



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 05:30 PM EST

PDB ID : 6DQJ  
EMDB ID : EMD-7978  
Title : Human type 3 1,4,5-inositol trisphosphate receptor in a ligand-free state  
Authors : Hite, R.K.; Paknejad, N.  
Deposited on : 2018-06-11  
Resolution : 3.49 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](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:

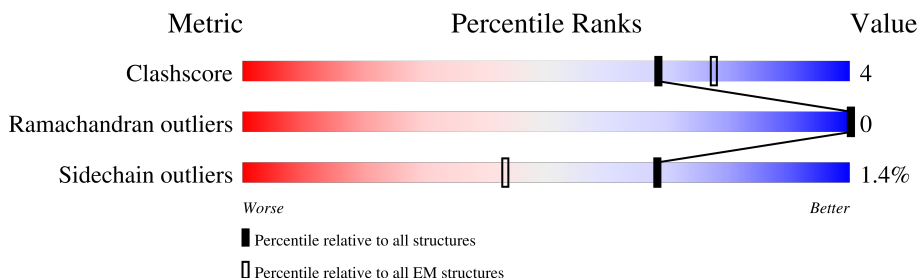
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 3.49 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  $\geq 3$ , 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	<p>68% 73% 9% 18%</p>
1	B	2671	<p>65% 72% 9% 18%</p>
1	C	2671	<p>65% 72% 9% 18%</p>
1	D	2671	<p>70% 73% 9% 18%</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 138477 atoms, of which 69265 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	2181	34618	11031	17316	2979	3188	104	0	0
1	B	2181	34619	11031	17317	2979	3188	104	0	0
1	C	2181	34618	11031	17316	2979	3188	104	0	0
1	D	2181	34618	11031	17316	2979	3188	104	0	0

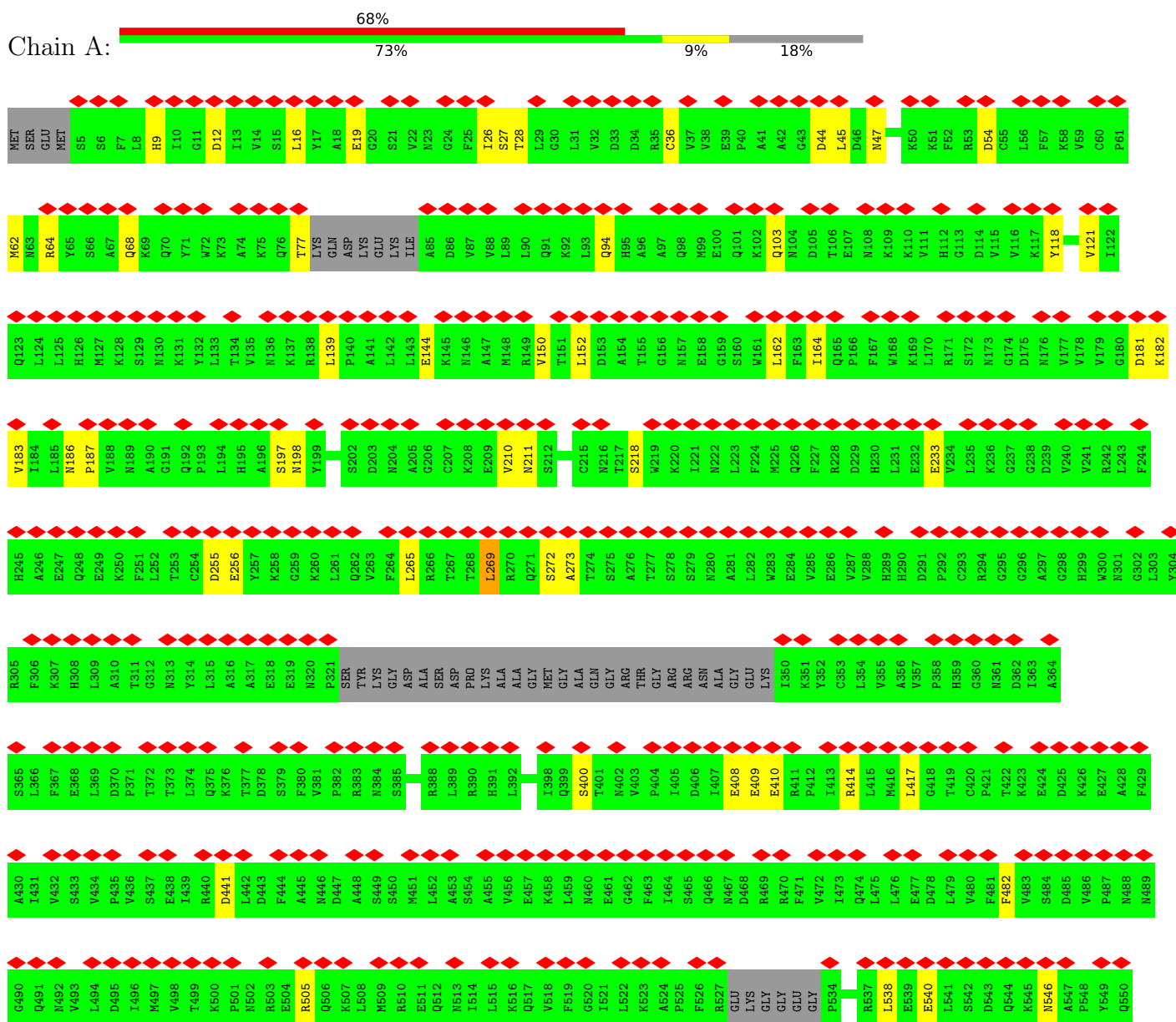
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

### 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



H561	M552	F553	R554	L555	C556	Y557	R558	V559	L560	R561	H562	E565	D566	Y567	R568	K569	M570	Q571	E572	H573	I574	A575	K576	Q577	F578	G579	M580	M581	Q582	S583	Q584	I585	G586	Y587	D588	I589	L590	A591	E592	D593	T594	L595	T596	A597	L598	L599	H600	M602	R603	K604	L605	L606	E607	K608	H609	I610	T611		
K612	V615	T617	F618	V619	S620	L621	V622	R623	K624	M625	R626	E627	P628	R629	F630	L631	D632	Y633	L634	S635	D636	L637	C638	V639	S640	M641	H642	I643	A644	I645	P646	V647	T648	Q649	E650	L651	I652	C653	C655	V656	L657	D658	P659	L660	K661	S662	D663	I664	L665	I666	R667	E668	E669	L670	R671	P672			
V673	K674	GLU	MET	ALA	GLN	SER	HIS	GLU	THR	LEU	SER	ILE	GLU	TYR	SER	GLU	E691	V692	W693	L694	T695	W696	T697	D698	A699	N700	N701	E702	H703	H704	E705	L706	S707	V708	R709	Q710	L711	A712	Q713	E714	R715	A717	G718	N719	H721	D722	P723	E723	N724	V725	L726	S727	L728	Y729	R730	Y731	Q732		
L733	K734	L735	F736	A737	R738	M739	C740	L741	E642	R743	Q744	Y745	L746	A747	I748	D749	E750	I751	S752	Q753	Q754	L755	G756	V757	D758	L759	H760	H761	L762	C763	M764	A765	D766	E767	M768	L769	P770	D771	L772	L773	A774	A775	S776	F777	H778	L779	L780	M781	L782	H783	S784	H785	V786	D787	R788	D789	P790	Q791	E792
L793	V794	T795	P796	F797	K798	F799	A800	MET	R801	L802	W803	T804	E805	I806	P807	T808	I810	T811	I812	K813	D814	Y815	D816	S817	N818	L819	M820	A821	S822	R823	D824	R825	K826	K827	L828	N829	K829	F830	A831	N832	T833	M834	E835	F836	V837	E838	D839	Y840	L841	N842	H843	Y844	V845	S846	A848	V849	P850	F851	A852
M853	E854	E855	K856	N857	K858	L859	T860	F861	E862	V863	V864	S865	L866	A867	H868	N869	L870	I871	Y872	F873	G874	F875	Y876	S877	F878	S879	E880	L881	L882	R883	L884	R885	R886	T887	L888	L889	G890	I891	I892	CYS	VAL	GLN	GLY	PRO	PRO	ALA	ALA	MET	LEU	GLN	ALA	TYR	GLU	ASP	PRO	GLY	GLY	LYS	ASN
VAL	ARG	ARG	ILE	GLN	GLY	VAL	HIS	MET	SER	THR	MET	THR	VAL	VAL	PHE	SER	ALA	PRO	SER	LEU	LEU	ALA	ALA	GLY	GLY	ALA	SER	ALA	GLU	ASP	LEU	ASP	ARG	SER	LYS	PHE	GLU	GLU	ASN	D961	I962	V963	Y964	M965	E966	T967	K968	L969	A970	I971	L972								
E973	I974	L975	Q976	I978	N980	V981	R982	L983	D984	Y985	R986	I987	S988	Y989	L990	L991	S992	V993	F994	K995	K996	E997	F998	V999	E1000	V1001	F1002	PRO	MET	GLN	ASP	SER	SER	GLY	ALA	ALA	ALA	PHE	GLU	GLU	ASN	GLU	D961	I962	V963	Y964	M965	E966	T967	K968	L969	A970	I971	L972					
E1033	A1034	M1035	F1036	G1037	VAL	GLY	LYS	THR	SER	S1043	M1044	L1045	E1046	V1047	D1048	D1049	E1050	G1051	G1052	R1053	M1054	F1055	L1056	L1057	V1058	L1059	I1060	H1061	L1062	T1063	M1064	H1065	D1066	Y1067	A1068	P1069	L1070	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	A1101	Q1102	D1103	V1104	E1105	N1106	Y1107	K1108	V1109	I1110	K1111	S1112	E1113	L1114	D1115	R1116	L1117	R1118	T1119	M1120	V1121	E1122	K1123	S1124	E1125	L1126	W1127	V1128	ASP	LYS	GLY	SER	GLY	LYS	GLY	LYS	GLY	GLU	VAL	GLU	ALA	ALA	LYS	ASP	LYS	GLU	ARG	PRO	THR			
ASP	GLU	GLU	PHE	LEU	HIS	PRO	GLU	GLY	LYS	SER	S1166	E1167	M1168	Y1169	Q1170	I1171	V1172	K1173	G1174	I1175	L1176	E1177	R1178	L1179	M1180	K1181	M1182	C1183	G1184	V1185	G1186	E1187	Q1188	M1189	R1190	K1191	K1192	Q1193	Q1194	R1195	L1196	L1197	K1198	M1199	M1200	D1201	A1202	H1203	K1204	V1205	M1206	L1207	D1208	L1209	L1210	Q1211	I1212		
P1213	Y1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	I1224	L1225	R1226	Y1227	T1228	H1229	Q1230	F1231	L1232	Q1233	K1234	F1235	C1236	A1237	G1238	M1239	P1240	G1241	M1242	Q1243	A1244	L1245	L1246	H1247	K1248	H1249	L1250	H1251	L1252	F1253	L1254	T1255	P1256	G1257	L1258	L1259	E1260	A1261	E1262	T1263	M1264	Q1265	H1266	I1267	F1268	L1269	M1270	M1271	Y1272
Q1273	L1274	C1275	S1276	E1277	I1278	S1279	E1280	P1281	V1282	L1283	K1284	H1285	F1286	V1287	H1288	L1289	L1290	A1291	T1292	H1293	G1294	R1295	H1296	V1297	Q1298	Y1299	L1300	D1301	F1302	L1303	H1304	T1305	V1306	I1307	K1308	A1309	E1310	G1311	K1312	Y1313	V1314	K1315	K1316	C1317	Q1318	D1319	M1320	I1321	M1322	T1323	E1324	L1325	T1326	M1327	A1328	G1329	D1330	L1331	V1332

L2056	L2057	L2058	Q2059	S2060	S2061	R2062	H2063	R2064	R2065	R2066	R2067	H2068	D2009	S2010	E2011	N2012	A2013	E2014	R2015	L2016	L2017	L2018	S2019	L2020	R2021	Q2022	Q2023	E2024	L2025	V2026	D2027	V2028	L2029	AS2030	K2031	A2032	Y2033	L2034	Q2035	E2036	E2037	E2038	R2039	E2040	N2041	S2042	E2043	V2044	S2045	P2046	R2047	E2048	V2049	G2050	H2051	N2052	L2053	Y2054	L2055		
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G1935	L1936	V1937	I1938	Q1939	T1940	L1941	E1942	T1943	L1944	T1945	E1946	Y1947	C1948	Q1949	C1952	H1953	E1954	M1955	Q1956	T1957	C1958	I1959	V1960	T1961	H1962	E1963	S1964	G1966	I1967	D1968	I1969	T1970	T1971	A1972	L1973	L1974	L1975	N1976	D1977	I1978	S1979	P1980	L1981	C1982	K1983	Y1984	L1985	M1986	D1987	L1988	V1989	L1990	Q1991	L1992	K1993	D1994	M1995				
I1873	L1874	R1875	F1876	L1877	Q1878	L1879	L1880	C1881	E1882	M1883	L1884	M1885	R1886	D1887	L1888	Q1889	M1890	F1891	L1892	C1894	Q1895	M1896	M1897	K1898	T1899	M1900	Y1901	M1902	L1903	V1904	C1905	E1906	T1907	L1908	F1909	L1910	L1911	M1914	C1915	G1916	T1919	G1920	G1921	L1922	G1923	L1924	L1925	G1926	L1927	Y1928	I1929	M1930	E1931	D1932	M1933	V1934					
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M1693	Y1694	L1695	Q1696	ASN	ARG	LYS	THR	SER	ASP	ARG	GLY	ASP	PRO	ASP	PRO	ILE	GLY	THR	GLY	LEU	ASP	PRO	D1717	M1718	S1719	I1720	I1721	A1722	E1658	E1659	K1660	L1661	C1662	I1663	K1664	V1665	L1666	K1667	E1731	G1732	A1733	T1734	K1735	L1736	V1737	C1738	D1739	L1740	I1741	T1742	S1743	T1744	K1745	M1746	K1748	I1749	F1750	Q1751	E1752		
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L1462	Q1463	Q1464	Q1465	H1466	K1467	S1469	V1470	E1471	A1472	C1473	I1474	R1475	T1476	L1477	M1479	V1480	A1481	K1482	G1483	R1484	A1490	I1491	L1492	P1494	M1495	D1496	L1497	D1498	A1499	H1500	I1501	S1502	S1503	M1504	L1505	S1506	G1508	A1515	S1516	C1517	A1518	A1519	A1520	Q1522	R1523	A1525	S1526	Y1528	K1529	A1530	T1531										
L1393	E1394	D1395	V1396	V1397	V1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	T1407	M1408	M1409	K1410	M1411	A1412	Y1413	V1414	N1415	F1416	V1417	V1418	H1419	C1420	P1361	L1362	M1363	Y1364	H1365	I1366	S1367	L1368	V1369	D1370	L1371	T1372	A1373	A1374	C1375	A1376	E1377	G1378	M1380	V1381	Y1382	E1384	I1385	K1386	C1387	T1388	S1389	L1390	P1392					
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	V1454	SER	SER	PRO	PHE	SER	GLU	ASN	GLN	THR	HIS	TYR	THR	THR	ASN	ASN	HIS	ILE	ILE	THR	THR	PHE	GLU	GLU	THR	THR	ASN	PHE	THR	THR	LEU	LEU	GLU	GLU	PRO

V2116	V2117	E2118	M2119	H2120	H2121	S2122	Q2123	E2124	E2125	I2126	V2127	R2128	Q2129	D2130	R2131	S2132	M2133	E2134	Q2135	I2136	V2137	F2138	P2139	V2140	F2141	G2142	I2143	C2144	Q2145	F2146	L2147	T2148	E2149	E2150	T2151	H2152	H2153	R2154	L2155	F2156	T2157	T2158	T2159	E2160	Q2161	D2162	E2163	Q2164	G2165	S2166	K2167	GLY	ALA	SER	THR	GLY	VAL	LEU	ASP	SER		
S2176	F2177	L2178	H2179	E2181	M2182	E2183	W2184	Q2185	R2186	K2187	L2188	S2189	S2190	M2191	P2192	L2193	I2194	Y2195	W2196	F2197	S2198	R2199	R2200	M2201	T2202	L2203	W2204	I2207	S2208	F2209	N2210	L2211	A2212	V2213	F2214	I2215	N2216	I2217	I2218	I2219	A2220	G2221	F2222	Y2223	P2224	Y2225	M2226	GLY	ALA	SER	THR	GLY	VAL	LEU	ASP	SER						
PRO	L2231	I2232	S2233	L2234	L2235	F2236	W2237	I2238	L2239	I2240	C2241	F2242	S2243	I2244	A2245	A2246	L2247	F2248	T2249	K2250	R2251	Y2252	S2260	I2261	V2266	A2267	L2268	I2269	L2270	R2271	L2272	S2273	I2274	Y2275	F2276	H2277	L2278	G2279	P2280	T2281	L2282	M2283	L2284	L2285	G2286	A2287	L2288	N2289	L2290	T2291	N2292	K2293	L2294	F2296								
V2297	V2298	S2299	F2300	G2301	V2302	M2303	R2304	G2305	T2306	F2307	L2308	G2309	Q2310	Y2311	K2312	A2313	L2314	V2315	M2316	D2317	M2318	E2319	F2320	L2321	R2322	H2323	V2324	G2325	Y2326	L2327	L2328	T2329	S2330	V2331	L2332	G2333	L2334	F2335	A2336	H2337	E2338	L2339	F2340	Y2341	S2342	I2343	L2344	L2345	L2346	D2347	L2348	I2349	Y2350	R2351	E2352	E2353	T2354	L2355	F2356			
M2357	V2358	I2359	K2360	S2361	V2362	T2363	R2364	N2365	G2366	R2367	S2368	I2369	L2370	L2371	T2372	A2373	M2374	L2375	A2376	L2377	L2378	L2379	V2380	Y2381	L2382	F2383	S2384	I2385	V2386	G2387	L2388	F2390	L2391	K2392	D2393	D2394	F2395	I2396	L2397	E2398	V2399	D2400	L2402	P2403	ASN	ASN	HIS	SER	THR	THR	ALA	ALA	SER	PRO	LEU	GLY	PRO	MET	HIS			
GLY	ALA	ALA	ALA	PHE	VAL	ASP	THR	CYS	SER	GLY	ASP	LYS	ASP	MET	ASP	CYS	VAL	VAL	F2490	P2491	A2492	R2493	V2494	V2495	Y2496	D2497	L2498	L2499	F2500	F2501	F2502	I2503	S2504	I2505	V2506	L2507	L2508	L2509	M2510	L2511	L2512	F2513	L2514	L2515	I2516	C2461	I2462	V2463	T2464	A2521	V2465	M2466	M2467	H2468	G2469	L2470	R2471	N2472	Q2473	G2474	G2475	W2476
G2477	D2478	I2479	L2480	R2481	K2482	P2483	S2484	K2485	D2486	K2487	F2488	D2489	F2490	P2491	A2492	R2493	V2494	V2495	Y2496	D2497	L2498	L2499	F2500	F2501	F2502	I2503	S2504	I2505	V2506	L2507	L2508	L2509	M2510	L2511	L2512	F2513	L2514	L2515	I2516	C2461	I2462	V2463	T2464	A2521	V2465	M2466	M2467	H2468	G2469	L2470	R2471	N2472	Q2473	G2474	G2475	W2476						
G2538	F2539	L2540	C2541	G2542	L2543	E2544	R2545	D2546	K2547	F2548	D2549	M2550	K2551	T2552	V2553	S2554	F2555	E2556	E2557	H2558	L2559	K2560	L2561	E2562	M2565	W2566	M2567	Y2568	L2569	V2570	F2571	L2572	V2573	L2574	V2575	R2576	V2577	K2578	M2579	K2580	T2581	D2582	Y2583	T2584	G2585	P2586	E2587	S2588	Y2589	V2590	A2591	Q2592	M2593	L2594	K2595	M2596	K2597	N2598				
L2599	D2600	W2601	M2605	K2606	A2607	M2608	S2609	L2610	V2611	SER	ASN	GLN	GLY	GLY	GLY	GLU	GLN	GLN	ASN	ASN	ILE	ARG	ILE	ILE	LEU	LEU	GLN	ASP	ASP	LYS	LEU	ASN	ASN	THR	MET	MET	LYS	LEU	VAL	SER	HIS	LEU	THR	ALA	GLN	ASN	GLU	LEU	LYS	LEU	GLY	GLU	MET	THR	THR	GLN	ARG	ARG	ARG	GLN	ARG	LEU
GLY	PHE	VAL	ASP	VAL	GLN	ASN	CYS	ILE	SER	ARG																																																				

