



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 07:08 PM EST

PDB ID : 6DR0
EMDB ID : EMD-7987
Title : Class 5 IP3-bound human type 3 1,4,5-inositol trisphosphate receptor
Authors : Hite, R.K.; Paknejad, N.
Deposited on : 2018-06-11
Resolution : 4.47 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.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

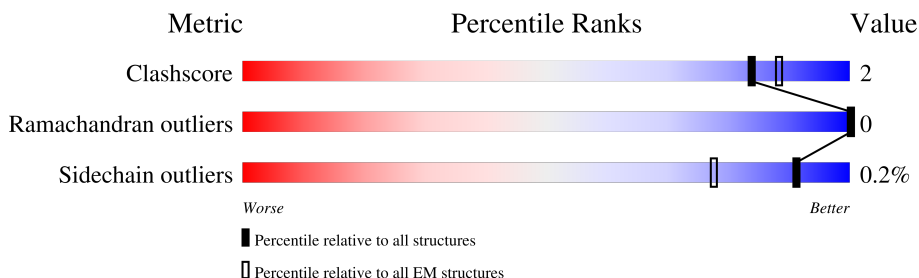
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.47 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 ≥ 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	<div> <div>31%</div> <div>76%</div> <div>6%</div> <div>18%</div> </div>
1	B	2671	<div> <div>39%</div> <div>76%</div> <div>6%</div> <div>18%</div> </div>
1	C	2671	<div> <div>51%</div> <div>76%</div> <div>6%</div> <div>18%</div> </div>
1	D	2671	<div> <div>45%</div> <div>76%</div> <div>5%</div> <div>18%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 140024 atoms, of which 70049 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.

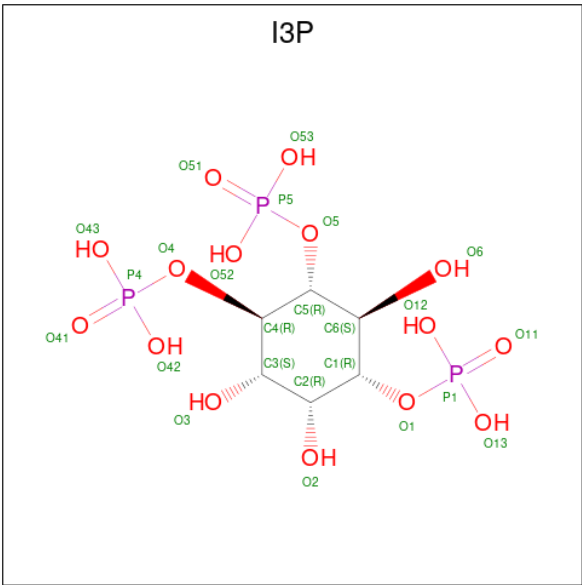
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2188	Total	C	H	N	O	S	0	0
			35063	11176	17553	3000	3228	106		
1	B	2188	Total	C	H	N	O	S	0	0
			35065	11176	17555	3000	3228	106		
1	C	2193	Total	C	H	N	O	S	0	0
			35140	11199	17593	3006	3236	106		
1	D	2181	Total	C	H	N	O	S	0	0
			34620	11035	17312	2979	3191	103		

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

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

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: C₆H₁₅O₁₅P₃).

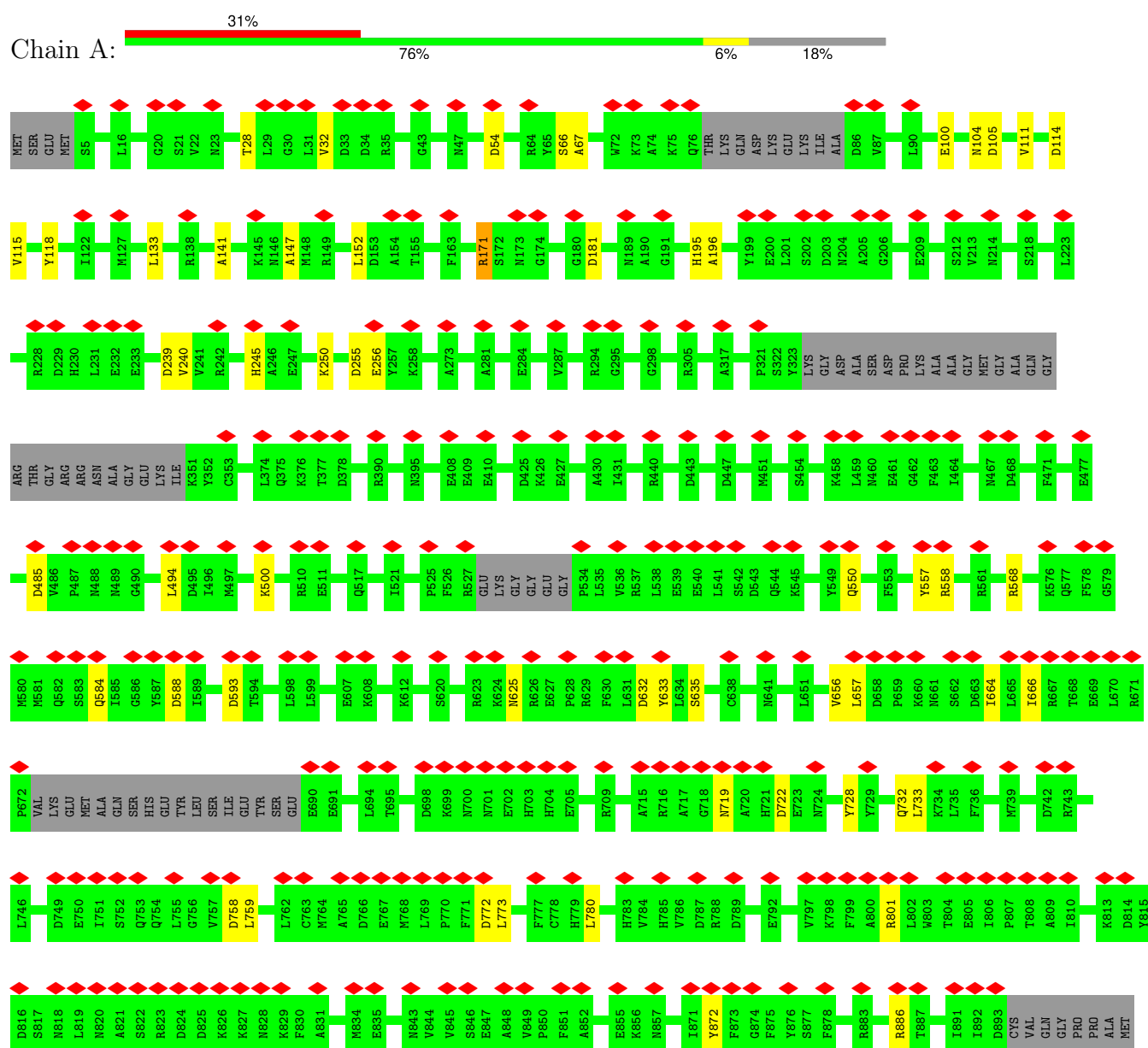


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

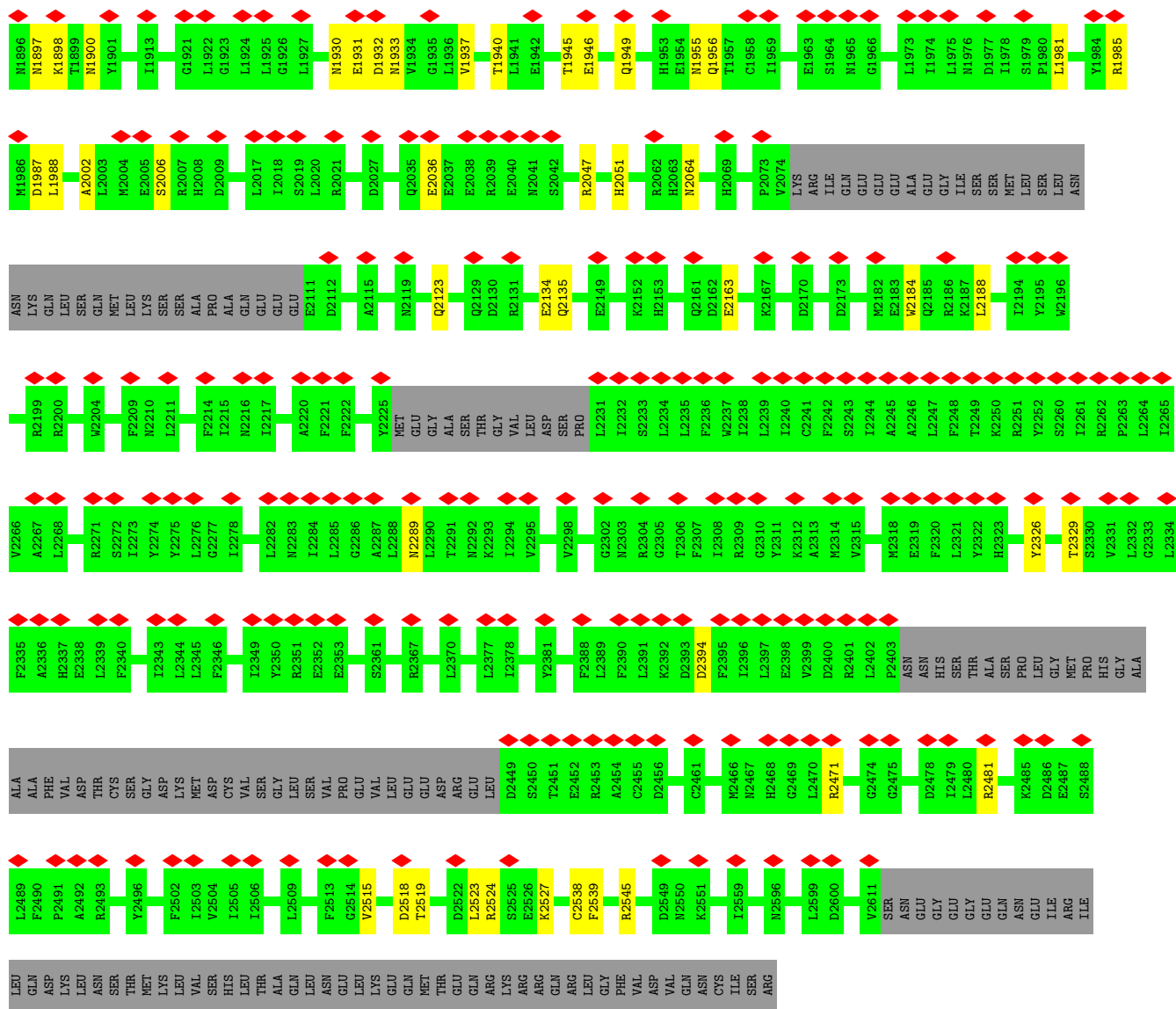
3 Residue-property plots

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.

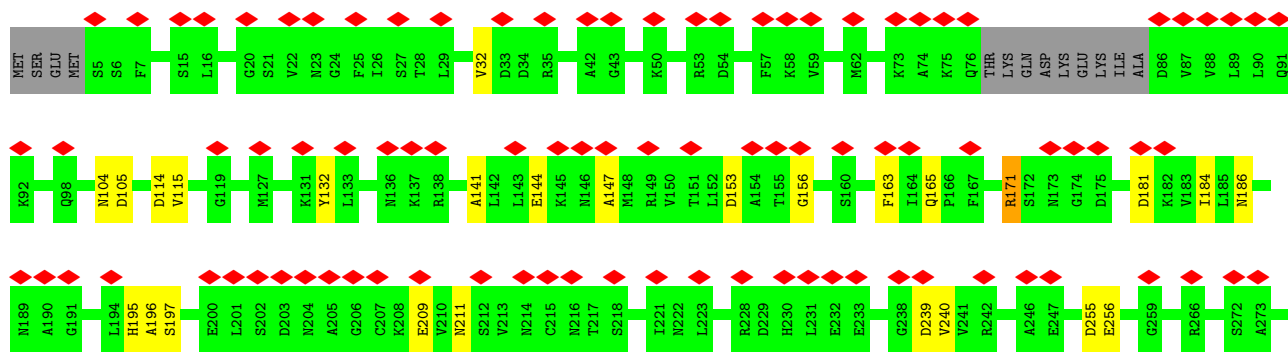
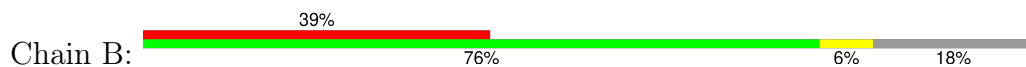
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

