



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 07:22 PM UTC

PDB ID : 9E19 / pdb_00009e19
EMDB ID : EMD-47386
Title : Structure of RyR1 in the open state in the presence of pentoxifylline
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 4.04 Å (reported)
Based on initial model : 7TZC

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

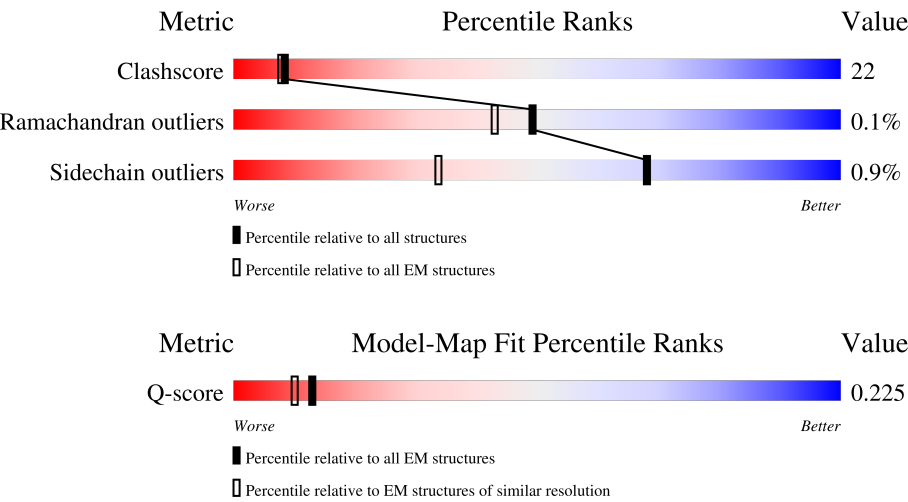
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.04 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6625 (3.54 - 4.54)

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

Mol	Chain	Length	Quality of chain
1	A	5037	41% 49%38%13%
1	B	5037	42% 49%38%13%
1	C	5037	41% 49%38%13%
1	D	5037	41% 49%37%13%

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Mol	Chain	Length	Quality of chain
2	E	108	82% 60%38%..
2	F	108	86% 60%38%..
2	G	108	83% 58%40%..
2	H	108	82% 56%42%..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 144136 atoms, of which 0 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	D	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	C	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	G	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	D	1	Total Ca 1 1	0
4	C	1	Total Ca 1 1	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

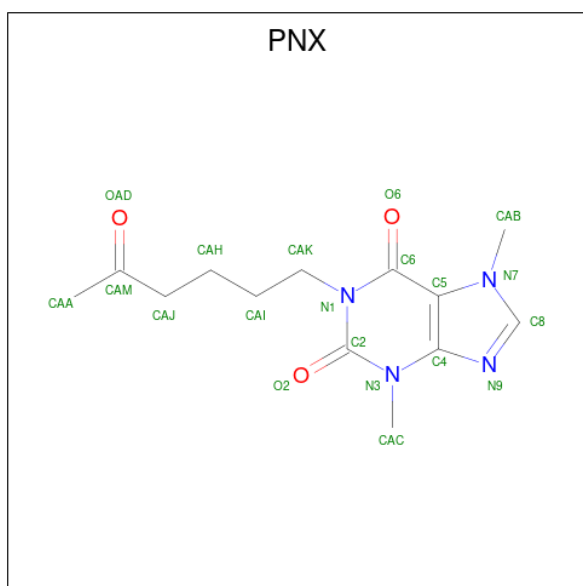
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

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

- Molecule 6 is 3,7-DIMETHYL-1-(5-OXOHEXYL)-3,7-DIHYDRO-1H-PURINE-2,6-DIONE (CCD ID: PNK) (formula: C₁₃H₁₈N₄O₃) (labeled as "Ligand of Interest" by depositor).

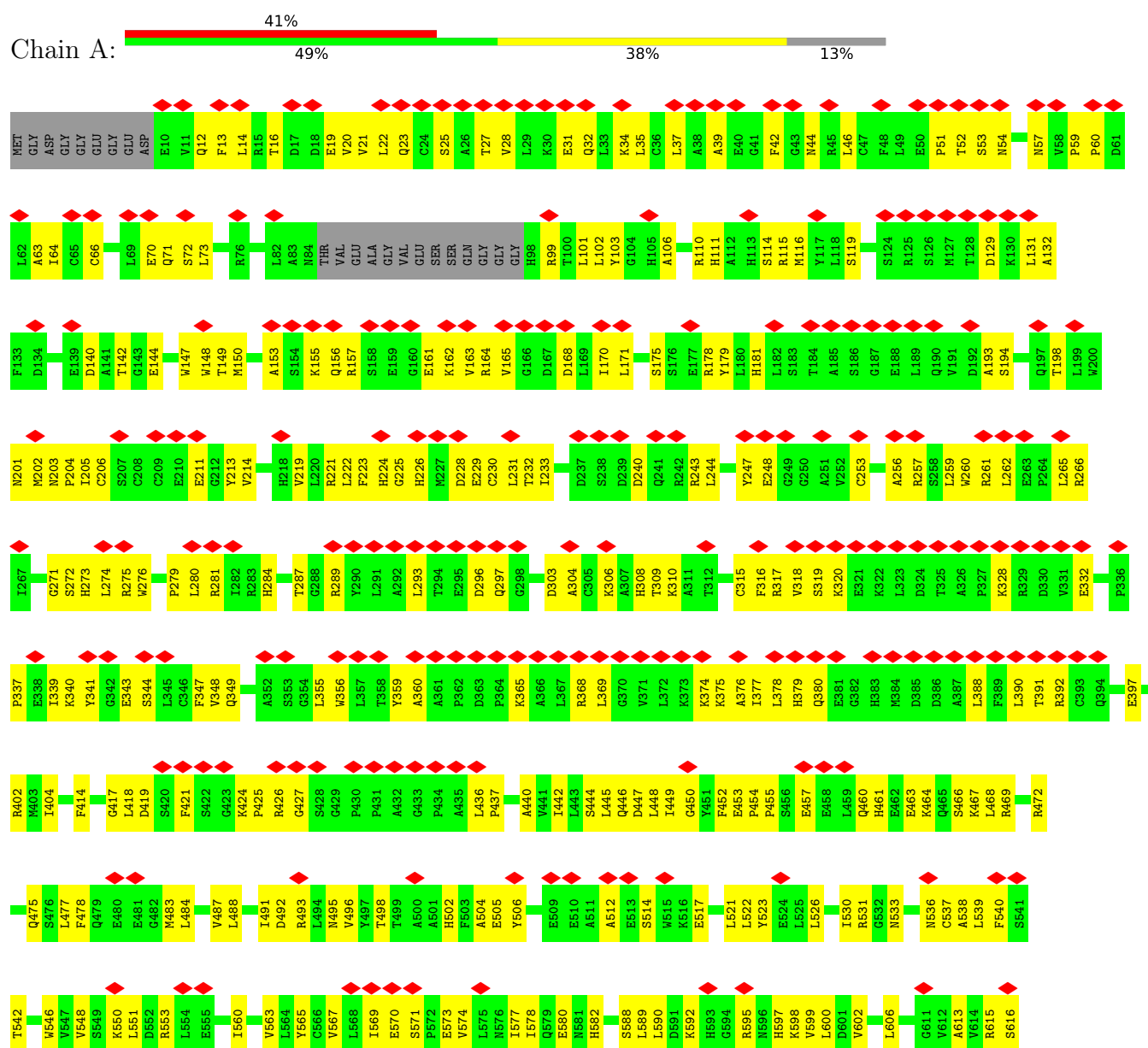


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			20	13	4	3	
6	B	1	Total	C	N	O	0
			20	13	4	3	
6	D	1	Total	C	N	O	0
			20	13	4	3	
6	C	1	Total	C	N	O	0
			20	13	4	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ryanodine receptor 1