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



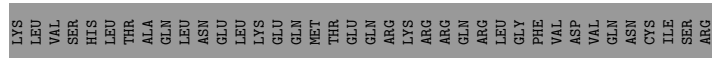
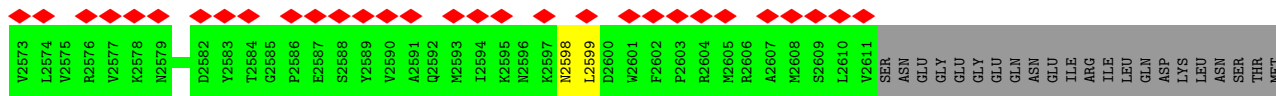
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765	866	867	068	869	070	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764
GLN	ASP	GLY	LYS	ILE	A85	D86	H87	H88	L89	L90	Q91	K92	L93	Q94	H95	A96	A97	Q98	H99	E100	P101	A102	Q103	M104	D105	T106	E107	M108	K109	K110	V111	H112	G113	D114	V115	L116	F117	Y118	G119	S120	P121	L122	Q123	L124															

LEU	D961	D962	V963	V964	M965	E966	T967	K968	L969	K970	L971	L972	E973	L974	L975	D976	F977	L978	L979	N980	V981	L982	L983	D984	R986	L987	S988	L989	L990	L991	S992	V993	F994	K995	K996	E997	F998	V999	E1000																						
L819	L820	A821	S822	R823	C763	M764	A765	D766	E767	M768	L769	P770	F771	D772	L773	R774	A775	S776	F777	C778	H779	L780	M781	L782	H783	V784	H785	V786	D787	R788	D789	P790	F791	A852	M853	E854	E855	K856	M857	K858	L859	T860	F861	E862	V863	V864	A867	H868	M869	L870	L871	I810	K813	D814	Y815	D816	S817	N818			
E880	L889	G890	L891	L892	L893	CYS	VAL	GLN	GLY	GLY	ASN	PRO	ALA	MET	LEU	GLN	ALA	PRO	ALA	LEU	GLN	TYR	GLU	ASP	PRO	GLY	GLY	LYS	ASN	VAL	S846	E847	A848	V849	P850	F851	A852	M853	E854	E855	K856	M857	K858	L859	T860	F861	E862	V863	V864	A867	H868	M869	L870	L871	I810	K813	D814	Y815	D816	S817	N818
L819	M820	A821	S822	R823	C763	M764	A765	D766	E767	M768	L769	P770	F771	D772	L773	R774	A775	S776	F777	C778	H779	L780	M781	L782	H783	V784	H785	V786	D787	R788	D789	P790	F791	A852	M853	E854	E855	K856	M857	K858	L859	T860	F861	E862	V863	V864	A867	H868	M869	L870	L871	I810	K813	D814	Y815	D816	S817	N818			
D698	K699	M700	M701	E702	H703	H704	E705	K706	S707	V708	R709	Q710	L711	A712	Q713	E714	A715	R716	A717	G718	M719	A720	H721	D722	E723	M724	V725	L726	S727	R728	Y729	R730	M731	Q732	L733	K734	T735	F736	A737	R738	M739	C740	L741	D742	R743	Q744	V745	L746	A747	P807	T808	D749	E750	L751	S752	Q753	Q754	L755	G756	V757	
D577	F578	G579	M580	M581	D582	S583	G584	I585	G586	Y587	D588	L589	A591	E592	D593	T594	T596	A597	L598	L599	H600	M601	N602	R603	K604	L605	L606	E607	K608	H609	L610	T611	K612	E614	V615	E616	E617	E618	E619	F618	M619	S620	L621	M622	R623	R626	E627	P628	R629	F630	L631	D632	V633	L634	S635	D636	L637				
M809	R810	E811	Q812	M813	L814	L815	L822	K823	F826	R827	GLU	LYS	GLY	GLY	GLU	GLY	P834	L835	V836	D837	L838	E839	E840	M841	S842	D843	D844	K845	N846	Q850	M851	M852	F853	R854	L855	C856	Y857	N858	G859	Q861	M862	L863	L864	L865	T866	V867	R868	T869	M869	S870	E871	S872	M873	L874	A875	K876	L877	A878	M879	E880	
A448	S449	S450	M451	L452	A453	S454	A455	V456	E457	M460	E461	F463	I464	S465	Q466	D468	R469	R470	F471	V472	I473	Q474	L475	L476	E477	D478	L479	V480	F481	F482	S484	D485	V486	P487	N488	N489	G490	Q491	M492	V493	L494	D495	I496	M497	V498	T499	K500	P501	N502	R503	E504	Y505	Q506	K507	L508						
M384	S385	Y386	V387	R390	H391	L392	N395	T396	W397	I398	Q399	S400	T401	M402	D406	I407	E408	E409	E410	M411	P412	I413	R414	L415	M416	Y417	G418	T419	C420	P421	K422	K423	E424	D425	K426	E427	A428	F429	A430	I431	V432	S433	V434	P435	V436	S437	E438	I439	R440	D441	L442	D443	F444	A445	M446	D447					
L125	H126	M127	K128	S129	M130	K131	Y132	L133	T134	V135	M136	K137	L138	R139	F140	A141	L142	L143	E144	K145	M148	R149	V150	T151	L152	A154	T155	G156	M157	E158	G159	S160	M161	L162	F163	I164	Q165	M168	K169	L170	R171	S172	M173	D175	M176	V177	L178	H245	A246	E247	D181	K182	V183	I184	L185	M186					
G191	L194	H195	A196	S197	M198	Y199	E200	L201	S202	D203	M204	A205	G206	R207	C208	E209	V210	N211	S212	V213	N214	C215	S218	V219	K220	I221	N222	L223	F224	P225	Q226	F227	R228	D229	H230	L231	E232	E233	V234	L235	D239	V240	V241	R242	L243	F244	H245	A246	E247	Q248	E249	K250	F251	L252							
D255	E256	Y257	K258	G259	K260	L261	Q262	L265	R266	T267	T268	L269	R270	Q271	S272	A273	T274	S275	A281	L282	V283	E284	V287	V288	H289	N290	N292	L293	D291	P292	C293	R294	A297	G298	H299	W300	N301	G302	L303	Y304	R305	H308	L309	G312	N313	Y314	L315	A316	A317	E318	E319	N320	P321	SER	TYR						
LYS	GLY	ALA	SER	ASP	PRO	LYS	ALA	ALA	GLY	MET	GLY	ALA	GLN	GLY	THR	GLY	ARG	ARG	ASN	ALA	GLY	GLU	LYS	I350	K351	Y352	C353	V355	A356	V357	P358	H359	G360	N361	D362	I363	A364	S365	F367	E368	D370	P371	T372	T373	L374	Q375	K376	T377	D378	S379	F380	V381	P382	K383							

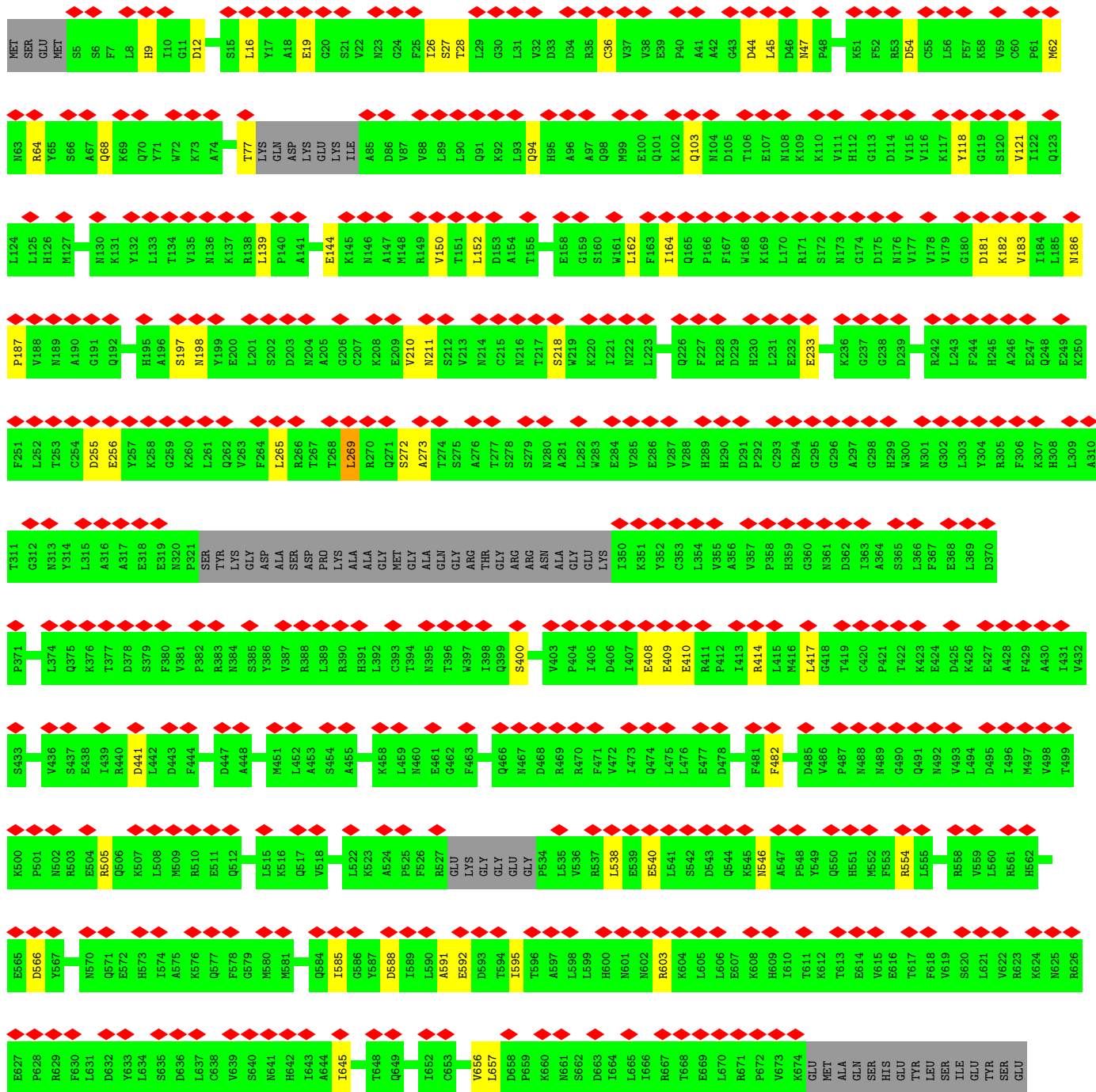
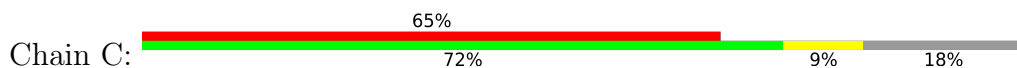


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H1061	T1063	M1064	H1065	Y1067	A1068	P1069	L1070	V1071	S1072	G1073	PHE	ASP	SER	THR	THR	ALA	ASN	K1080	H1081	F1082	S1083	Q1084	R1085	Q1086	E1087	A1088	M1089	H1090	T1091	F1092	K1093	Q1094	V1095	Q1096	L1097	L1098	I1099	S1100	A1101	Q1102	V1047	Q1170	I1171	V1172	K1173	G1174	I1175	L1176	E1177	R1178	K1111	S1112	E1113	D1114	D1115	R1116	L1117	T1119	M1120		
V1121	E1122	K1123	S1124	E1125	L1126	W1127	ASP	LYS	LYS	GLY	SER	GLY	LYS	GLY	VAL	VAL	GLU	GLY	ALA	ALA	LYS	ASP	LYS	LYS	GLU	ARG	PRO	THR	ASP	GLU	GLY	PHE	HIS	PRO	PRO	GLY	LYS	THR	SER	S1166	E1167	M1168	Y1169	Q1170	I1171	V1172	K1173	G1174	I1175	L1176	E1177	R1178	L1179	M1180							
K1181	M1182	C1183	G1184	V1185	G1186	E1187	Q1188	M1189	R1190	K1191	K1192	L1252	F1253	L1254	T1255	P1256	G1257	L1258	L1259	M1200	A1201	A1202	H1203	K1204	V1205	M1206	L1207	D1208	L1209	L1210	Q1211	I1212	P1213	I1214	D1215	K1216	E1217	G1217	D1218	A1219	K1220	M1221	M1222	L1223	I1224	L1225	R1226	Y1227	L1228	H1229	Q1230	F1231	L1232	Q1233	K1234	F1235	C1236	A1237	G1238	M1239	P1240
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Y1421	V1422	D1423	THR	VAL	GLU	MET	LYS	GLU	ILE	TYR	THR	SER	ASN	HIS	ILE	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	THR	THR	THR	ARG	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	PHE	SER	GLU	ASN	SER	SER	GLU	GLN	THR	HIS	GLN	THR	ILE	VAL	VAL	GLN	LEU	LEU	GLN	SER	THR	THR	THR	THR	ARG	ARG	GLU	LYS	ARG	VAL	A1462	Q1463	Q1464	Q1465	H1466	K1467	G1468	S1469	V1470	E1471	A1472	C1473	I1474	R1475	T1476	L1477	A1478	M1479	V1480	A1481	K1482	G1483	L1484	A1489	I1491	L1492	L1493			
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A1601	L1602	E1603	E1604	R1605	L1606	K1607	P1608	L1609	V1610	Q1611	L1612	E1613	L1614	S1615	V1616	L1617	V1618	V1619	Y1620	L1621	H1622	M1623	P1624	E1625	L1626	L1627	F1628	L1629	E1630	G1631	E1632	E1633	A1634	Y1635	Q1636	R1637	C1638	E1639	S1640	G1641	G1642	F1643	L1644	S1645	K1646	L1647	I1648	Y1651	K1652	D1653	L1654	M1655	E1656	S1657	E1658	E1659	K1660	L1661			
C1662	I1663	K1664	V1665	L1666	R1667	T1668	L1669	Q1670	Q1671	M1672	L1673	L1674	K1675	K1676	T1677	K1678	Y1679	G1680	D1681	R1682	G1683	M1684	Q1685	L1686	R1687	K1688	M1689	L1690	L1691	Q1692	M1693	Y1694	L1695	ASN	ARG	LYS	SER	THR	ARG	ARG	GLY	ASP	LEU	PRO	PRO	PRO	ILE	GLY	THR	GLY	LEU	ASP	PRO	D1717	W1718	S1719	A1720	I1721			
A1722	A1723	T1724	Q1725	C1726	R1727	L1728	D1729	K1730	E1731	G1732	A1733	T1734	K1735	L1736	V1737	C1738	D1739	L1740	I1741	T1744	K1745	M1746	E1747	K1748	I1749	F1750	Q1751	E1752	S1753	G1754	G1755	L1756	A1757	I1758	H1759	L1760	L1761	D1762	G1763	G1764	M1765	T1766	E1767	I1768	Q1769	K1770	S1771	F1772	M1773	N1774	L1775	M1776	M1777	S1778	D1779	K1780	K1781	S1782			

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SER	LEU	GLY	PRO	SER	LEU	ARG	ARG	GLY	HIS	GLU	VAL	SER	SER	GLU	ARG	VAL	VAL	GLN	SER	SER	GLU	M1863	G1864	S1865	V1866	I1867	L1868	M1870	Q1871	P1872	I1873	L1874	R1875	Q1878	L1879	L1880	C1881	E1882	N1883	H1884	N1885	R1886	D1887	L1888	Q1889	N1890	F1891	L1892	R1893	C1894	Q1895	N1896	N1897	K1898	T1899	N1900	L1903	V1904							
C1905	E1906	T1907	L1908	Q1909	F1910	L1911	D1912	I1913	M1914	L1915	G1916	S1917	T1918	T1919	G1920	G1921	L1922	G1923	L1924	L1925	G1926	L1927	Y1928	I1929	M1930	I1931	D1932	M1933	V1934	G1935	L1936	V1937	I1938	L1941	E1942	T1943	L1944	L1945	E1946	C1948	Q1949	G1950	P1951	C1952	H1953	E1954	Q1956	G1957	C1958	I1959	V1960	T1961	H1962	E1963	S1964	N1965									
G1966	I1967	D1968	I1969	I1970	T1971	A1972	L1973	I1974	L1975	M1976	D1977	I1978	S1979	P1980	L1981	C1982	K1983	Y1984	R1985	M1986	D1987	L1988	Y1989	L1990	Q1991	L1992	K1993	L1994	D1995	N1996	S1997	L1998	L1999	L2000	L2001	A2002	L2003	M2004	S2006	R2007	H2008	D2009	G1950	P1951	C1952	H1953	E1954	Q1956	G1957	C1958	I1959	V1960	T1961	H1962	E1963	S1964	N1965								
D2027	V2028	I2029	K2030	K2031	A2032	Y2033	L2034	Q2035	E2036	E2037	E2038	R2039	E2040	N2041	S2042	E2043	V2044	S2045	P2046	R2047	E2048	V2049	G2050	H2051	M2052	I2053	Y2054	I2055	L2056	A2057	Q2058	L2059	S2061	R2062	H2063	N2064	K2065	L2066	L2067	Q2068	H2069	L2070	L2071	K2072	P2073	V2074	ARG	LYS	ILE	GLN	GLU	GLU	ALA	GLY	SER										
SER	MET	LEU	SER	LEU	ASN	ASN	LYS	GLN	LEU	SER	GLN	MET	LEU	LYS	SER	ALA	PRO	ALA	GLN	GLU	GLU	E2111	D2112	P2113	L2114	A2115	Y2116	Y2117	E2118	M2119	H2120	L2121	S2122	N2123	T2124	E2125	R2128	Q2129	R2130	R2131	S2132	M2133	E2134	Q2135	L2136	V2137	F2138	P2139	V2140	T2141	G2142	L2143	C2144	Q2145	F2146	L2147									
T2148	E2149	E2150	L2151	K2152	H2153	R2154	L2155	F2156	T2157	T2158	L2159	E2160	Q2161	D2162	E2163	Q2164	G2165	S2166	K2167	V2168	S2169	D2170	F2171	F2172	L2173	Q2174	F2177	L2178	H2179	N2180	E2181	M2182	E2183	W2184	Q2185	R2186	K2187	L2188	R2189	S2190	M2191	P2192	L2193	I2194	V2195	W2196	F2197	S2198	R2199	R2200	M2201	T2202	L2203	Q2204	G2205	A2206	I2207	S2208							
F2209	N2210	L2211	A2212	V2213	F2214	L2215	M2216	L2217	L2218	L2219	A2220	F2221	F2222	Y2223	P2224	Y2225	M2226	GLU	GLY	ALA	SER	THR	VAL	LEU	ASP	SER	PRO	L2231	L2232	S2233	L2234	L2235	F2236	W2237	L2238	L2239	L2240	C2241	F2242	S2243	A2244	A2245	A2246	L2247	F2248	T2249	K2250	R2251	Y2252	S2253	S2254	L2255	R2256	A2257	L2258	L2259	L2260	L2261	R2262	P2263	L2264	L2265	V2266	A2267	L2268
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S2330	V2331	L2332	G2333	L2334	F2335	A2336	H2337	E2338	L2339	F2340	Y2341	S2342	I2343	L2344	L2345	F2346	D2347	L2348	I2349	Y2350	R2351	E2352	E2353	T2354	L2355	L2356	M2357	V2358	I2359	K2360	S2361	V2362	L2363	R2364	N2365	G2366	R2367	S2368	I2369	L2370	L2371	T2372	A2373	L2374	L2375	L2376	A2377	L2378	L2379	V2380	Y2381	L2382	F2383	S2384	I2385	V2386	G2387	F2388	L2389						
F2390	L2391	K2392	D2393	D2394	F2395	L2396	L2397	E2398	V2399	D2400	R2401	L2402	P2403	ASN	ASN	HIS	THR	ALA	ALA	PRO	PRO	GLY	MET	PRO	HIS	GLY	ALA	ALA	PHE	VAL	ASP	THR	CYS	SER	GLY	ASP	LYS	MET	ASP	CYS	VAL	SER	GLY	LEU	SER	VAL	PRO	GLU	VAL	LEU	GLU	ASP	ARG	GLU	LEU	D2449									
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I2512	F2513	G2514	V2515	L2516	L2517	D2518	F2519	F2520	A2521	D2522	L2523	R2524	S2525	E2526	K2527	O2528	K2529	G2530	E2531	E2532	L2533	L2534	K2535	T2536	T2537	C2538	F2539	I2540	C2541	G2542	L2543	E2544	R2545	D2546	K2547	F2548	D2549	N2550	K2551	T2552	V2553	F2554	E2555	E2556	E2557	L2558	I2559	K2560	L2561	E2562	H2563	N2564	M2565	W2566	N2567	Y2568	L2569	L2572							