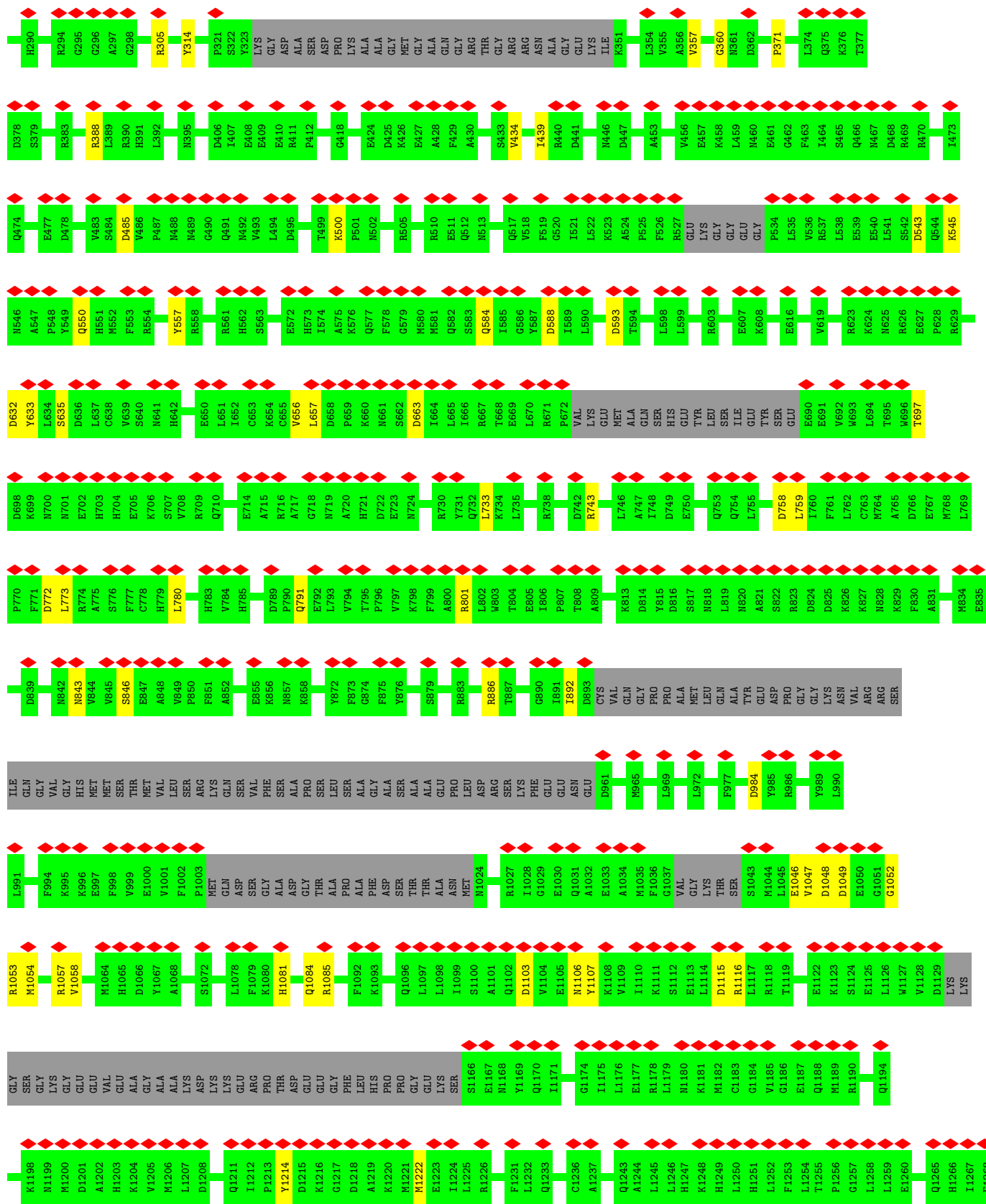




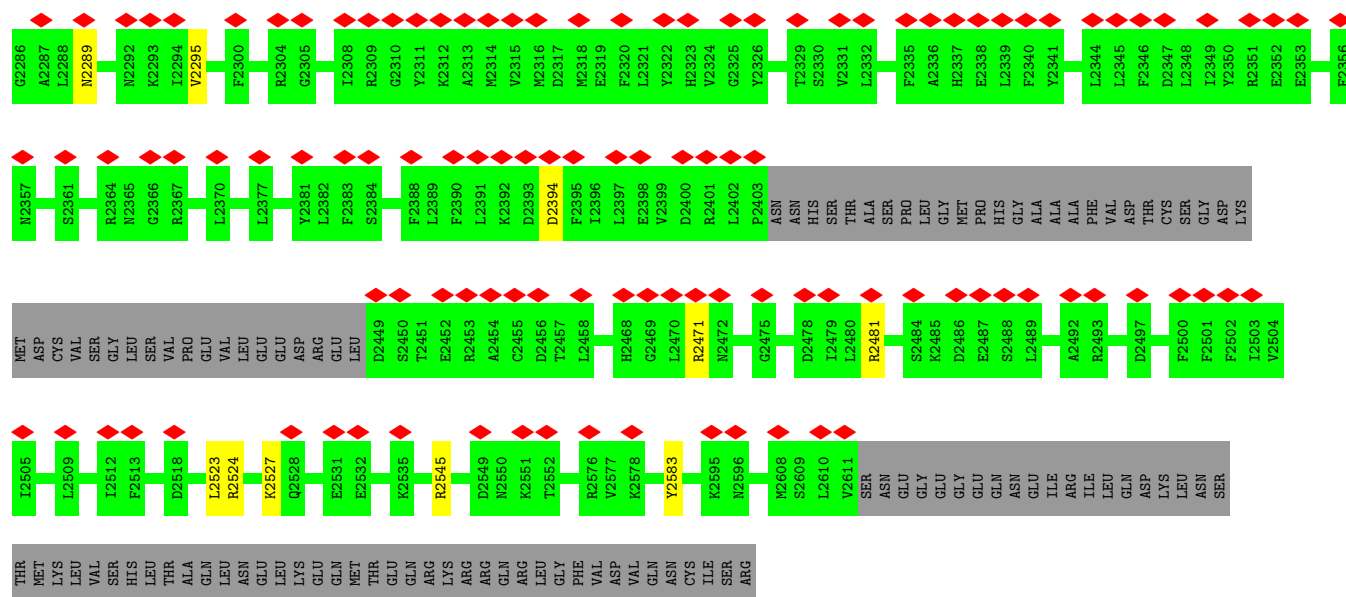


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

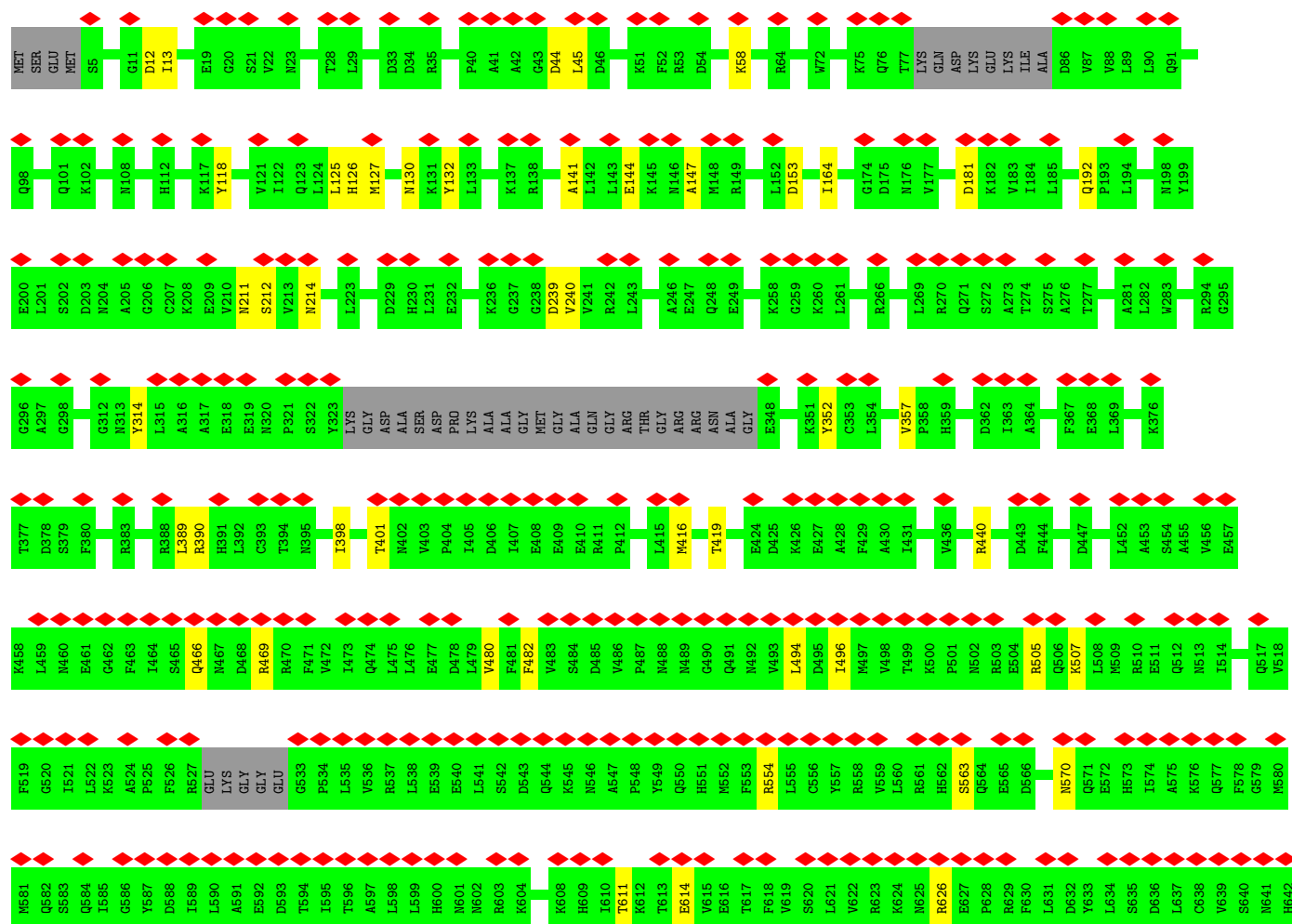
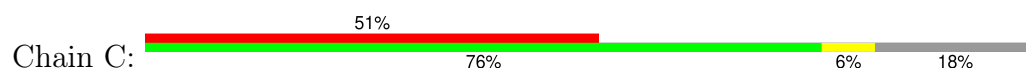




F2221	Y2225	MET	GLU	GLU	GLY	ALA	THR	GLY	VAL	LEU	ASP	SER	PRO	L2231	L2232	S2233	L2234	Q2145	F2146	L2235	F2236	W2237	L2238	L2239	L2240	C2241	F2242	S2243	L2244	A2245	A2246	L2247	F2248	T2249	K2250	R2251	V2252	S2190	M2191	F2197	S2198	R2199	R2200	M2201	T2202	L2203	W2204	G2205	F2209	N2210	L2211	A2212	SER	SER	ALA	F2214	A2220
Q2035	E2036	E2037	E2038	R2039	E2040	N2041	S2042	E2043	R2047	H2051	N2052	L2053	Y2054	L2055	L2056	A2057	R2062	H2063	N2064	K2065	H2069	P2073	V2074	LYS	ILE	GLN	GLU	GLU	ALA	GLU	GLY	ILE	SER	SER	MET	LEU	SER	LEU	ASN	ASN	LYS	GLN	SER	GLN	MET	LEU	LYS	SER	LEU	LYS	SER	LEU	LYS	LEU	LEU	ALA	
K1770	H1773	M1777	S1778	D1779	R1784	F1785	F1786	K1787	D1791	A1796	E1799	T1800	K1801	S1802	T1803	V1804	ALA	VAL	ASN	ASN	ASP	GLY	LEU	GLY	THR	GLY	LEU	ASP	PRO	ILE	GLN	PRO	ASP	W1718	S1719	A1720	A1723	D1729	K1730	E1731	K1735	C1738	D1739	S1743	E1747	E1752	G1755	D1762	K1675	K1676	T1677						
K1678	Y1679	G1680	D1681	Q1685	K1688	M1689	Q1692	M1693	Q1696	ASN	ARG	LYS	SER	THR	ARG	GLY	ASP	LEU	PRO	ASP	PRO	ILE	GLY	THR	GLY	LEU	ASP	PRO	ASP	Q1636	R1637	C1638	E1639	S1640	G1641	G1642	F1643	K1646	L1647	I1648	D1653	L1654	M1655	E1656	S1657	E1658	I1663	K1664	V1665	L1666	R1667						
V1552	D1587	Y1588	I1591	I1592	E1593	K1594	L1595	Q1596	D1597	A1601	E1604	R1605	V1610	E1613	V1616	H1622	L1627	F1628	L1629	E1630	G1631	Q1636	R1637	C1638	E1639	S1640	A1521	Q1522	R1523	N1524	A1525	S1526	S1527	Y1528	K1529	A1530	T1531	T1532	R1533	A1541	F1542	P1543	R1544	V1545	T1546	P1547	T1548	A1549	N1550	Q1551							
ILE	ARG	THR	LEU	M1490	V1492	A1493	K1494	G1495	R1496	A1497	L1498	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	N1524	A1525	S1526	S1527	Y1528	K1529	A1530	T1531	T1532	R1533	A1541	F1542	P1543	R1544	V1545	T1546	P1547	T1548	A1549	N1550	Q1551
K1466	Y1467	L1468	L1469	S1470	V1471	V1472	L1473	D1474	T1475	I1476	M1477	A1478	F1479	S1481	S1482	P1483	PHE	SER	GLU	ASN	SER	THR	SER	LEU	GLN	THR	HIS	GLN	THR	ILE	VAL	VAL	GLN	LEU	GLN	SER	THR	ARG	LEU	LEU	CYS	PRO	TRP	LEU	GLN	GLN	HIS	LYS	GLY	SER	VAL	GLU	ALA	CYS			
E1403	D1404	C1405	I1406	T1407	E1408	V1409	K1410	M1411	A1412	Y1413	V1414	H1418	H1419	C1420	Y1421	V1422	D1423	T1424	E1425	V1426	E1427	M1428	K1429	E1430	T1433	S1434	M1435	H1436	I1437	W1438	T1439	L1440	F1441	E1442	M1443	F1444	T1445	L1446	D1447	M1448	A1449	R1450	V1451	C1452	S1453	K1454	R1455	GLU	LYS	ARG	VAL	ALA	ASP	PRO	T1463	L1464	E1465
Y1336	N1337	D1338	K1339	A1340	S1341	L1342	A1343	H1344	L1345	L1346	D1347	M1348	M1349	K1350	A1351	A1352	R1353	D1354	G1355	V1356	A1357	D1358	H1359	H1365	I1366	S1367	D1370	L1371	L1372	A1373	A1374	C1375	A1376	E1377	G1378	K1379	N1380	V1381	Y1382	T1383	E1384	I1385	K1386	C1387	L1390	L1391	E1394	D1395	V1396	V1397	S1398	V1399	T1400	T1401	H1402		
L1269	H1270	Q1273	L1274	C1275	S1276	E1277	E1280	P1281	V1282	H1285	F1286	V1287	H1288	L1289	L1290	H1293	G1294	R1295	H1296	V1297	Q1298	Y1299	F1302	L1303	H1304	T1305	K1308	A1309	E1310	G1311	K1312	Y1313	V1314	K1315	K1316	C1317	Q1318	D1319	M1320	I1321	M1322	T1323	E1324	M1327	A1328	G1329	D1330	D1331	V1332	V1333	V1334	F1335					