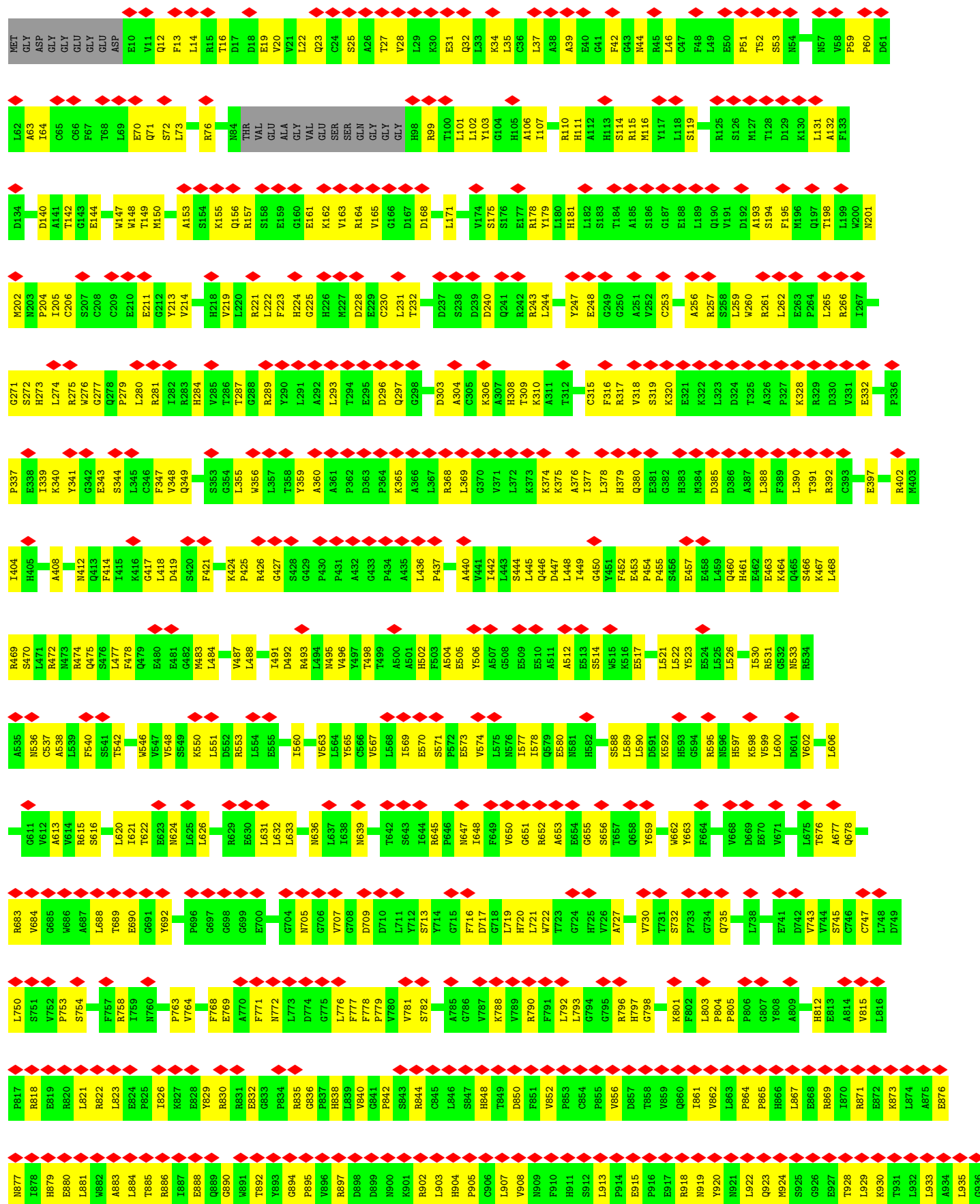
PHE	L620	G691	F757	E824	I1009	W1069	G1135	R1271	ASP
LYS	I621	Y692	R758	P825	V1010	D1070	S1136	Q1196	TTR
LYS	T622	S693	I759	I826	Q1011	R1071	E1137	V1199	GLU
LYS	E623	P694	N760	K827	I1012	V1072	F1138	G1200	ASN
ALA	M624	Y695	P763	R830	I1013	R1073	F1139	H1201	LEU
ALA	L626	P696	P764	R831	I1014	K951	G1140	L1202	ARG
MET	R629	G697	F768	R832	A1015	K952	R1141	G1205	ARG
THR	E630	G698	E769	E832	A1016	T953	F1142	Q1206	ALA
GLN	L631	G699	A770	G832	R1017	K954	W1077	D1207	ALA
PRO	L632	E700	F771	P834	M1018	L955	E1078	Q1210	GLY
ALA	L633	G703	N772	R835	M1019	P956	K1079	S1210	GLY
ALA	M636	G704	L773	G836	R1020	K957	Y1081	L1211	GLY
THR	L637	G705	L774	P837	L1021	T958	Q1084	R1212	ALA
ALA	L638	N705	D774	H838	L1022	Y959	G1084	F1213	GLU
PRO	M639	G706	L775	P842	P1023	M660	R1087	W1214	GLY
LYS	T642	G707	G776	S843	Y1024	M661	Y1088	A1215	LYS
LYS	S643	G708	F777	R844	L1026	S962	Y1089	I1216	GLU
GLY	L644	D709	F778	C945	L1027	N963	F1090	Q1220	GLY
GLY	R645	D710	F779	L846	D1028	G964	E1091	E1221	THR
PRO	L646	L711	V781	S847	E1029	Y965	F1092	G1222	ALA
GLY	N647	L712	S782	H848	A1030	K966	E1093	F1223	GLY
GLY	P648	S713	Y714	T949	T1031	P667	A1094	E1224	THR
THR	L648	G715	A785	D850	K1032	A968	Y1095	P1225	ALA
PRO	F649	F716	G786	R851	R1033	P669	E1099	I1159	GLY
PRO	V650	D717	K788	V852	S1034	L970	M1100	I1160	GLY
GLY	G651	L719	V789	P853	N1035	D971	R1101	I1161	THR
R652	L720	L721	R790	C854	D1036	L972	Y1102	F1162	PRO
A653	W722	W723	F791	P855	D1037	S973	G1103	T1163	PRO
E654	G724	G725	L792	V856	S1038	H974	W1104	L1164	GLY
G655	H726	G794	L793	D857	A1039	V975	M1105	M1165	VAL
S656	Y726	G795	L794	T858	G1040	R976	E1107	E1166	GLU
T857	A727	G796	R796	V859	Q1041	L977	P1107	V1168	ALA
Q658	V730	R797	H797	Q860	A1042	T978	E1108	L1169	GLN
Y659	T731	G801	K812	I861	V1043	P979	L1109	M1170	VAL
W662	S732	F802	E913	V862	R1044	A880	D1112	S1171	ARG
Y663	P733	L803	A814	L863	T1045	Q981	V1113	D1172	ALA
F664	G734	P804	V815	P864	L1046	T982	E1114	S1173	GLU
D669	Q735	P905	R818	P865	L1047	T983	L1115	G1174	LYS
E670	H736	P906	R819	H866	G1048	L984	G1116	S1175	ASP
E671	E741	G907	E919	L867	Y1049	V885	A1117	E1176	ALA
L675	D742	Y808	R820	E925	G1050	D986	D1118	T1177	THR
T676	V743	A909	R821	G926	V1051	R987	E1119	A1178	THR
A677	S744	G908	L821	E927	N1052	L988	L1120	Y1255	GLU
Q678	C745	Y809	R822	E928	L1053	E989	A1121	F1179	LYS
R683	D747	V815	L884	K873	E1054	N991	F1124	R1180	ASN
G685	L748	R818	T885	L874	P1055	G992	N1125	E1181	LYS
W686	D749	R819	E942	A875	Q1056	H993	H1126	I1182	LYS
A687	L750	R820	A944	E876	Q1057	N994	H1127	E1183	ARG
L688	L751	R821	E945	N877	Q1058	A997	R1128	G1185	ALA
T689	S752	R822	A946	R878	E1059	D998	G1129	H1127	ALA
E690	P754	L823		I879	P1060	D999	Q1130	G1187	GLU
				L880	S1061	R1000	R1131	F1188	ASP
				L881	Q1062	V1001	W1132	L1189	PRO
				W882	V1063	A1002	H1133	S1193	
				A883	E1064	Q1003	L1134	L1194	
				L884	W1005	G1004		G1195	
				T885	S1008	W1005		P1196	
				R886					

S2300	F2235	G2171	P2091	C2021	H1953	R1797	D1649	A1578	G1517	D1456
A2303	L2236	P2172	Q2092	P2022	R1954	L1798	I1650	M1579	C1518	Q1459
G2304	C2237	E2175	S2093	L2023	R1955	A1801	L1651	F1580	D1521	H1460
C2305	Y2238	G2176	L2094	P2024	E1956	R1808	E1652	S1582	L1522	D1461
L2307	F2239	L2177	Q2095	E2025	D1809	R1809	S1654	E1583	A1523	M1462
Q2308	C2240	M2178	E2096	I2027	D1810	K1810	R1656	M1584	G1526	L1463
S2243	S2243	L2179	V2098	L2031	F1961	R1813	L1657	K1585	M1527	F1464
R2244	Q2244	S2181	M2101	Q2032	R1964	R1813	D1658	P1589	T1528	D1465
Q2245	Q2245	L2182	V2102	A2040	Y1965	M1814	L1659	Q1590	F1529	L1466
N2246	N2246	G2183	V2103	L2044	V1966	L1815	Q1660	C1591	T1530	S1467
Q2247	Q2247	L2185	A2106	Q2045	D1967	V1819	R1661	P1592	N1532	K1468
S2249	S2249	K2189	Q2107	Q2045	K1968	R1820	L1667	P1593	G1533	V1469
A2315	M2250	V2190	E2108	L2046	L1969	D1821	L1668	R1594	K1534	R1470
R2316	F2251	F2191	Q1970	GLU	Q1970	G1822	L1671	L1595	E1535	A1471
D2252	D2252	Y2192	R1976	GLY	R1976	P1748	I1676	Q1598	N1537	V1472
H2253	H2253	Q2193	Y1977	GLY	A1978	P1749	Y1670	M1601	T1538	V1474
L2254	L2254	H2194	A1978	GLU	L1980	P1750	R1670	P1602	M1476	T1475
S2255	S2255	P2195	L1979	GLU	S1833	G1751	R1671	V1603	F1539	G1477
Y2256	Y2256	M2198	L1980	PRO	F1836	K1753	H1683	S1604	F1540	D1478
L2257	L2257	R2199	M1981	GLU	V1839	G1754	A1684	L1685	Q1541	E1479
L2258	L2258	E2205	R1982	GLU	P1840	G1755	C1686	S1606	V1542	Q1480
E2259	E2259	L2201	A1983	GLU	L1844	A1757	D1690	M1608	E1543	G1481
G2262	G2262	G2202	A1984	GLU	L1849	R1758	Q1691	F1612	N1545	N1482
Q2263	Q2263	H2204	F1984	THR	V1850	R1759	A1692	L1613	T1546	V1483
G2264	G2264	E2206	T1985	SER	M1851	H1760	Q1693	Q1614	K1547	H1484
L2265	L2265	V2207	M1986	SER	G1852	G1761	L1694	V1615	L1548	S1485
G2266	G2266	W2208	S1987	ARG	I1854	L1762	L1695	V1616	F1549	S1486
R2267	R2267	E2209	A1988	LEU	F1854	P1763	H1696	E1618	P1550	L1487
Q2268	Q2268	V2210	A1989	SER	E1857	G1764	L1698	R1618	A1551	L1488
G2269	G2269	M2212	E1990	LEU	D1858	V1765	E1699	R1619	V1552	C1489
S2270	S2270	N2213	T1991	LEU	V1859	R1772	D1700	A1620	F1554	S1490
T2271	T2271	Q2214	A1992	GLU	K1860	P1773	A1701	C1621	L1555	N1491
P2272	P2272	L2215	R1993	THR	M1865	P1774	H1702	E1622	T1557	C1492
L2273	L2273	G2216	R1994	VAL	I1866	H1775	L1703	R1623	H1558	Y1493
D2274	D2274	Q2217	T1995	ARG	E1867	S1778	G1705	L1624	Q1559	M1494
V2275	V2275	G2218	R1996	LEU	P1868	P1779	P1706	G1625	N1560	V1495
A2278	A2278	E2219	E1997	VAL	E1869	P1780	L1707	W1626	V1561	L1496
S2279	S2279	T2220	F1998	LYS	V1870	C1781	R1708	A1627	T1562	D1499
D2282	D2282	Q2221	S2000	GLU	F1871	F1782	A1709	V1628	Q1563	F1500
N2283	N2283	L2223	Q2003	LYS	T1872	V1783	G1710	Q1629	E1565	V1501
E2284	E2284	T2224	E2004	PRO	E1873	A1784	Y1711	C1630	L1566	S1502
L2286	L2286	E2157	Q2005	GLU	E1874	A1785	D1713	Q1631	G1567	P1503
A2287	A2287	C2158	M1939	GLU	GLU	L1786	L1715	D1632	K1568	G1504
L2288	L2288	L2159	L2009	LEU	GLU	P1787	D1714	A1638	Q1569	Q1505
A2289	A2289	G2160	L2010	PRO	GLU	A1788	L1716	L1639	K1570	Q1506
L2290	L2290	Q2161	L2011	ALA	GLU	A1789	E1721	H1640	N1571	G1507
Q2291	Q2291	Q2161	H2011	GLU	GLU	G1790	S1722	I1641	I1572	R1508
E2292	E2292	S2164	T2012	GLU	GLU	A1792	C1724	E1644	M1573	T1509
Q2293	Q2293	L2165	K2013	E2088	GLU	G1791	E1793	N1645	P1574	S1510
D2294	D2294	M2170	D2014	K2089	GLU	V1791	A1794	R1646	S1576	H1511
K2297	K2297		E2015	K2090	GLU	A1792	P1795	M1648	A1577	T1512
V2298	V2298		A2016		GLU	A1792				D1513
V2299	V2299		D2017		GLU	A1794				L1514
			E2018		GLU	P1795				V1515
			E2019		GLU	A1796				T1516
			D2020		GLU					

