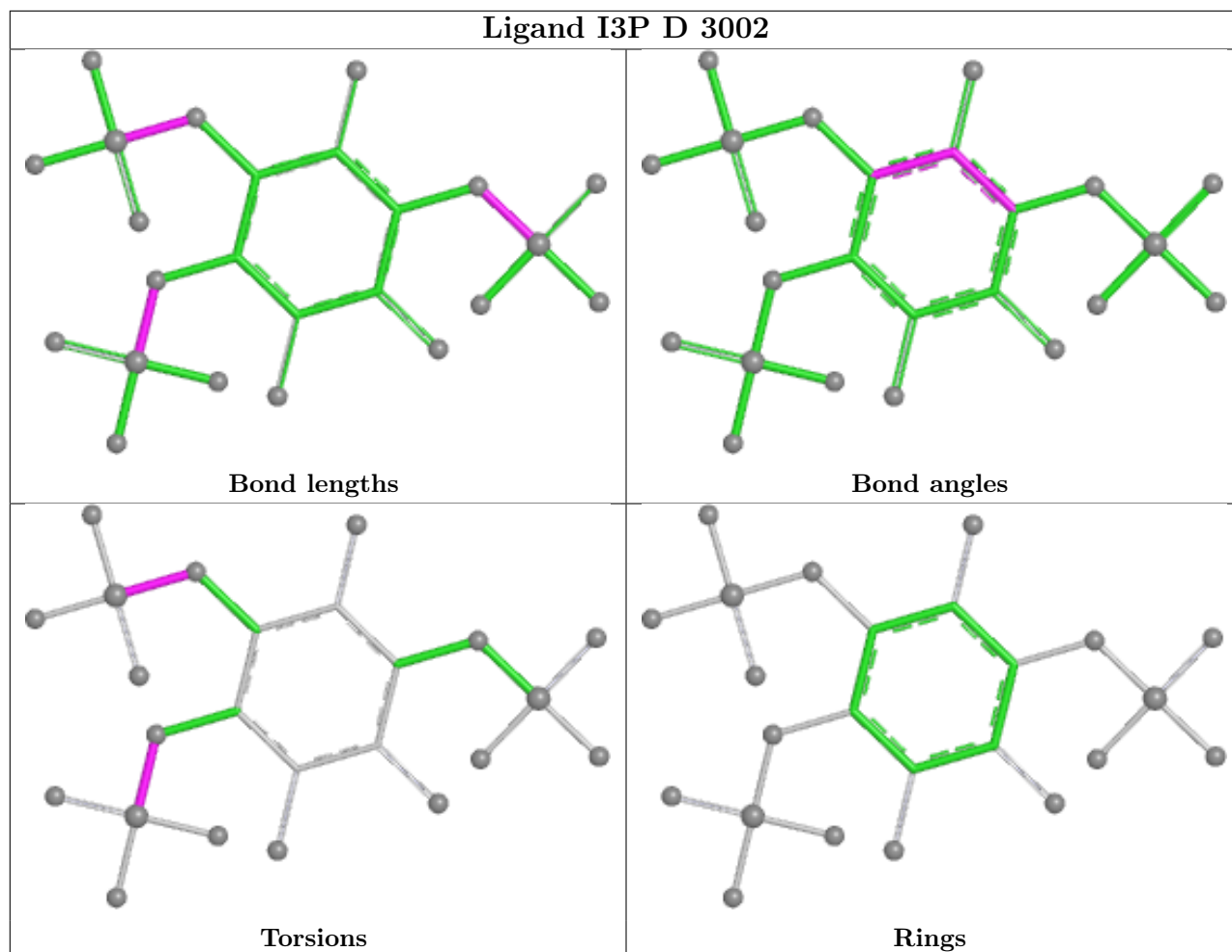
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	A	5
1	B	5
1	C	5
1	D	5

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1552:TRP	C	1587:ASP	N	47.85

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1552:TRP	C	1587:ASP	N	47.85
1	C	1552:TRP	C	1587:ASP	N	47.85
1	D	1552:TRP	C	1587:ASP	N	47.85
1	B	1484:ARG	C	1490:ALA	N	16.56