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

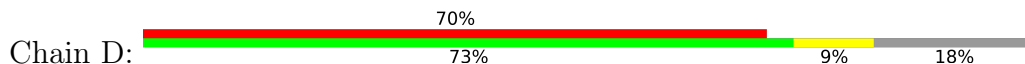


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S752	Q753	Q754	L755	G756	D758	L759	I760	F761	L762	C763	M764	A765	D766	E767	M768	L769	P770	F771	D772	L773	R774	A775	C778	H779	L780	M781	L782	H783	V784	H785	V786	D787	R788	D789	P790	Q791	E792	L793	V794	T795	P796	K797	K798	F799	A800	R801	L802	V803	T804	E805	I806	P807	T808	A809	I810	T811	I812			
K814	D814	Y815	D816	S817	N818	L819	N820	A821	S822	R823	D824	D825	K826	K827	N828	K829	F830	A831	N832	T833	M834	E835	F836	V837	E838	D839	Y840	L841	N842	N843	V844	V845	S846	E847	A848	V849	F851	A852	N853	E854	E855	K856	N857	T860	F861	E862	V863	V864	S865	L866	A867	H868	I871	Y872	F873					
Y876	S877	F878	S879	E880	L881	L882	R883	L884	T885	R886	T887	L888	L889	G890	I891	I892	D893	CYS	VAL	GLN	GLY	PRO	ALA	LEU	GLN	ALA	TVR	GLU	ASP	PRO	GLY	LYS	ASN	VAL	ARG	ARG	ARG	ILE	GLY	VAL	GLY	HIS	MET	MET	SER	THR	MET	VAL	LEU	SER	ARG	GLN	SER	VAL						
PHE	SER	ALA	PRO	SER	LEU	SER	ALA	ALA	ALA	GLU	PRO	LEU	ASP	ARG	SER	LYS	PHE	GLU	GLU	ASN	D961	I962	V963	V964	H965	K968	L969	K970	I971	L972	L975	Q976	F977	I978	L979	N980	L983	D984	Y985	R986	I987	S988	Y989	L990	V993	F994	K995	K996	E997	F998	V999									
E1000	V1001	F1002	PRO	MET	GLN	ASP	SER	GLY	ALA	ALA	ASP	THR	ALA	PRO	PHE	ASP	SER	THR	THR	ALA	M1024	L1025	D1026	R1027	I1028	E1029	E1030	E1033	A1034	M1035	F1036	G1037	VAL	GLY	GLY	THR	SER	S1043	M1044	L1045	E1046	V1047	D1048	D1049	E1050	G1051	G1052	R1053	M1054	F1055	L1056	R1057	V1058	L1059	I1060					
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V1121	E1122	K1123	S1124	H1125	L1126	V1127	ASP	LYS	GLY	GLY	SER	GLY	GLY	GLY	GLU	VAL	ALA	ALA	ASP	ASP	H1203	K1204	V1205	M1206	L1207	D1208	L1209	L1210	Q1211	I1212	P1213	Y1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	I1224	L1225	R1226	G1174	I1175	L1176	E1177	R1178	L1179	Q1233	K1234	F1235	G1236	P1240	G1241	M1242			
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Q1243	A1244	L1245	L1246	H1247	K1248	H1249	L1250	H1251	L1252	F1253	L1254	T1255	P1256	G1257	L1258	L1259	E1260	A1261	E1262	T1263	M1264	Q1265	H1266	I1267	F1268	Y1272	Q1273	L1274	C1275	S1276	E1277	I1278	S1279	E1280	F1281	V1282	L1283	Q1284	H1285	F1286	V1287	H1288	L1289	L1290	A1291	T1292	H1293	G1294	R1295	L1296	V1297	Q1298	Y1299	L1300	L1303	H1304				
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S1367	L1368	V1369	D1370	L1371	L1372	A1373	A1374	C1375	A1376	E1377	G1378	K1379	M1380	V1381	Y1382	T1383	E1384	I1385	K1386	T1387	L1388	S1389	L1390	L1391	P1392	L1393	E1394	D1395	V1396	S1397	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	L1406	D1407	E1408	Y1409	K1410	M1411	A1412	F1413	Y1414	N1415	F1416	V1417	M1418	H1419	H1359	S1360	P1361	L1362	M1363	Y1364	H1365	I1366
GLU	MET	LYS	GLU	ILE	TYR	THR	SER	ASN	HIS	TRP	THR	LEU	PHE	GLU	ASN	PHE	THR	LEU	ASP	MET	ARG	VAL	VAL	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		

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Q1464	THR	Q1464
Q1465	LEU	Q1465
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K1467	THR	K1467
G1468	LEU	G1468
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V1470	GLY	V1470
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A1472	ASP	A1472
C1473	ARG	C1473
I1474	LEU	I1474
R1475	THR	R1475
T1476	PRO	T1476
L1477	LEU	L1477
A1478	GLY	A1478
M1479	GLU	M1479
V1480	THR	V1480
A1481	SER	A1481
K1482	GLN	K1482
G1483	GLY	G1483
R1484	GLU	R1484
I1490	LEU	I1490
I1491	THR	I1491
L1492	SER	L1492
E1593	ASP	E1593
L1494	GLU	L1494
P1494	PRO	P1494
M1495	GLY	M1495
D1496	LEU	D1496
L1497	THR	L1497
D1498	GLY	D1498
A1499	GLU	A1499
H1500	THR	H1500
I1501	ARG	I1501
S1502	GLY	S1502
S1503	HIS	S1503
M1504	GLN	M1504
L1505	VAL	L1505
S1506	GLU	S1506
S1507	THR	S1507
G1508	ILE	G1508
A1510	VAL	A1510
S1516	VAL	S1516
C1517	GLN	C1517
A1518	LEU	A1518
A1519	GLN	A1519
A1520	SER	A1520
A1521	THR	A1521
Q1522	ARG	Q1522
R1523	LEU	R1523
N1524	LEU	N1524
A1525	GLY	A1525
S1526	PRO	S1526
S1527	THR	S1527
Y1528	GLY	Y1528
K1529	LEU	K1529
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T1532	GLU	T1532
R1533	GLY	R1533
A1541	ARG	A1541
F1542	LYS	F1542
P1543	ASP	P1543
R1544	THR	R1544
V1545	ARG	V1545
T1546	GLY	T1546
P1547	ASP	P1547
T1548	LEU	T1548
A1549	ASP	A1549
N1550	PRO	N1550
Q1551	ILE	Q1551
W1552	THR	W1552
D1587	GLY	D1587
K1588	LEU	K1588
G1589	GLY	G1589
N1590	PRO	N1590
I1591	ARG	I1591
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L1594	LEU	L1594
K1589	GLY	K1589
L1595	PRO	L1595
Q1596	ASP	Q1596
D1597	PRO	D1597
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I1599	GLY	I1599
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L1602	THR	L1602
E1603	LEU	E1603
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L1606	SER	L1606
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V1610	GLY	V1610
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D1619	LEU	D1619
L1620	GLN	L1620
L1621	GLN	L1621
H1622	THR	H1622
W1623	THR	W1623
P1624	ARG	P1624
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L1626	LEU	L1626
L1627	GLU	L1627
F1628	THR	F1628
L1629	LEU	L1629
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G1631	GLY	G1631
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L1635	GLY	L1635
Q1636	ARG	Q1636
R1637	ARG	R1637
C1638	LYS	C1638
E1639	SER	E1639
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G1641	ARG	G1641
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F1643	ASP	F1643
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L1789	THR	L1789
H1790	THR	H1790
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M1792	THR	M1792
M1793	THR	M1793
K1794	THR	K1794
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A1796	THR	A1796
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V1804	THR	V1804
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VAL	THR	VAL
ASN	THR	ASN
MET	THR	MET
ASN	THR	ASN
ASP	THR	ASP
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L1691	THR	L1691
Q1692	THR	Q1692
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ARG	THR	ARG
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THR	THR	THR
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ARG	THR	ARG
GLY	THR	GLY
ASP	THR	ASP
PRO	THR	PRO
LEU	THR	LEU
ALA	THR	ALA
GLU	THR	GLU
GLY	THR	GLY
VAL	THR	VAL
PRO	THR	PRO
PHE	THR	PHE
SER	THR	SER
ILE	THR	ILE
PRO	THR	PRO
GLY	THR	GLY
SER	THR	SER
PRO	THR	PRO
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Q1725	THR	Q1725
C1726	THR	C1726
R1727	THR	R1727
L1901	THR	L1901
N1902	THR	N1902
L1903	THR	L1903
V1904	THR	V1904
C1905	THR	C1905
E1906	THR	E1906
T1907	THR	T1907
L1908	THR	L1908
Q1909	THR	Q1909
F1910	THR	F1910
L1911	THR	L1911
D1912	THR	D1912
A1913	THR	A1913
M1914	THR	M1914
C1915	THR	C1915
G1916	THR	G1916
S1917	THR	S1917
T1918	THR	T1918
T1919	THR	T1919
G1920	THR	G1920
G1921	THR	G1921
L1922	THR	L1922
G1923	THR	G1923
L1924	THR	L1924
L1925	THR	L1925
G1926	THR	G1926
L1927	THR	L1927
Y1928	THR	Y1928
I1929	THR	I1929
M1930	THR	M1930
E1931	THR	E1931
D1932	THR	D1932
M1933	THR	M1933
V1934	THR	V1934
G1935	THR	G1935
L1936	THR	L1936
Y1937	THR	Y1937
I1938	THR	I1938
Q1939	THR	Q1939
T1940	THR	T1940
L1941	THR	L1941
E1942	THR	E1942
T1943	THR	T1943
L1944	THR	L1944
T1945	THR	T1945
E1946	THR	E1946
Y1947	THR	Y1947
C1948	THR	C1948
Q1949	THR	Q1949
G1950	THR	G1950
P1951	THR	P1951
C1952	THR	C1952
H1953	THR	H1953
E1954	THR	E1954
N1955	THR	N1955
Q1956	THR	Q1956
T1957	THR	T1957
C1958	THR	C1958
I1959	THR	I1959
V1960	THR	V1960
T1961	THR	T1961
H1962	THR	H1962
E1963	THR	E1963
S1964	THR	S1964
N1965	THR	N1965
G1966	THR	G1966
T1967	THR	T1967
D1968	THR	D1968
T1969	THR	T1969
T1970	THR	T1970
T1971	THR	T1971
L1972	THR	L1972
L1973	THR	L1973
I1974	THR	I1974
L1975	THR	L1975
N1976	THR	N1976
D1977	THR	D1977
I1978	THR	I1978
S1979	THR	S1979
F1980	THR	F1980
L1981	THR	L1981
C1982	THR	C1982
K1983	THR	K1983
Y1984	THR	Y1984
R1985	THR	R1985
M1986	THR	M1986
D1987	THR	D1987
L1988	THR	L1988
V1989	THR	V1989
Q1991	THR	Q1991
L1992	THR	L1992
K1993	THR	K1993
D1994	THR	D1994
M1995	THR	M1995
A1996	THR	A1996
S1997	THR	S1997
K1998	THR	K1998
L1999	THR	L1999
L2000	THR	L2000
L2001	THR	L2001
A2002	THR	A2002
L2003	THR	L2003
M2004	THR	M2004
E2005	THR	E2005
S2006	THR	S2006
R2007	THR	R2007
H2008	THR	H2008
D2009	THR	D2009
S2010	THR	S2010
E2011	THR	E2011
M2012	THR	M2012
A2013	THR	A2013
E2014	THR	E2014
R2015	THR	R2015
T2016	THR	T2016
L2017	THR	L2017
T2018	THR	T2018
I1959	THR	I1959
L2020	THR	L2020
R2021	THR	R2021
P2022	THR	P2022
Q2023	THR	Q2023
E2024	THR	E2024
L2025	THR	L2025
V2026	THR	V2026
V2028	THR	V2028
I2029	THR	I2029
K2030	THR	K2030
K2031	THR	K2031
A2032</		

L2270	R2271	S2272	I2273	V2274	Y2275	L2276	G2277	I2278	G2279	F2280	T2281	L2282	N2283	I2284	L2285	G2286	A2287	L2288	N2289	L2290	T2291	N2292	K2293	L2294	V2295	F2296	V2297	V2298	S2299	F2300	V2301	G2302	N2303	R2304	G2305	T2306	F2307	I2308	R2309	G2310	Y2311	K2312	A2313	M2314	V2315	M2316	D2317	M2318	E2319	F2320	L2321	Y2322	H2323	G2325	Y2326	L2327	L2328	T2329				
S2330	V2331	L2332	G2333	L2334	F2335	A2336	H2337	E2338	L2339	F2340	Y2341	S2342	ASN	I2343	L2344	L2345	F2346	D2347	L2348	I2349	Y2350	R2351	E2352	E2353	T2354	L2355	F2356	N2357	V2358	I2359	K2360	S2361	V2362	T2363	R2364	N2365	G2366	R2367	S2368	I2369	L2370	L2371	T2372	A2373	L2374	L2375	V2376	A2377	L2378	M2379	V2380	Y2381	L2382	F2383	V2386	G2387	F2388	L2389	F2390			
L2391	K2392	D2393	D2394	F2395	L2396	L2397	F2398	V2399	D2400	R2401	L2402	P2403	ASN	HIS	L2404	SER	THR	ALA	SER	PRO	LEU	GLY	MET	PRO	HIS	GLY	ALA	ALA	ALA	PHE	VAL	ASP	THR	CYS	SER	GLY	ASP	LYS	MET	LYS	ASP	CYS	VAL	GLY	SER	LEU	SER	VAL	PRO	GLU	VAL	VAL	LEU	LEU	GLU	GLU	ASP	ARG	GLU	LEU	D2449	S2450
T2451	E2452	R2453	A2454	C2455	D2456	T2457	L2458	L2459	M2460	C2461	I2462	V2463	T2464	V2465	M2466	N2467	H2468	G2469	L2470	R2471	N2472	G2473	G2474	G2475	V2476	G2477	D2478	I2479	L2480	R2481	K2482	P2483	S2484	K2485	D2486	E2487	S2488	L2489	F2490	F2491	A2492	R2493	V2494	V2495	Y2496	D2497	L2498	L2499	F2500	F2501	F2502	I2503	V2504	I2505	I2506	I2507	V2508	L2509	M2510			
L2511	I2512	F2513	G2514	V2515	I2516	I2517	D2518	T2519	F2520	A2521	D2522	L2523	R2524	S2525	E2526	K2527	Q2528	K2529	K2530	E2531	E2532	I2533	L2534	K2535	T2536	T2537	C2538	F2539	I2540	C2541	G2542	L2543	E2544	R2545	D2546	K2547	S2548	D2549	N2550	K2551	T2552	V2553	S2554	F2555	E2556	E2557	H2558	I2559	K2560	L2561	E2562	H2563	N2564	M2565	Y2566	L2569	Y2570	F2571				
I2572	V2573	L2574	V2575	V2576	V2577	K2578	N2579	K2580	L2581	D2582	L2583	T2584	G2585	E2586	F2587	S2588	Y2589	V2590	A2591	Q2592	N2593	I2594	K2595	N2596	K2597	N2598	L2599	D2600	M2601	F2602	P2603	R2604	M2605	R2606	A2607	M2608	L2610	V2611	SER	ASN	GLU	GLY	GLU	GLY	GLN	ASN	GLU	ASN	GLU	ILE	SER	ARG										
THR	MET	LYS	LEU	VAL	SER	HIS	LEU	THR	ALA	GLN	LEU	ASN	GLU	LEU	GLN	MET	THR	GLU	GLN	ARG	LYS	ARG	ARG	GLM	ASP	VAL	VAL	GLN	ASN	CYS	ILE	SER	ARG																													

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



MET	SER	GLU	MET	S5	L8	H9	I10	G11	D12	I13	V14	S15	L16	Y17	A18	E19	G20	S21	V22	M23	G24	F25	I26	S27	T28	L29	G30	L31	V32	D33	D34	R35	C36	V37	V38	E39	P40	A41	A42	G43	D44	L45	D46	N47	P48	P49	K109	K110	K51	F52	R53	D54	G55	L56	F57	R58	K59	C60	P61
M62	M63	R64	V65	S66	A67	Q68	K69	Q70	Y71	W72	K73	A74	K75	Q76	T77	LYS	GLN	ASP	LYS	GLU	LYS	ILE	A85	D86	W87	V88	L89	L90	Q91	R92	L93	Q94	H95	A96	Q98	M99	E100	Q101	K102	Q103	M104	D105	T106	E107	M108	K109	K168	L170	V111	H112	G113	D114	V115	V116	K117	Y118	G119	S120	V121
I122	Q123	L124	L125	H126	M127	K128	S129	M130	K131	Y132	L133	T134	V135	M136	K137	R138	L139	P140	L201	A141	L142	L143	E144	K145	N146	A147	M148	R149	V150	T151	L152	D153	M154	L155	L156	M157	E158	G159	S160	W161	L162	F163	I164	Q165	P166	F167	W168	K169	L170	R171	S172	M173	G174	D175	M176	V177	V178	G180	D181
K182	V183	I184	L185	N186	P187	V188	M189	A190	G191	P192	L193	L194	H195	A196	S197	N198	Y199	E200	L201	S202	D203	M204	A205	G206	C207	K208	E209	V210	M211	S212	L213	M214	C215	M216	T217	S218	I221	N222	L223	F224	M225	Q226	F227	R228	D229	H230	L231	E232	E233	V234	L235	K236	G237	G238	D239	V240	V241	R242	
L243	F244	H245	A246	E249	K250	F251	L252	T253	C254	D255	E256	Y257	K258	G259	K260	L261	Q262	V263	F264	L265	R266	T267	T268	L269	R270	Q271	S272	A273	T274	S275	A276	T277	S278	S279	N280	A281	L282	W283	E284	V285	E286	V287	V288	H289	H290	D291	P292	C293	R294	G295	G296	A297	M300	N301	G302	L303	Y304		