G3113	G3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	V3064	V3065	N3066	C3067	L3128	T3130	V3131	T3132	T3133	T3134	L3135	L3136	L3137	P3138	V3139	L3140	T3141	V3080	K3081	K3082	S3083	G3084	P3085	E3086	I3087	V3088	K3151	F3152	G3091	L3092	R3093	S3094	F3095	F3096			S3100	S3101	D3102	I3103	E3104	K3105	T3168	L3169	C3170	S3171	L3172	V3173	S3174
H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3061	P3062	A3063	V3064	V3065	N3066	C3067	L3068	H3069	I3070	L3071	A3072	R3073	S3074	L3075	D3076	A3077	R3078	T3079	V3080	K3081	K3082	S3083	G3084	P3085	E3086	I3087	V3088	K3151	F3152	G3091	L3092	R3093	S3094	F3095	F3096			S3100	S3101	D3102	I3103	E3104	K3105	T3168	L3169	C3170	S3171	L3172	V3173	S3174		
E2992	Q2993	E2994	I2995	K2996	F2997	G2998	A2999	K3000	I3001	L3002	L3003	P3004	L3005	I3006	N3007	Q3008	Y3009	F3010	T3011	N3012	H3013	C3014	L3015	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	S3032	N3033	K3034	E3035	K3036	E3037	N3038	I3039	T3040	L3041	L3042	F3043	C3044	K3045	L3046	A3047	A3048	L3049	V3050	R3051		
K2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	I2951	E2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	L2960	Q2961	Q2962	L2963	L2964	R2965	W2966	M2967	D2968	I2969	S2970	Q2971	E2972	F2973	I2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991		
Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	E2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	L2903	L2904	L2905	V2906	P2907	P2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	R2918	D2919	K2920	E2921	K2922	A2923	Q2924	E2925	L2926	K2927	K2928	F2929	L2930	Q2931			
S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	THR	ARG	GLY	LYS	LYS	LYS	THR	LYS	LYS	ILE	SER	GLN	ALA	ALA	GLN	THR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871				
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	F3880	I3662	I3662	R3594	R3594	R3594	K3534	D3473	P3410	R3350	A3291	I3229
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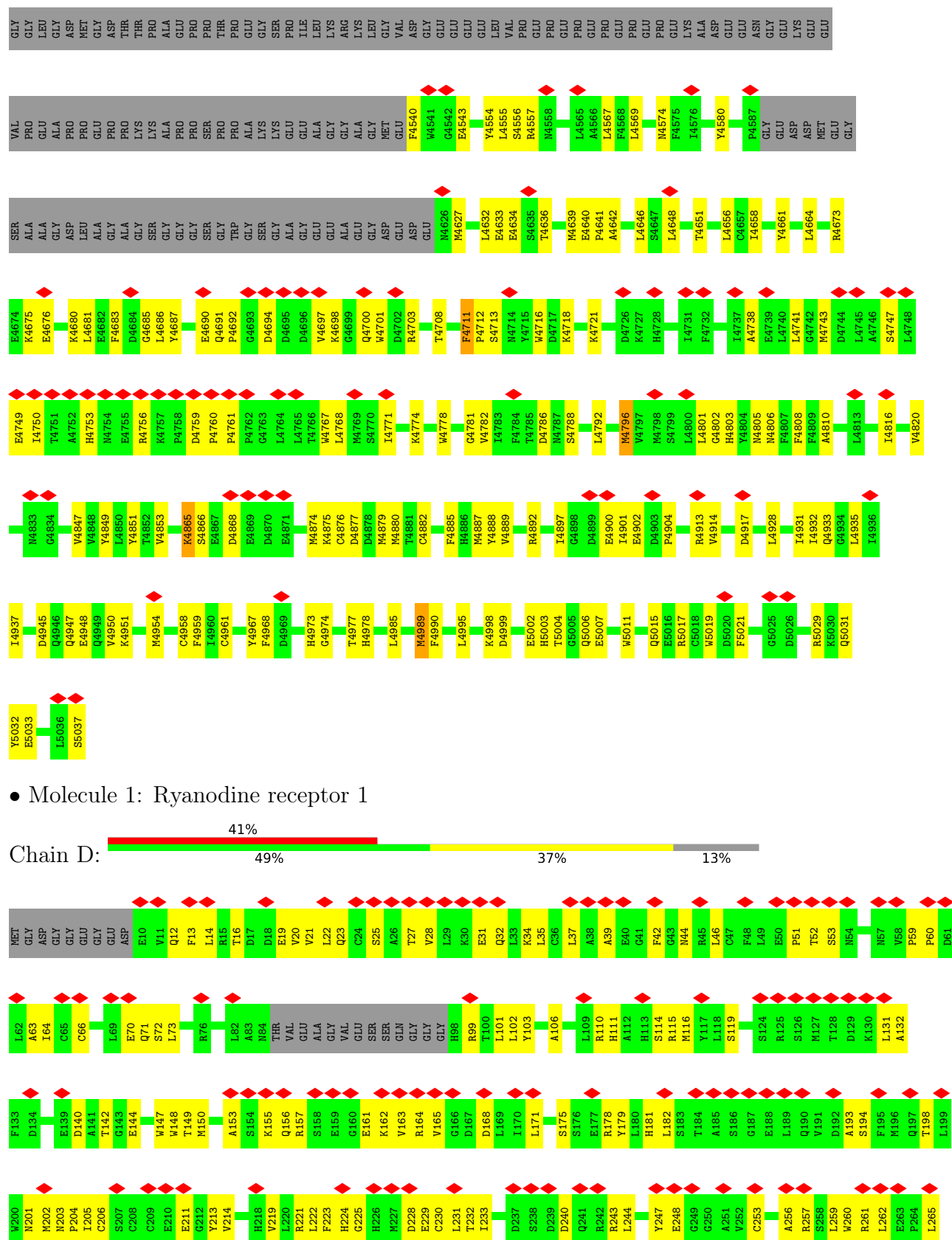


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	N1645	L1515		V1453	LEU	PRO	PRO	G1195	H1133	N1066	G1006	E944
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	L1651	D1521	E1583	D1461	ALA	ALA	ALA	G1200	F1138	R1071	D1012	N949
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	T1666	N1532			PRO	ARG	GLU	R1214	G1150		R1025	M960
A1744	L1667	G1533			ARG	GLY	GLY	A1215	C1151		L1026	M961
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F2636	A2576	L2512	G2448	L2376	Q2308	S2243	Q2180	Q2095	L2023	E1956	GLU	A1901
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F3435	N3313	S3314	I3253	S3314	T3133	A3072	N3012	K2891	GLU	I2771	P2712
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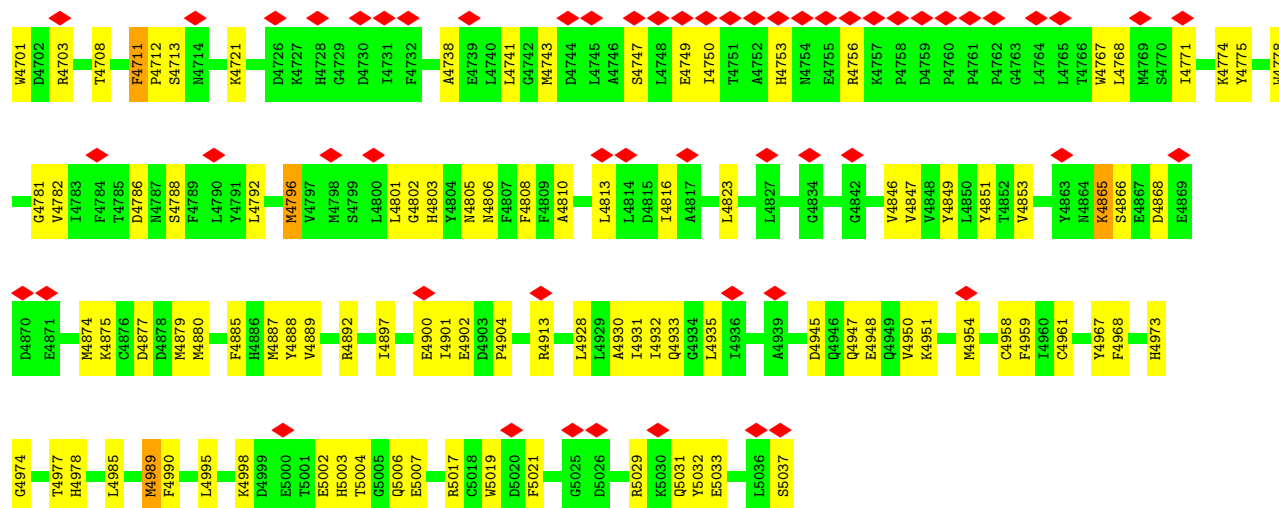