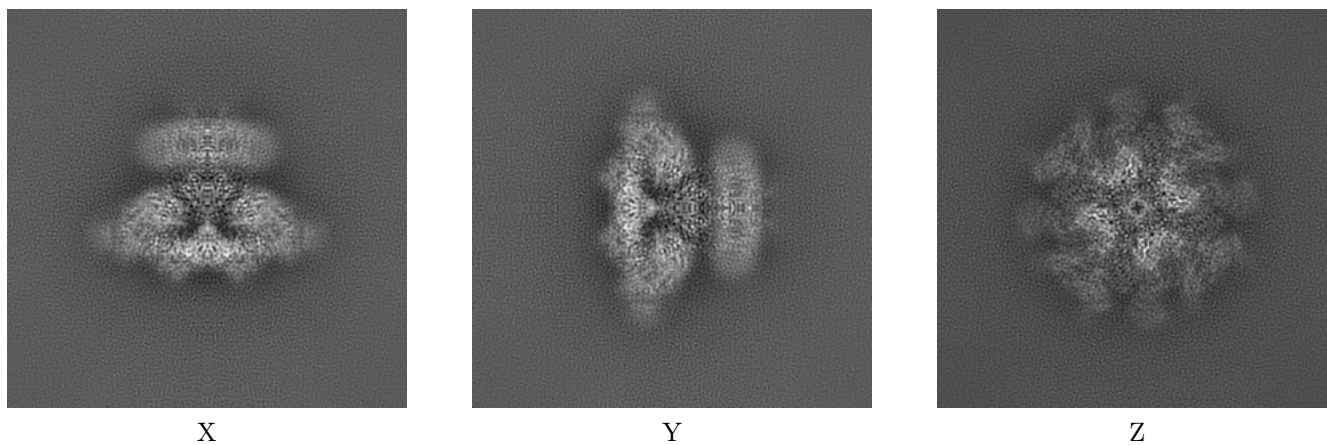
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7981. 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](#)

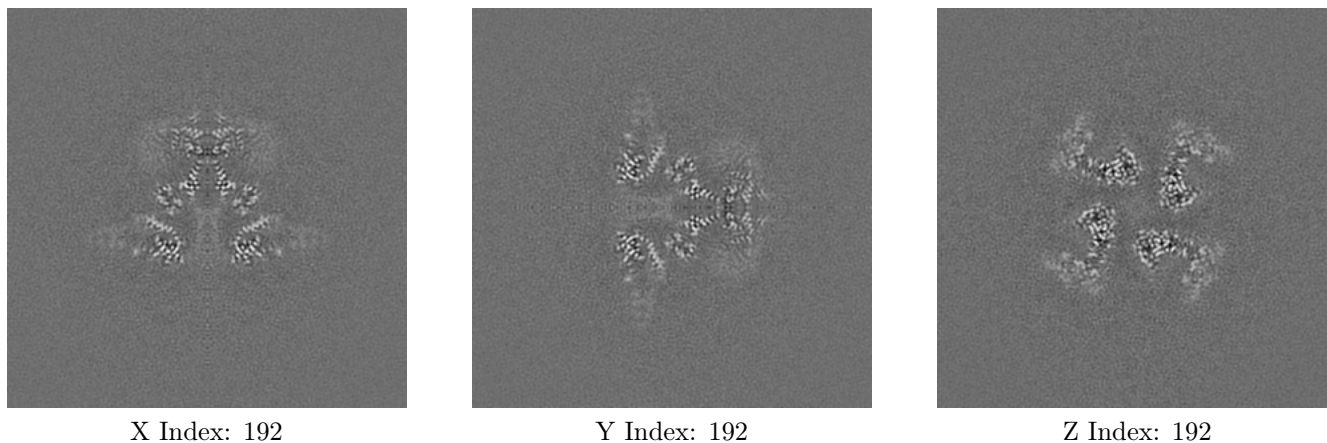
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

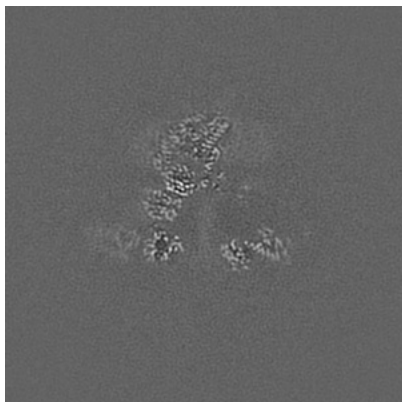
#### 6.2.1 Primary map



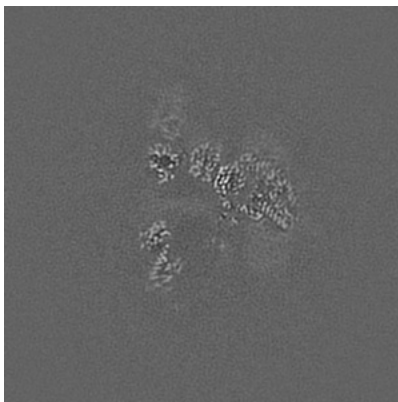
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