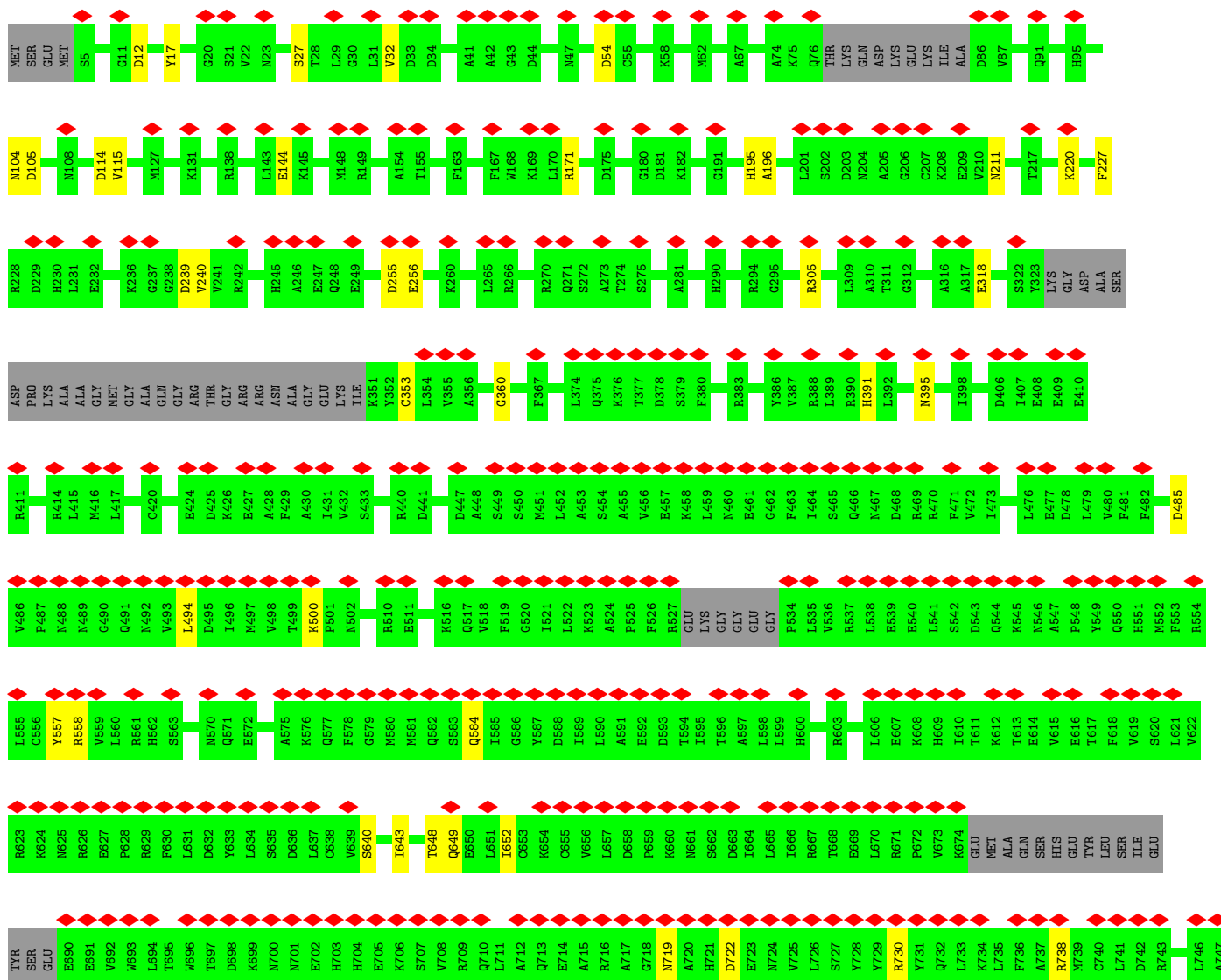
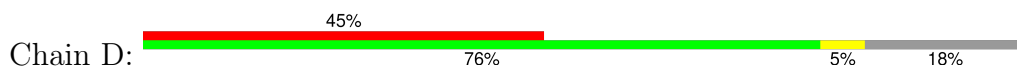
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





E1442	M1443	F1444	T1445	L1446	D1447	M1448	A1449	R1450	V1451	C1452	S1453	K1454	R1455	GLU	LYS	ARG	VAL	ALA	ASP	PRO	T1463	L1464	E1465	K1466	V1467	V1468	L1469	S1470	V1471	V1472	L1473	D1474	T1475	I1476	M1477	A1478	F1479	F1480	S1481	S1482	P1483	PHE	SER	GLU	ASN	THR	SER	LEU	GLN	THR	HIS	GLN	THR	ILE	VAL	VAL	GLN	LEU
L1627	F1628	R1629	E1630	G1631	S1632	E1633	Y1634	A1635	Q1636	R1637	C1638	E1639	S1640	G1641	G1642	F1643	K1646	L1647	I1648	Q1649	H1650	T1651	K1652	D1653	L1654	M1655	E1656	S1657	E1658	E1659	I1663	K1664	R1667	Q1671	M1672	L1673	L1674	K1675	K1676	T1677	K1678	Y1679	G1680	D1681	R1682	G1683	N1684	Q1685	L1686	R1687	K1688	M1689	N1693	Y1694				
L1695	Q1696	ASN	ARG	LYS	THR	SER	ARG	GLY	ASP	LEU	PRO	ASP	ILE	THR	GLY	ASP	W1718	S1719	A1720	A1723	L1728	D1729	K1730	E1731	G1732	K1735	L1736	V1737	C1738	D1739	L1740	I1741	T1742	S1743	T1744	K1745	M1746	E1747	K1748	I1749	F1750	S1753	I1754	G1755	D1762	G1763	G1764											
F1772	H1773	N1774	L1775	M1776	M1777	S1778	D1779	K1780	R1784	F1785	R1792	M1793	K1794	R1796	A1796	E1799	S1802	T1803	V1804	ALA	VAL	ASN	MET	ASN	ASP	LEU	GLY	SER	GLN	PRO	HIS	GLU	ASP	ARG	GLU	PRO	VAL	ARG	VAL	ALA	SER	PHE	SER	ILE	PRO	GLY	SER	SER										
ARG	TYR	SER	GLY	PRO	SER	LEU	ARG	GLY	HIS	GLU	GLU	VAL	GLN	SER	SER	GLU	M1863	G1864	T1865	S1866	V1867	R1875	F1876	L1877	Q1878	R1886	Q1889	N1890	F1891	L1892	R1893	C1894	Q1895	N1896	N1897	K1898	Y1901	E1906	D1912	I1913	T1918	T1919	L1922	G1923	L1924	L1925												
G1926	L1927	M1930	E1931	D1932	N1933	V1934	G1935	L1936	V1937	I1938	Q1939	T1940	E1946	Y1947	C1948	Q1949	H1953	Q1956	T1961	H1962	E1963	S1964	N1965	G1966	A1972	L1973	I1974	L1975	N1976	D1977	L1981	C1982	K1983	Y1984	R1985	M1986	L1992	K1998	L2001	A2002	L2003	M2004	E2005	S2006	R2007	H2008	D2009	S2010										
A2013	E2014	R2015	I2018	R2021	P2022	Q2023	E2024	D2027	K2031	A2032	Y2033	L2034	Q2035	E2036	E2037	E2038	R2039	E2040	S2042	E2043	H2051	L2058	Q2059	R2062	H2063	N2064	K2065	Q2068	H2069	P2073	V2074	LYS	ARG	ILE	GLN	GLU	GLU	ALA	GLU	GLY	ILE	SER	MET	LEU	SER	LEU	ASN											
ASN	LYS	GLN	LEU	SER	GLN	MET	LEU	LYS	SER	ALA	ALA	GLN	GLU	GLU	GLU	E2111	A2115	Y2116	N2119	Q2123	Q2129	D2130	R2131	E2134	Q2135	F2146	L2147	T2148	E2149	E2150	T2151	K2152	H2153	T2158	Q2161	D2162	E2163	K2167	D2170	D2173	F2177	L2178	H2179	W2182														
E2183	S2190	M2191	P2192	L2193	T2194	Y2195	W2196	F2197	S2198	R2199	R2200	M2201	W2204	F2209	A2212	V2213	F2214	L2215	N2216	T2217	L2218	L2219	A2220	F2221	F2222	Y2225	GLU	ALA	SER	THR	GLY	VAL	LEU	ASP	SER	PRO	L2231	L2232	S2233	L2234	L2235	F2236	W2237	L2238	L2239	I2240	C2241	F2242	S2243	I2244	A2245	A2246						
L2247	F2248	T2249	K2250	R2251	Y2252	S2260	P2263	L2264	A2267	L2268	R2271	S2272	I2273	Y2274	L2276	Q2277	L2278	Q2279	P2280	T2281	L2282	N2283	L2284	G2285	A2287	L2288	N2289	I2294	V2295	F2296	V2297	V2298	G2302	N2303	R2304	Q2305	L2306	F2307	I2308	R2309	Q2310	Y2311	K2312	A2313	M2314	V2315	R2401	L2402	P2403	ASN	ASN	HIS						
Y2322	H2323	V2324	G2325	V2331	L2332	F2335	A2336	H2337	E2338	L2339	F2340	Y2341	L2344	L2345	F2346	D2347	L2348	I2349	Y2350	L2351	E2352	E2353	F2356	K2360	S2361	R2364	R2367	A2373	L2374	L2377	L2378	Y2381	F2388	K2392	D2393	D2394	F2395	L2396	V2399	P2400	R2401	L2402	P2403	ASN	ASN	HIS												

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







ARG
LYS
ARG
ARG
GLN
ARG
LEU
GLY
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, Not provided	
Number of particles used	27334	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	11.858	Depositor
Minimum map value	-6.272	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.551	Depositor
Recommended contour level	3.06	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

5.1 Standard geometry

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	0.26	0/17827	0.47	3/24087 (0.0%)
1	B	0.25	0/17827	0.47	3/24087 (0.0%)
1	C	0.25	0/17864	0.46	3/24137 (0.0%)
1	D	0.25	0/17613	0.47	4/23801 (0.0%)
All	All	0.25	0/71131	0.47	13/96112 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1547	PRO	N-CA-CB	5.71	110.15	103.30
1	C	1547	PRO	N-CA-CB	5.66	110.09	103.30
1	C	1501	PRO	N-CA-CB	5.61	110.04	103.30
1	C	1543	PRO	N-CA-CB	5.61	110.03	103.30
1	B	1547	PRO	N-CA-CB	5.61	110.03	103.30
1	D	1436	PRO	N-CA-CB	5.59	110.01	103.30
1	D	1494	PRO	N-CA-CB	5.58	109.99	103.30
1	A	1547	PRO	N-CA-CB	5.57	109.99	103.30
1	A	1501	PRO	N-CA-CB	5.57	109.99	103.30
1	D	1543	PRO	N-CA-CB	5.56	109.97	103.30
1	A	1543	PRO	N-CA-CB	5.53	109.94	103.30
1	B	1501	PRO	N-CA-CB	5.51	109.92	103.30
1	B	1543	PRO	N-CA-CB	5.51	109.91	103.30

There are no chirality outliers.

There are no planarity outliers.