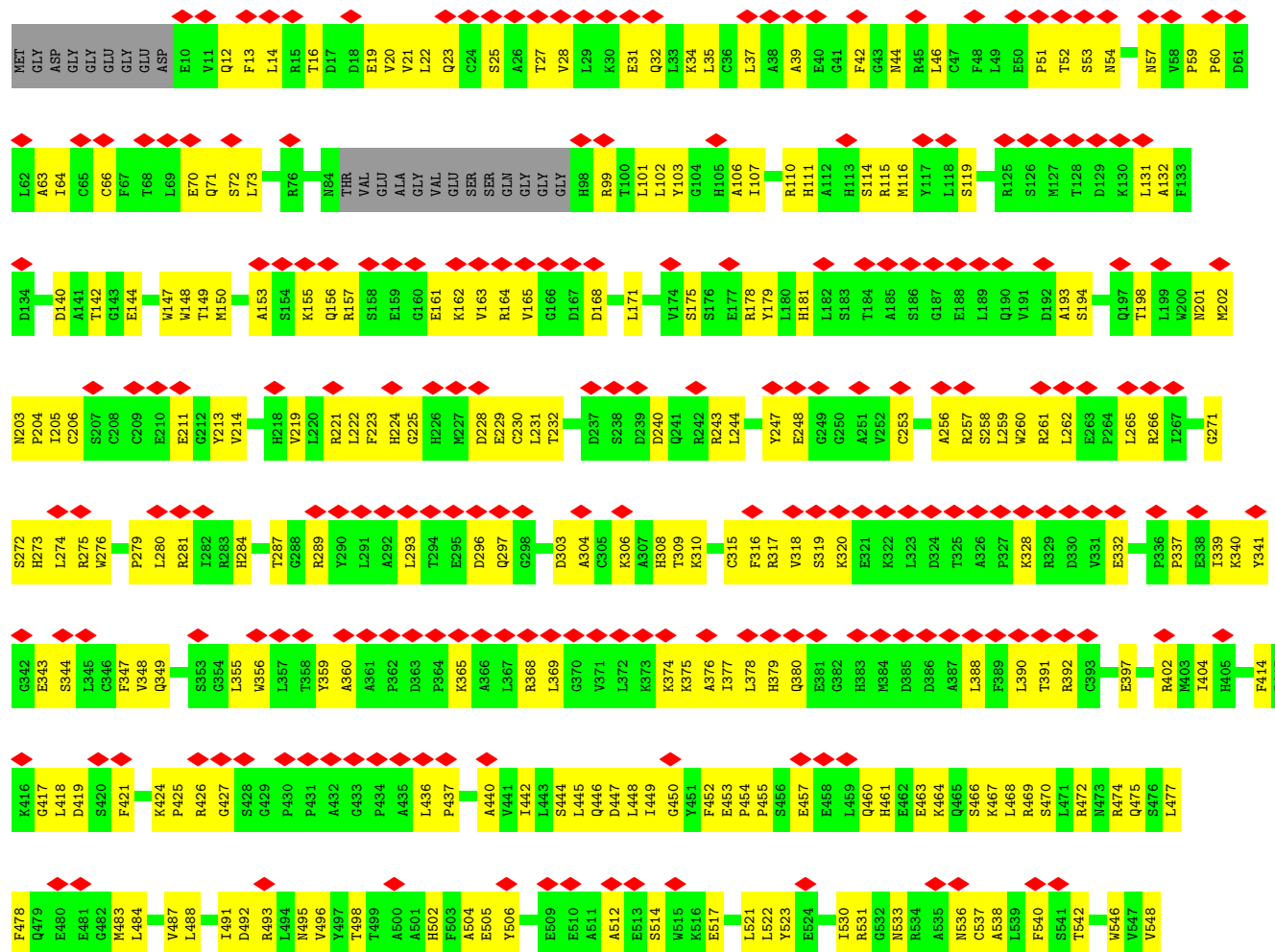
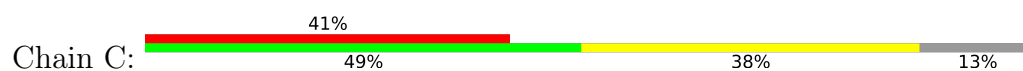


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LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	ASP	GLN	GLU	ARG	LYS	LYS	R3498	R3499	D3501	R3502	Y3503	S3504	V3505	Q3506	T3507	S3508	L3509	T3510	V3511	A3512	T3513	L3514	K3515	K3516	M3517	L3518	L3522	N3523	N3524	C3525	A3526	P3527	T3528	D3529	Q3530	D3531	L3532	L3533	M3534	L3535	A3536	K3537	T3538	R3539	Y3540	A3541																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					





• Molecule 1: Ryanodine receptor 1





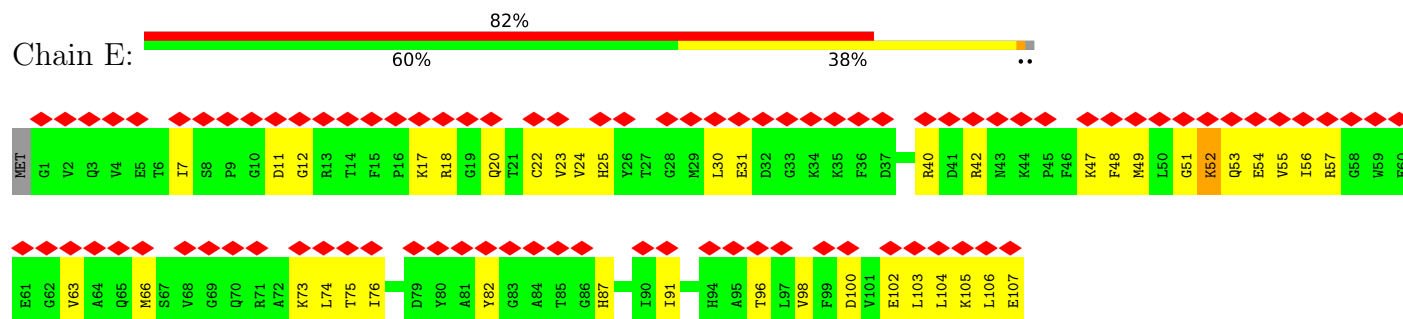




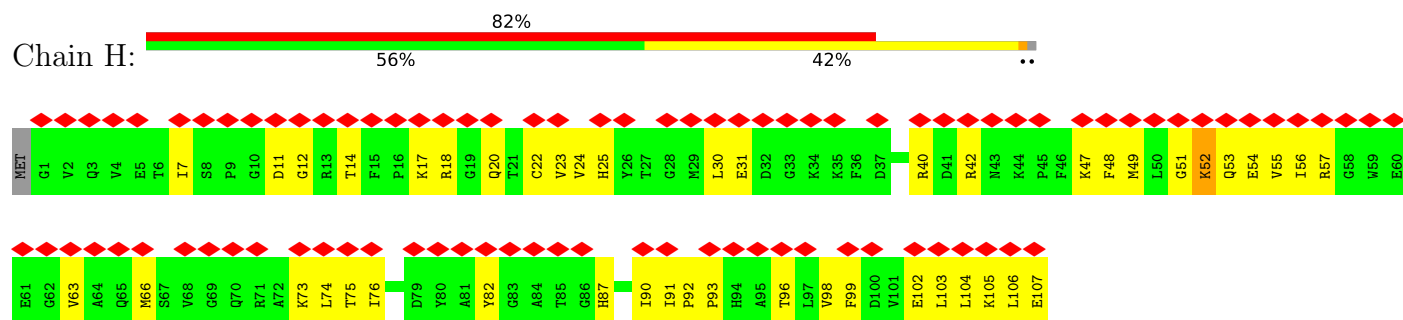
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G3855	G3855	E3760	E3692	H3558	V3439	E3377	A3195	G3255	V3134	V3134
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N3860	N3860	E3765	E3565	E3565	Y3444	A3382	M3201	R3262	V3139	V3139
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G3867	G3867	E3772	R3578	R3578	F3451	E3390	P3208	V3269	H3146	H3146
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L3873	L3873	E3778	L3582	G3582	V3457	E3396	N3214	P3275	G3153	G3153
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D3875	D3875	E3780	E3584	E3584	V3459	F3398	C3216	L3277	D3155	D3155
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R3877	R3877	E3782	E3586	E3586	E3461	V3400	V3218	S3279	I3157	I3157
G3878	G3878	E3783	E3587	E3587	Q3462	L3401	V3280	Y3280	L3158	L3158
L3879	L3879	E3784	E3588	E3588	E3463	C3402	L3281	L3281	D3159	D3159
V3880	V3880	E3785	E3589	E3589	E3464	R3403	P3282	P3282	D3160	D3160
R3881	R3881	E3786	E3590	E3590	E3465	E3404	K3283	W3284	V3161	V3161
Q3882	Q3882	E3787	E3591	E3591	E3466	L3405	S3224	W3285	P3162	P3162
L3883	L3883	E3788	E3592	E3592	E3467	Y3406	P3225	R3286	R3167	R3167
M3884	M3884	E3789	E3593	E3593	E3468	F3407	E3226	E3287	T3168	T3168
N3885	N3885	E3790	E3594	E3594	E3469	A3408	R3287	R3287	C3170	C3170
G3886	G3886	E3791	E3595	E3595	E3470	E3409	P3289	P3289	SS171	SS171
L3887	L3887	E3792	E3596	E3596	E3471	P3410	E3290	E3290	SS172	SS172
V3888	V3888	E3793	E3597	E3597	E3472	L3411	A3291	A3291	T3173	T3173
K3889	K3889	E3794	E3598	E3598	E3473	L3412	P3293	P3293	SS174	SS174
G3890	G3890	E3795	E3599	E3599	E3474	I3413	L3294	L3294	L3175	L3175
L3891	L3891	E3796	E3600	E3600	E3475	R3414	A3295	A3295	G3176	G3176
M3892	M3892	E3797	E3601	E3601	E3476	V3415	L3296	L3296		
N3893	N3893	E3798	E3602	E3602	E3477	D3417				
R3894	R3894	E3799	E3603	E3603	E3478					
G3895	G3895	E3800	E3604	E3604	E3479					
L3896	L3896	E3801	E3605	E3605	E3480					
V3897	V3897	E3802	E3606	E3606	E3481					
K3898	K3898	E3803	E3607	E3607	E3482					
L3899	L3899	E3804	E3608	E3608	E3483					
M3900	M3900	E3805	E3609	E3609	E3484					
N3901	N3901	E3806	E3610	E3610	E3485					
R3902	R3902	E3807	E3611	E3611	E3486					
G3903	G3903	E3808	E3612	E3612	E3487					
L3904	L3904	E3809	E3613	E3613	E3488					
V3905	V3905	E3810	E3614	E3614	E3489					
K3906	K3906	E3811	E3615	E3615	E3490					
L3907	L3907	E3812	E3616	E3616	E3491					
M3908	M3908	E3813	E3617	E3617	E3492					
N3909	N3909	E3814	E3618	E3618	E3493					
R3910	R3910	E3815	E3619	E3619	E3494					
G3911	G3911	E3816	E3620	E3620	E3495					
L3912	L3912	E3817	E3621	E3621	E3496					
M3913	M3913	E3818	E3622	E3622	E3497					
N3914	N3914	E3819	E3623	E3623	E3498					
R3915	R3915	E3820	E3624	E3624	E3499					
G3916	G3916	E3821	E3625	E3625	E3500					
L3917	L3917	E3822	E3626	E3626	E3501					
M3918	M3918	E3823	E3627	E3627	E3502					
N3919	N3919	E3824	E3628	E3628	E3503					
R3920	R3920	E3825	E3629	E3629	E3504					
G3921	G3921	E3826	E3630	E3630	E3505					
L3922	L3922	E3827	E3631	E3631	E3506					
M3923	M3923	E3828	E3632	E3632	E3507					
N3924	N3924	E3829	E3633	E3633	E3508					
R3925	R3925	E3830	E3634	E3634	E3509					
G3926	G3926	E3831	E3635	E3635	E3510					
L3927	L3927	E3832	E3636	E3636	E3511					
M3928	M3928	E3833	E3637	E3637	E3512					
N3929	N3929	E3834	E3638	E3638	E3513					
R3930	R3930	E3835	E3639	E3639	E3514					
G3931	G3931	E3836	E3640	E3640	E3515					
L3932	L3932	E3837	E3641	E3641	E3516					
M3933	M3933	E3838	E3642	E3642	E3517					
N3934	N3934	E3839	E3643	E3643	E3518					
R3935	R3935	E3840	E3644	E3644	E3519					
G3936	G3936	E3841	E3645	E3645	E3520					
L3937	L3937	E3842	E3646	E3646	E3521					
M3938	M3938	E3843	E3647	E3647	E3522					
N3939	N3939	E3844	E3648	E3648	E3523					
R3940	R3940	E3845	E3649	E3649	E3524					
G3941	G3941	E3846	E3650	E3650	E3525					
L3942	L3942	E3847	E3651	E3651	E3526					
M3943	M3943	E3848	E3652	E3652	E3527					
N3944	N3944	E3849	E3653	E3653	E3528					
R3945	R3945	E3850	E3654	E3654	E3529					
G3946	G3946	E3851	E3655	E3655	E3530					
L3947	L3947	E3852	E3656	E3656	E3531					
M3948	M3948	E3853	E3657	E3657	E3532					
N3949	N3949	E3854	E3658	E3658	E3533					
R3950	R3950	E3855	E3659	E3659	E3534					
G3951	G3951	E3856	E3660	E3660	E3535					
L3952	L3952	E3857	E3661	E3661	E3536					
M3953	M3953	E3858	E3662	E3662	E3537					
N3954	N3954	E3859	E3663	E3663	E3538					
R3955	R3955	E3860	E3664	E3664	E3539					
G3956	G3956	E3861	E3665	E3665	E3540					
L3957	L3957	E3862	E3666	E3666	E3541					
M3958	M3958	E3863	E3667	E3667	E3542					
N3959	N3959	E3864	E3668	E3668	E3543					
R3960	R3960	E3865	E3669	E3669	E3544					
G3961	G3961	E3866	E3670	E3670	E3545					
L3962	L3962	E3867	E3671	E3671	E3546					
M3963	M3963	E3868	E3672	E3672	E3547					
N3964	N3964	E3869	E3673	E3673	E3548					
R3965	R3965	E3870	E3674	E3674	E3549					
G3966	G3966	E3871	E3675	E3675	E3550					
L3967	L3967	E3872	E3676	E3676	E3551					
M3968	M3968	E3873	E3677	E3677	E3552					
N3969	N3969	E3874	E3678	E3678	E3553					
R3970	R3970	E3875	E3679	E3679	E3554					
G3971	G3971	E3876	E3680	E3680	E3555					
L3972	L3972	E3877	E3681	E3681	E3556					
M3973	M3973	E3878	E3682	E3682	E3557					
N3974	N3974	E3879	E3683	E3683	E3558			</		