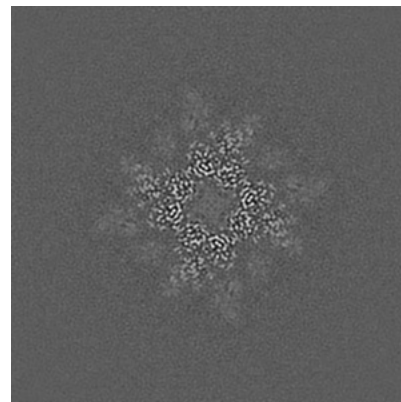
### 6.3.1 Primary map



X Index: 202



Y Index: 202

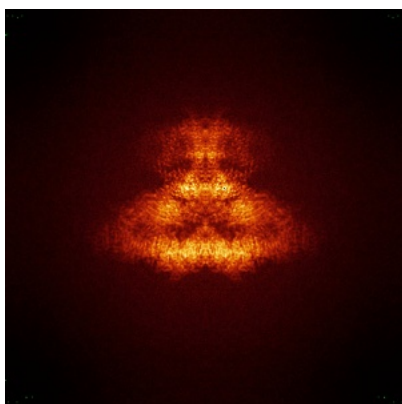


Z Index: 149

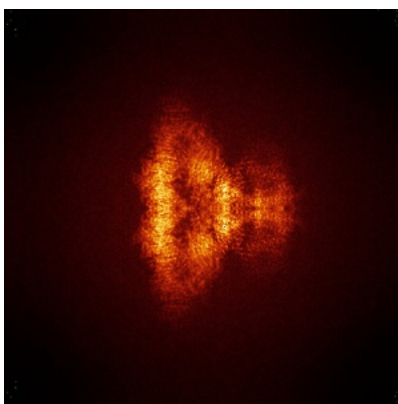
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