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	17510	17553	17452	77	0
1	B	17510	17555	17453	75	0
1	C	17547	17593	17492	85	0
1	D	17308	17312	17141	74	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	1	0
3	B	24	9	9	0	0
3	C	24	9	9	1	0
3	D	24	9	9	0	0
All	All	69975	70049	69574	304	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 (304) 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:1054:MET:SD	1:A:1057:ARG:NH2	2.59	0.75
1:C:2163:GLU:O	1:D:2545:ARG:NH1	2.21	0.74
1:A:1085:ARG:NH1	1:A:1613:GLU:OE2	2.20	0.74
1:A:2545:ARG:NH1	1:D:2163:GLU:O	2.22	0.73
1:D:749:ASP:O	1:D:753:GLN:NE2	2.22	0.73
1:D:1987:ASP:OD1	1:D:2042:SER:OG	2.06	0.72
1:B:1085:ARG:NH1	1:B:1613:GLU:OE2	2.23	0.72
1:C:401:THR:OG1	1:C:416:MET:O	2.08	0.71
1:C:1956:GLN:NE2	1:C:2002:ALA:O	2.24	0.70
1:C:2394:ASP:OD1	1:C:2481:ARG:NH2	2.25	0.70
1:B:171:ARG:NH1	1:B:181:ASP:OD2	2.24	0.70
1:A:1889:GLN:NE2	1:A:1946:GLU:O	2.25	0.70
1:A:2394:ASP:OD1	1:A:2481:ARG:NH2	2.25	0.70
1:B:557:TYR:OH	1:B:584:GLN:OE1	2.08	0.69
1:C:1735:LYS:NZ	1:C:1739:ASP:OD2	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1053:ARG:NE	1:D:1693:ASN:O	2.25	0.69
1:B:733:LEU:HD12	1:B:780:LEU:HD22	1.75	0.69
1:B:2394:ASP:OD1	1:B:2481:ARG:NH2	2.25	0.69
1:B:743:ARG:NH2	1:B:791:GLN:O	2.26	0.69
1:D:649:GLN:NE2	1:D:738:ARG:O	2.26	0.68
1:D:12:ASP:OD1	1:D:227:PHE:N	2.26	0.68
1:B:1054:MET:SD	1:B:1057:ARG:NH2	2.67	0.68
1:A:1214:TYR:OH	1:A:1222:MET:SD	2.51	0.68
1:C:127:MET:O	1:C:440:ARG:NH2	2.27	0.68
1:C:611:THR:OG1	1:C:614:GLU:OE1	2.10	0.67
1:C:1054:MET:SD	1:C:1057:ARG:NH2	2.67	0.67
1:C:1949:GLN:NE2	1:C:2583:TYR:O	2.27	0.67
1:C:743:ARG:NH2	1:C:791:GLN:O	2.27	0.67
1:D:1725:GLN:NE2	1:D:1759:HIS:O	2.28	0.67
1:C:806:ILE:O	1:C:995:LYS:NZ	2.23	0.66
1:D:2038:GLU:OE2	1:D:2042:SER:OG	2.12	0.66
1:D:2394:ASP:OD1	1:D:2481:ARG:NH2	2.28	0.66
1:B:1956:GLN:NE2	1:B:2002:ALA:O	2.28	0.66
1:B:2163:GLU:O	1:C:2545:ARG:NH1	2.29	0.66
1:B:1214:TYR:OH	1:B:1222:MET:SD	2.50	0.65
1:A:118:TYR:OH	1:A:181:ASP:OD2	2.14	0.65
1:A:733:LEU:HD12	1:A:780:LEU:HD22	1.79	0.65
1:A:632:ASP:O	1:A:635:SER:OG	2.08	0.65
1:C:663:ASP:OD1	1:C:697:THR:OG1	2.14	0.65
1:B:2123:GLN:OE1	1:B:2135:GLN:NE2	2.30	0.64
1:A:886:ARG:NH1	1:A:1047:VAL:O	2.31	0.64
1:B:1937:VAL:O	1:B:1940:THR:OG1	2.10	0.64
1:B:1787:LYS:NZ	1:B:1791:ASP:OD2	2.31	0.64
1:A:1937:VAL:O	1:A:1940:THR:OG1	2.11	0.64
1:D:1735:LYS:NZ	1:D:1739:ASP:OD2	2.19	0.64
1:D:1235:PHE:O	1:D:1242:ASN:ND2	2.31	0.64
1:A:195:HIS:ND1	1:A:196:ALA:O	2.31	0.63
1:A:557:TYR:OH	1:A:584:GLN:OE1	2.17	0.63
1:C:507:LYS:NZ	3:C:2702:I3P:O53	2.27	0.63
1:C:2123:GLN:OE1	1:C:2135:GLN:NE2	2.31	0.62
1:C:192:GLN:O	1:C:212:SER:OG	2.17	0.62
1:B:886:ARG:NH1	1:B:1047:VAL:O	2.32	0.62
1:D:1107:TYR:OH	1:D:1200:MET:SD	2.50	0.62
1:B:2187:LYS:O	1:B:2190:SER:OG	2.14	0.62
1:C:1878:GLN:OE1	1:C:1939:GLN:NE2	2.31	0.62
1:D:195:HIS:ND1	1:D:196:ALA:O	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:GLU:OE2	1:C:211:ASN:ND2	2.33	0.61
1:C:1385:ILE:O	1:C:1388:THR:OG1	2.18	0.61
1:B:144:GLU:OE2	1:B:211:ASN:ND2	2.33	0.61
1:A:2163:GLU:O	1:B:2545:ARG:NH1	2.34	0.61
1:A:1385:ILE:O	1:A:1388:THR:OG1	2.15	0.61
1:A:485:ASP:OD2	1:A:500:LYS:NZ	2.35	0.60
1:A:1254:LEU:O	1:A:1285:HIS:NE2	2.35	0.59
1:A:1243:GLN:OE1	1:A:1271:ASN:ND2	2.36	0.59
1:D:1350:LYS:O	1:D:1353:ARG:NH1	2.37	0.58
1:B:892:ILE:HG21	1:B:1058:VAL:HG13	1.85	0.58
1:C:2010:SER:O	1:C:2014:GLU:N	2.35	0.58
1:B:1735:LYS:NZ	1:B:1739:ASP:OD2	2.36	0.58
1:C:1890:ASN:OD1	1:C:1893:ARG:NH2	2.36	0.58
1:D:2123:GLN:OE1	1:D:2135:GLN:NE2	2.37	0.57
1:B:1890:ASN:OD1	1:B:1893:ARG:NH2	2.36	0.57
1:D:1945:THR:O	1:D:1949:GLN:N	2.37	0.57
1:A:1490:ALA:O	1:A:1494:LYS:N	2.38	0.57
1:B:195:HIS:ND1	1:B:196:ALA:O	2.37	0.57
1:C:2367:ARG:NE	1:D:2352:GLU:OE2	2.37	0.57
1:C:626:ARG:NH2	1:C:663:ASP:OD2	2.37	0.57
1:C:656:VAL:HG13	1:C:657:LEU:HD22	1.87	0.57
1:D:2523:LEU:O	1:D:2527:LYS:N	2.38	0.57
1:C:314:TYR:N	1:C:357:VAL:O	2.38	0.57
1:C:389:LEU:HB2	1:C:398:ILE:HD12	1.86	0.57
1:B:163:PHE:N	1:B:186:ASN:O	2.35	0.56
1:B:1889:GLN:NE2	1:B:1946:GLU:O	2.38	0.56
1:B:656:VAL:HG13	1:B:657:LEU:HD22	1.87	0.56
1:D:1937:VAL:O	1:D:1940:THR:OG1	2.21	0.56
1:D:1782:SER:OG	1:D:1897:ASN:OD1	2.21	0.56
1:D:1178:ARG:O	1:D:1182:MET:N	2.39	0.56
1:B:1391:LEU:O	1:B:1421:TYR:OH	2.24	0.55
1:A:1890:ASN:OD1	1:A:1893:ARG:NH2	2.39	0.55
1:C:1397:VAL:O	1:C:1401:THR:OG1	2.17	0.55
1:D:640:SER:O	1:D:643:ILE:N	2.39	0.55
1:D:1951:PRO:O	1:D:1956:GLN:NE2	2.40	0.55
1:A:1391:LEU:O	1:A:1421:TYR:OH	2.24	0.55
1:B:1893:ARG:NH1	1:B:1955:ASN:OD1	2.39	0.55
1:D:1764:GLY:O	1:D:1883:ASN:ND2	2.39	0.55
1:C:886:ARG:NH1	1:C:1047:VAL:O	2.40	0.55
1:A:1787:LYS:NZ	1:A:1791:ASP:OD2	2.40	0.55
1:D:27:SER:OG	1:D:54:ASP:OD2	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2123:GLN:OE1	1:A:2135:GLN:NE2	2.41	0.54
1:C:1085:ARG:NH1	1:C:1613:GLU:OE2	2.40	0.54
1:C:1087:GLU:O	1:C:1091:THR:OG1	2.18	0.54
1:C:1103:ASP:OD2	1:C:1192:LYS:NZ	2.39	0.54
1:A:171:ARG:NH1	1:A:181:ASP:OD2	2.41	0.54
1:C:2523:LEU:O	1:C:2527:LYS:N	2.39	0.54
1:A:1783:GLU:OE1	1:A:1897:ASN:ND2	2.41	0.54
1:D:827:LYS:O	1:D:831:ALA:N	2.39	0.54
1:C:2360:LYS:O	1:C:2364:ARG:N	2.39	0.53
1:A:656:VAL:HG13	1:A:657:LEU:HD22	1.91	0.53
1:A:1956:GLN:NE2	1:A:2002:ALA:O	2.42	0.53
1:A:2524:ARG:NE	1:D:2518:ASP:OD2	2.43	0.52
1:C:1254:LEU:O	1:C:1285:HIS:NE2	2.43	0.52
1:D:1953:HIS:NE2	1:D:2006:SER:O	2.43	0.52
1:A:2184:TRP:O	1:A:2188:LEU:N	2.43	0.51
1:A:664:ILE:O	1:A:728:TYR:OH	2.20	0.51
1:B:1319:ASP:OD1	1:B:1380:ASN:ND2	2.44	0.51
1:C:2006:SER:OG	1:C:2134:GLU:OE1	2.22	0.51
1:D:1889:GLN:NE2	1:D:1946:GLU:O	2.44	0.51
1:C:1103:ASP:O	1:C:1107:TYR:N	2.42	0.51
1:D:391:HIS:O	1:D:395:ASN:N	2.43	0.50
1:A:568:ARG:NH2	3:A:2702:I3P:O11	2.45	0.50
1:B:663:ASP:OD1	1:B:697:THR:OG1	2.13	0.50
1:D:2003:LEU:O	1:D:2012:ASN:ND2	2.44	0.50
1:A:1103:ASP:OD2	1:A:1192:LYS:NZ	2.44	0.50
1:C:314:TYR:O	1:C:357:VAL:N	2.45	0.50
1:C:1747:GLU:OE1	1:C:1792:ARG:NH1	2.45	0.50
1:A:1981:LEU:O	1:A:1985:ARG:N	2.43	0.50
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.44	0.50
1:B:104:ASN:OD1	1:B:105:ASP:N	2.44	0.49
1:B:1103:ASP:O	1:B:1107:TYR:N	2.46	0.49
1:D:2006:SER:OG	1:D:2134:GLU:OE1	2.20	0.49
1:D:730:ARG:NH2	1:D:772:ASP:OD2	2.45	0.49
1:C:482:PHE:O	1:C:505:ARG:NH1	2.46	0.49
1:D:1928:TYR:O	1:D:1933:ASN:ND2	2.45	0.49
1:C:563:SER:O	1:C:570:ASN:ND2	2.46	0.49
1:B:153:ASP:OD2	1:B:156:GLY:N	2.43	0.49
1:D:2401:ARG:NE	1:D:2449:ASP:OD2	2.45	0.49
1:B:1046:GLU:OE2	1:B:1052:GLY:N	2.45	0.49
1:C:58:LYS:N	1:C:125:LEU:O	2.45	0.48
1:D:1965:ASN:OD1	1:D:2015:ARG:NH2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2047:ARG:O	1:A:2051:HIS:ND1	2.46	0.48
1:C:118:TYR:OH	1:C:181:ASP:OD2	2.31	0.48
1:D:719:ASN:ND2	1:D:722:ASP:OD2	2.45	0.48
1:D:1280:GLU:OE2	1:D:1284:GLN:NE2	2.46	0.48
1:D:1878:GLN:OE1	1:D:1939:GLN:NE2	2.43	0.48
1:D:485:ASP:OD2	1:D:500:LYS:NZ	2.43	0.48
1:D:872:TYR:OH	1:D:973:GLU:O	2.31	0.48
1:D:557:TYR:OH	1:D:584:GLN:OE1	2.32	0.48
1:D:1932:ASP:OD1	1:D:1933:ASN:N	2.47	0.48
1:B:1337:ASN:OD1	1:B:1338:ASP:N	2.46	0.48
1:C:1223:GLU:OE1	1:C:1226:ARG:NH2	2.46	0.48
1:A:2518:ASP:OD2	1:B:2524:ARG:NE	2.45	0.48
1:C:1932:ASP:OD1	1:C:1933:ASN:N	2.47	0.48
1:B:1081:HIS:O	1:B:1084:GLN:NE2	2.46	0.47
1:C:352:TYR:O	1:C:419:THR:OG1	2.27	0.47
1:C:12:ASP:OD1	1:C:13:ILE:N	2.48	0.47
1:D:104:ASN:OD1	1:D:105:ASP:N	2.47	0.47
1:A:1337:ASN:OD1	1:A:1338:ASP:N	2.47	0.47
1:B:255:ASP:OD1	1:B:256:GLU:N	2.48	0.47
1:B:1397:VAL:O	1:B:1401:THR:OG1	2.16	0.47
1:D:17:TYR:O	1:D:220:LYS:N	2.47	0.47
1:B:314:TYR:N	1:B:357:VAL:O	2.45	0.47
1:B:2047:ARG:O	1:B:2051:HIS:ND1	2.44	0.47
1:D:114:ASP:OD1	1:D:115:VAL:N	2.47	0.47
1:B:434:VAL:HG11	1:B:439:ILE:HD11	1.97	0.46
1:C:892:ILE:HG21	1:C:1058:VAL:HG13	1.96	0.46
1:C:988:SER:O	1:C:992:SER:OG	2.31	0.46
1:C:2007:ARG:O	1:C:2062:ARG:NH2	2.48	0.46
1:D:758:ASP:OD1	1:D:759:LEU:N	2.48	0.46
1:D:1048:ASP:OD1	1:D:1049:ASP:N	2.48	0.46
1:B:305:ARG:NE	1:B:360:GLY:O	2.48	0.46
1:B:1930:ASN:OD1	1:B:1931:GLU:N	2.49	0.46
1:A:1893:ARG:NH1	1:A:1955:ASN:OD1	2.48	0.46
1:A:2326:TYR:O	1:A:2329:THR:OG1	2.32	0.46
1:B:543:ASP:OD2	1:B:545:LYS:NZ	2.49	0.46
1:B:114:ASP:OD1	1:B:115:VAL:N	2.47	0.46
1:B:758:ASP:OD1	1:B:759:LEU:N	2.49	0.46
1:C:758:ASP:OD1	1:C:759:LEU:N	2.49	0.46
1:B:1048:ASP:OD1	1:B:1049:ASP:N	2.49	0.46
1:C:466:GLN:OE1	1:C:469:ARG:NH2	2.48	0.46
1:A:66:SER:N	1:A:100:GLU:OE2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:O	1:B:184:ILE:N	2.45	0.46
1:A:104:ASN:OD1	1:A:105:ASP:N	2.49	0.45
1:A:239:ASP:OD1	1:A:240:VAL:N	2.49	0.45
1:A:255:ASP:OD1	1:A:256:GLU:N	2.47	0.45
1:C:1337:ASN:OD1	1:C:1338:ASP:N	2.49	0.45
1:A:114:ASP:OD1	1:A:115:VAL:N	2.49	0.45
1:A:1048:ASP:OD1	1:A:1049:ASP:N	2.49	0.45
1:B:371:PRO:O	1:B:388:ARG:NH1	2.50	0.45
1:C:1048:ASP:OD1	1:C:1049:ASP:N	2.49	0.45
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.47	0.45
1:A:2036:GLU:OE2	1:A:2047:ARG:NH2	2.49	0.45
1:B:1981:LEU:O	1:B:1985:ARG:N	2.47	0.45
1:C:132:TYR:N	1:C:153:ASP:O	2.50	0.45
1:D:305:ARG:NE	1:D:360:GLY:O	2.49	0.45
1:A:32:VAL:HG12	1:A:32:VAL:O	2.17	0.45
1:B:132:TYR:N	1:B:153:ASP:O	2.50	0.45
1:D:882:LEU:O	1:D:885:THR:OG1	2.25	0.45
1:A:1109:VAL:O	1:A:1113:GLU:N	2.49	0.45
1:C:1889:GLN:NE2	1:C:1946:GLU:O	2.50	0.45
1:A:494:LEU:O	1:A:558:ARG:NH2	2.50	0.45
1:A:1932:ASP:OD1	1:A:1933:ASN:N	2.50	0.45
1:C:1319:ASP:OD1	1:C:1380:ASN:ND2	2.49	0.45
1:D:32:VAL:HG12	1:D:32:VAL:O	2.17	0.45
1:B:2151:THR:HG23	1:B:2154:ARG:HH21	1.82	0.45
1:D:2058:LEU:O	1:D:2061:SER:OG	2.28	0.45
1:B:1887:ASP:O	1:B:1891:PHE:N	2.49	0.44
1:C:764:MET:O	1:C:774:ARG:NH2	2.49	0.44
1:C:1391:LEU:O	1:C:1421:TYR:OH	2.35	0.44
1:A:141:ALA:N	1:A:147:ALA:O	2.47	0.44
1:C:141:ALA:N	1:C:147:ALA:O	2.44	0.44
1:B:239:ASP:OD1	1:B:240:VAL:N	2.50	0.44
1:D:1783:GLU:OE1	1:D:1899:THR:OG1	2.34	0.44
1:A:758:ASP:OD1	1:A:759:LEU:N	2.50	0.44
1:A:1894:CYS:SG	1:A:1900:ASN:ND2	2.91	0.44
1:C:164:ILE:HG23	1:C:164:ILE:O	2.17	0.44
1:C:1033:GLU:OE2	1:C:1085:ARG:NH2	2.51	0.44
1:C:1523:ARG:O	1:C:1527:SER:N	2.49	0.44
1:A:1897:ASN:OD1	1:A:1898:LYS:N	2.51	0.44
1:C:1981:LEU:O	1:C:1985:ARG:N	2.46	0.44
1:B:141:ALA:N	1:B:147:ALA:O	2.48	0.44
1:A:2515:VAL:O	1:A:2519:THR:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HG12	1:B:32:VAL:O	2.16	0.44
1:C:44:ASP:OD1	1:C:45:LEU:N	2.50	0.44
1:C:1891:PHE:O	1:C:1895:GLN:NE2	2.50	0.44
1:D:1681:ASP:OD1	1:D:1682:ARG:N	2.51	0.44
1:A:1735:LYS:NZ	1:A:1739:ASP:OD2	2.51	0.44
1:A:1749:ILE:O	1:A:1753:SER:N	2.50	0.44
1:B:632:ASP:O	1:B:635:SER:OG	2.22	0.44
1:B:1115:ASP:OD1	1:B:1116:ARG:N	2.50	0.44
1:D:1736:LEU:O	1:D:1740:LEU:N	2.46	0.44
1:D:2296:PHE:O	1:D:2300:PHE:N	2.48	0.44
1:D:2552:THR:HG23	1:D:2553:VAL:HG13	2.00	0.44
1:C:126:HIS:O	1:C:130:ASN:N	2.47	0.44
1:D:494:LEU:O	1:D:558:ARG:NH2	2.51	0.44
1:B:485:ASP:OD2	1:B:500:LYS:NZ	2.50	0.43
1:C:2218:ILE:HG21	1:C:2282:LEU:HD21	2.00	0.43
1:B:1932:ASP:OD1	1:B:1933:ASN:N	2.52	0.43
1:D:2590:VAL:O	1:D:2593:MET:N	2.51	0.43
1:A:666:ILE:HG22	1:A:732:GLN:HG2	2.01	0.43
1:C:1115:ASP:OD1	1:C:1116:ARG:N	2.52	0.43
1:C:1930:ASN:OD1	1:C:1931:GLU:N	2.52	0.43
1:D:239:ASP:OD1	1:D:240:VAL:N	2.50	0.43
1:D:1290:LEU:HD23	1:D:1332:VAL:HG13	2.00	0.43
1:B:1970:ILE:HG21	1:B:2000:LEU:HD21	2.00	0.43
1:D:255:ASP:OD1	1:D:256:GLU:N	2.49	0.43
1:A:2538:CYS:SG	1:A:2539:PHE:N	2.92	0.43
1:B:593:ASP:OD1	1:B:633:TYR:OH	2.19	0.43
1:B:2006:SER:OG	1:B:2134:GLU:OE1	2.30	0.43
1:C:1740:LEU:O	1:C:1744:THR:HG22	2.18	0.43
1:A:2523:LEU:O	1:A:2527:LYS:N	2.48	0.43
1:A:1053:ARG:NH2	1:A:1627:LEU:O	2.52	0.43
1:A:67:ALA:N	1:A:100:GLU:OE1	2.50	0.43
1:A:1987:ASP:OD1	1:A:1988:LEU:N	2.52	0.43
1:B:843:ASN:O	1:B:846:SER:OG	2.32	0.43
1:C:239:ASP:OD1	1:C:240:VAL:N	2.53	0.42
1:D:1068:ALA:HB3	1:D:1069:PRO:HD3	2.00	0.42
1:A:872:TYR:OH	1:A:973:GLU:O	2.36	0.42
1:C:1897:ASN:OD1	1:C:1898:LYS:N	2.50	0.42
1:D:648:THR:HG22	1:D:652:ILE:HD12	2.01	0.42
1:A:1286:PHE:O	1:A:1290:LEU:N	2.50	0.42
1:A:1930:ASN:OD1	1:A:1931:GLU:N	2.51	0.42
1:D:2260:SER:OG	1:D:2261:ILE:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ASN:ND2	1:A:722:ASP:OD2	2.52	0.42
1:A:550:GLN:OE1	1:A:588:ASP:OD2	2.38	0.42
1:A:772:ASP:OD1	1:A:773:LEU:N	2.53	0.42
1:B:1897:ASN:OD1	1:B:1898:LYS:N	2.52	0.42
1:D:968:LYS:HA	1:D:971:ILE:HD12	2.00	0.42
1:C:1937:VAL:O	1:C:1940:THR:OG1	2.29	0.42
1:A:1945:THR:O	1:A:1949:GLN:N	2.45	0.41
1:C:192:GLN:NE2	1:C:214:ASN:OD1	2.51	0.41
1:C:480:VAL:HG12	1:C:496:ILE:HD11	2.02	0.41
1:A:593:ASP:OD1	1:A:633:TYR:OH	2.23	0.41
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.46	0.41
1:B:550:GLN:OE1	1:B:588:ASP:OD2	2.38	0.41
1:B:197:SER:OG	1:B:209:GLU:O	2.27	0.41
1:B:1053:ARG:NH2	1:B:1627:LEU:O	2.53	0.41
1:B:2523:LEU:O	1:B:2527:LYS:N	2.49	0.41
1:D:2012:ASN:O	1:D:2016:ILE:HD12	2.21	0.41
1:B:2053:ILE:O	1:B:2057:ALA:N	2.51	0.41
1:C:2401:ARG:NE	1:C:2449:ASP:OD2	2.53	0.41
1:D:2498:LEU:HD12	1:D:2502:PHE:HE2	1.85	0.41
1:A:133:LEU:HA	1:A:152:LEU:HD23	2.02	0.41
1:B:1949:GLN:NE2	1:B:2583:TYR:O	2.54	0.41
1:C:494:LEU:HD21	1:C:554:ARG:HB3	2.02	0.41
1:C:1043:SER:OG	1:C:1044:MET:N	2.53	0.41
1:C:1749:ILE:O	1:C:1753:SER:N	2.53	0.41
1:D:318:GLU:O	1:D:353:CYS:N	2.54	0.41
1:A:111:VAL:O	1:A:111:VAL:HG12	2.21	0.41
1:A:245:HIS:N	1:A:250:LYS:O	2.54	0.41
1:C:871:ILE:HD13	1:C:974:ILE:HG23	2.03	0.41
1:D:144:GLU:OE2	1:D:211:ASN:ND2	2.48	0.41
1:D:1225:LEU:O	1:D:1228:THR:OG1	2.28	0.41
1:A:28:THR:N	1:A:54:ASP:OD2	2.54	0.40
1:A:2006:SER:OG	1:A:2134:GLU:OE1	2.28	0.40
1:C:1930:ASN:N	1:C:1933:ASN:OD1	2.50	0.40
1:B:772:ASP:OD1	1:B:773:LEU:N	2.54	0.40
1:D:2237:TRP:O	1:D:2241:CYS:N	2.51	0.40
1:B:2007:ARG:O	1:B:2062:ARG:NH2	2.54	0.40
1:C:2148:THR:HG1	1:C:2151:THR:HG1	1.67	0.40
1:C:2192:PRO:O	1:C:2196:TRP:N	2.51	0.40
1:B:1891:PHE:O	1:B:1895:GLN:NE2	2.55	0.40
1:B:2204:TRP:CE2	1:B:2295:VAL:HG11	2.57	0.40
1:C:772:ASP:OD1	1:C:773:LEU:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:ALA:HB3	1:A:1312:LYS:O	2.21	0.40
1:C:882:LEU:O	1:C:885:THR:OG1	2.29	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	2148/2671 (80%)	2067 (96%)	81 (4%)	0	100	100
1	B	2148/2671 (80%)	2067 (96%)	81 (4%)	0	100	100
1	C	2153/2671 (81%)	2070 (96%)	83 (4%)	0	100	100
1	D	2139/2671 (80%)	2063 (96%)	76 (4%)	0	100	100
All	All	8588/10684 (80%)	8267 (96%)	321 (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	1924/2385 (81%)	1919 (100%)	5 (0%)	91	91
1	B	1924/2385 (81%)	1919 (100%)	5 (0%)	91	91
1	C	1928/2385 (81%)	1924 (100%)	4 (0%)	92	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	1875/2385 (79%)	1870 (100%)	5 (0%)	91	91
All	All	7651/9540 (80%)	7632 (100%)	19 (0%)	91	93