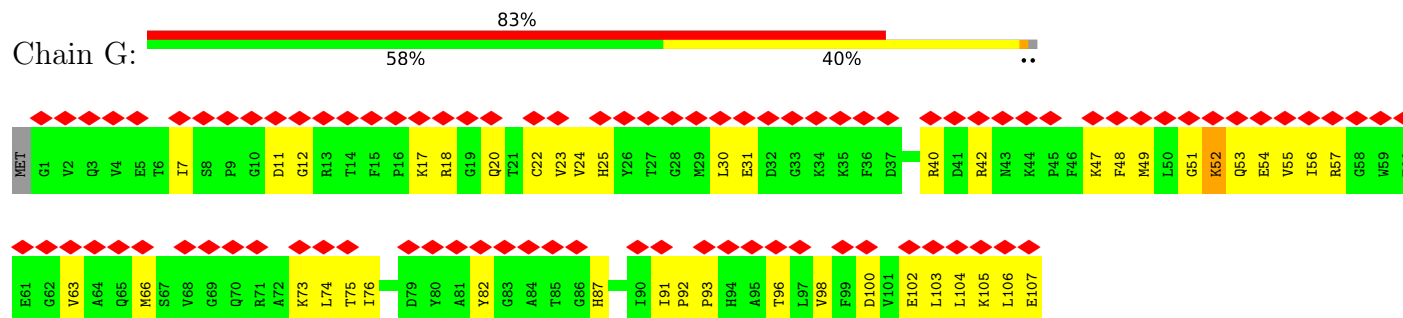
● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



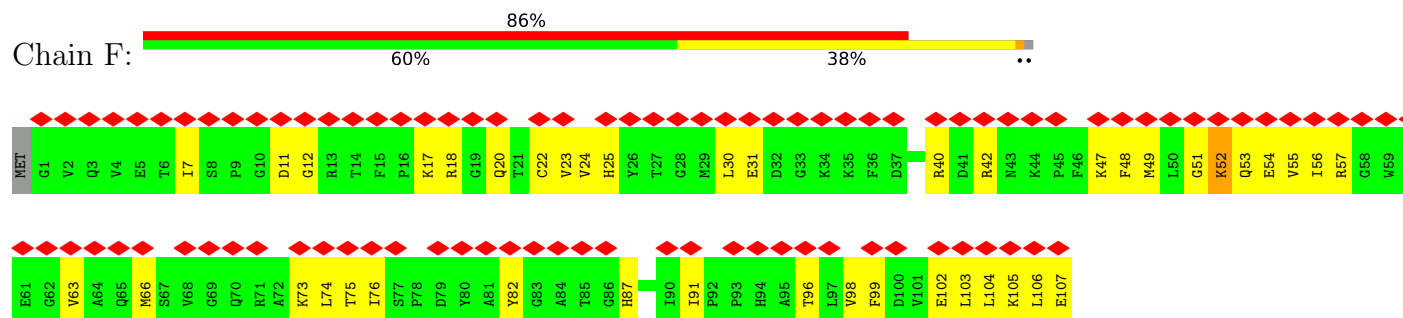
● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3336	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.283	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, CA, PNX

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	0.17	0/35977	0.47	10/48726 (0.0%)
1	B	0.18	0/35977	0.47	10/48726 (0.0%)
1	C	0.18	0/35977	0.47	10/48726 (0.0%)
1	D	0.18	0/35977	0.47	10/48726 (0.0%)
2	E	0.17	0/850	0.51	0/1146
2	F	0.17	0/850	0.51	0/1146
2	G	0.17	0/850	0.51	0/1146
2	H	0.17	0/850	0.51	0/1146
All	All	0.18	0/147308	0.47	40/199488 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2578	MET	CB-CG-SD	8.39	137.88	112.70
1	A	2578	MET	CB-CG-SD	8.38	137.85	112.70
1	B	2578	MET	CB-CG-SD	8.38	137.85	112.70
1	C	2578	MET	CB-CG-SD	8.38	137.83	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1071	ARG	CA-CB-CG	7.72	129.54	114.10

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1608	MET	Peptide
1	A	4189	ARG	Sidechain
1	B	1608	MET	Peptide
1	B	4189	ARG	Sidechain
1	D	1608	MET	Peptide

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	35150	0	34793	1543	0
1	B	35150	0	34793	1545	0
1	C	35150	0	34793	1531	0
1	D	35150	0	34793	1504	0
2	E	831	0	831	32	0
2	F	831	0	831	29	0
2	G	831	0	831	32	0
2	H	831	0	831	33	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	20	0	18	2	0
6	C	20	0	18	1	0
6	D	20	0	18	1	0
All	All	144136	0	142616	6164	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 22.

The worst 5 of 6164 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2639:MET:HG2	1:B:2640:PRO:HD3	1.47	0.97
1:C:2639:MET:HG2	1:C:2640:PRO:HD3	1.47	0.96
1:D:2639:MET:HG2	1:D:2640:PRO:HD3	1.47	0.96
1:A:2639:MET:HG2	1:A:2640:PRO:HD3	1.47	0.96
1:A:4061:PHE:HA	1:A:4064:MET:HE2	1.50	0.93

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	4385/5037 (87%)	4260 (97%)	121 (3%)	4 (0%)	48	80
1	B	4385/5037 (87%)	4260 (97%)	121 (3%)	4 (0%)	48	80
1	C	4385/5037 (87%)	4260 (97%)	121 (3%)	4 (0%)	48	80
1	D	4385/5037 (87%)	4261 (97%)	120 (3%)	4 (0%)	48	80
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17960/20580 (87%)	17449 (97%)	495 (3%)	16 (0%)	49	80

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	908	VAL
1	A	3300	ALA
1	A	4711	PHE
1	B	908	VAL
1	B	3300	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	3836/4276 (90%)	3795 (99%)	41 (1%)	65	74
1	B	3836/4276 (90%)	3795 (99%)	41 (1%)	65	74
1	C	3836/4276 (90%)	3795 (99%)	41 (1%)	65	74
1	D	3836/4276 (90%)	3795 (99%)	41 (1%)	65	74
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	64
2	F	89/90 (99%)	87 (98%)	2 (2%)	45	64
2	G	89/90 (99%)	87 (98%)	2 (2%)	45	64
2	H	89/90 (99%)	87 (98%)	2 (2%)	45	64
All	All	15700/17464 (90%)	15528 (99%)	172 (1%)	68	74

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2932	MET
1	C	2268[A]	GLN
1	D	3422[A]	HIS
1	D	4989	MET

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Mol	Chain	Res	Type
1	C	2584[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2029	GLN
1	C	255	HIS
1	D	2187	ASN
1	D	3465	ASN
1	C	597	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	C	5301	-	32,33,33	0.28	0	48,52,52	0.42	0
6	PNX	D	5304	-	21,21,21	1.43	4 (19%)	30,30,30	2.01	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PNX	B	5304	-	21,21,21	1.44	4 (19%)	30,30,30	2.03	10 (33%)
6	PNX	A	5304	-	21,21,21	1.44	5 (23%)	30,30,30	2.02	10 (33%)
3	ATP	B	5301	-	32,33,33	0.28	0	48,52,52	0.42	0
3	ATP	A	5301	-	32,33,33	0.28	0	48,52,52	0.42	0
6	PNX	C	5304	-	21,21,21	1.43	4 (19%)	30,30,30	2.02	10 (33%)
3	ATP	D	5301	-	32,33,33	0.28	0	48,52,52	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	C	5301	-	-	6/22/38/38	0/3/3/3
6	PNX	D	5304	-	-	4/7/7/7	0/2/2/2
6	PNX	B	5304	-	-	4/7/7/7	0/2/2/2
6	PNX	A	5304	-	-	4/7/7/7	0/2/2/2
3	ATP	B	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	A	5301	-	-	6/22/38/38	0/3/3/3
6	PNX	C	5304	-	-	4/7/7/7	0/2/2/2
3	ATP	D	5301	-	-	6/22/38/38	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5304	PNX	C6-N1	-4.18	1.32	1.40
6	A	5304	PNX	C6-N1	-4.17	1.33	1.40
6	D	5304	PNX	C6-N1	-4.15	1.33	1.40
6	C	5304	PNX	C6-N1	-4.13	1.33	1.40
6	B	5304	PNX	C2-N1	-2.15	1.35	1.38