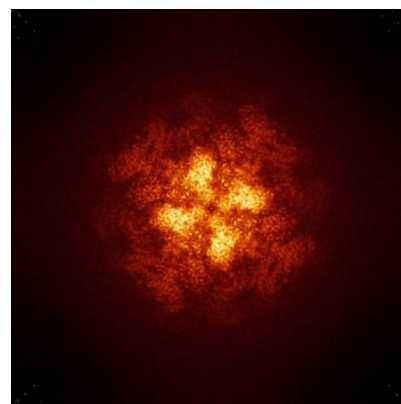
### 6.4.1 Primary map



X



Y

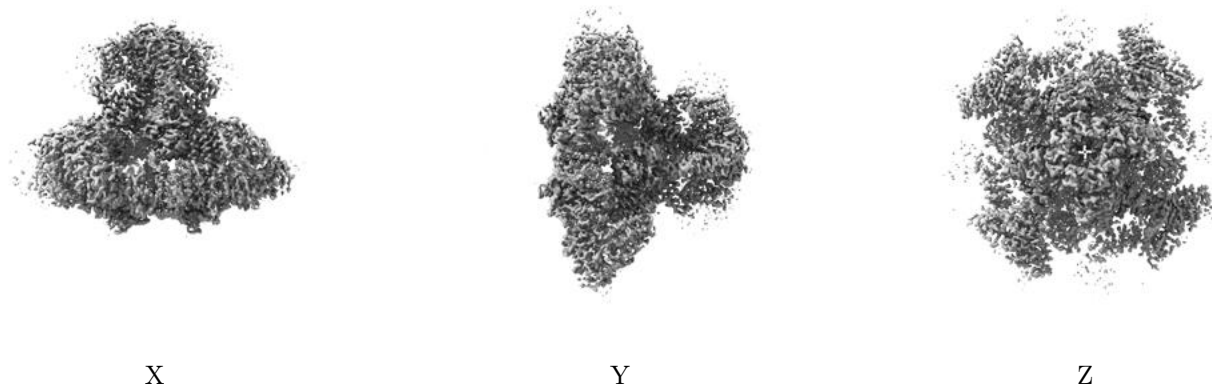


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

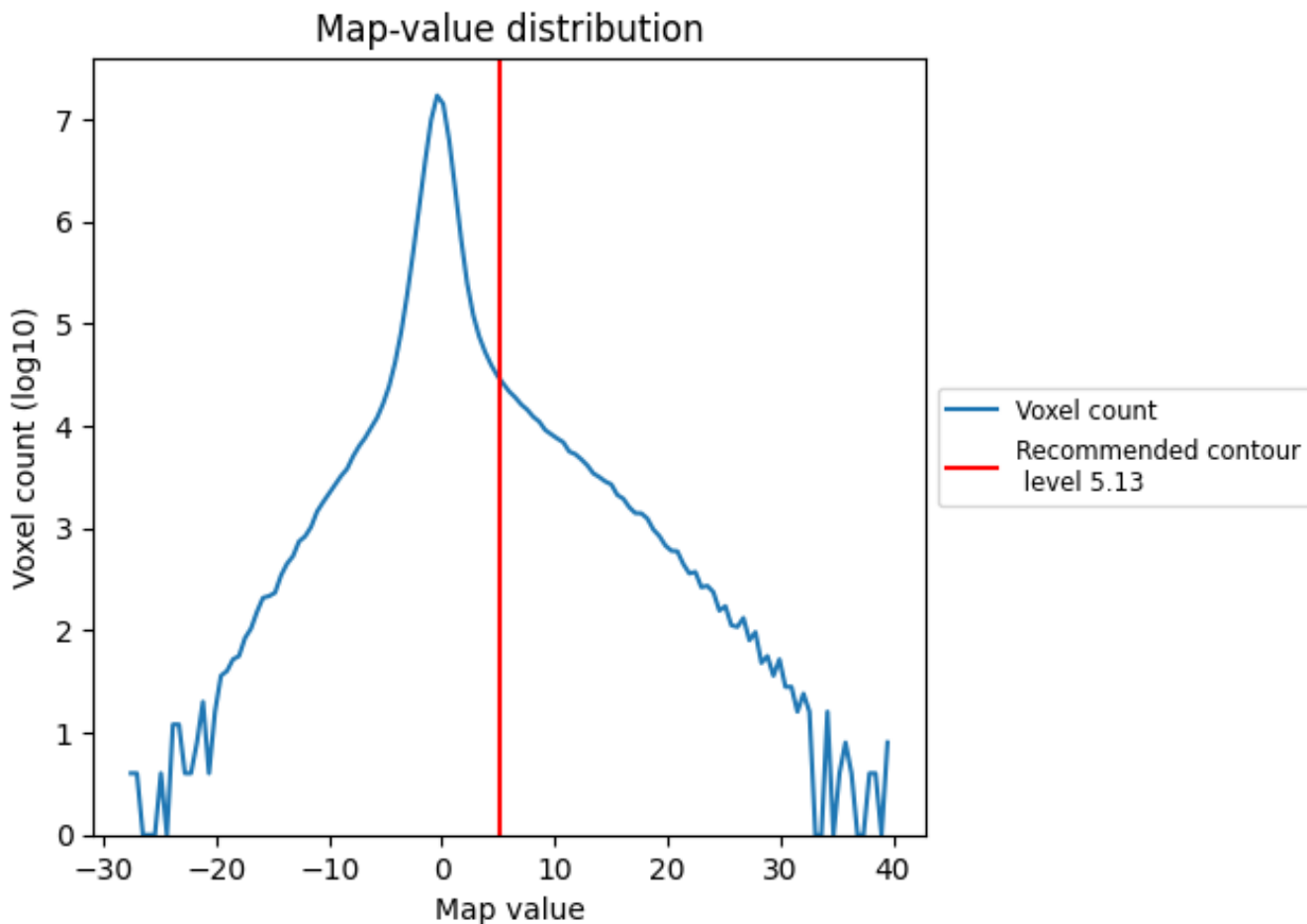
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