R305	F306	K307	H308	L309	A310	T311	G312	N313	Y314	E318	E319	N320	SER	TYR	LYS	GLY	ASP	ALA	SER	ASP	PRO	LYS	ALA	ALA	GLY	MET	GLY	ALA	GLN	GLY	ARG	ARG	ASN	ALA	GLY	GLU	L350	K351	L354	V355	A356	V357	P358	H359	G360	N361	D362	I363	A364	S365	L366	F367								
E368	L369	D370	P371	T372	T373	L374	Q375	K376	T377	D378	S379	F380	V381	P382	R383	N384	S385	A448	Y386	V387	R388	L389	R390	H391	L392	C393	T394	N395	T396	V397	I398	Q399	S400	T401	M402	V403	P404	I405	D406	I407	E408	E409	E410	R411	P412	I413	R414	L415	M416	L417	G418	T419	C420	K423	E424	D425	E427			
A428	F429	A430	P435	V436	S437	E438	I439	R440	D441	L442	D443	F444	A445	N446	D447	S448	S449	S450	M451	L452	A453	S454	A455	V456	E457	K458	L459	M460	E461	G462	F463	I464	S465	Q466	D468	R469	R470	F471	V472	I473	Q474	L475	L476	E477	D478	L479	V480	F481	F482	V483	S484	D485	V486	P487	M488	M489	G490			
Q491	M492	V493	L494	D495	M497	V498	T499	K500	P501	N502	R503	E504	Q505	Q506	K507	L508	M509	R510	E511	Q512	N513	I514	L515	K516	Q517	V518	L519	G520	I521	L522	K523	P525	F526	GLU	LYS	GLY	GLY	GLY	P534	L535	V536	R537	L538	E539	E540	L541	N601	S642	D543	Q544	K545	N546	A547	P548	Y549	Q550				
H551	M552	F553	R554	L555	C556	Y557	R558	V559	L560	H561	H562	S563	Q564	F565	D566	Y567	R568	K569	N570	Q571	E572	H573	I574	A575	K576	Q577	F578	G579	M580	M581	Q582	S583	Q584	I585	G586	Y587	D588	I589	L590	A591	E592	D593	T594	I595	T596	A597	L598	L599	H600	N601	N602	R603	K604	L605	L606	E607	K608	H609	I610	
T611	K612	T613	E616	T617	F618	V619	S620	L621	V622	R623	K624	N625	R626	E627	P628	R629	F630	L631	D632	V633	L634	S635	D636	L637	C638	V639	S640	N641	H642	I643	A644	I645	P646	V647	T648	Q649	L651	I652	C653	K654	C655	V656	L657	D658	P659	K660	N661	S662	D663	I664	L665	I666	T667	E668	S669	L670	R671			
P672	V673	K674	GLU	MET	ALA	GLN	SER	HIS	A800	TYR	LEU	SER	ILE	GLU	TYR	SER	GLU	GLU	E691	V692	M693	L694	T695	V696	L697	L700	L701	E702	H703	H704	E705	K706	S707	V708	R709	Q710	L711	A712	E714	A715	R716	A717	G718	M719	A720	H721	D722	E723	N724	V725	L726	S727	Y728	Y729	R730	Y731				
Q732	L733	K734	L735	F736	A737	R738	M739	C740	L741	D742	R743	V745	L746	A747	L748	D749	E750	I751	S752	T753	Q754	L755	D758	L759	I760	F761	L762	C763	M764	A765	D766	E767	M768	L769	P770	F771	D772	L773	R774	A775	S776	F777	C778	H779	L780	M781	L782	H783	V784	H785	V786	D787	R788	D789	Q791	E792				
L793	W794	T795	P796	K798	F799	A800	R801	L802	H803	T804	E805	L806	P807	T808	I810	T811	L812	K813	F814	Y815	D816	S817	N818	L819	I820	A821	S822	R823	D824	D825	K826	K827	L828	G829	I831	H832	T833	H834	E835	F836	H837	E838	D839	Y840	L841	N842	H843	V844	H845	S846	E847	A848	V849	P850	F851	A852				
M853	E854	E855	K856	N857	K858	L859	T860	F861	E862	V863	V864	S865	L866	A867	L870	I871	V872	F873	G874	F875	Y876	S877	R878	S879	E880	L881	L882	L884	T885	T887	L888	L889	G890	I891	I892	D893	V963	V964	M965	E966	T967	K968	L969	K970	I971	L972	E973													
ARG	ARG	SER	ILE	GLN	GLY	VAL	GLY	HIS	MET	SER	THR	MET	VAL	LEU	SER	ARG	LYS	GLN	SER	VAL	PHE	SER	ALA	PRO	LEU	LEU	ASP	ARG	SER	LYS	PHE	GLU	GLU	ASN	D961	I962	V963	V964	M965	E966	T967	K968	L969	K970	I971	L972	E973													
I974	L975	Q976	F977	I978	L979	N980	V981	L983	D984	R985	R986	I987	S988	Y989	L990	L991	S992	V993	F994	K995	X996	F997	F998	V999	E1000	V1001	F1002	PRO	MET	GLN	ASP	GLY	ALA	ASP	GLY	ALA	THR	THR	ALA	ASN	PRO	ALA	PHE	ASP	SER	THR	THR	ALA	ASN	MET	M1024	L1025	D1026	I1027	I1028	G1029	E1030	Q1031	M1032	M1033
A1034	M1035	F1036	G1037	VAL	GLY	LYS	THR	SER	M1043	M1044	L1045	E1046	V1047	D1048	D1049	E1050	R1053	M1054	F1055	L1056	R1057	V1058	L1059	I1060	H1061	L1062	T1063	M1064	H1065	D1066	Y1067	A1068	P1069	L1070	V1071	S1072	G1073	A1074	L1075	Q1076	L1077	L1078	F1079	K1080	H1081	F1082	S1083	Q1084	R1085	Q1086	E1087	M1088	H1089	T1091	F1092	K1093	Q1094			

PRO	GLU	GLY	PHE	LEU	PRO	PRO	GLY	SER	S1166	GLU	D1215	C1275	F1335	D1395	ARG	Q1463	A1541	Y1635	L1695	G1755	M1863
HIS	GLY	GLU	ASP	LEU	PRO	PRO	GLY	SER	E1167	GLY	K1216	S1276	S1335	V1395	GLU	Q1464	F1542	Q1635	Q1696	L1755	G1864
ASP	PHE	LEU	HIS	LEU	PRO	PRO	GLY	SER	E1167	GLU	G1217	S1277	M1337	V1397	LYS	Q1465	F1543	R1637	Q1697	L1756	G1984
GLU	PHE	LEU	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	D1218	I1278	M1338	S1398	VAL	H1466	R1544	C1638	ASN	A1757	M1984
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	A1219	I1278	K1339	V1399	VAL	K1467	R1545	E1639	ARG	A1758	M1985
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	A1220	I1279	K1340	V1400	VAL	K1468	R1546	E1640	THR	A1759	M1986
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	M1221	V1282	S1341	T1401	VAL	V1469	T1548	G1641	THR	A1760	M1987
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	M1222	V1283	S1342	T1402	VAL	V1470	T1549	G1642	THR	A1761	M1988
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	E1223	L1283	A1343	H1403	VAL	E1471	A1549	F1643	THR	A1762	M1989
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1224	Q1284	H1344	D1404	VAL	E1472	M1550	L1644	THR	A1763	M1990
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1225	H1285	L1345	C1405	VAL	I1474	V1552	S1645	PRO	A1764	M1991
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1226	F1286	D1346	C1405	VAL	I1474	V1552	S1646	PRO	A1765	M1992
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	R1226	F1287	D1347	C1405	VAL	I1474	V1552	S1647	PRO	A1766	M1993
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1227	H1288	D1348	C1405	VAL	I1474	V1552	S1648	PRO	A1767	M1994
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	T1228	L1289	M1349	C1405	VAL	I1474	V1552	S1649	PRO	A1768	M1995
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	H1229	L1290	M1349	C1405	VAL	I1474	V1552	S1650	PRO	A1769	M1996
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	Q1230	A1291	M1350	C1405	VAL	I1474	V1552	S1651	PRO	A1770	M1997
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	F1231	T1292	M1350	C1405	VAL	I1474	V1552	S1652	PRO	A1771	M1998
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	F1232	H1293	M1351	C1405	VAL	I1474	V1552	S1653	PRO	A1772	M1999
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	Q1233	H1293	M1352	C1405	VAL	I1474	V1552	S1654	PRO	A1773	M2000
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	K1234	G1294	M1353	C1405	VAL	I1474	V1552	S1655	PRO	A1774	M2001
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	F1235	R1295	M1354	C1405	VAL	I1474	V1552	S1656	PRO	A1775	M2002
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	C1236	H1296	M1355	C1405	VAL	I1474	V1552	S1657	PRO	A1776	M2003
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	A1237	V1297	M1356	C1405	VAL	I1474	V1552	S1658	PRO	A1777	M2004
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	G1238	Y1299	M1357	C1405	VAL	I1474	V1552	S1659	PRO	A1778	M2005
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	M1239	L1300	M1358	C1405	VAL	I1474	V1552	S1660	PRO	A1779	M2006
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	P1240	D1301	M1359	C1405	VAL	I1474	V1552	S1661	PRO	A1780	M2007
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	G1241	F1302	M1360	C1405	VAL	I1474	V1552	S1662	PRO	A1781	M2008
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	G1242	L1303	M1361	C1405	VAL	I1474	V1552	S1663	PRO	A1782	M2009
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	Q1243	L1303	M1362	C1405	VAL	I1474	V1552	S1664	PRO	A1783	M2010
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	A1244	H1304	M1363	C1405	VAL	I1474	V1552	S1665	PRO	A1784	M2011
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1245	T1305	M1364	C1405	VAL	I1474	V1552	S1666	PRO	A1785	M2012
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1246	V1306	M1365	C1405	VAL	I1474	V1552	S1667	PRO	A1786	M2013
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1247	I1307	M1366	C1405	VAL	I1474	V1552	S1668	PRO	A1787	M2014
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	H1247	K1308	M1367	C1405	VAL	I1474	V1552	S1669	PRO	A1788	M2015
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	K1248	A1309	M1368	C1405	VAL	I1474	V1552	S1670	PRO	A1789	M2016
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	H1249	H1310	M1369	C1405	VAL	I1474	V1552	S1671	PRO	A1790	M2017
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	H1250	E1311	M1370	C1405	VAL	I1474	V1552	S1672	PRO	A1791	M2018
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1252	L1312	M1371	C1405	VAL	I1474	V1552	S1673	PRO	A1792	M2019
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	F1253	Y1313	M1372	C1405	VAL	I1474	V1552	S1674	PRO	A1793	M2020
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1254	V1314	M1373	C1405	VAL	I1474	V1552	S1675	PRO	A1794	M2021
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	T1255	K1315	M1374	C1405	VAL	I1474	V1552	S1676	PRO	A1795	M2022
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	P1256	K1316	M1375	C1405	VAL	I1474	V1552	S1677	PRO	A1796	M2023
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	P1257	C1317	M1376	C1405	VAL	I1474	V1552	S1678	PRO	A1797	M2024
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1258	Q1318	M1377	C1405	VAL	I1474	V1552	S1679	PRO	A1798	M2025
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1259	D1319	M1378	C1405	VAL	I1474	V1552	S1680	PRO	A1799	M2026
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1260	M1320	M1379	C1405	VAL	I1474	V1552	S1681	PRO	A1800	M2027
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	A1261	I1321	M1380	C1405	VAL	I1474	V1552	S1682	PRO	A1801	M2028
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	E1262	M1322	M1381	C1405	VAL	I1474	V1552	S1683	PRO	A1802	M2029
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	T1263	L1323	M1382	C1405	VAL	I1474	V1552	S1684	PRO	A1803	M2030
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	M1264	E1324	M1383	C1405	VAL	I1474	V1552	S1685	PRO	A1804	M2031
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	Q1265	L1325	M1384	C1405	VAL	I1474	V1552	S1686	PRO	A1805	M2032
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	H1266	T1326	M1385	C1405	VAL	I1474	V1552	S1687	PRO	A1806	M2033
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	I1267	M1327	M1386	C1405	VAL	I1474	V1552	S1688	PRO	A1807	M2034
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	I1268	A1328	M1387	C1405	VAL	I1474	V1552	S1689	PRO	A1808	M2035
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1269	G1329	M1388	C1405	VAL	I1474	V1552	S1690	PRO	A1809	M2036
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	M1270	D1330	M1389	C1405	VAL	I1474	V1552	S1691	PRO	A1810	M2037
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	M1271	D1331	M1390	C1405	VAL	I1474	V1552	S1692	PRO	A1811	M2038
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	V1272	V1332	M1391	C1405	VAL	I1474	V1552	S1693	PRO	A1812	M2039
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	Q1273	V1333	M1392	C1405	VAL	I1474	V1552	S1694	PRO	A1813	M2040
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	L1274	V1334	M1393	C1405	VAL	I1474	V1552	S1695	PRO	A1814	M2041
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	ASP	ASP	M1863	C1405	VAL	I1474	V1552	S1696	PRO	A1815	M2042
GLY	PRO	PRO	PRO	PRO	PRO	PRO	GLY	SER	E1167	GLU	LYS	LYS	G1864	C1405	VAL	I1474	V1552	S1697			



R1875	F1876	L1877	Q1878	L1879	C1881	E1882	H1883	H1884	H1885	R1886	D1887	L1888	Q1889	H1890	F1891	L1892	R1893	C1894	Q1895	H1896	H1897	K1898	T1899	H1900	Y1901	H1902	L1903	H1904	C1905	E1906	T1907	L1908	Q1909	F1910	L1911	D1912	I1913	H1914	G1915	G1916	S1917	T1918	T1919	G1920	G1921	L1922	G1923	L1924	L1925	G1926	L1927	I1928	I1929	H1930	E1931	D1932	H1933	Y1934				
G1935	L1936	Y1937	I1938	Q1939	L1941	E1942	T1943	L1944	T1945	E1946	Y1947	C1948	Q1949	G1950	P1951	C1952	H1953	E1954	H1955	Q1956	T1957	C1958	I1959	V1960	T1961	H1962	E1963	L1964	H1965	G1966	I1967	D1968	L1969	I1970	F1971	A1972	L1973	I1974	L1975	N1976	D1977	R2008	E2009	P1980	L1981	G1920	C1982	L1983	Y1984	R1985	H1986	D1987	L1988	V1989	L1990	Q1991	L1992	K1993	D1994			
M1995	K1996	L2000	L2001	A2002	L2003	M2004	E2005	S2006	R2007	H2008	D2009	S2010	E2011	N2012	A2013	E2014	R2015	I2016	L2017	I2018	S2019	L2020	R2021	P2022	Q2023	E2024	L2025	V2026	D2027	V2028	I2029	K2030	L2031	A2032	Y2033	L2034	Q2035	E2036	E2037	E2038	R2039	E2040	N2041	E2042	S2043	V2044	S2045	P2046	R2047	E2048	V2049	G2050	H2051	N2052	L1992	Y2054	I2055					
L2056	A2057	L2058	L2060	S2061	H2062	M2064	K2065	Q2066	Q2067	Q2068	H2069	L2070	L2071	K2072	P2073	V2074	LYS	ARG	ILE	GLN	GLU	S2019	L2020	GLU	GLY	ILE	Q2023	SER	MET	LEU	SER	LEU	ASN	LYS	GLN	SER	GLN	MET	L2034	L2035	L2036	SER	ALA	PRO	E2111	D2112	A2115	Y2116														
Y2117	E2118	N2119	H2120	T2121	S2122	Q2123	I2124	E2125	I2126	R2127	Q2128	Q2129	D2130	R2131	S2132	M2133	E2134	Q2135	I2136	V2137	F2138	P2139	V2140	P2141	G2142	I2143	C2144	Q2145	L2147	T2148	E2149	E2150	T2151	K2152	H2153	R2154	L2155	F2156	T2157	T2158	T2159	E2160	Q2161	D2162	E2163	Q2164	G2165	K2166	S2167	V2168	S2169	D2170	F2171	D2172	D2173	Q2174	S2175	S2176				
F2177	L2178	H2179	N2180	E2181	N2182	E2183	N2184	Q2185	R2186	K2187	L2188	L2189	S2190	N2191	P2192	L2193	I2194	Y2195	N2196	F2197	S2198	R2199	R2200	H2201	T2202	L2203	W2204	G2205	S2206	I2207	S2208	F2209	N2210	L2211	A2212	I2215	N2216	I2217	I2218	I2219	A2220	F2221	F2222	V2223	P2224	V2225	N2226	GLU	GLY	ALA	SER	THR	VAL	LEU	ASP	PRO						
L2231	I2232	S2233	L2234	L2235	F2236	W2237	I2238	L2239	I2240	C2241	F2242	S2243	I2244	A2245	A2246	L2247	F2248	T2249	K2250	R2251	Y2252	S2260	I2261	R2262	P2263	L2264	I2265	V2266	A2267	L2268	I2269	L2270	R2271	S2272	I2273	Y2274	I2275	L2276	G2277	I2278	P2280	L2281	N2283	I2284	L2285	G2286	A2287	L2288	N2289	L2290	T2291	N2292	K2293	L2294	V2295	F2296	V2297					
V2298	S2299	F2300	V2301	G2302	N2303	R2304	G2305	T2306	F2307	I2308	R2309	G2310	Y2311	K2312	A2313	M2314	V2315	M2316	T2317	M2318	E2319	F2320	L2321	Y2322	H2323	V2324	G2325	Y2326	L2327	L2328	T2329	S2330	V2331	L2332	G2333	L2334	F2335	A2336	H2337	E2338	L2339	F2340	Y2341	S2342	L2343	L2344	L2345	F2346	D2347	L2348	I2349	Y2350	N2351	E2352	E2353	T2354	L2355	F2356	N2357			
V2358	I2359	K2360	S2361	V2362	T2363	R2364	N2365	G2366	R2367	S2368	I2369	L2370	L2371	T2372	A2373	L2374	L2375	A2376	L2377	I2378	L2379	V2380	Y2381	L2382	F2383	S2384	L2385	V2386	G2387	F2388	L2389	F2390	L2391	K2392	D2393	D2394	F2395	I2396	L2397	E2398	V2399	D2400	R2401	L2402	P2403	ASN	ASN	HIS	SER	THR	ALA	SER	PRO	PRO	LEU	GLY	MET	PRO	HIS	L2355	F2356	N2357
ALA	ALA	ALA	PHE	VAL	ASP	THR	CYS	SER	GLY	ASP	LYS	ASP	ASP	CYS	VAL	GLY	LEU	VAL	PRO	GLU	VAL	LEU	GLU	GLU	D2449	D2450	T2451	E2452	R2453	A2454	C2455	D2456	T2457	L2458	L2459	M2460	C2461	I2462	V2463	T2464	V2465	M2466	N2467	H2468	G2469	L2470	R2471	N2472	G2473	G2474	G2475	V2476	G2477									
D2478	I2479	L2480	R2481	K2482	P2483	S2484	K2485	D2486	E2487	S2488	L2489	F2490	P2491	A2492	R2493	V2494	V2495	Y2496	D2497	L2498	L2499	F2500	F2501	F2502	I2503	V2504	I2505	L2506	I2507	V2508	L2509	N2510	L2511	L2512	F2513	G2514	V2515	L2516	L2517	D2518	T2519	F2520	A2521	R2522	L2523	R2524	S2525	E2526	K2527	Q2528	K2529	K2530	E2531	E2532	L2533	L2534	K2535	T2536	T2537			
C2538	P2539	I2540	C2541	G2542	L2543	E2544	R2545	D2546	K2547	F2548	D2549	N2550	K2551	T2552	V2553	S2554	F2555	E2556	I2559	K2560	H2563	N2564	M2565	W2566	N2567	Y2568	L2569	Y2570	F2571	I2572	V2573	L2574	V2575	R2576	V2577	K2578	N2579	K2580	T2581	D2582	Y2583	T2584	E2587	S2588	Y2589	V2590	A2591	Q2592	M2593	I2594	K2595	N2596	K2597	N2598	L2599	D2600						
W2601	F2602	P2603	R2604	N2605	R2606	A2607	N2608	S2609	L2610	L2611	SER	ASN	GLY	GLU	GLY	GLY	GLU	ASN	GLU	ILE	ARG	ILE	LEU	GLN	ASP	LYS	LEU	ASN	THR	MET	LYS	LEU	VAL	SER	HIS	LEU	THR	ALA	GLN	LEU	ASN	GLU	GLY	LEU	THR	GLN	ARG	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, C4	Depositor
Number of particles used	26325	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	Not provided	
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	34.630	Depositor
Minimum map value	-19.505	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.473	Depositor
Recommended contour level	5.72	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

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	0.38	0/17606	0.51	4/23791 (0.0%)
1	B	0.38	0/17606	0.51	4/23791 (0.0%)
1	C	0.38	0/17606	0.51	4/23791 (0.0%)
1	D	0.38	0/17606	0.51	4/23791 (0.0%)
All	All	0.38	0/70424	0.51	16/95164 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1494	PRO	N-CA-CB	5.60	110.02	103.30
1	C	1494	PRO	N-CA-CB	5.60	110.02	103.30
1	A	1547	PRO	N-CA-CB	5.59	110.00	103.30
1	D	1494	PRO	N-CA-CB	5.57	109.99	103.30
1	B	1547	PRO	N-CA-CB	5.57	109.98	103.30
1	C	1547	PRO	N-CA-CB	5.57	109.98	103.30
1	D	1547	PRO	N-CA-CB	5.57	109.98	103.30
1	A	1494	PRO	N-CA-CB	5.55	109.96	103.30
1	B	1543	PRO	N-CA-CB	5.37	109.74	103.30
1	C	1543	PRO	N-CA-CB	5.37	109.74	103.30
1	D	1543	PRO	N-CA-CB	5.37	109.74	103.30
1	A	1543	PRO	N-CA-CB	5.36	109.73	103.30
1	A	1436	PRO	N-CA-CB	5.10	109.42	103.30
1	B	1436	PRO	N-CA-CB	5.10	109.42	103.30
1	C	1436	PRO	N-CA-CB	5.10	109.42	103.30
1	D	1436	PRO	N-CA-CB	5.10	109.42	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	17302	17316	17145	132	0
1	B	17302	17317	17145	136	0
1	C	17302	17316	17145	135	0
1	D	17302	17316	17145	131	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
All	All	69212	69265	68580	520	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 4.