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5304	PNX	C5-C6-N1	4.30	120.32	112.23
6	C	5304	PNX	C5-C6-N1	4.28	120.28	112.23
6	A	5304	PNX	C5-C6-N1	4.28	120.28	112.23
6	D	5304	PNX	C5-C6-N1	4.25	120.23	112.23
6	B	5304	PNX	C6-C5-C4	-3.98	117.91	122.92

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

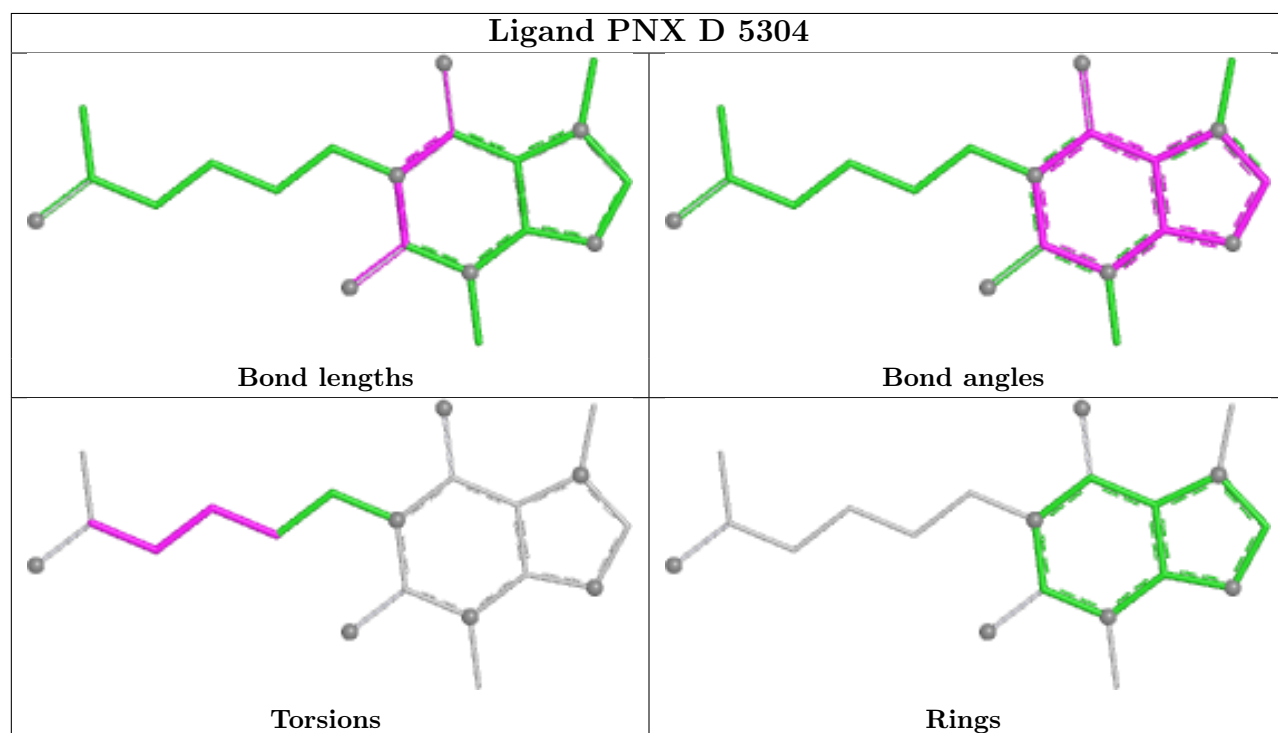
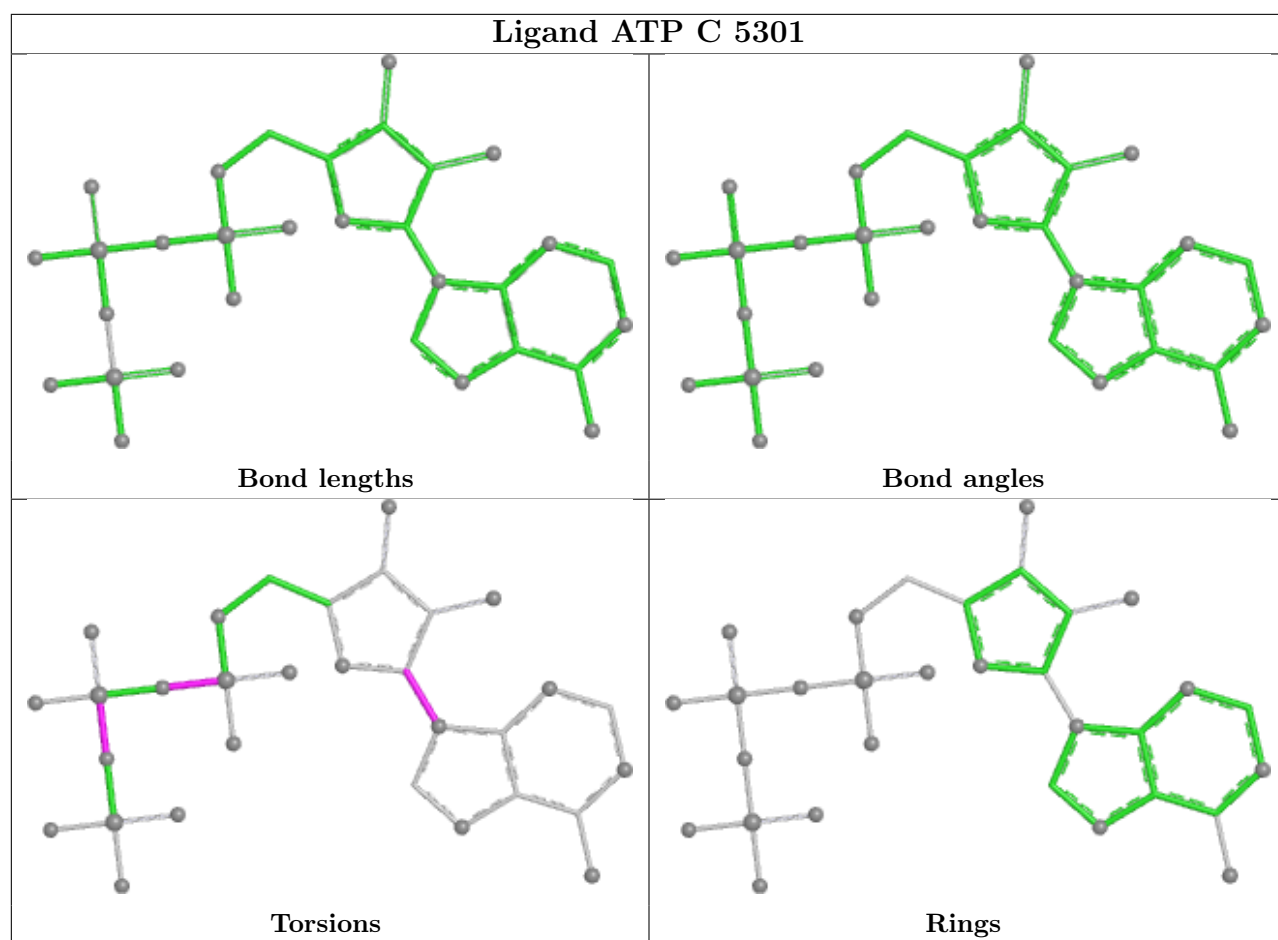
Mol	Chain	Res	Type	Atoms
6	A	5304	PNX	CAI-CAH-CAJ-CAM
6	B	5304	PNX	CAI-CAH-CAJ-CAM
6	D	5304	PNX	CAI-CAH-CAJ-CAM
6	C	5304	PNX	CAI-CAH-CAJ-CAM
6	A	5304	PNX	CAH-CAJ-CAM-OAD