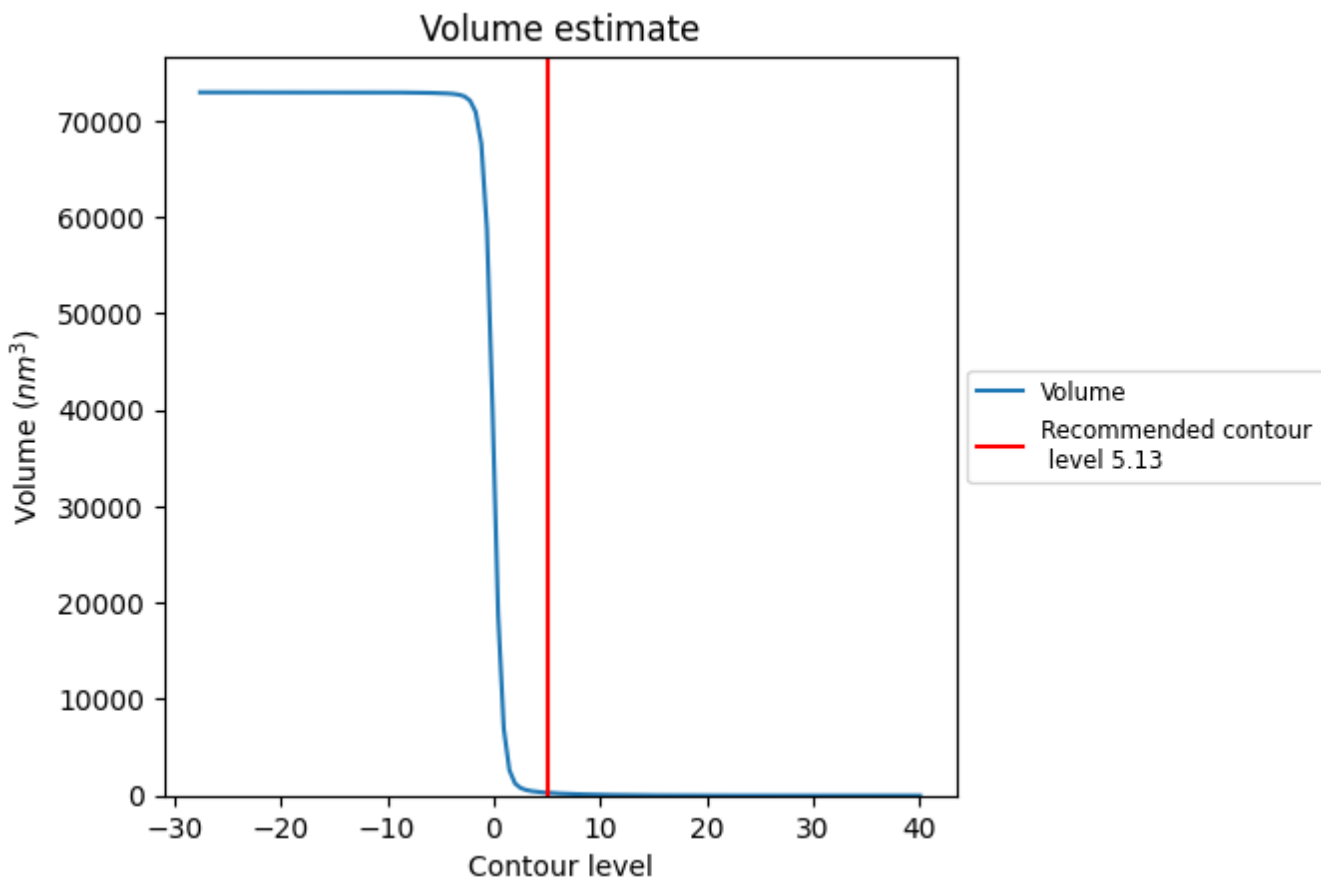
This section contains the results of statistical analysis of the map.