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

Mol	Chain	Res	Type
1	A	171	ARG
1	A	625	ASN
1	A	2064	ASN
1	A	2289	ASN
1	A	2471	ARG
1	B	171	ARG
1	B	1106	ASN
1	B	2064	ASN
1	B	2289	ASN
1	B	2471	ARG
1	C	390	ARG
1	C	2064	ASN
1	C	2289	ASN
1	C	2471	ARG
1	D	171	ARG
1	D	1897	ASN
1	D	1976	ASN
1	D	2289	ASN
1	D	2471	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	2702	-	24,24,24	1.32	3 (12%)	39,39,39	0.81	1 (2%)
3	I3P	D	2702	-	24,24,24	1.34	3 (12%)	39,39,39	0.83	2 (5%)
3	I3P	A	2702	-	24,24,24	1.30	3 (12%)	39,39,39	0.83	2 (5%)
3	I3P	C	2702	-	24,24,24	1.33	3 (12%)	39,39,39	0.87	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	2702	-	-	1/15/39/39	0/1/1/1
3	I3P	D	2702	-	-	2/15/39/39	0/1/1/1
3	I3P	A	2702	-	-	0/15/39/39	0/1/1/1
3	I3P	C	2702	-	-	0/15/39/39	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2702	I3P	P4-O4	3.34	1.65	1.59
3	D	2702	I3P	P1-O1	3.27	1.65	1.59
3	C	2702	I3P	P1-O1	3.26	1.65	1.59
3	C	2702	I3P	P4-O4	3.23	1.65	1.59
3	A	2702	I3P	P1-O1	3.22	1.65	1.59
3	B	2702	I3P	P1-O1	3.22	1.65	1.59
3	B	2702	I3P	P4-O4	3.21	1.65	1.59
3	A	2702	I3P	P4-O4	3.17	1.65	1.59
3	C	2702	I3P	P5-O5	3.16	1.65	1.59
3	D	2702	I3P	P5-O5	3.11	1.65	1.59
3	B	2702	I3P	P5-O5	3.07	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2702	I3P	P5-O5	3.00	1.64	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2702	I3P	P5-O5-C5	-2.21	117.53	123.43
3	C	2702	I3P	C5-C6-C1	2.18	113.53	109.11
3	A	2702	I3P	P5-O5-C5	-2.15	117.69	123.43
3	B	2702	I3P	P5-O5-C5	-2.12	117.78	123.43
3	A	2702	I3P	P4-O4-C4	-2.09	117.86	123.43
3	D	2702	I3P	P1-O1-C1	-2.04	117.98	123.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

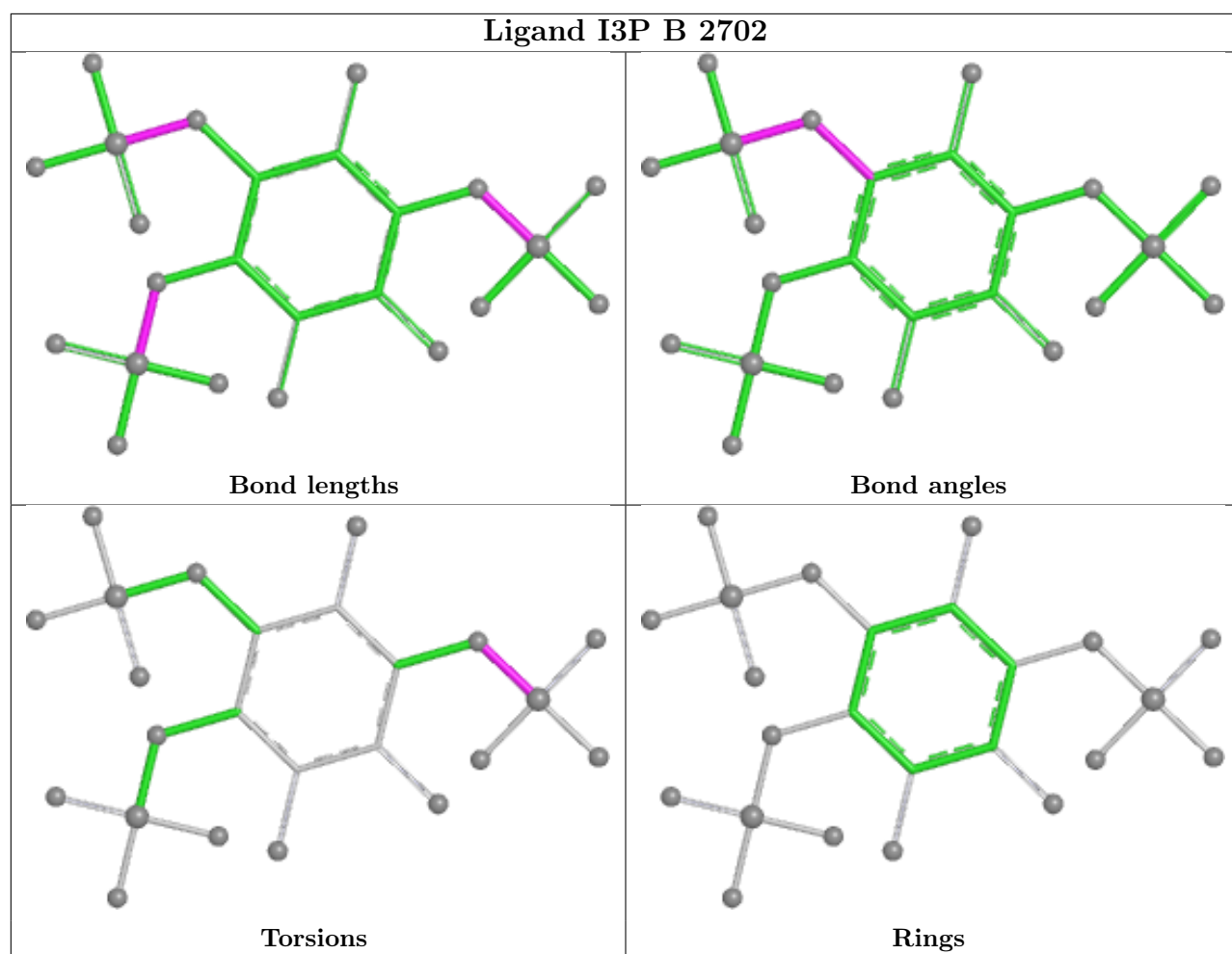
Mol	Chain	Res	Type	Atoms
3	D	2702	I3P	C4-O4-P4-O43
3	B	2702	I3P	C1-O1-P1-O11
3	D	2702	I3P	C3-C4-O4-P4