All (520) 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:764:MET:O	1:A:774:ARG:NH1	2.20	0.74
1:C:764:MET:O	1:C:774:ARG:NH1	2.20	0.74
1:C:1619:ASP:OD2	1:C:1687:ARG:NH2	2.20	0.74
1:B:764:MET:O	1:B:774:ARG:NH1	2.20	0.74
1:D:764:MET:O	1:D:774:ARG:NH1	2.20	0.74
1:A:1619:ASP:OD2	1:A:1687:ARG:NH2	2.20	0.73
1:C:144:GLU:OE2	1:C:211:ASN:ND2	2.22	0.73
1:D:1619:ASP:OD2	1:D:1687:ARG:NH2	2.20	0.73
1:B:1619:ASP:OD2	1:B:1687:ARG:NH2	2.20	0.73
1:A:144:GLU:OE2	1:A:211:ASN:ND2	2.22	0.73
1:D:144:GLU:OE2	1:D:211:ASN:ND2	2.22	0.73
1:C:27:SER:OG	1:C:54:ASP:OD2	2.06	0.73
1:B:27:SER:OG	1:B:54:ASP:OD2	2.06	0.72
1:C:743:ARG:NH2	1:C:788:ARG:O	2.23	0.72
1:B:144:GLU:OE2	1:B:211:ASN:ND2	2.22	0.72
1:A:1735:LYS:NZ	1:A:1779:ASP:OD2	2.23	0.71
1:D:743:ARG:NH2	1:D:788:ARG:O	2.23	0.71
1:B:743:ARG:NH2	1:B:788:ARG:O	2.23	0.71
1:D:1735:LYS:NZ	1:D:1779:ASP:OD2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1735:LYS:NZ	1:B:1779:ASP:OD2	2.23	0.71
1:C:1735:LYS:NZ	1:C:1779:ASP:OD2	2.23	0.71
1:A:27:SER:OG	1:A:54:ASP:OD2	2.06	0.71
1:A:743:ARG:NH2	1:A:788:ARG:O	2.23	0.70
1:D:798:LYS:O	1:D:801:ARG:NH1	2.24	0.70
1:D:27:SER:OG	1:D:54:ASP:OD2	2.06	0.70
1:D:540:GLU:O	1:D:546:ASN:ND2	2.25	0.70
1:B:798:LYS:O	1:B:801:ARG:NH1	2.24	0.70
1:A:540:GLU:O	1:A:546:ASN:ND2	2.25	0.70
1:C:540:GLU:O	1:C:546:ASN:ND2	2.25	0.70
1:C:798:LYS:O	1:C:801:ARG:NH1	2.24	0.70
1:B:1783:GLU:OE1	1:B:1899:THR:OG1	2.10	0.70
1:D:1783:GLU:OE1	1:D:1899:THR:OG1	2.10	0.69
1:C:1783:GLU:OE1	1:C:1899:THR:OG1	2.10	0.69
1:A:798:LYS:O	1:A:801:ARG:NH1	2.24	0.69
1:D:2467:ASN:OD1	1:D:2471:ARG:NH1	2.26	0.69
1:A:1783:GLU:OE1	1:A:1899:THR:OG1	2.10	0.69
1:B:2467:ASN:OD1	1:B:2471:ARG:NH1	2.26	0.69
1:A:886:ARG:NE	1:A:1049:ASP:OD1	2.26	0.69
1:B:540:GLU:O	1:B:546:ASN:ND2	2.25	0.68
1:C:886:ARG:NE	1:C:1049:ASP:OD1	2.26	0.68
1:C:2467:ASN:OD1	1:C:2471:ARG:NH1	2.26	0.68
1:A:2467:ASN:OD1	1:A:2471:ARG:NH1	2.26	0.68
1:B:886:ARG:NE	1:B:1049:ASP:OD1	2.26	0.67
1:D:886:ARG:NE	1:D:1049:ASP:OD1	2.26	0.67
1:B:1895:GLN:O	1:B:1900:ASN:ND2	2.27	0.67
1:C:410:GLU:OE1	1:C:410:GLU:N	2.27	0.67
1:C:1895:GLN:O	1:C:1900:ASN:ND2	2.27	0.67
1:D:1895:GLN:O	1:D:1900:ASN:ND2	2.27	0.67
1:A:410:GLU:N	1:A:410:GLU:OE1	2.27	0.67
1:D:410:GLU:N	1:D:410:GLU:OE1	2.27	0.67
1:B:19:GLU:OE1	1:B:182:LYS:NZ	2.20	0.67
1:C:19:GLU:OE1	1:C:182:LYS:NZ	2.20	0.67
1:C:1180:ASN:O	1:C:1234:LYS:NZ	2.28	0.67
1:A:1895:GLN:O	1:A:1900:ASN:ND2	2.27	0.67
1:B:410:GLU:N	1:B:410:GLU:OE1	2.27	0.66
1:B:233:GLU:OE1	1:B:233:GLU:N	2.29	0.66
1:A:1180:ASN:O	1:A:1234:LYS:NZ	2.28	0.66
1:D:19:GLU:OE1	1:D:182:LYS:NZ	2.20	0.66
1:B:1180:ASN:O	1:B:1234:LYS:NZ	2.28	0.66
1:A:233:GLU:N	1:A:233:GLU:OE1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1180:ASN:O	1:D:1234:LYS:NZ	2.28	0.66
1:D:233:GLU:OE1	1:D:233:GLU:N	2.29	0.65
1:C:233:GLU:N	1:C:233:GLU:OE1	2.29	0.65
1:A:2163:GLU:O	1:B:2545:ARG:NH1	2.31	0.64
1:C:2484:SER:HB2	1:D:2399:VAL:HG21	1.82	0.62
1:C:2358:VAL:O	1:C:2361:SER:OG	2.08	0.62
1:A:2545:ARG:NH1	1:D:2163:GLU:O	2.33	0.61
1:C:2163:GLU:O	1:D:2545:ARG:NH1	2.33	0.61
1:D:2024:GLU:OE1	1:D:2024:GLU:N	2.34	0.61
1:C:2024:GLU:N	1:C:2024:GLU:OE1	2.34	0.61
1:B:2163:GLU:O	1:C:2545:ARG:NH1	2.33	0.61
1:B:2484:SER:HB2	1:C:2399:VAL:HG21	1.82	0.61
1:C:1307:ILE:HD11	1:C:1318:GLN:HB3	1.83	0.61
1:A:2024:GLU:N	1:A:2024:GLU:OE1	2.34	0.60
1:A:2484:SER:HB2	1:B:2399:VAL:HG21	1.83	0.60
1:B:1203:HIS:CE1	1:B:1245:LEU:HD21	2.36	0.60
1:D:1307:ILE:HD11	1:D:1318:GLN:HB3	1.83	0.60
1:C:255:ASP:OD1	1:C:256:GLU:N	2.35	0.60
1:A:1307:ILE:HD11	1:A:1318:GLN:HB3	1.83	0.60
1:B:2024:GLU:OE1	1:B:2024:GLU:N	2.34	0.60
1:D:255:ASP:OD1	1:D:256:GLU:N	2.35	0.60
1:A:1203:HIS:CE1	1:A:1245:LEU:HD21	2.36	0.60
1:C:1203:HIS:CE1	1:C:1245:LEU:HD21	2.36	0.60
1:C:19:GLU:O	1:C:218:SER:OG	2.20	0.60
1:B:16:LEU:HD12	1:B:26:ILE:HD12	1.84	0.59
1:B:1307:ILE:HD11	1:B:1318:GLN:HB3	1.83	0.59
1:C:68:GLN:N	1:C:68:GLN:OE1	2.35	0.59
1:C:482:PHE:O	1:C:505:ARG:NH1	2.35	0.59
1:D:1203:HIS:CE1	1:D:1245:LEU:HD21	2.36	0.59
1:D:19:GLU:O	1:D:218:SER:OG	2.20	0.59
1:B:68:GLN:OE1	1:B:68:GLN:N	2.35	0.59
1:B:19:GLU:O	1:B:218:SER:OG	2.20	0.59
1:C:16:LEU:HD12	1:C:26:ILE:HD12	1.85	0.59
1:A:68:GLN:N	1:A:68:GLN:OE1	2.35	0.59
1:B:482:PHE:O	1:B:505:ARG:NH1	2.35	0.59
1:D:482:PHE:O	1:D:505:ARG:NH1	2.35	0.59
1:A:255:ASP:OD1	1:A:256:GLU:N	2.35	0.58
1:D:16:LEU:HD12	1:D:26:ILE:HD12	1.85	0.58
1:A:482:PHE:O	1:A:505:ARG:NH1	2.35	0.58
1:A:1767:GLU:N	1:A:1767:GLU:OE1	2.36	0.58
1:B:854:GLU:N	1:B:854:GLU:OE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1767:GLU:N	1:C:1767:GLU:OE1	2.36	0.58
1:D:1767:GLU:OE1	1:D:1767:GLU:N	2.36	0.58
1:A:854:GLU:N	1:A:854:GLU:OE1	2.37	0.58
1:B:255:ASP:OD1	1:B:256:GLU:N	2.35	0.58
1:D:68:GLN:OE1	1:D:68:GLN:N	2.35	0.58
1:A:16:LEU:HD12	1:A:26:ILE:HD12	1.84	0.58
1:A:19:GLU:OE1	1:A:182:LYS:NZ	2.20	0.58
1:A:19:GLU:O	1:A:218:SER:OG	2.20	0.58
1:C:854:GLU:OE1	1:C:854:GLU:N	2.37	0.57
1:A:2399:VAL:HG21	1:D:2484:SER:HB2	1.86	0.57
1:B:1767:GLU:N	1:B:1767:GLU:OE1	2.36	0.57
1:D:854:GLU:N	1:D:854:GLU:OE1	2.37	0.57
1:A:2518:ASP:OD1	1:B:2524:ARG:NE	2.34	0.57
1:B:408:GLU:N	1:B:408:GLU:OE1	2.38	0.57
1:C:408:GLU:OE1	1:C:408:GLU:N	2.38	0.57
1:D:408:GLU:N	1:D:408:GLU:OE1	2.38	0.57
1:C:2037:GLU:N	1:C:2037:GLU:OE1	2.38	0.56
1:D:2037:GLU:OE1	1:D:2037:GLU:N	2.38	0.56
1:A:2037:GLU:N	1:A:2037:GLU:OE1	2.38	0.56
1:A:400:SER:HA	1:A:417:LEU:HD12	1.88	0.56
1:D:400:SER:HA	1:D:417:LEU:HD12	1.88	0.56
1:B:2037:GLU:N	1:B:2037:GLU:OE1	2.38	0.56
1:A:2269:ILE:CD1	1:A:2285:LEU:HD11	2.36	0.56
1:C:2269:ILE:CD1	1:C:2285:LEU:HD11	2.36	0.56
1:C:400:SER:HA	1:C:417:LEU:HD12	1.88	0.56
1:C:2518:ASP:OD1	1:D:2524:ARG:NE	2.37	0.56
1:A:408:GLU:OE1	1:A:408:GLU:N	2.38	0.55
1:B:2269:ILE:CD1	1:B:2285:LEU:HD11	2.36	0.55
1:C:691:GLU:N	1:C:691:GLU:OE1	2.40	0.55
1:A:691:GLU:N	1:A:691:GLU:OE1	2.40	0.55
1:A:1911:LEU:HD23	1:A:1937:VAL:HG23	1.89	0.55
1:C:1911:LEU:HD23	1:C:1937:VAL:HG23	1.89	0.55
1:D:1336:TYR:HB2	1:D:1345:LEU:HD22	1.89	0.55
1:B:28:THR:OG1	1:B:54:ASP:OD1	2.22	0.55
1:D:2317:ASP:OD1	1:D:2318:MET:N	2.40	0.55
1:A:1336:TYR:HB2	1:A:1345:LEU:HD22	1.89	0.55
1:B:1298:GLN:OE1	1:B:1298:GLN:N	2.40	0.55
1:C:2064:ASN:OD1	1:C:2067:LEU:N	2.40	0.55
1:D:1911:LEU:HD23	1:D:1937:VAL:HG23	1.89	0.55
1:D:2269:ILE:CD1	1:D:2285:LEU:HD11	2.36	0.55
1:B:400:SER:HA	1:B:417:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1911:LEU:HD23	1:B:1937:VAL:HG23	1.89	0.55
1:D:2358:VAL:O	1:D:2361:SER:OG	2.08	0.55
1:A:2317:ASP:OD1	1:A:2318:MET:N	2.40	0.54
1:B:1336:TYR:HB2	1:B:1345:LEU:HD22	1.89	0.54
1:B:2064:ASN:OD1	1:B:2067:LEU:N	2.40	0.54
1:B:2518:ASP:OD1	1:C:2524:ARG:NE	2.37	0.54
1:B:691:GLU:OE1	1:B:691:GLU:N	2.40	0.54
1:C:1336:TYR:HB2	1:C:1345:LEU:HD22	1.89	0.54
1:C:591:ALA:O	1:C:595:ILE:HG22	2.08	0.54
1:D:691:GLU:N	1:D:691:GLU:OE1	2.40	0.54
1:D:1298:GLN:OE1	1:D:1298:GLN:N	2.40	0.54
1:A:2358:VAL:O	1:A:2361:SER:OG	2.08	0.54
1:D:591:ALA:O	1:D:595:ILE:HG22	2.08	0.54
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.40	0.54
1:A:591:ALA:O	1:A:595:ILE:HG22	2.08	0.54
1:D:28:THR:OG1	1:D:54:ASP:OD1	2.22	0.54
1:B:591:ALA:O	1:B:595:ILE:HG22	2.08	0.53
1:A:2064:ASN:OD1	1:A:2067:LEU:N	2.40	0.53
1:C:1298:GLN:N	1:C:1298:GLN:OE1	2.40	0.53
1:D:1755:GLY:O	1:D:1759:HIS:ND1	2.41	0.53
1:C:2317:ASP:OD1	1:C:2318:MET:N	2.40	0.53
1:B:1954:GLU:OE1	1:B:1954:GLU:N	2.42	0.53
1:D:118:TYR:OH	1:D:181:ASP:OD2	2.26	0.53
1:D:2064:ASN:OD1	1:D:2067:LEU:N	2.40	0.53
1:A:118:TYR:OH	1:A:181:ASP:OD2	2.26	0.52
1:C:1755:GLY:O	1:C:1759:HIS:ND1	2.41	0.52
1:A:47:ASN:O	1:A:47:ASN:ND2	2.43	0.52
1:B:47:ASN:ND2	1:B:47:ASN:O	2.43	0.52
1:B:2317:ASP:OD1	1:B:2318:MET:N	2.40	0.52
1:D:47:ASN:ND2	1:D:47:ASN:O	2.43	0.52
1:B:1932:ASP:OD1	1:B:1933:ASN:N	2.43	0.52
1:D:1932:ASP:OD1	1:D:1933:ASN:N	2.43	0.52
1:A:28:THR:OG1	1:A:54:ASP:OD1	2.22	0.52
1:B:2006:SER:OG	1:B:2134:GLU:OE1	2.20	0.52
1:A:1954:GLU:OE1	1:A:1954:GLU:N	2.42	0.52
1:C:1954:GLU:OE1	1:C:1954:GLU:N	2.42	0.52
1:A:1932:ASP:OD1	1:A:1933:ASN:N	2.43	0.52
1:A:2524:ARG:NE	1:D:2518:ASP:OD1	2.39	0.51
1:B:1755:GLY:O	1:B:1759:HIS:ND1	2.41	0.51
1:C:28:THR:OG1	1:C:54:ASP:OD1	2.22	0.51
1:C:1932:ASP:OD1	1:C:1933:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:GLU:N	1:A:750:GLU:OE1	2.43	0.51
1:A:2147:LEU:HD23	1:A:2152:LYS:CE	2.41	0.51
1:B:118:TYR:OH	1:B:181:ASP:OD2	2.26	0.51
1:C:47:ASN:O	1:C:47:ASN:ND2	2.43	0.51
1:A:1633:GLU:OE1	1:A:1633:GLU:N	2.43	0.51
1:B:2020:LEU:HD22	1:B:2025:LEU:HD21	1.93	0.51
1:C:2020:LEU:HD22	1:C:2025:LEU:HD21	1.93	0.51
1:A:1755:GLY:O	1:A:1759:HIS:ND1	2.41	0.51
1:B:1633:GLU:OE1	1:B:1633:GLU:N	2.43	0.51
1:D:2147:LEU:HD23	1:D:2152:LYS:CE	2.41	0.51
1:C:118:TYR:OH	1:C:181:ASP:OD2	2.26	0.51
1:D:750:GLU:OE1	1:D:750:GLU:N	2.43	0.51
1:A:2124:ILE:HD11	1:A:2568:TYR:CD1	2.46	0.51
1:D:1633:GLU:OE1	1:D:1633:GLU:N	2.43	0.51
1:B:750:GLU:OE1	1:B:750:GLU:N	2.43	0.51
1:B:1254:LEU:O	1:B:1285:HIS:NE2	2.44	0.51
1:B:2124:ILE:HD11	1:B:2568:TYR:CD1	2.46	0.51
1:B:2147:LEU:HD23	1:B:2152:LYS:CE	2.41	0.51
1:D:1954:GLU:N	1:D:1954:GLU:OE1	2.42	0.51
1:C:2124:ILE:HD11	1:C:2568:TYR:CD1	2.46	0.50
1:C:750:GLU:N	1:C:750:GLU:OE1	2.43	0.50
1:C:1254:LEU:O	1:C:1285:HIS:NE2	2.44	0.50
1:D:2549:ASP:OD1	1:D:2550:ASN:N	2.45	0.50
1:A:1218:ASP:OD1	1:A:1219:ALA:N	2.44	0.50
1:A:1254:LEU:O	1:A:1285:HIS:NE2	2.44	0.50
1:C:409:GLU:OE2	1:C:414:ARG:NH1	2.45	0.50
1:D:2020:LEU:HD22	1:D:2025:LEU:HD21	1.93	0.50
1:D:2054:TYR:CE2	1:D:2058:LEU:HD11	2.47	0.50
1:D:2124:ILE:HD11	1:D:2568:TYR:CD1	2.46	0.50
1:B:782:LEU:HD23	1:B:782:LEU:O	2.12	0.50
1:B:1218:ASP:OD1	1:B:1219:ALA:N	2.44	0.50
1:C:2054:TYR:CE2	1:C:2058:LEU:HD11	2.47	0.50
1:D:1218:ASP:OD1	1:D:1219:ALA:N	2.44	0.50
1:B:733:LEU:CD1	1:B:780:LEU:HD22	2.42	0.50
1:C:782:LEU:HD23	1:C:782:LEU:O	2.12	0.50
1:D:782:LEU:O	1:D:782:LEU:HD23	2.12	0.50
1:A:409:GLU:OE2	1:A:414:ARG:NH1	2.45	0.50
1:A:733:LEU:CD1	1:A:780:LEU:HD22	2.42	0.50
1:A:2054:TYR:CE2	1:A:2058:LEU:HD11	2.47	0.50
1:C:2147:LEU:HD23	1:C:2152:LYS:CE	2.41	0.50
1:B:409:GLU:OE2	1:B:414:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.44	0.49
1:D:1254:LEU:O	1:D:1285:HIS:NE2	2.44	0.49
1:A:197:SER:OG	1:A:198:ASN:N	2.46	0.49
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.44	0.49
1:A:2020:LEU:HD22	1:A:2025:LEU:HD21	1.93	0.49
1:C:197:SER:OG	1:C:198:ASN:N	2.46	0.49
1:B:197:SER:OG	1:B:198:ASN:N	2.46	0.49
1:C:733:LEU:CD1	1:C:780:LEU:HD22	2.42	0.49
1:C:1633:GLU:N	1:C:1633:GLU:OE1	2.43	0.49
1:D:409:GLU:OE2	1:D:414:ARG:NH1	2.45	0.49
1:B:2549:ASP:OD1	1:B:2550:ASN:N	2.45	0.49
1:B:2054:TYR:CE2	1:B:2058:LEU:HD11	2.47	0.49
1:B:2358:VAL:O	1:B:2361:SER:OG	2.08	0.48
1:C:1218:ASP:OD1	1:C:1219:ALA:N	2.44	0.48
1:C:2549:ASP:OD1	1:C:2550:ASN:N	2.45	0.48
1:D:733:LEU:CD1	1:D:780:LEU:HD22	2.42	0.48
1:B:2390:PHE:O	1:B:2391:LEU:HD23	2.14	0.48
1:C:272:SER:OG	1:C:273:ALA:N	2.46	0.48
1:A:2549:ASP:OD1	1:A:2550:ASN:N	2.45	0.48
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.44	0.48
1:C:2390:PHE:O	1:C:2391:LEU:HD23	2.14	0.48
1:A:2364:ARG:CD	1:A:2523:LEU:HD21	2.44	0.48
1:A:782:LEU:O	1:A:782:LEU:HD23	2.12	0.48
1:D:2364:ARG:CD	1:D:2523:LEU:HD21	2.44	0.48
1:A:976:GLN:OE1	1:A:980:ASN:ND2	2.46	0.48
1:B:272:SER:OG	1:B:273:ALA:N	2.46	0.48
1:D:272:SER:OG	1:D:273:ALA:N	2.46	0.48
1:C:976:GLN:OE1	1:C:980:ASN:ND2	2.46	0.48
1:C:1229:HIS:NE2	1:C:1260:GLU:OE2	2.47	0.48
1:C:2364:ARG:CD	1:C:2523:LEU:HD21	2.44	0.48
1:D:769:LEU:HD12	1:D:770:PRO:O	2.14	0.48
1:D:2390:PHE:O	1:D:2391:LEU:HD23	2.14	0.48
1:B:769:LEU:HD12	1:B:770:PRO:O	2.14	0.48
1:B:1117:LEU:HD21	1:B:1175:ILE:HG21	1.96	0.48
1:D:976:GLN:OE1	1:D:980:ASN:ND2	2.46	0.48
1:A:1117:LEU:HD21	1:A:1175:ILE:HG21	1.96	0.47
1:C:769:LEU:HD12	1:C:770:PRO:O	2.14	0.47
1:A:2390:PHE:O	1:A:2391:LEU:HD23	2.14	0.47
1:C:1097:LEU:HD12	1:C:1595:LEU:HD22	1.96	0.47
1:D:197:SER:OG	1:D:198:ASN:N	2.46	0.47
1:B:2364:ARG:CD	1:B:2523:LEU:HD21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1337:ASN:ND2	1:B:1395:ASP:OD2	2.47	0.47
1:D:1229:HIS:NE2	1:D:1260:GLU:OE2	2.47	0.47
1:D:1256:PRO:HA	1:D:1289:LEU:HD21	1.96	0.47
1:D:1337:ASN:ND2	1:D:1395:ASP:OD2	2.47	0.47
1:A:1229:HIS:NE2	1:A:1260:GLU:OE2	2.47	0.47
1:B:1097:LEU:HD12	1:B:1595:LEU:HD22	1.96	0.47
1:B:2364:ARG:HD3	1:B:2523:LEU:HD21	1.97	0.47
1:C:2364:ARG:HD3	1:C:2523:LEU:HD21	1.97	0.47
1:D:1617:LEU:HD23	1:D:1621:LEU:HD23	1.97	0.47
1:D:1647:LEU:O	1:D:1651:THR:OG1	2.32	0.47
1:A:1256:PRO:HA	1:A:1289:LEU:HD21	1.96	0.47
1:B:1229:HIS:NE2	1:B:1260:GLU:OE2	2.47	0.47
1:A:769:LEU:HD12	1:A:770:PRO:O	2.14	0.47
1:D:1097:LEU:HD12	1:D:1595:LEU:HD22	1.96	0.47
1:D:1280:GLU:OE2	1:D:1284:GLN:NE2	2.48	0.47
1:D:2364:ARG:HD3	1:D:2523:LEU:HD21	1.97	0.47
1:A:1280:GLU:OE2	1:A:1284:GLN:NE2	2.48	0.47
1:A:1337:ASN:ND2	1:A:1395:ASP:OD2	2.48	0.46
1:B:1647:LEU:O	1:B:1651:THR:OG1	2.32	0.46
1:C:1256:PRO:HA	1:C:1289:LEU:HD21	1.96	0.46
1:D:1616:VAL:HG21	1:D:1690:LEU:HD23	1.97	0.46
1:B:164:ILE:HD11	1:B:183:VAL:HG21	1.97	0.46
1:B:1280:GLU:OE2	1:B:1284:GLN:NE2	2.48	0.46
1:C:1616:VAL:HG21	1:C:1690:LEU:HD23	1.97	0.46
1:D:164:ILE:HD11	1:D:183:VAL:HG21	1.97	0.46
1:C:64:ARG:NH2	1:C:103:GLN:OE1	2.47	0.46
1:C:1337:ASN:ND2	1:C:1395:ASP:OD2	2.47	0.46
1:C:1394:GLU:N	1:C:1394:GLU:OE1	2.49	0.46
1:A:272:SER:OG	1:A:273:ALA:N	2.46	0.46
1:A:2364:ARG:HD3	1:A:2523:LEU:HD21	1.97	0.46
1:C:1617:LEU:HD23	1:C:1621:LEU:HD23	1.97	0.46
1:D:1117:LEU:HD21	1:D:1175:ILE:HG21	1.96	0.46
1:C:1280:GLU:OE2	1:C:1284:GLN:NE2	2.48	0.46
1:B:1256:PRO:HA	1:B:1289:LEU:HD21	1.96	0.46
1:B:1394:GLU:N	1:B:1394:GLU:OE1	2.49	0.46
1:C:1117:LEU:HD21	1:C:1175:ILE:HG21	1.96	0.46
1:A:1325:LEU:HD13	1:A:1325:LEU:O	2.16	0.46
1:B:1325:LEU:HD13	1:B:1325:LEU:O	2.16	0.46
1:B:1410:LYS:O	1:B:1414:VAL:HG23	2.16	0.46
1:D:1325:LEU:HD13	1:D:1325:LEU:O	2.16	0.46
1:A:1394:GLU:OE1	1:A:1394:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1617:LEU:HD23	1:B:1621:LEU:HD23	1.97	0.46
1:C:164:ILE:HD11	1:C:183:VAL:HG21	1.97	0.46
1:C:1647:LEU:O	1:C:1651:THR:OG1	2.32	0.46
1:D:1394:GLU:OE1	1:D:1394:GLU:N	2.49	0.46
1:A:1617:LEU:HD23	1:A:1621:LEU:HD23	1.97	0.46
1:A:2552:THR:HG23	1:A:2553:VAL:HG13	1.98	0.46
1:B:64:ARG:NH2	1:B:103:GLN:OE1	2.47	0.46
1:C:1325:LEU:HD13	1:C:1325:LEU:O	2.16	0.46
1:A:1097:LEU:HD12	1:A:1595:LEU:HD22	1.96	0.45
1:A:1616:VAL:HG21	1:A:1690:LEU:HD23	1.97	0.45
1:B:603:ARG:NH1	1:B:645:ILE:HD13	2.31	0.45
1:C:1410:LYS:O	1:C:1414:VAL:HG23	2.16	0.45
1:D:1866:SER:HA	1:D:1869:ILE:HG22	1.98	0.45
1:C:2147:LEU:HD23	1:C:2152:LYS:HE2	1.98	0.45
1:B:1616:VAL:HG21	1:B:1690:LEU:HD23	1.97	0.45
1:D:1116:ARG:O	1:D:1119:THR:OG1	2.30	0.45
1:A:164:ILE:HD11	1:A:183:VAL:HG21	1.97	0.45
1:A:2147:LEU:HD23	1:A:2152:LYS:HE2	1.98	0.45
1:B:1866:SER:HA	1:B:1869:ILE:HG22	1.98	0.45
1:C:1866:SER:HA	1:C:1869:ILE:HG22	1.98	0.45
1:D:1410:LYS:O	1:D:1414:VAL:HG23	2.16	0.45
1:C:603:ARG:NH1	1:C:645:ILE:HD13	2.31	0.45
1:D:603:ARG:NH1	1:D:645:ILE:HD13	2.31	0.45
1:D:2147:LEU:HD23	1:D:2152:LYS:HE2	1.98	0.45
1:D:2552:THR:HG23	1:D:2553:VAL:HG13	1.98	0.45
1:A:44:ASP:OD1	1:A:45:LEU:N	2.50	0.45
1:B:2215:ILE:HD12	1:B:2341:TYR:CD2	2.52	0.45
1:A:265:LEU:HD11	1:A:417:LEU:HD13	1.99	0.45
1:A:603:ARG:NH1	1:A:645:ILE:HD13	2.31	0.45
1:B:2552:THR:HG23	1:B:2553:VAL:HG13	1.98	0.45
1:D:64:ARG:NH2	1:D:103:GLN:OE1	2.47	0.45
1:A:9:HIS:N	1:A:12:ASP:OD2	2.49	0.44
1:A:1410:LYS:O	1:A:1414:VAL:HG23	2.16	0.44
1:B:1725:GLN:HB2	1:B:1760:LEU:HD13	1.98	0.44
1:C:1725:GLN:HB2	1:C:1760:LEU:HD13	1.98	0.44
1:C:2215:ILE:HD12	1:C:2341:TYR:CD2	2.52	0.44
1:D:36:CYS:SG	1:D:152:LEU:HD21	2.58	0.44
1:A:1725:GLN:HB2	1:A:1760:LEU:HD13	1.98	0.44
1:A:1866:SER:HA	1:A:1869:ILE:HG22	1.98	0.44
1:B:44:ASP:OD1	1:B:45:LEU:N	2.50	0.44
1:B:976:GLN:OE1	1:B:980:ASN:ND2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2147:LEU:HD23	1:B:2152:LYS:HE2	1.98	0.44
1:C:968:LYS:O	1:C:972:LEU:HD23	2.17	0.44
1:C:44:ASP:OD1	1:C:45:LEU:N	2.50	0.44
1:C:2552:THR:HG23	1:C:2553:VAL:HG13	1.98	0.44
1:D:2215:ILE:HD12	1:D:2341:TYR:CD2	2.52	0.44
1:A:64:ARG:NH2	1:A:103:GLN:OE1	2.47	0.44
1:A:2215:ILE:HD12	1:A:2341:TYR:CD2	2.52	0.44
1:D:44:ASP:OD1	1:D:45:LEU:N	2.50	0.44
1:D:961:ASP:OD1	1:D:962:ILE:N	2.50	0.44
1:D:968:LYS:O	1:D:972:LEU:HD23	2.17	0.44
1:D:1725:GLN:HB2	1:D:1760:LEU:HD13	1.98	0.44
1:A:1307:ILE:HD11	1:A:1318:GLN:CB	2.47	0.44
1:A:1056:LEU:HD22	1:A:1694:TYR:HD1	1.83	0.44
1:A:1235:PHE:O	1:A:1242:ASN:ND2	2.48	0.44
1:C:1258:LEU:HD23	1:C:1298:GLN:NE2	2.33	0.44
1:C:2006:SER:OG	1:C:2134:GLU:OE1	2.20	0.44
1:A:1116:ARG:O	1:A:1119:THR:OG1	2.30	0.44
1:B:265:LEU:HD11	1:B:417:LEU:HD13	1.99	0.44
1:B:968:LYS:O	1:B:972:LEU:HD23	2.17	0.44
1:C:150:VAL:HG21	1:C:210:VAL:HG12	2.00	0.44
1:D:1056:LEU:HD22	1:D:1694:TYR:HD1	1.83	0.44
1:A:1258:LEU:HD23	1:A:1298:GLN:NE2	2.33	0.44
1:B:1056:LEU:HD22	1:B:1694:TYR:HD1	1.83	0.44
1:B:1258:LEU:HD23	1:B:1298:GLN:NE2	2.33	0.44
1:C:36:CYS:SG	1:C:152:LEU:HD21	2.58	0.44
1:C:961:ASP:OD1	1:C:962:ILE:N	2.50	0.44
1:D:265:LEU:HD11	1:D:417:LEU:HD13	1.99	0.44
1:A:2367:ARG:NH2	1:B:2352:GLU:OE2	2.47	0.44
1:C:721:HIS:O	1:C:725:VAL:HG23	2.18	0.44
1:B:9:HIS:N	1:B:12:ASP:OD2	2.49	0.43
1:A:36:CYS:SG	1:A:152:LEU:HD21	2.57	0.43
1:A:961:ASP:OD1	1:A:962:ILE:N	2.50	0.43
1:A:2124:ILE:HD11	1:A:2568:TYR:CE1	2.53	0.43
1:B:36:CYS:SG	1:B:152:LEU:HD21	2.58	0.43
1:C:265:LEU:HD11	1:C:417:LEU:HD13	1.99	0.43
1:C:1056:LEU:HD22	1:C:1694:TYR:HD1	1.83	0.43
1:C:2261:ILE:HG22	1:C:2265:ILE:HD12	2.01	0.43
1:C:2598:ASN:OD1	1:C:2599:LEU:N	2.51	0.43
1:D:1258:LEU:HD23	1:D:1298:GLN:NE2	2.33	0.43
1:B:2261:ILE:HG22	1:B:2265:ILE:HD12	2.00	0.43
1:D:810:ILE:HD11	1:D:989:TYR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:HG21	1:B:210:VAL:HG12	2.00	0.43
1:D:2261:ILE:HG22	1:D:2265:ILE:HD12	2.01	0.43
1:D:2598:ASN:OD1	1:D:2599:LEU:N	2.51	0.43
1:B:554:ARG:NH2	1:B:588:ASP:OD2	2.52	0.43
1:A:2598:ASN:OD1	1:A:2599:LEU:N	2.51	0.43
1:B:2124:ILE:HD11	1:B:2568:TYR:CE1	2.53	0.43
1:C:810:ILE:HD11	1:C:989:TYR:HA	2.00	0.43
1:D:150:VAL:HG21	1:D:210:VAL:HG12	2.00	0.43
1:D:721:HIS:O	1:D:725:VAL:HG23	2.18	0.43
1:A:2261:ILE:HG22	1:A:2265:ILE:HD12	2.01	0.43
1:A:769:LEU:HD13	1:A:773:LEU:HD23	2.01	0.43
1:B:810:ILE:HD11	1:B:989:TYR:HA	2.00	0.43
1:A:721:HIS:O	1:A:725:VAL:HG23	2.18	0.43
1:A:810:ILE:HD11	1:A:989:TYR:HA	2.00	0.43
1:D:1076:GLN:NE2	1:D:1658:GLU:OE1	2.52	0.43
1:D:1880:LEU:CD1	1:D:1888:LEU:HD13	2.49	0.43
1:A:968:LYS:O	1:A:972:LEU:HD23	2.17	0.43
1:B:1076:GLN:NE2	1:B:1658:GLU:OE1	2.52	0.43
1:B:2598:ASN:OD1	1:B:2599:LEU:N	2.51	0.43
1:C:1880:LEU:CD1	1:C:1888:LEU:HD13	2.49	0.43
1:D:554:ARG:NH2	1:D:588:ASP:OD2	2.52	0.43
1:A:554:ARG:NH2	1:A:588:ASP:OD2	2.51	0.42
1:A:1880:LEU:CD1	1:A:1888:LEU:HD13	2.49	0.42
1:B:721:HIS:O	1:B:725:VAL:HG23	2.18	0.42
1:C:1076:GLN:NE2	1:C:1658:GLU:OE1	2.52	0.42
1:D:729:TYR:O	1:D:733:LEU:HD23	2.19	0.42
1:D:769:LEU:HD13	1:D:773:LEU:HD23	2.01	0.42
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.44	0.42
1:D:1645:SER:N	1:D:1731:GLU:OE1	2.52	0.42
1:C:2365:ASN:OD1	1:C:2368:SER:OG	2.34	0.42
1:A:150:VAL:HG21	1:A:210:VAL:HG12	2.00	0.42
1:B:729:TYR:O	1:B:733:LEU:HD23	2.19	0.42
1:B:1235:PHE:O	1:B:1242:ASN:ND2	2.48	0.42
1:C:9:HIS:N	1:C:12:ASP:OD2	2.49	0.42
1:C:554:ARG:NH2	1:C:588:ASP:OD2	2.52	0.42
1:C:1054:MET:O	1:C:1058:VAL:HG23	2.20	0.42
1:D:1092:PHE:O	1:D:1095:VAL:HG12	2.19	0.42
1:D:2124:ILE:HD11	1:D:2568:TYR:CE1	2.53	0.42
1:C:729:TYR:O	1:C:733:LEU:HD23	2.19	0.42
1:B:961:ASP:OD1	1:B:962:ILE:N	2.50	0.42
1:B:1880:LEU:CD1	1:B:1888:LEU:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2009:ASP:OD1	1:B:2010:SER:N	2.53	0.42
1:B:2147:LEU:HD23	1:B:2152:LYS:HE3	2.00	0.42
1:D:2147:LEU:HD23	1:D:2152:LYS:HE3	2.00	0.42
1:A:1076:GLN:NE2	1:A:1658:GLU:OE1	2.52	0.42
1:A:1092:PHE:O	1:A:1095:VAL:HG12	2.19	0.42
1:B:769:LEU:HD13	1:B:773:LEU:HD23	2.01	0.42
1:B:1092:PHE:O	1:B:1095:VAL:HG12	2.19	0.42
1:B:1307:ILE:HD11	1:B:1318:GLN:CB	2.47	0.42
1:C:2147:LEU:HD23	1:C:2152:LYS:HE3	2.00	0.42
1:D:1054:MET:O	1:D:1058:VAL:HG23	2.20	0.42
1:B:441:ASP:OD2	1:B:505:ARG:NE	2.53	0.42
1:B:1645:SER:N	1:B:1731:GLU:OE1	2.52	0.42
1:B:1746:ASN:HB2	1:B:1749:ILE:HD12	2.02	0.42
1:C:1092:PHE:O	1:C:1095:VAL:HG12	2.19	0.42
1:C:1645:SER:N	1:C:1731:GLU:OE1	2.52	0.42
1:A:729:TYR:O	1:A:733:LEU:HD23	2.19	0.42
1:B:1867:VAL:O	1:B:1936:LEU:HD11	2.20	0.42
1:C:769:LEU:HD13	1:C:773:LEU:HD23	2.01	0.42
1:C:2124:ILE:HD11	1:C:2568:TYR:CE1	2.53	0.42
1:D:441:ASP:OD2	1:D:505:ARG:NE	2.53	0.42
1:A:1054:MET:O	1:A:1058:VAL:HG23	2.20	0.42
1:A:2536:THR:O	1:A:2536:THR:HG22	2.20	0.42
1:C:1746:ASN:HB2	1:C:1749:ILE:HD12	2.02	0.42
1:A:269:LEU:HD13	1:A:269:LEU:O	2.20	0.42
1:B:62:MET:SD	1:B:121:VAL:HG11	2.60	0.42
1:B:2536:THR:HG22	1:B:2536:THR:O	2.20	0.42
1:C:1307:ILE:HD11	1:C:1318:GLN:CB	2.47	0.42
1:A:441:ASP:OD2	1:A:505:ARG:NE	2.53	0.41
1:A:1867:VAL:O	1:A:1936:LEU:HD11	2.20	0.41
1:B:1116:ARG:O	1:B:1119:THR:OG1	2.30	0.41
1:B:2365:ASN:OD1	1:B:2368:SER:OG	2.34	0.41
1:C:62:MET:SD	1:C:121:VAL:HG11	2.60	0.41
1:A:1645:SER:N	1:A:1731:GLU:OE1	2.52	0.41
1:A:2009:ASP:OD1	1:A:2010:SER:N	2.53	0.41
1:C:441:ASP:OD2	1:C:505:ARG:NE	2.53	0.41
1:C:2536:THR:O	1:C:2536:THR:HG22	2.20	0.41
1:D:269:LEU:HD13	1:D:269:LEU:O	2.20	0.41
1:A:1293:HIS:ND1	1:A:1293:HIS:O	2.54	0.41
1:D:2536:THR:HG22	1:D:2536:THR:O	2.20	0.41
1:B:269:LEU:HD13	1:B:269:LEU:O	2.20	0.41
1:B:1224:ILE:O	1:B:1228:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:HD13	1:C:269:LEU:O	2.20	0.41
1:C:840:TYR:O	1:C:844:VAL:HG23	2.20	0.41
1:D:62:MET:SD	1:D:121:VAL:HG11	2.60	0.41
1:D:1293:HIS:O	1:D:1293:HIS:ND1	2.54	0.41
1:A:62:MET:SD	1:A:121:VAL:HG11	2.60	0.41
1:A:1746:ASN:HB2	1:A:1749:ILE:HD12	2.02	0.41
1:A:2365:ASN:O	1:A:2368:SER:OG	2.39	0.41
1:C:1235:PHE:O	1:C:1242:ASN:ND2	2.48	0.41
1:D:2183:GLU:OE1	1:D:2186:ARG:NH2	2.48	0.41
1:B:1054:MET:O	1:B:1058:VAL:HG23	2.20	0.41
1:C:2365:ASN:O	1:C:2368:SER:OG	2.39	0.41
1:D:1746:ASN:HB2	1:D:1749:ILE:HD12	2.02	0.41
1:D:1867:VAL:O	1:D:1936:LEU:HD11	2.20	0.41
1:A:2147:LEU:HD23	1:A:2152:LYS:HE3	2.00	0.41
1:C:1867:VAL:O	1:C:1936:LEU:HD11	2.20	0.41
1:B:585:ILE:HG23	1:B:592:GLU:HG3	2.02	0.41
1:C:585:ILE:HG23	1:C:592:GLU:HG3	2.02	0.41
1:C:766:ASP:O	1:C:774:ARG:NH1	2.54	0.41
1:C:1224:ILE:O	1:C:1228:THR:HG23	2.21	0.41
1:D:162:LEU:HD23	1:D:187:PRO:HA	2.03	0.41
1:D:840:TYR:O	1:D:844:VAL:HG23	2.20	0.41
1:A:585:ILE:HG23	1:A:592:GLU:HG3	2.02	0.41
1:A:656:VAL:HG13	1:A:657:LEU:HD22	2.03	0.41
1:B:656:VAL:HG13	1:B:657:LEU:HD22	2.03	0.41
1:B:766:ASP:O	1:B:774:ARG:NH1	2.54	0.41
1:B:1293:HIS:ND1	1:B:1293:HIS:O	2.54	0.41
1:C:162:LEU:HD23	1:C:187:PRO:HA	2.03	0.41
1:A:162:LEU:HD23	1:A:187:PRO:HA	2.03	0.41
1:B:2365:ASN:O	1:B:2368:SER:OG	2.39	0.41
1:C:656:VAL:HG13	1:C:657:LEU:HD22	2.03	0.41
1:D:656:VAL:HG13	1:D:657:LEU:HD22	2.03	0.41
1:B:655:CYS:O	1:B:661:ASN:ND2	2.53	0.40
1:C:1203:HIS:NE2	1:C:1245:LEU:HD21	2.36	0.40
1:D:1203:HIS:NE2	1:D:1245:LEU:HD21	2.36	0.40
1:A:1203:HIS:NE2	1:A:1245:LEU:HD21	2.36	0.40
1:B:1911:LEU:O	1:B:1911:LEU:HD22	2.22	0.40
1:C:1911:LEU:O	1:C:1911:LEU:HD22	2.22	0.40
1:C:2009:ASP:OD1	1:C:2010:SER:N	2.53	0.40
1:D:197:SER:HG	1:D:199:TYR:HD2	1.67	0.40
1:D:2365:ASN:O	1:D:2368:SER:OG	2.39	0.40
1:C:1293:HIS:O	1:C:1293:HIS:ND1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:TYR:O	1:A:844:VAL:HG23	2.20	0.40
1:B:840:TYR:O	1:B:844:VAL:HG23	2.20	0.40
1:B:1043:SER:OG	1:B:1044:MET:N	2.54	0.40
1:C:2367:ARG:NH2	1:D:2352:GLU:OE2	2.50	0.40
1:D:1224:ILE:O	1:D:1228:THR:HG23	2.21	0.40
1:A:766:ASP:O	1:A:774:ARG:NH1	2.54	0.40
1:A:1097:LEU:C	1:A:1098:LEU:HD12	2.42	0.40
1:D:766:ASP:O	1:D:774:ARG:NH1	2.54	0.40
1:D:1056:LEU:HD22	1:D:1694:TYR:CD1	2.57	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	2139/2671 (80%)	2043 (96%)	96 (4%)	0	100	100
1	B	2139/2671 (80%)	2042 (96%)	97 (4%)	0	100	100
1	C	2139/2671 (80%)	2042 (96%)	97 (4%)	0	100	100
1	D	2139/2671 (80%)	2042 (96%)	97 (4%)	0	100	100
All	All	8556/10684 (80%)	8169 (96%)	387 (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	1874/2385 (79%)	1848 (99%)	26 (1%)	67	85
1	B	1874/2385 (79%)	1848 (99%)	26 (1%)	67	85
1	C	1874/2385 (79%)	1848 (99%)	26 (1%)	67	85
1	D	1874/2385 (79%)	1848 (99%)	26 (1%)	67	85
All	All	7496/9540 (79%)	7392 (99%)	104 (1%)	68	85