### 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.

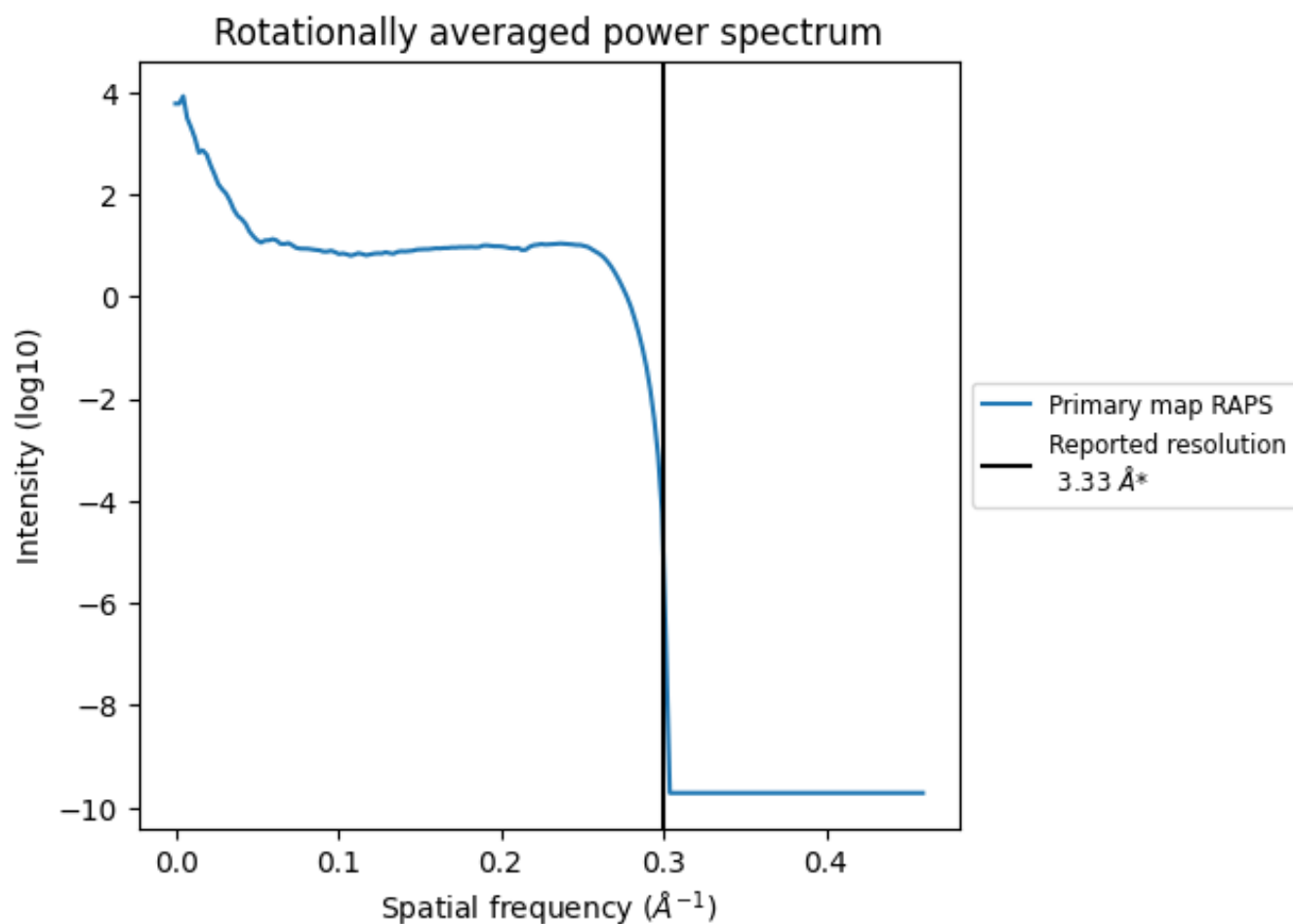
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 280 nm<sup>3</sup>; this corresponds to an approximate mass of 253 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  $0.300 \text{\AA}^{-1}$