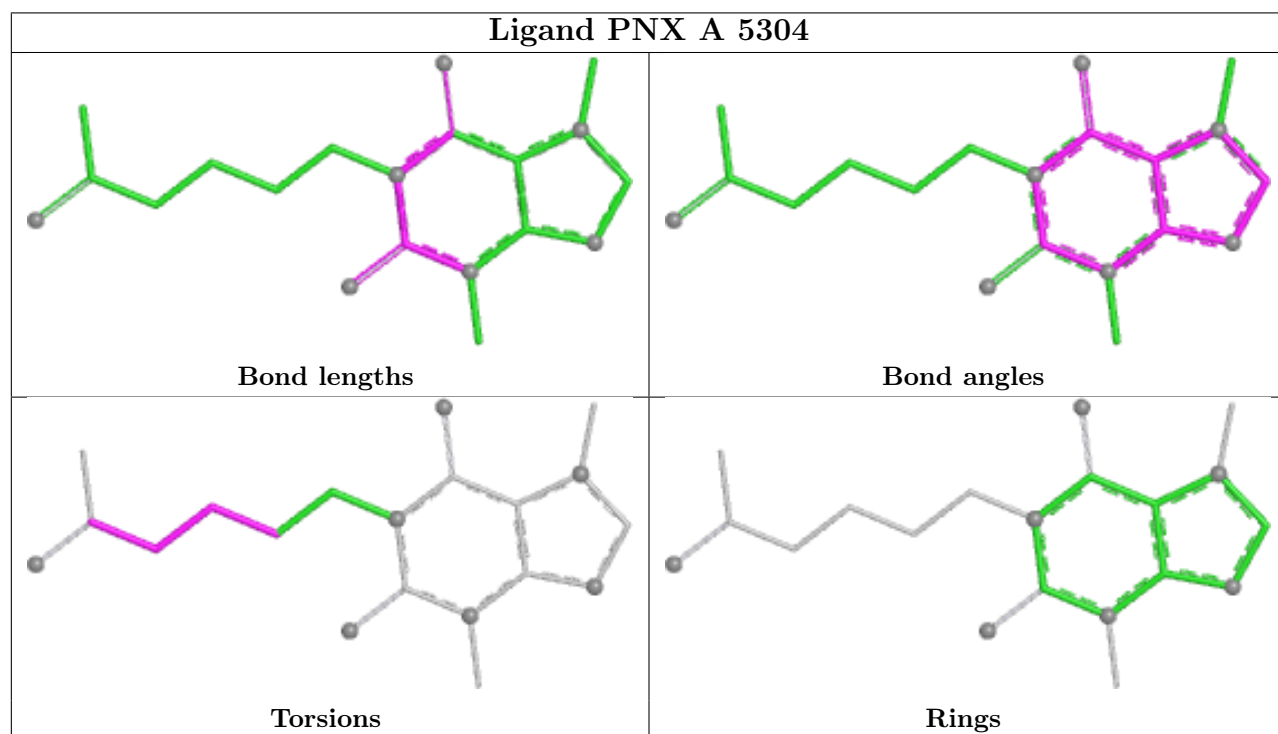
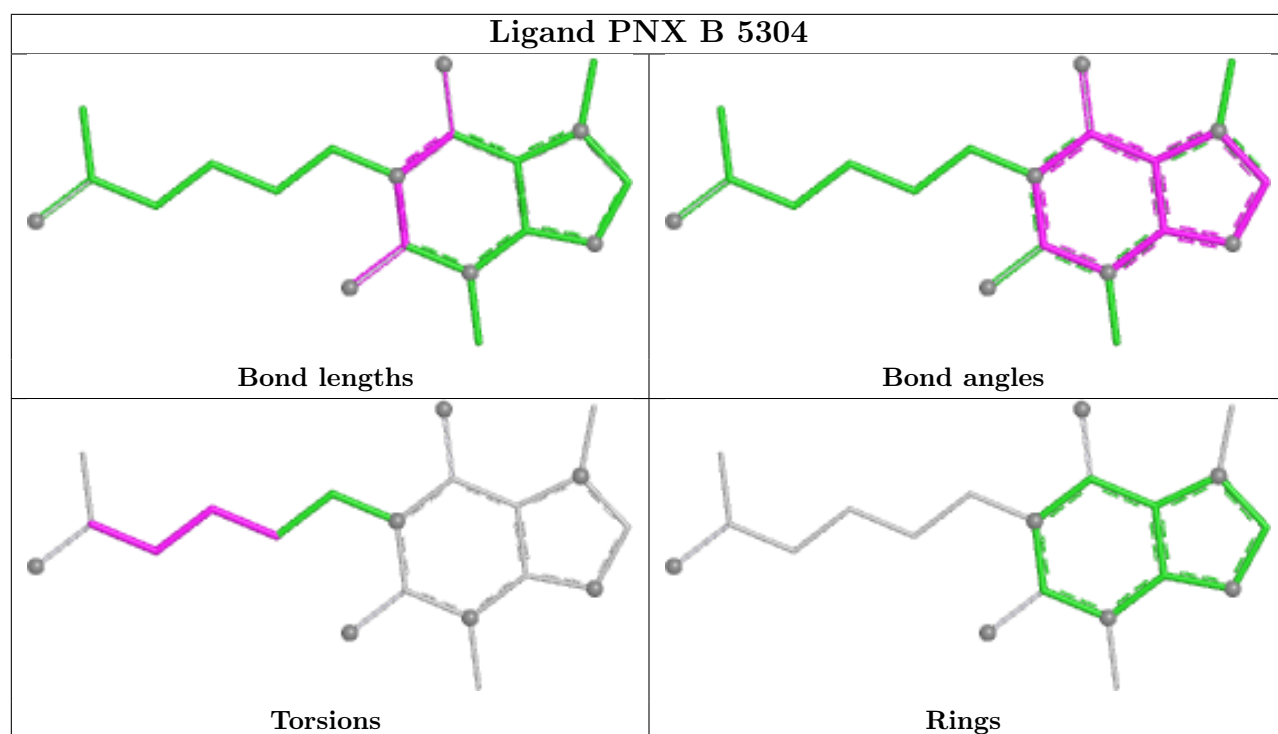
There are no ring outliers.

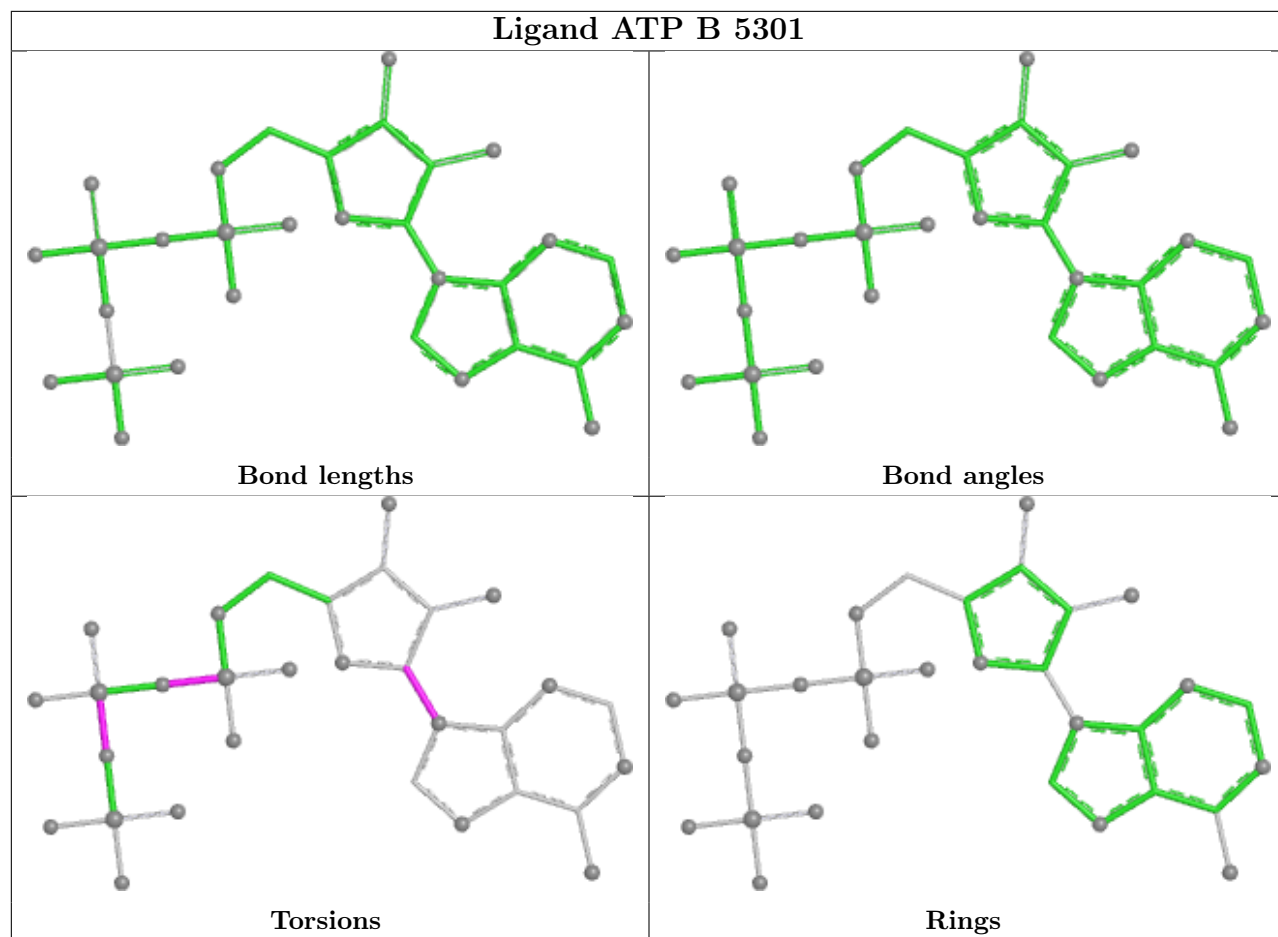
8 monomers are involved in 10 short contacts:

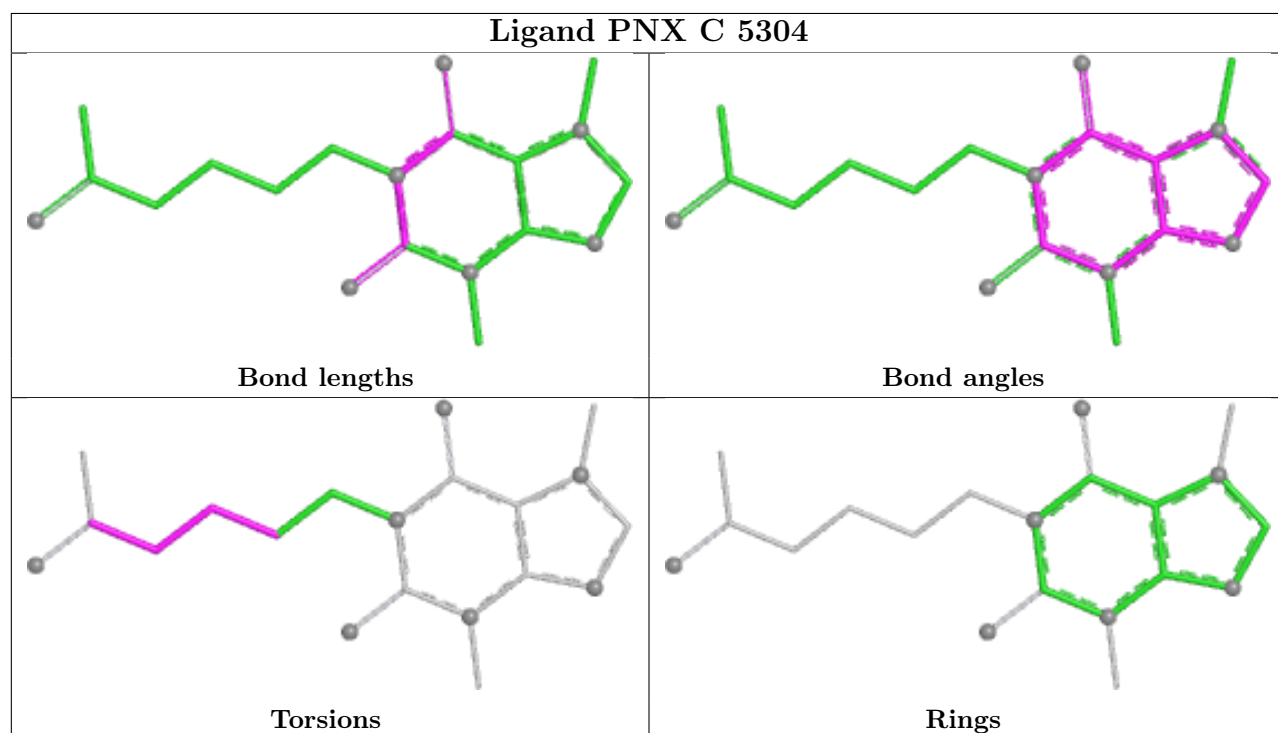
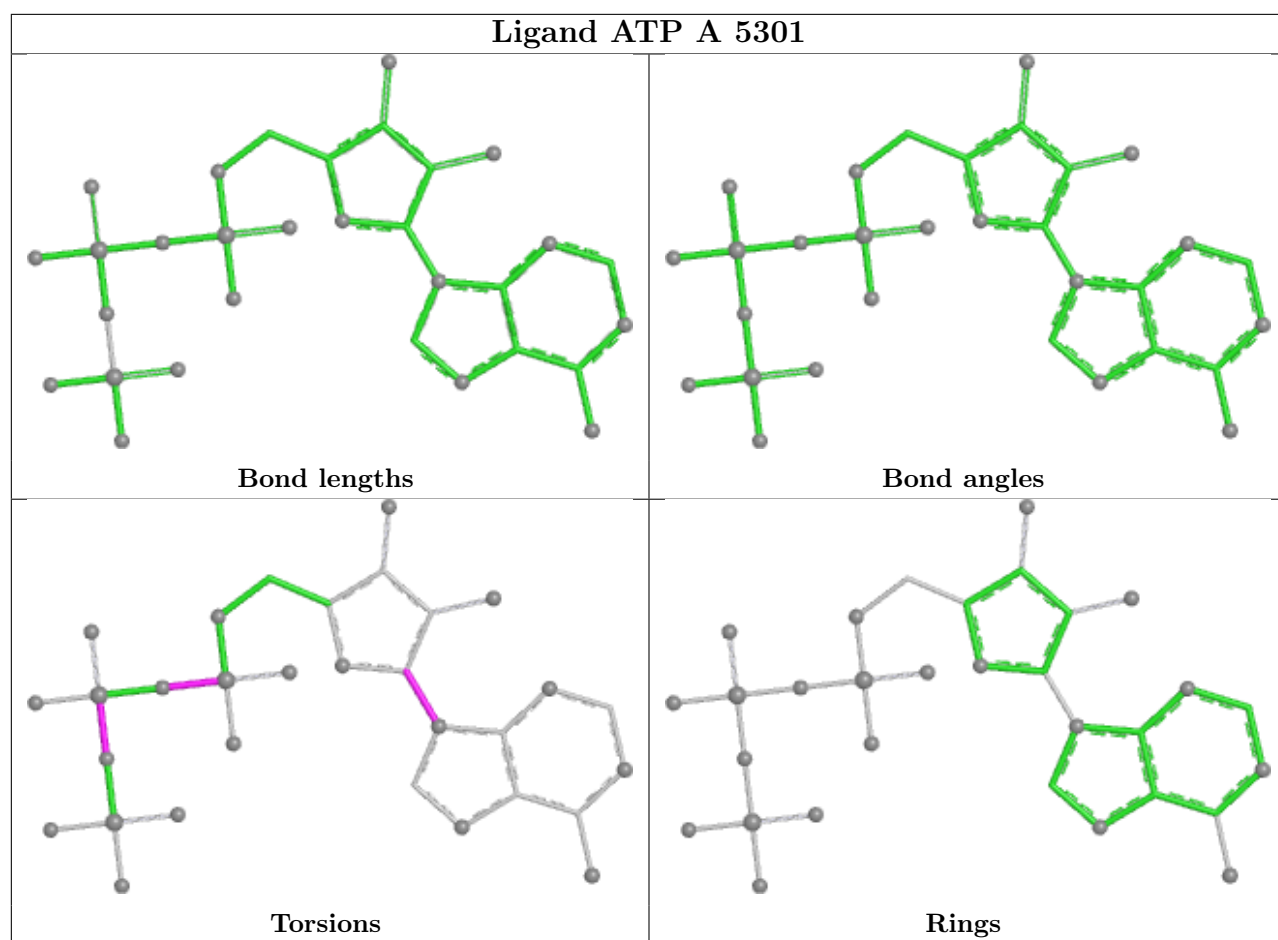
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5301	ATP	1	0
6	D	5304	PNX	1	0
6	B	5304	PNX	2	0
6	A	5304	PNX	2	0
3	B	5301	ATP	1	0
3	A	5301	ATP	1	0
6	C	5304	PNX	1	0
3	D	5301	ATP	1	0