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	94	GLN
1	A	139	LEU
1	A	186	ASN
1	A	269	LEU
1	A	538	LEU
1	A	566	ASP
1	A	787	ASP
1	A	862	GLU
1	A	1024	ASN
1	A	1055	PHE
1	A	1300	LEU
1	A	1622	HIS
1	A	1691	LEU
1	A	1760	LEU
1	A	1911	LEU
1	A	2008	HIS
1	A	2051	HIS
1	A	2121	THR
1	A	2222	PHE
1	A	2282	LEU
1	A	2402	LEU
1	A	2502	PHE
1	A	2520	PHE
1	A	2541	CYS
1	A	2554	SER
1	B	77	THR
1	B	94	GLN
1	B	139	LEU
1	B	186	ASN
1	B	269	LEU
1	B	538	LEU
1	B	566	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	787	ASP
1	B	862	GLU
1	B	1024	ASN
1	B	1055	PHE
1	B	1300	LEU
1	B	1622	HIS
1	B	1691	LEU
1	B	1760	LEU
1	B	1911	LEU
1	B	2008	HIS
1	B	2051	HIS
1	B	2121	THR
1	B	2222	PHE
1	B	2282	LEU
1	B	2402	LEU
1	B	2502	PHE
1	B	2520	PHE
1	B	2541	CYS
1	B	2554	SER
1	C	77	THR
1	C	94	GLN
1	C	139	LEU
1	C	186	ASN
1	C	269	LEU
1	C	538	LEU
1	C	566	ASP
1	C	787	ASP
1	C	862	GLU
1	C	1024	ASN
1	C	1055	PHE
1	C	1300	LEU
1	C	1622	HIS
1	C	1691	LEU
1	C	1760	LEU
1	C	1911	LEU
1	C	2008	HIS
1	C	2051	HIS
1	C	2121	THR
1	C	2222	PHE
1	C	2282	LEU
1	C	2402	LEU
1	C	2502	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	2520	PHE
1	C	2541	CYS
1	C	2554	SER
1	D	77	THR
1	D	94	GLN
1	D	139	LEU
1	D	186	ASN
1	D	269	LEU
1	D	538	LEU
1	D	566	ASP
1	D	787	ASP
1	D	862	GLU
1	D	1024	ASN
1	D	1055	PHE
1	D	1300	LEU
1	D	1622	HIS
1	D	1691	LEU
1	D	1760	LEU
1	D	1911	LEU
1	D	2008	HIS
1	D	2051	HIS
1	D	2121	THR
1	D	2222	PHE
1	D	2282	LEU
1	D	2402	LEU
1	D	2502	PHE
1	D	2520	PHE
1	D	2541	CYS
1	D	2554	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	869	ASN
1	A	1199	ASN
1	A	1288	HIS
1	A	1337	ASN
1	B	869	ASN
1	B	1199	ASN
1	B	1288	HIS
1	B	1337	ASN
1	C	402	ASN