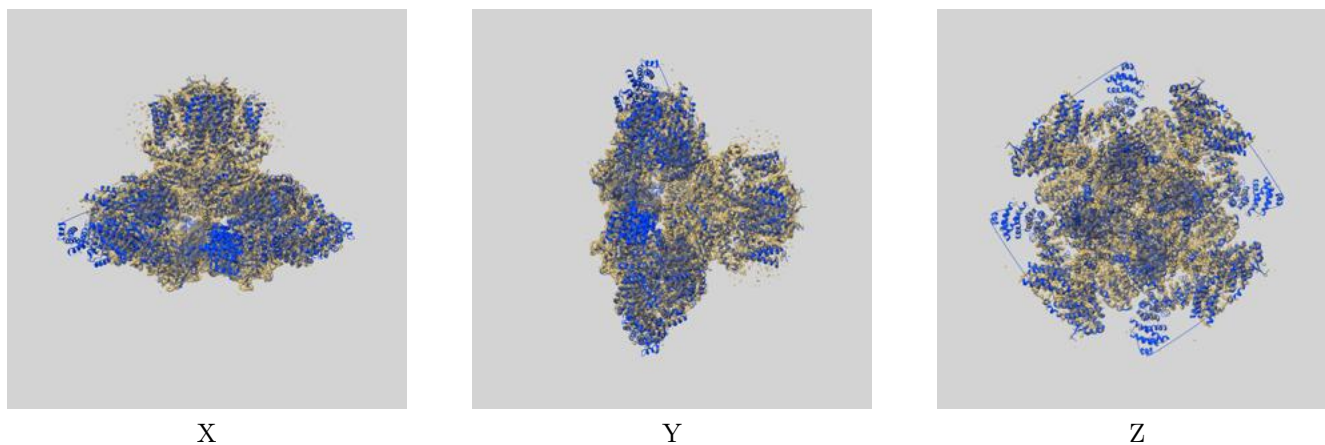
## 8 Fourier-Shell correlation

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-7981 and PDB model 6DQN. Per-residue inclusion information can be found in section [3](#) on page [5](#).

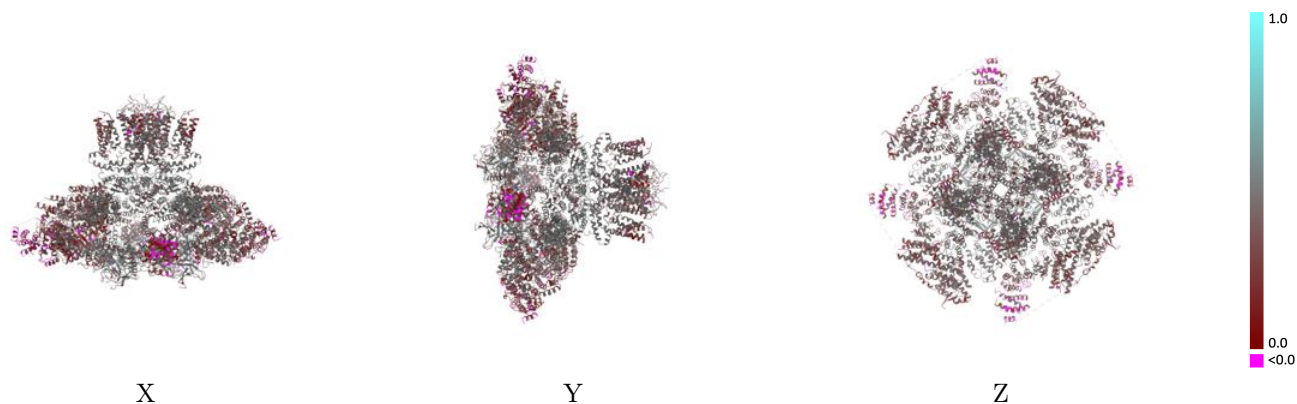
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 5.13 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.