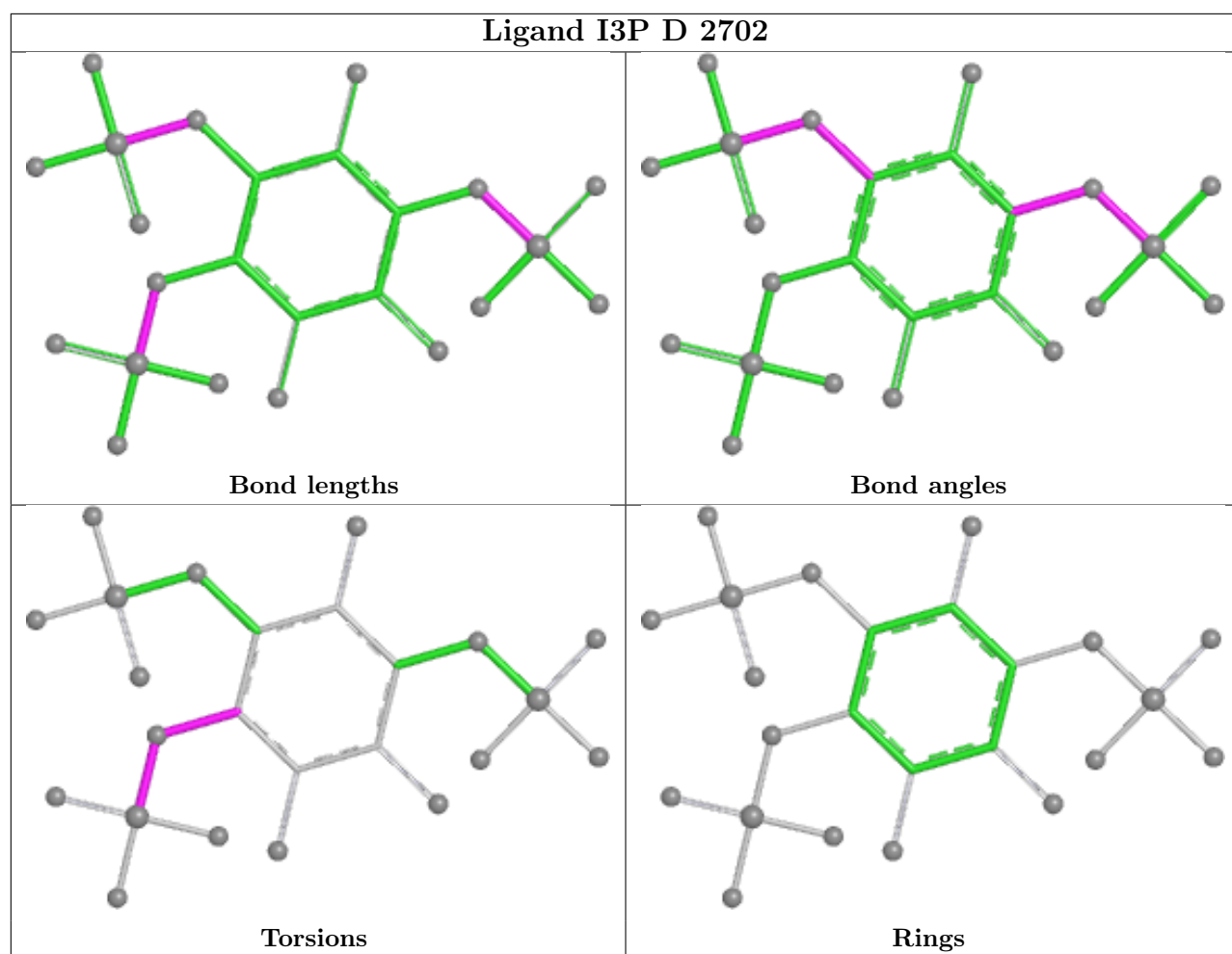
There are no ring outliers.

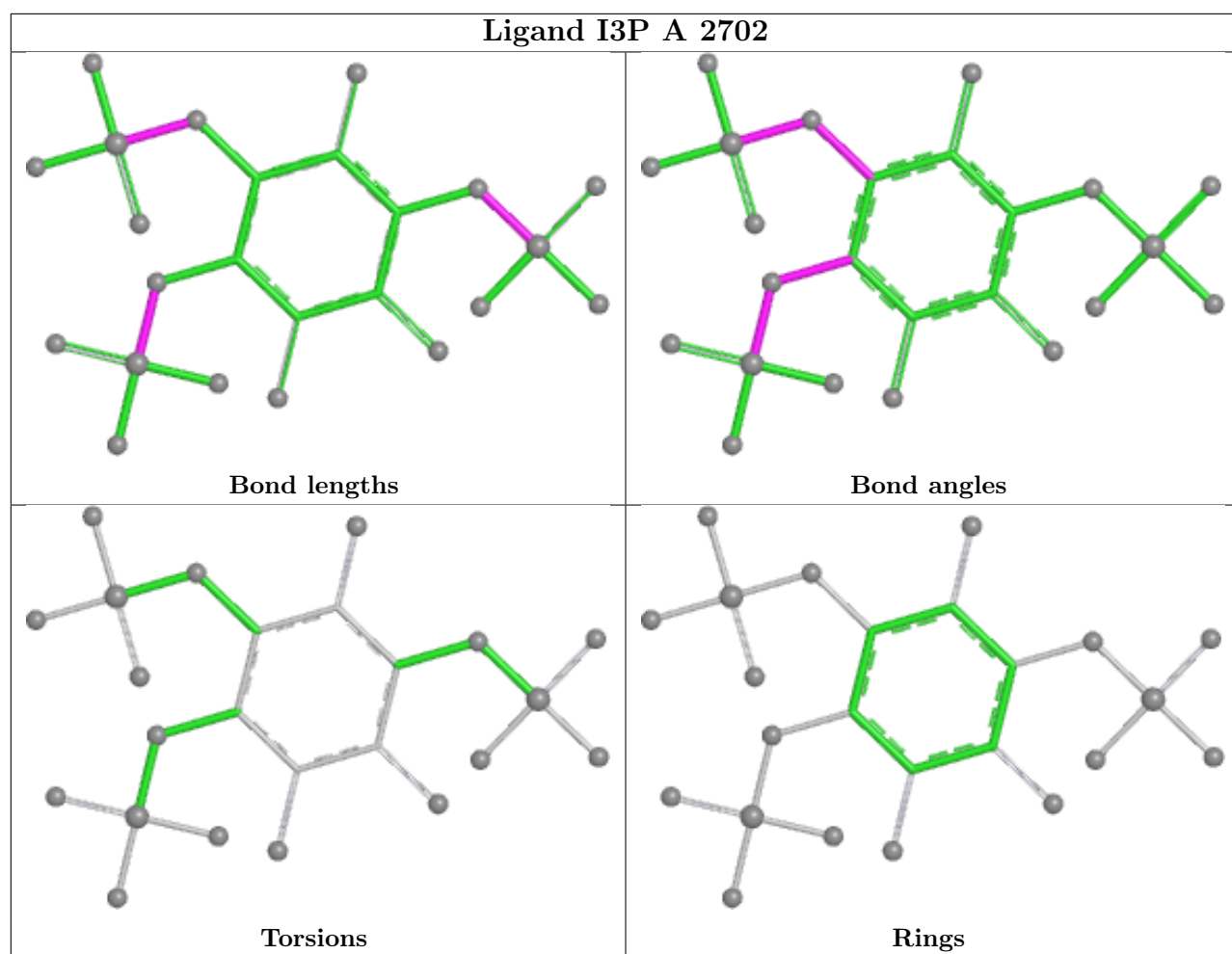
2 monomers are involved in 2 short contacts:

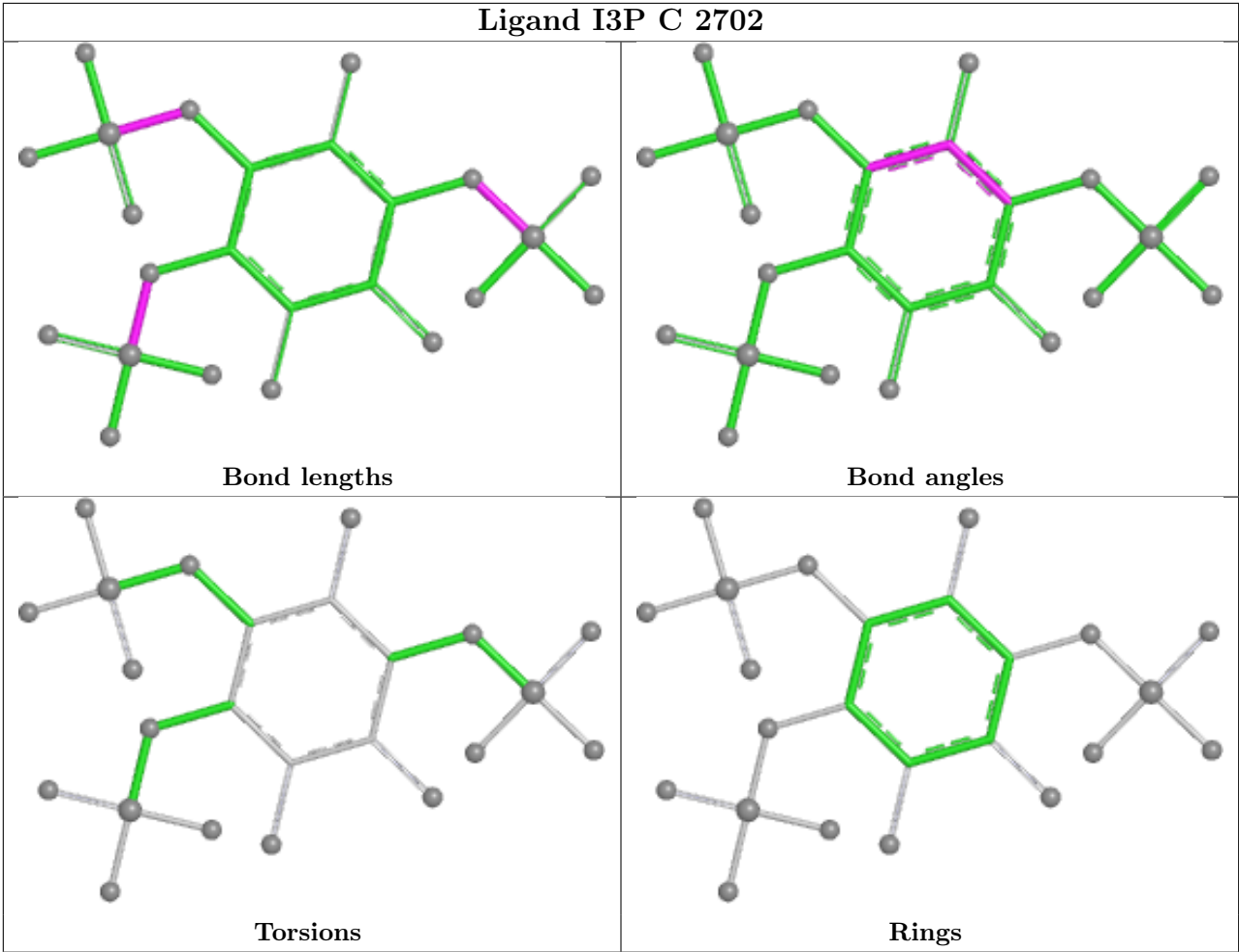
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2702	I3P	1	0
3	C	2702	I3P	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All 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	50.16

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1552:TRP	C	1587:ASP	N	50.02
1	C	1552:TRP	C	1587:ASP	N	48.78
1	B	1552:TRP	C	1587:ASP	N	48.53
1	D	1484:ARG	C	1490:ALA	N	15.83
1	A	1533:ARG	C	1541:ALA	N	15.74
1	B	1533:ARG	C	1541:ALA	N	15.65
1	D	1533:ARG	C	1541:ALA	N	15.40
1	C	1533:ARG	C	1541:ALA	N	14.97
1	D	1508:GLY	C	1515:ALA	N	7.98
1	C	2252:TYR	C	2260:SER	N	6.60
1	D	2252:TYR	C	2260:SER	N	6.26
1	A	2252:TYR	C	2260:SER	N	6.08
1	B	2252:TYR	C	2260:SER	N	5.65

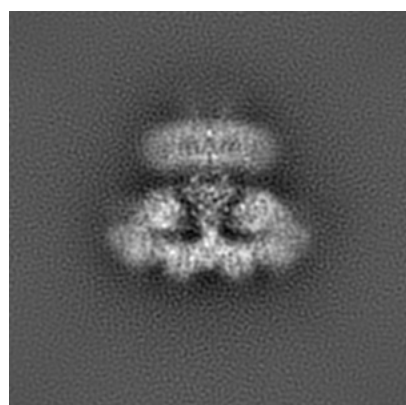
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7987. These allow visual inspection of the internal detail of the map and identification of artifacts.