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Mol	Chain	Res	Type
1	C	869	ASN
1	C	1076	GLN
1	C	1199	ASN
1	C	1288	HIS
1	C	1337	ASN
1	C	1773	HIS
1	D	402	ASN
1	D	869	ASN
1	D	1199	ASN
1	D	1288	HIS

### 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

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

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	49.53
1	B	1552:TRP	C	1587:ASP	N	49.53
1	C	1552:TRP	C	1587:ASP	N	49.53
1	D	1552:TRP	C	1587:ASP	N	49.53
1	A	1484:ARG	C	1490:ALA	N	15.78
1	B	1484:ARG	C	1490:ALA	N	15.78
1	C	1484:ARG	C	1490:ALA	N	15.78
1	D	1484:ARG	C	1490:ALA	N	15.78
1	A	1533:ARG	C	1541:ALA	N	15.69
1	B	1533:ARG	C	1541:ALA	N	15.69
1	C	1533:ARG	C	1541:ALA	N	15.69
1	D	1533:ARG	C	1541:ALA	N	15.69
1	A	2252:TYR	C	2260:SER	N	7.83
1	B	2252:TYR	C	2260:SER	N	7.83
1	C	2252:TYR	C	2260:SER	N	7.83
1	D	2252:TYR	C	2260:SER	N	7.83
1	A	1508:GLY	C	1515:ALA	N	7.09
1	B	1508:GLY	C	1515:ALA	N	7.09
1	C	1508:GLY	C	1515:ALA	N	7.09
1	D	1508:GLY	C	1515:ALA	N	7.09

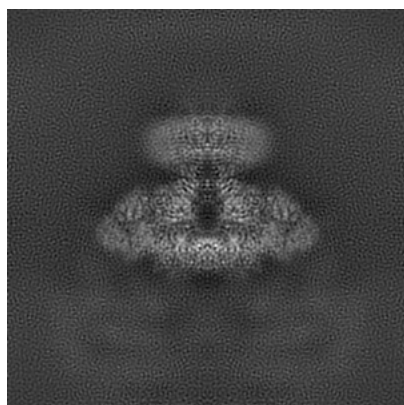
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7978. These allow visual inspection of the internal detail of the map and identification of artifacts.

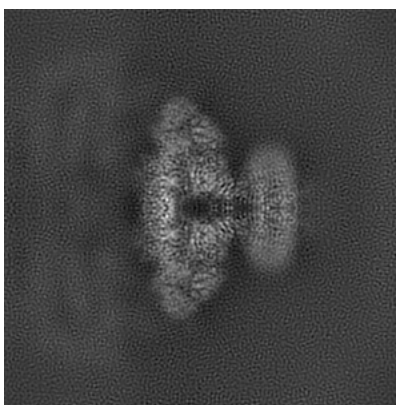
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

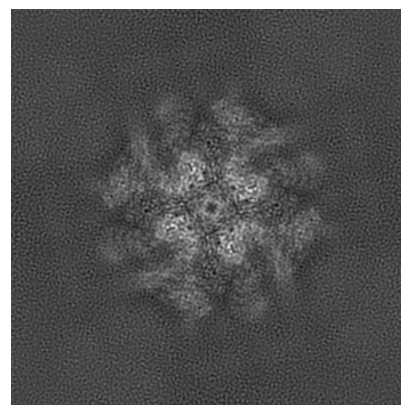
#### 6.1.1 Primary map



X



Y

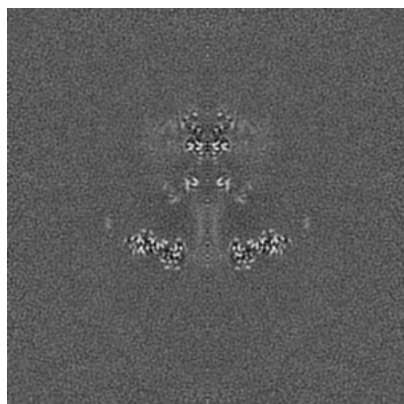


Z

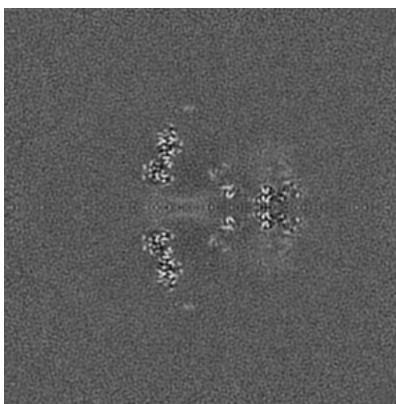
The images above show the map projected in three orthogonal directions.

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

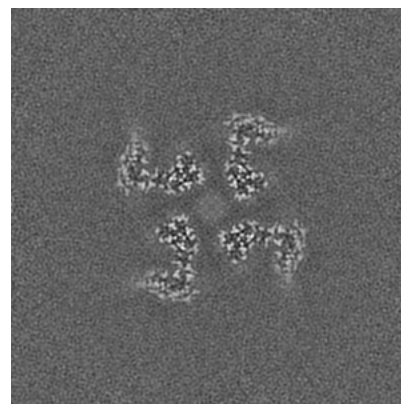
#### 6.2.1 Primary map



X Index: 192



Y Index: 192



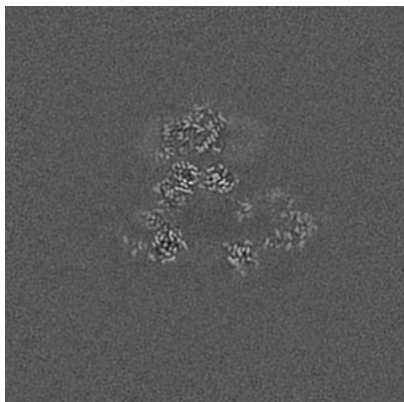
Z Index: 192



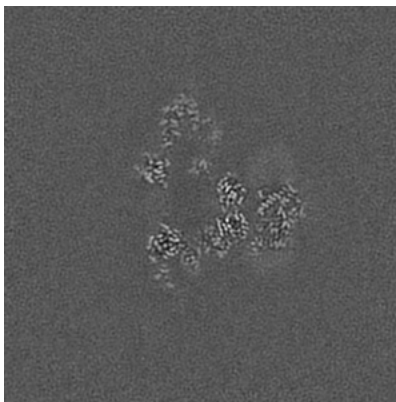
The images above show central slices of the map in three orthogonal directions.

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

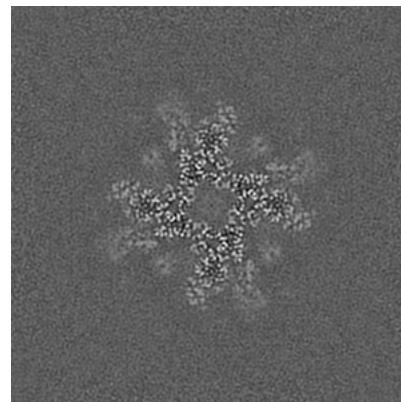
### 6.3.1 Primary map



X Index: 207



Y Index: 177

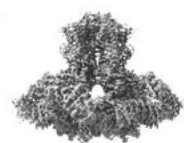


Z Index: 155

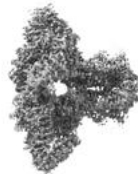
The images above show the largest variance slices of the map in three orthogonal directions.