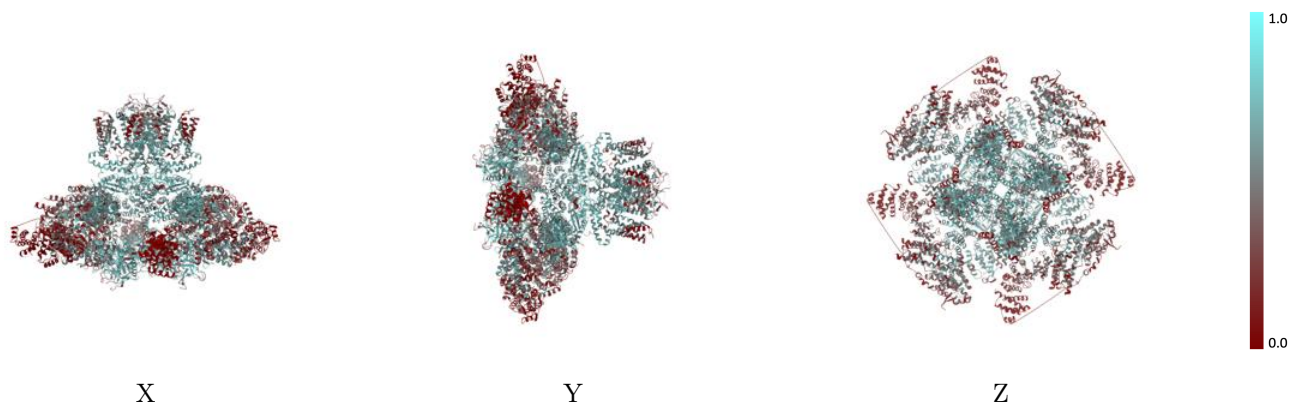


## 9.2 Q-score mapped to coordinate model [i](#)



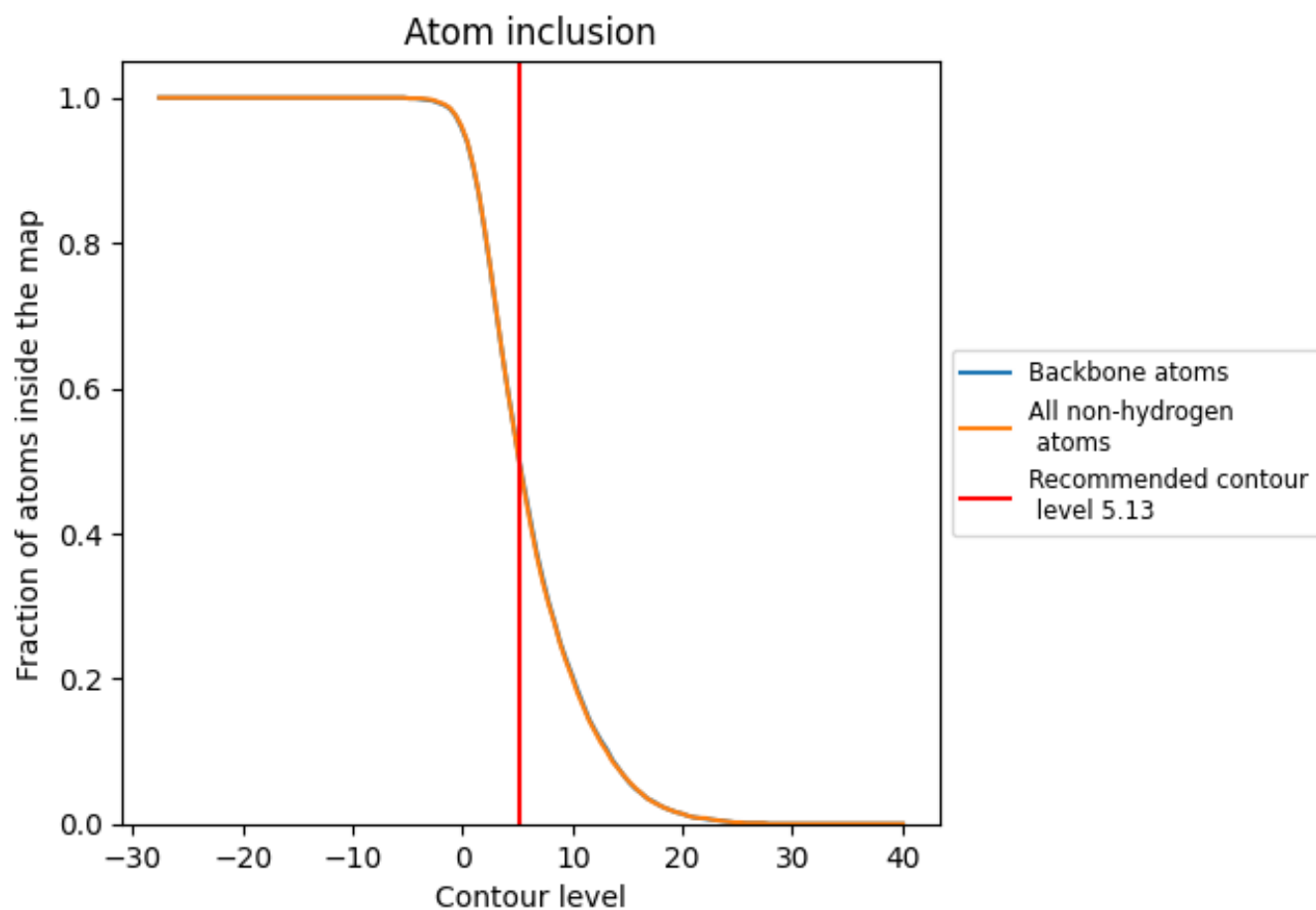
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.13).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 50% 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 (5.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	█ 0.5000	█ 0.3870
A	█ 0.5040	█ 0.3870
B	█ 0.5040	█ 0.3860
C	█ 0.5040	█ 0.3870
D	█ 0.5040	█ 0.3870