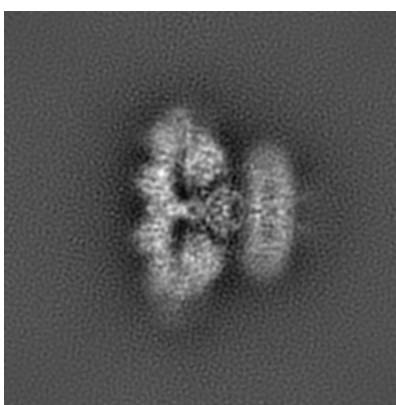
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

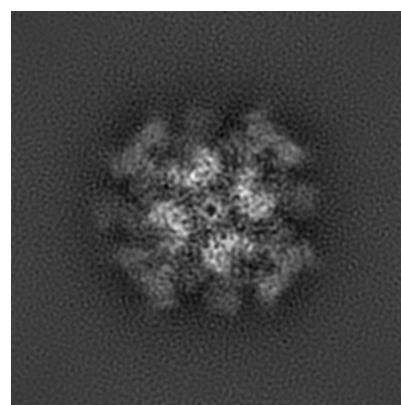
6.1.1 Primary map



X



Y

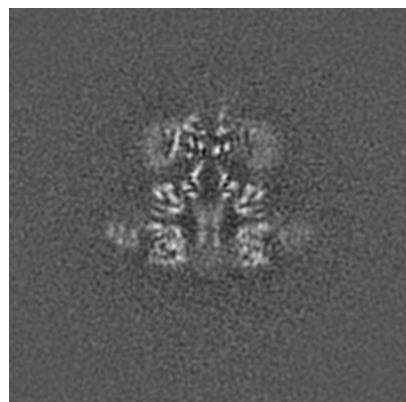


Z

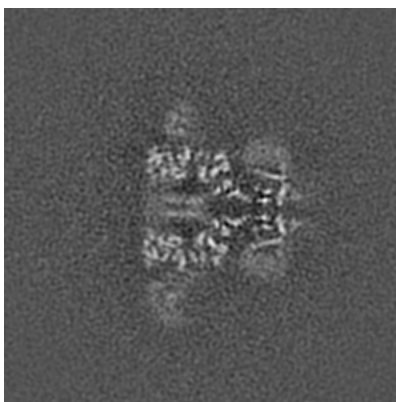
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

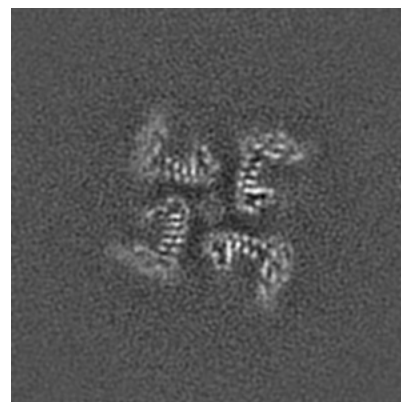
6.2.1 Primary map



X Index: 192



Y Index: 192

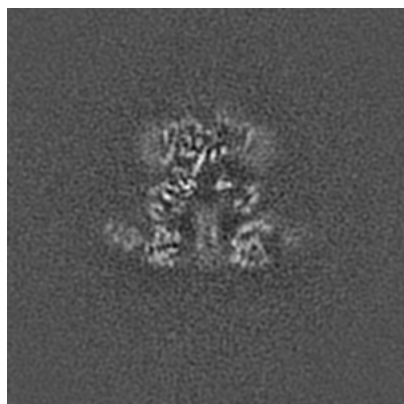


Z Index: 192

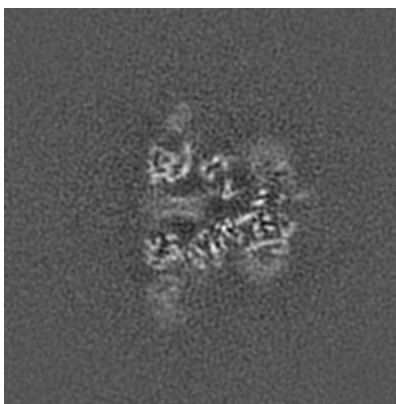
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

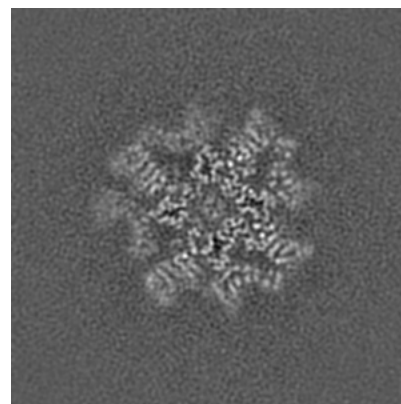
6.3.1 Primary map



X Index: 195



Y Index: 189

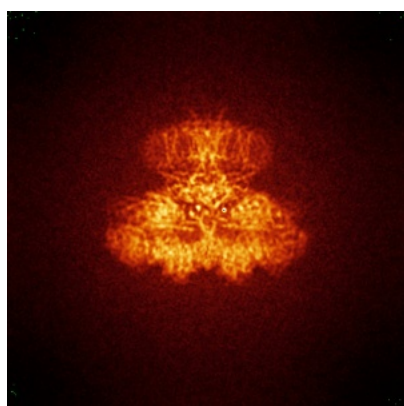


Z Index: 155

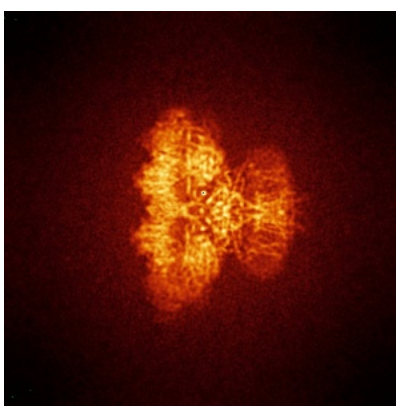
The images above show the largest variance slices of the map in three orthogonal directions.

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

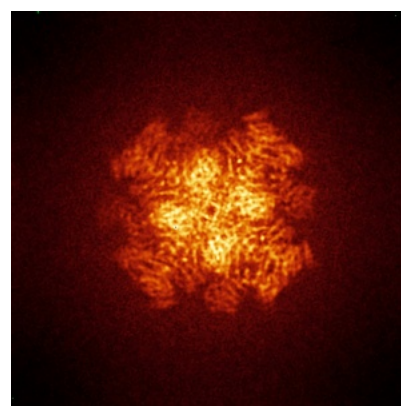
6.4.1 Primary map



X



Y

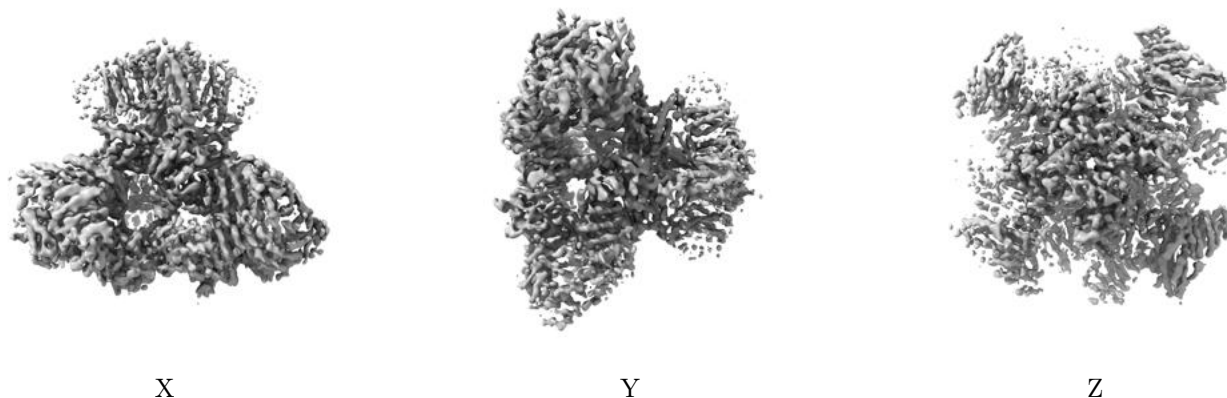


Z

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 3.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

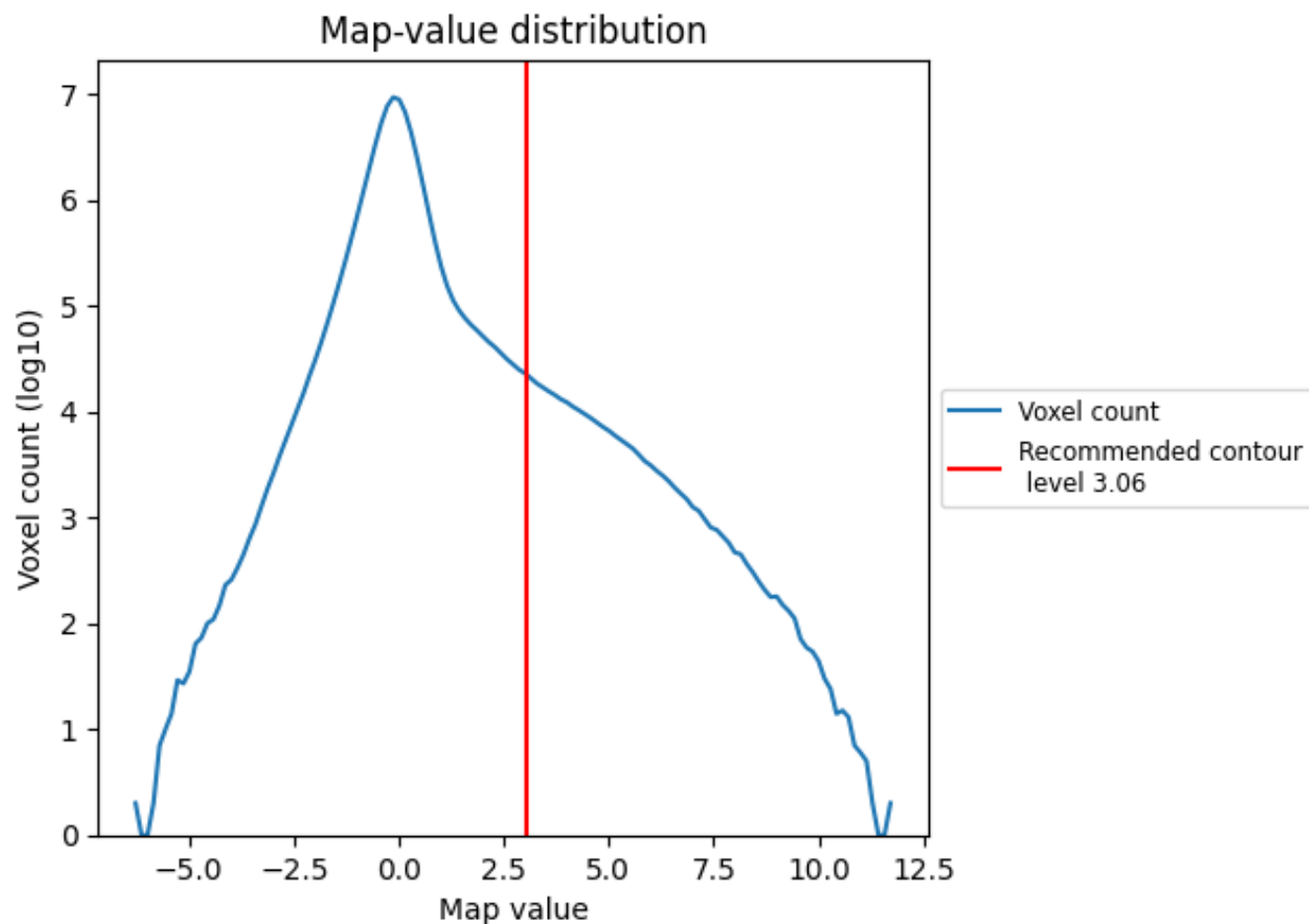
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

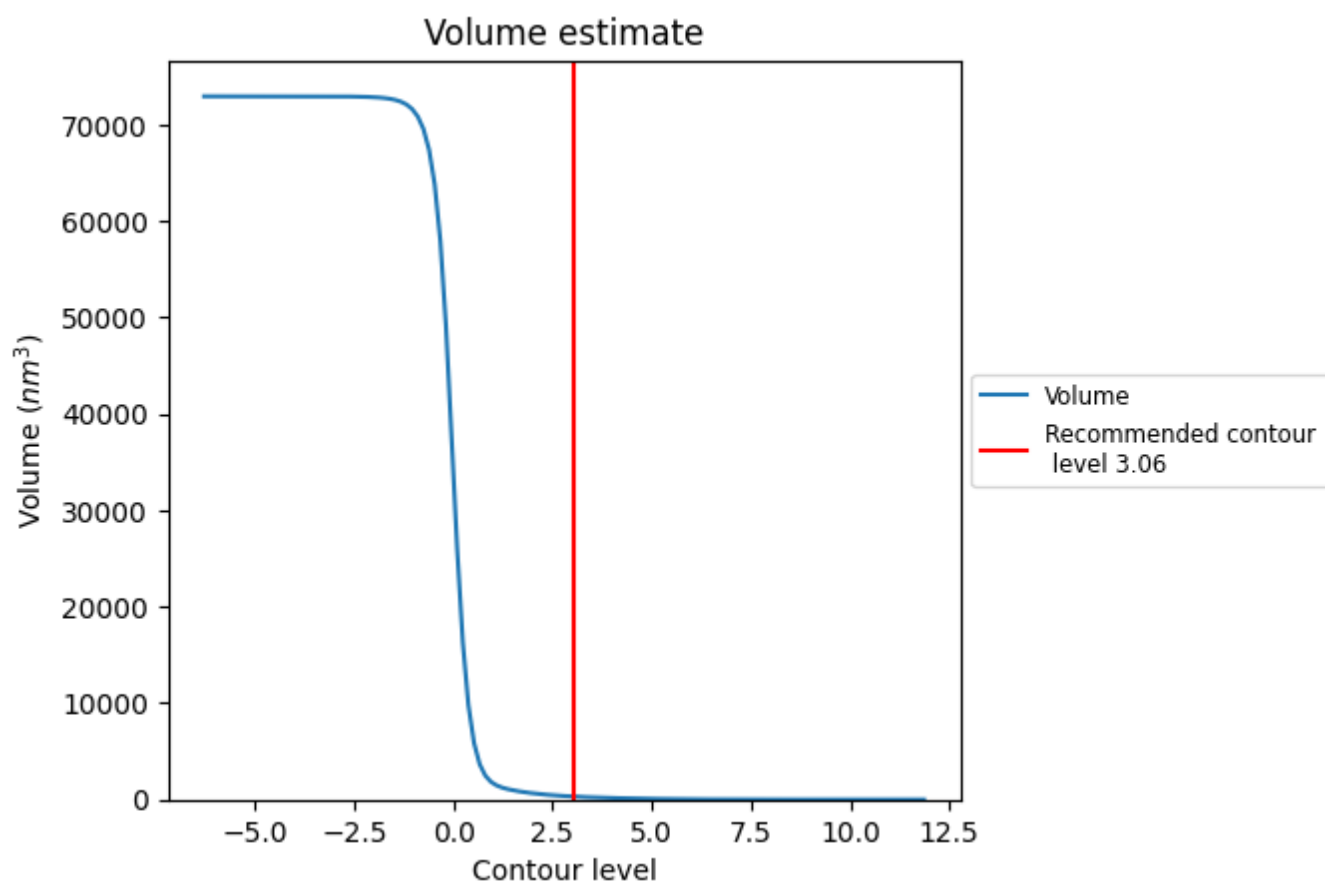
This section contains the results of statistical analysis of the map.