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

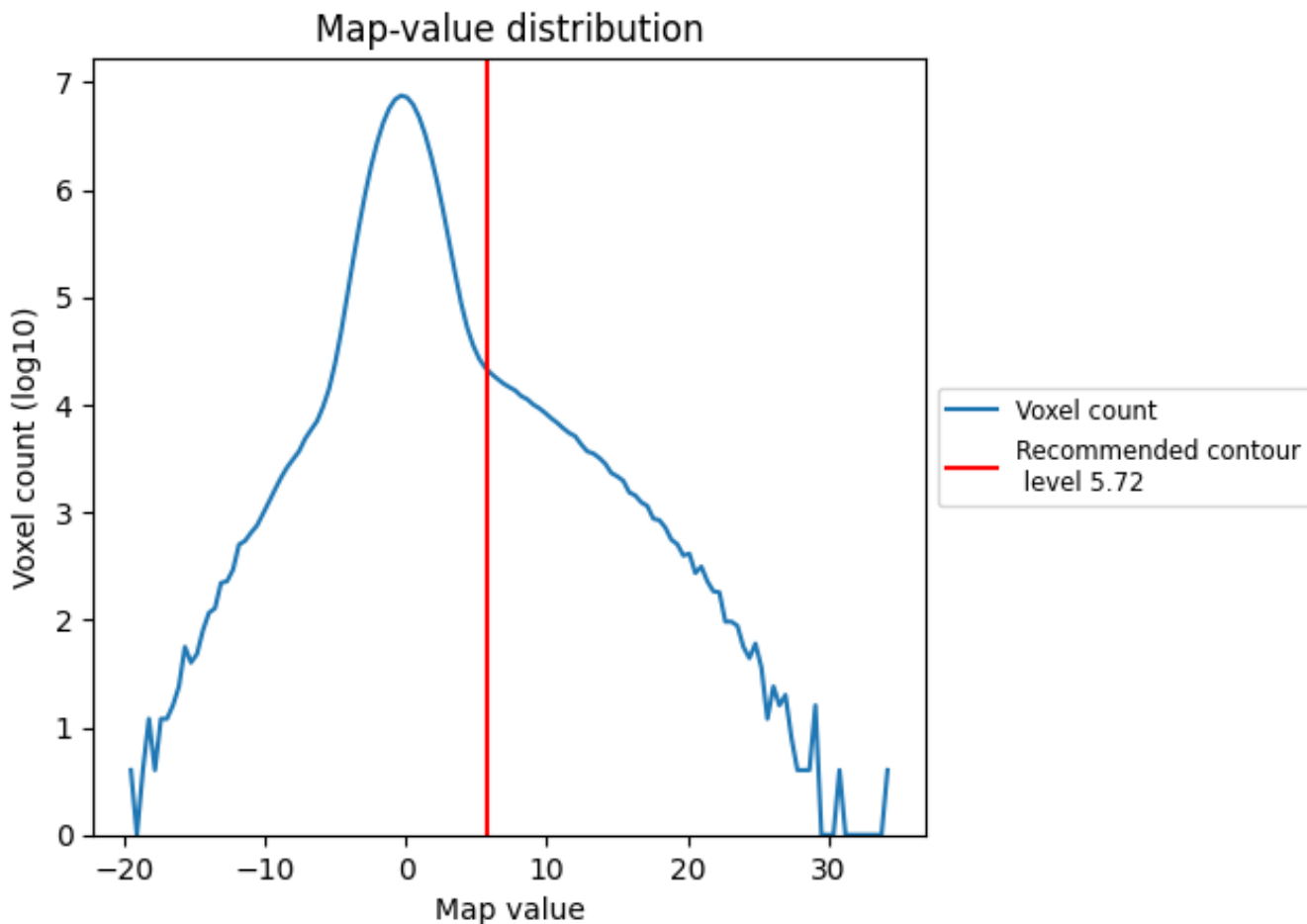
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

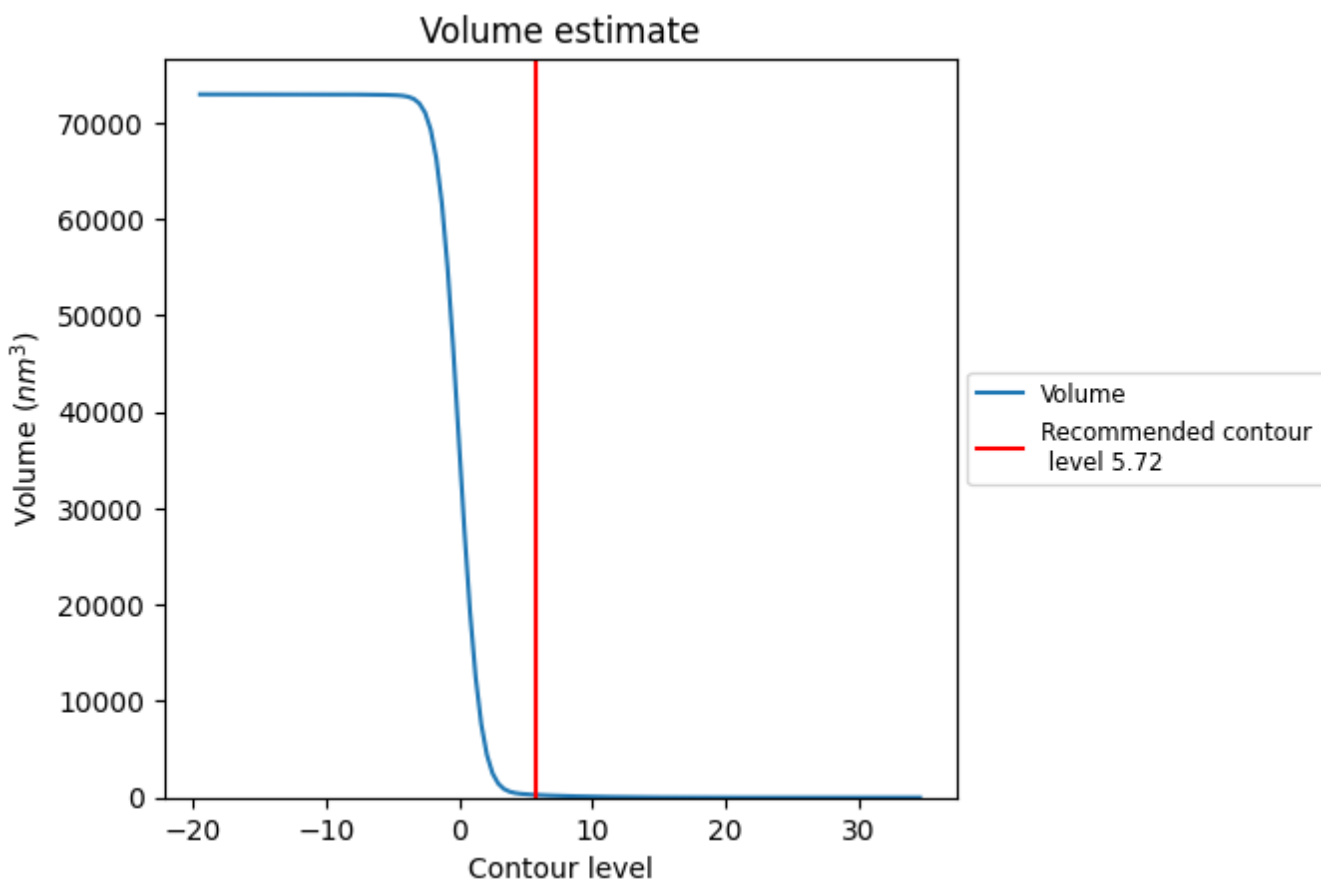
This section contains the results of statistical analysis of the map.

### 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.

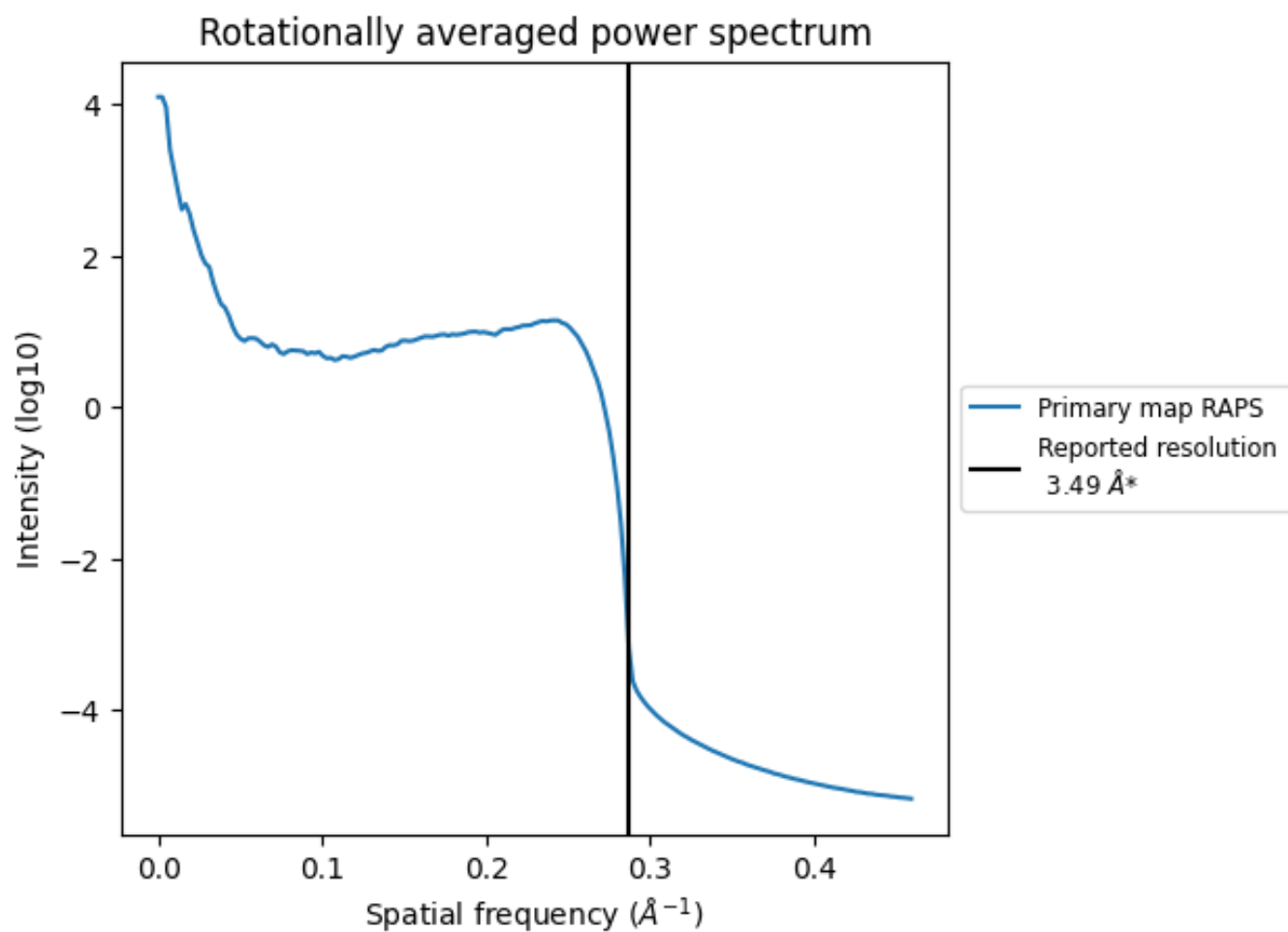
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm<sup>3</sup>; this corresponds to an approximate mass of 252 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  $0.287 \text{\AA}^{-1}$

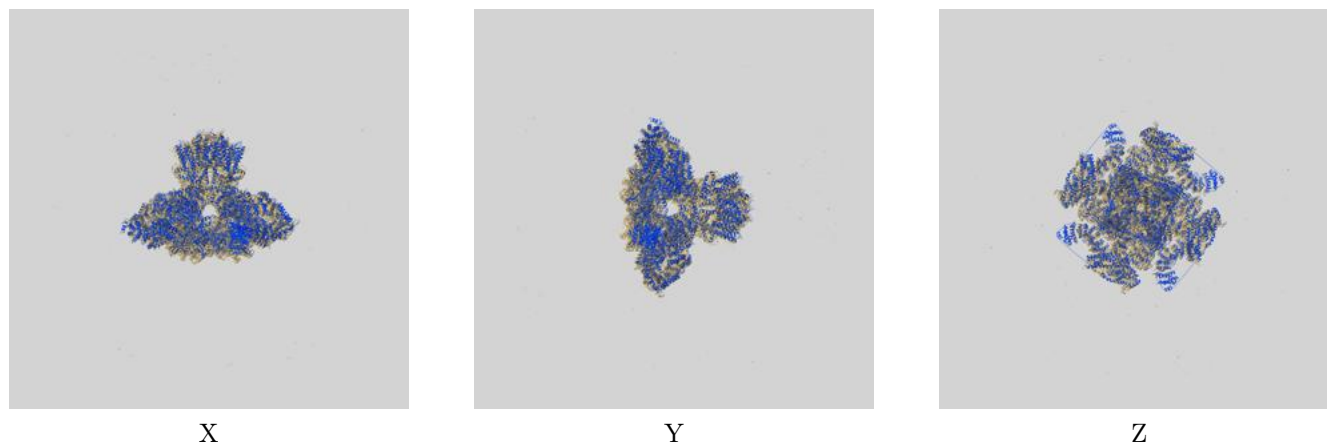
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

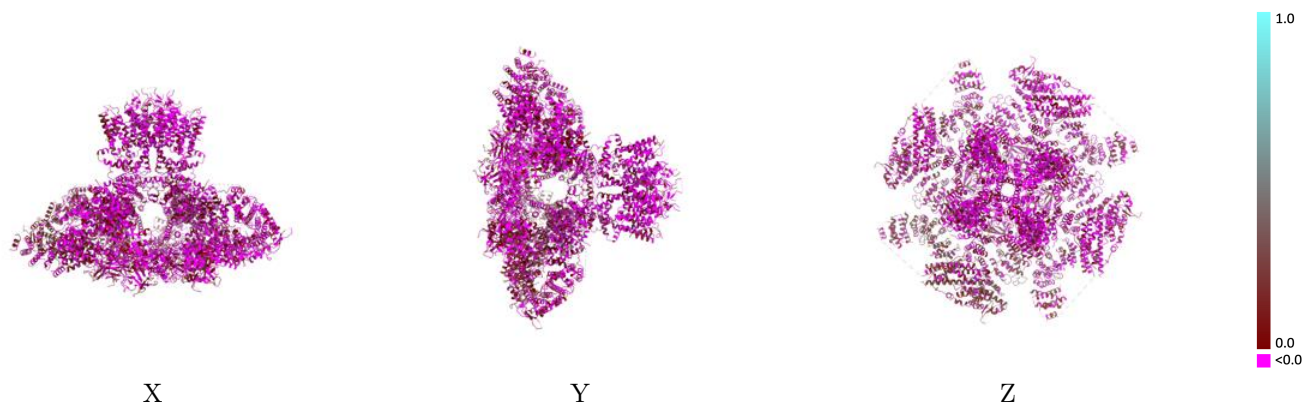
This section contains information regarding the fit between EMDB map EMD-7978 and PDB model 6DQJ. Per-residue inclusion information can be found in section 3 on page 4.

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



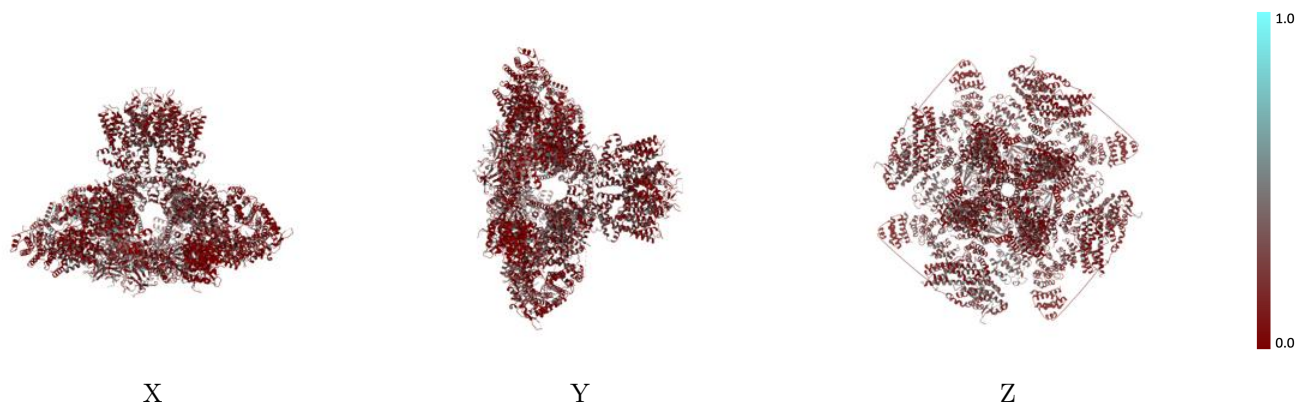
The images above show the 3D surface view of the map at the recommended contour level 5.72 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

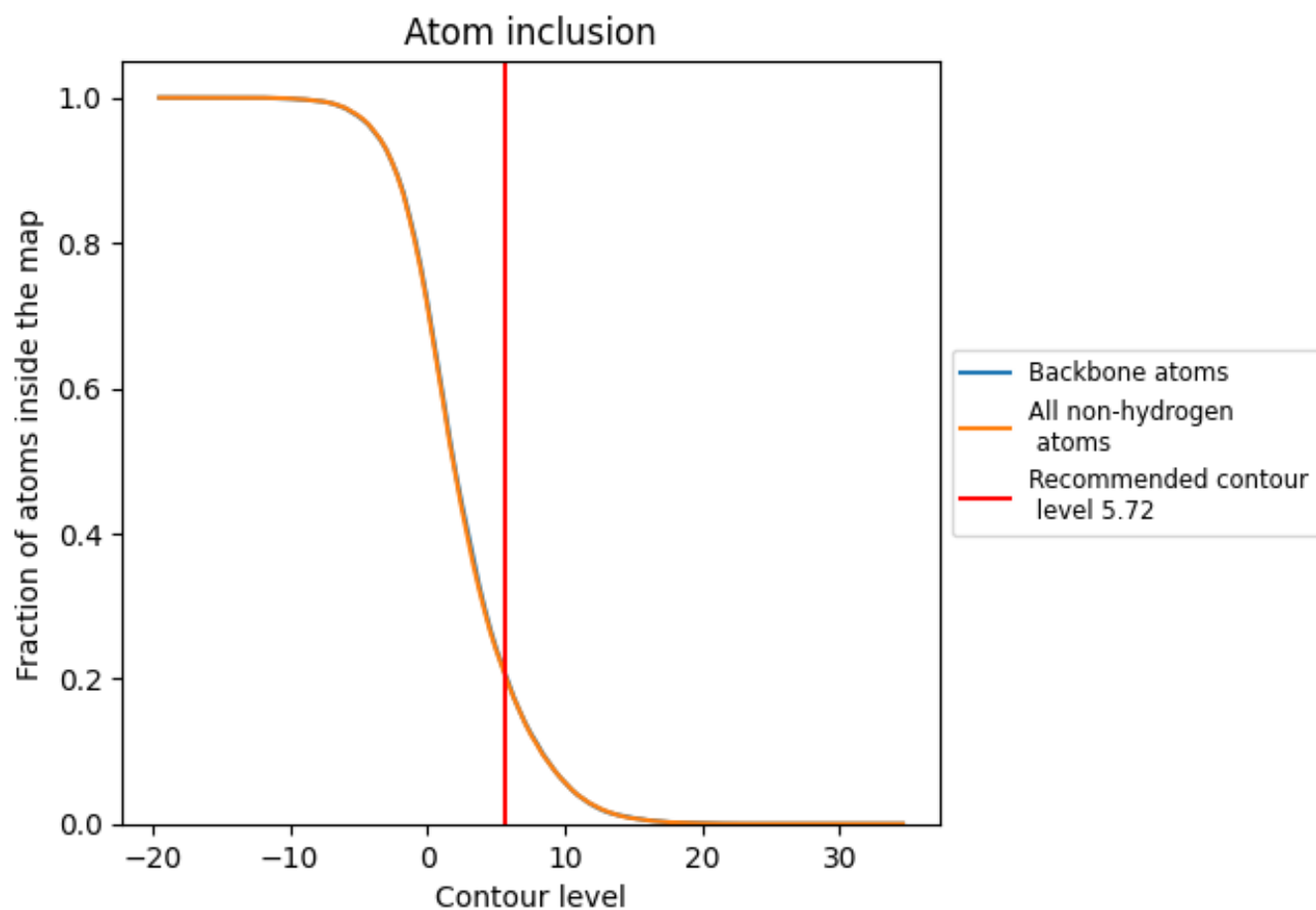
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (5.72).













## 9.4 Atom inclusion [i](#)



At the recommended contour level, 20% of all backbone atoms, 20% 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 (5.72) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2016	 0.0040
A	 0.1846	 -0.0320
B	 0.2121	 0.0190
C	 0.2355	 0.0570
D	 0.1845	 -0.0260