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.

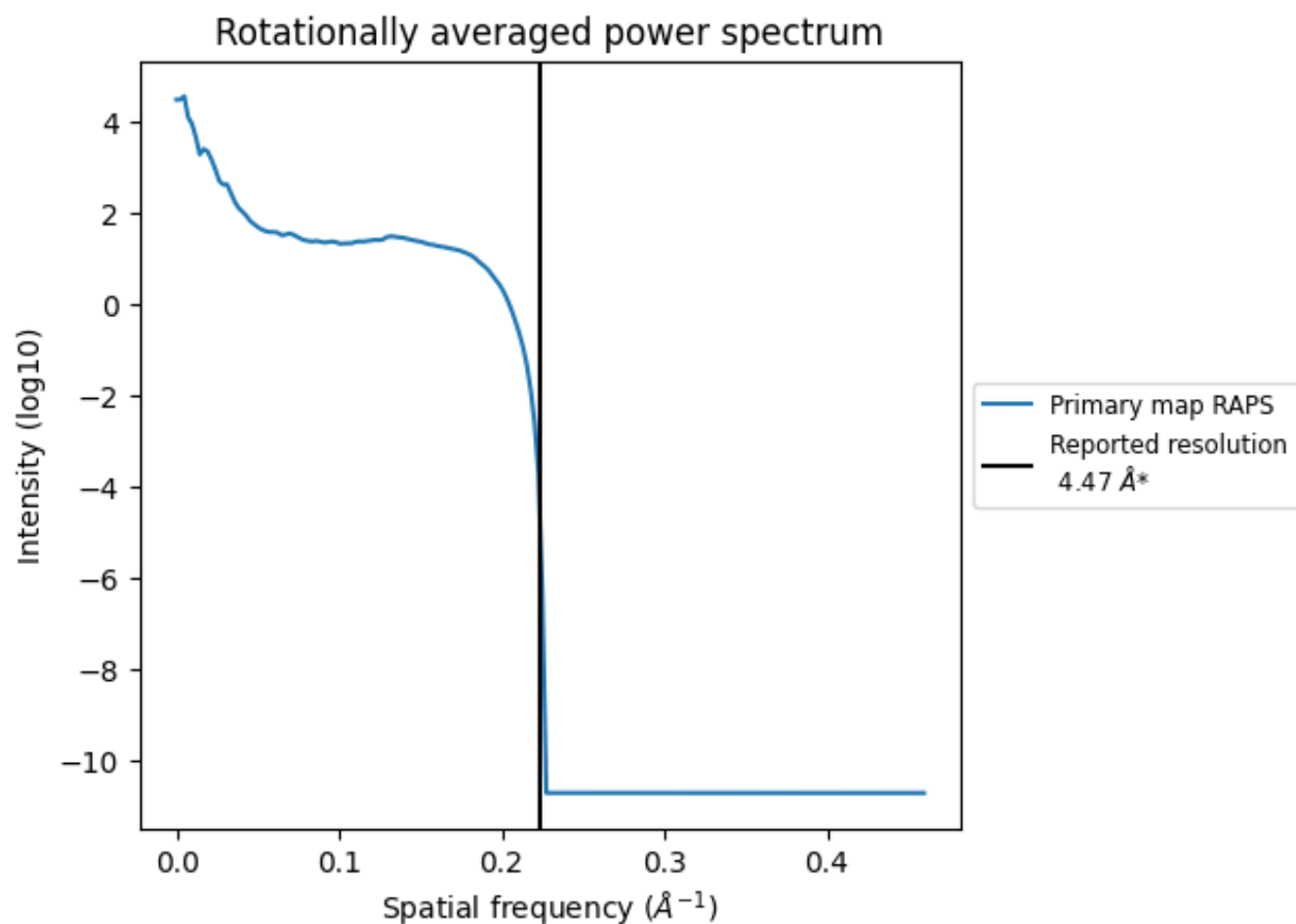
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm³; this corresponds to an approximate mass of 278 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.224 Å⁻¹

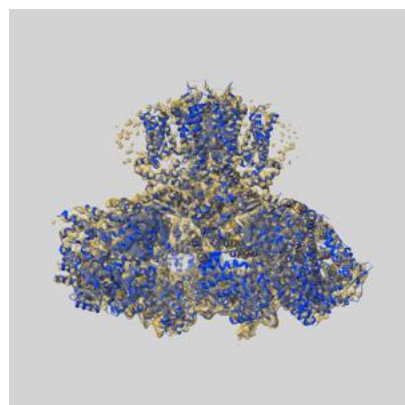
8 Fourier-Shell correlation ⓘ

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

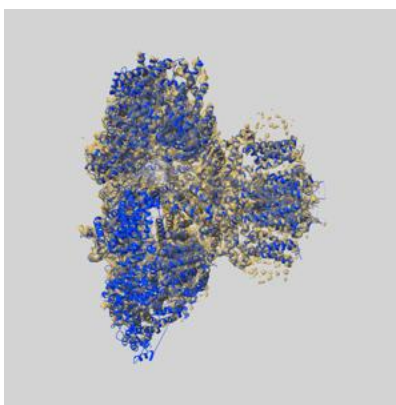
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7987 and PDB model 6DR0. Per-residue inclusion information can be found in section [3](#) on page [5](#).

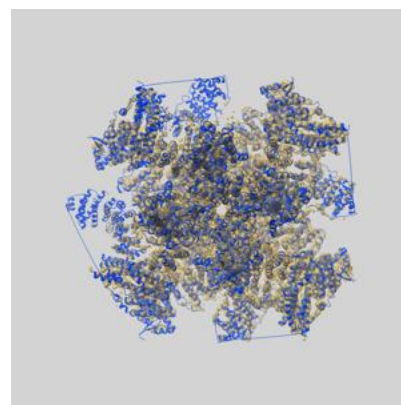
9.1 Map-model overlay [i](#)



X



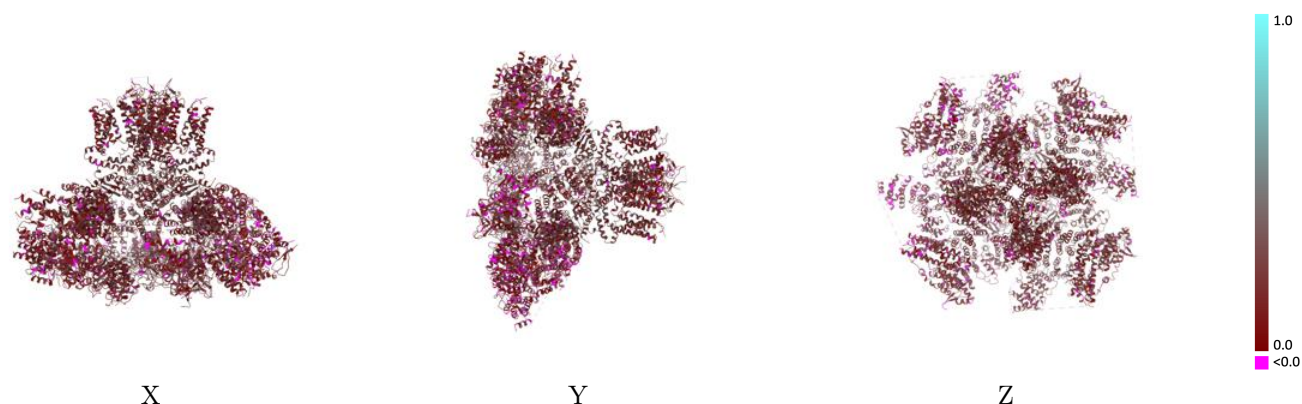
Y



Z

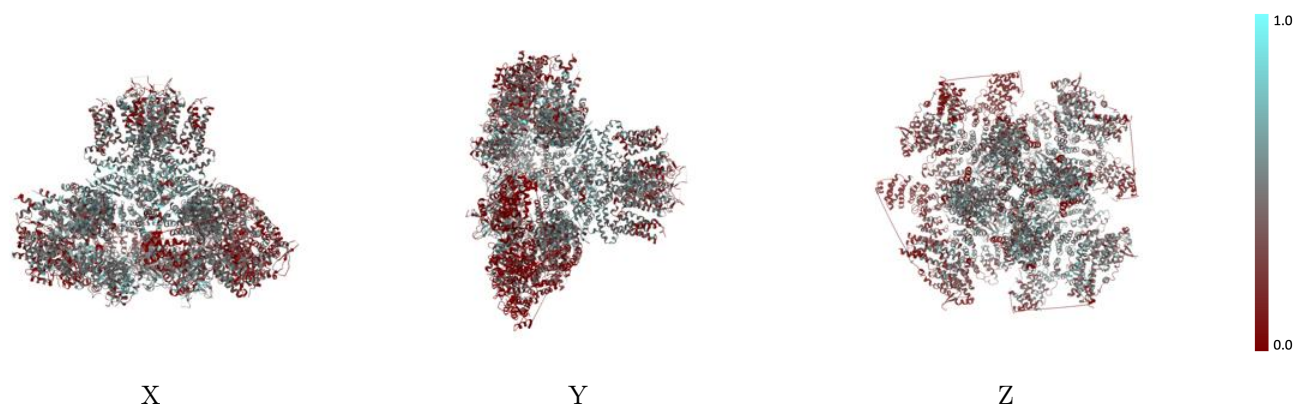
The images above show the 3D surface view of the map at the recommended contour level 3.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



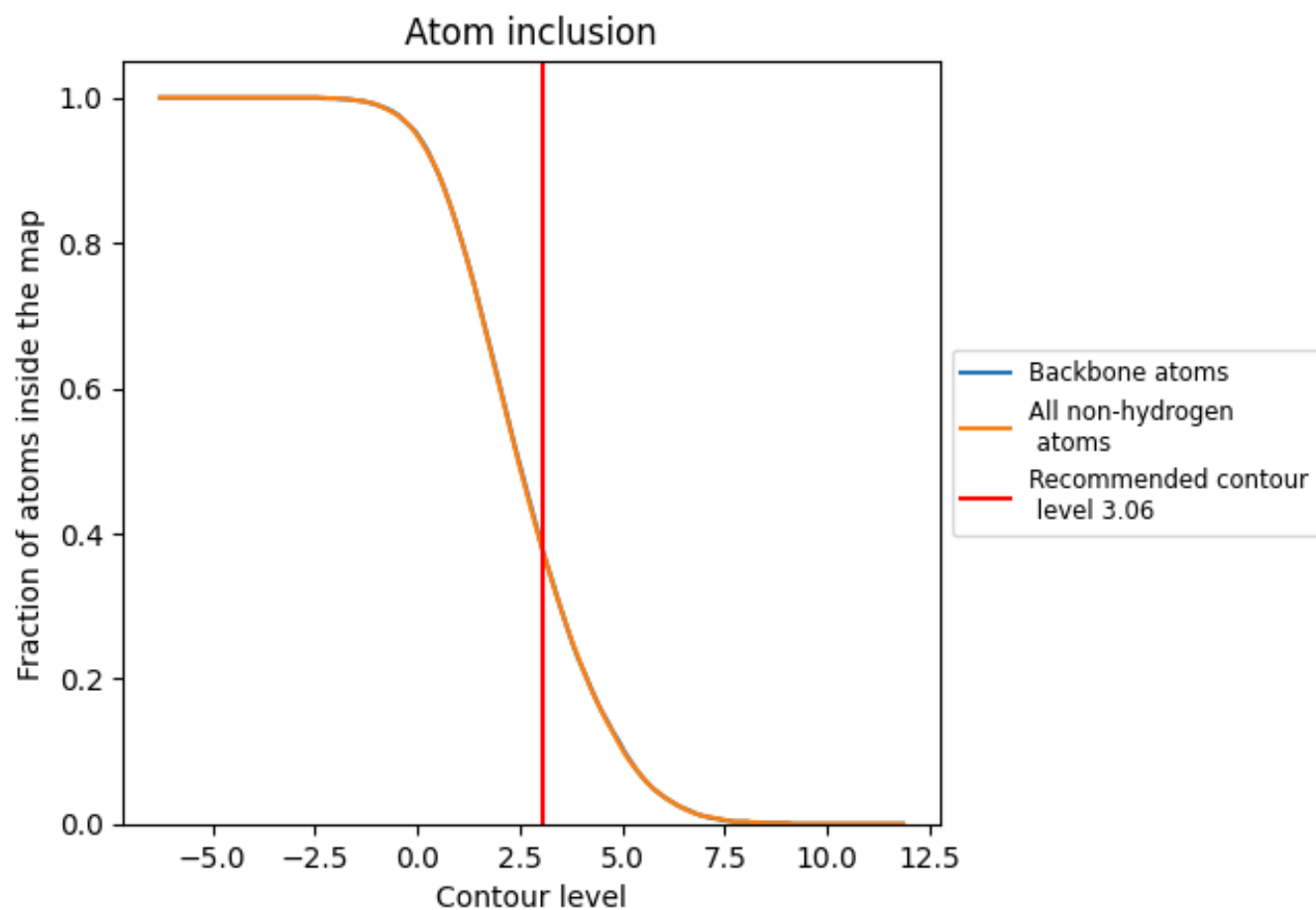
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3760	<div></div> 0.1920
A	<div></div> 0.4510	<div></div> 0.2070
B	<div></div> 0.4070	<div></div> 0.2020
C	<div></div> 0.3120	<div></div> 0.1760
D	<div></div> 0.3520	<div></div> 0.1850