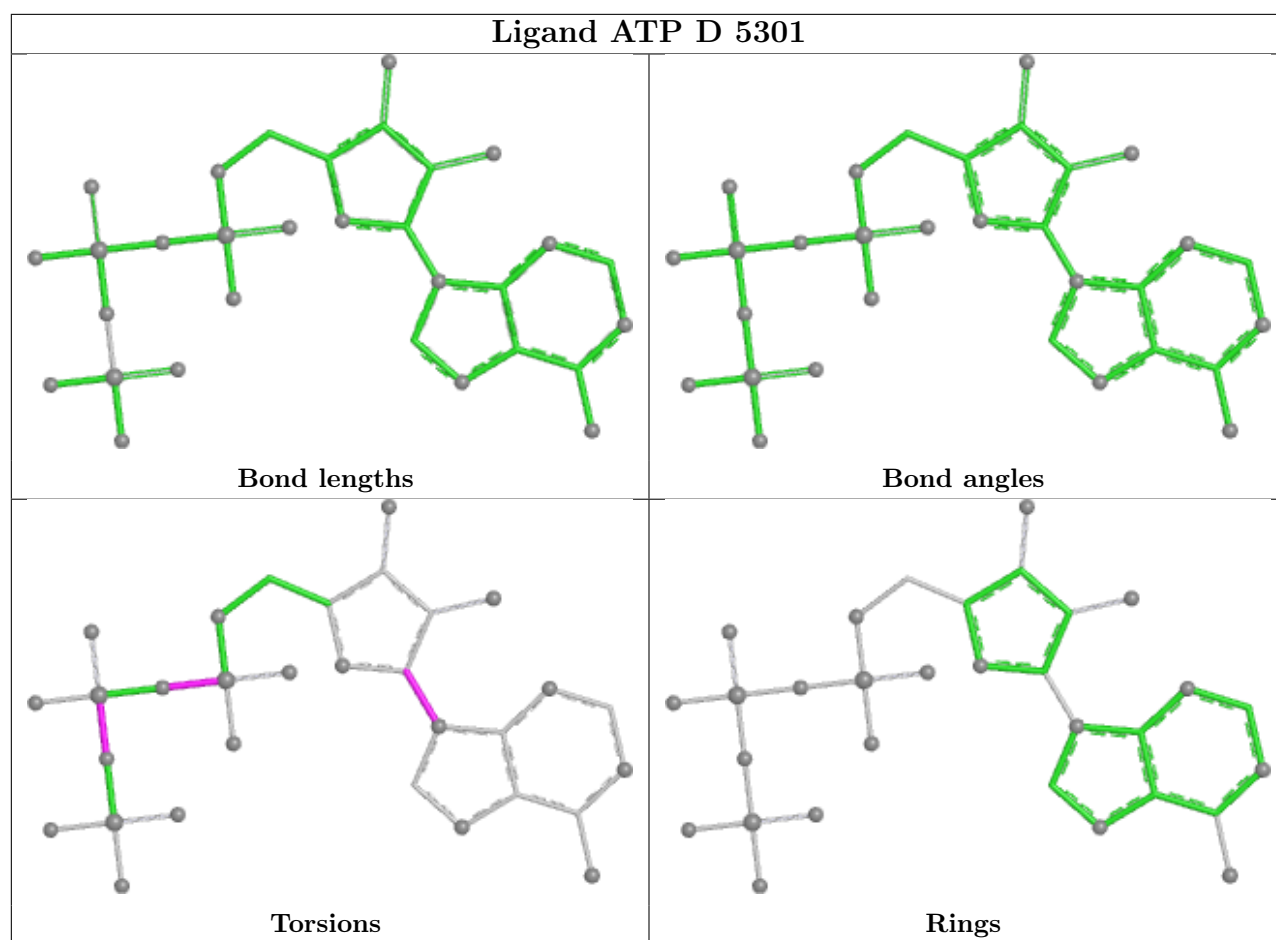
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

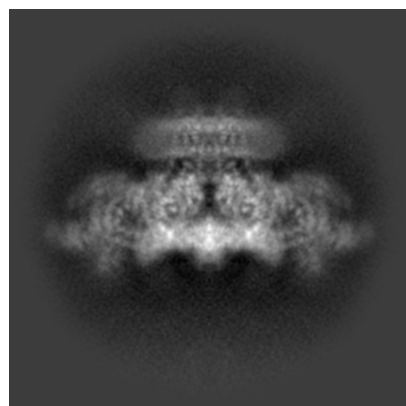
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47386. These allow visual inspection of the internal detail of the map and identification of artifacts.

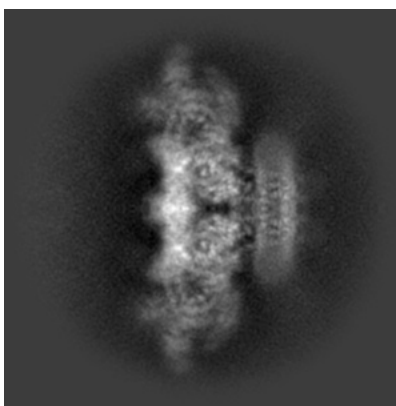
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

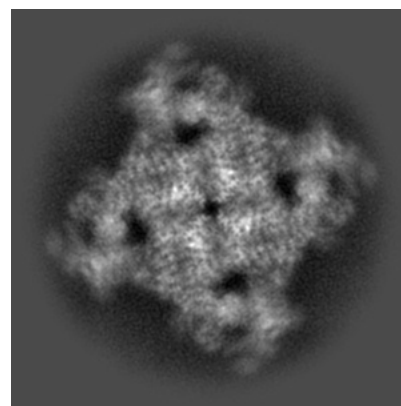
6.1.1 Primary map



X

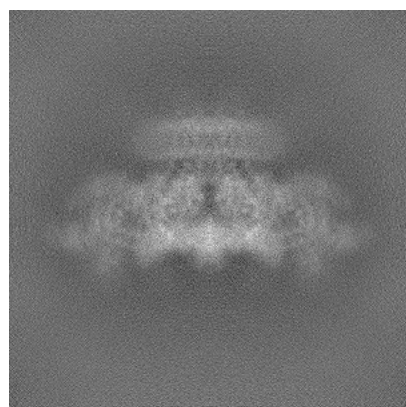


Y

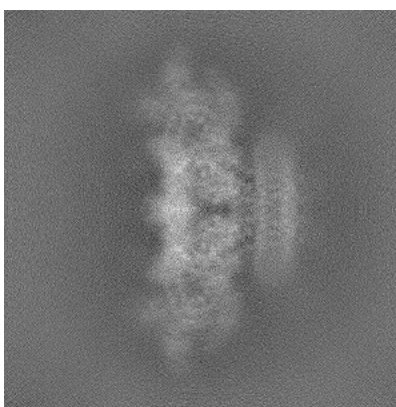


Z

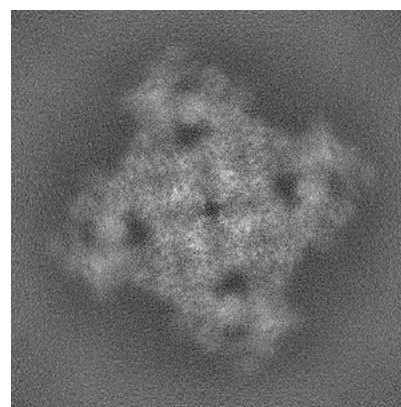
6.1.2 Raw map



X



Y

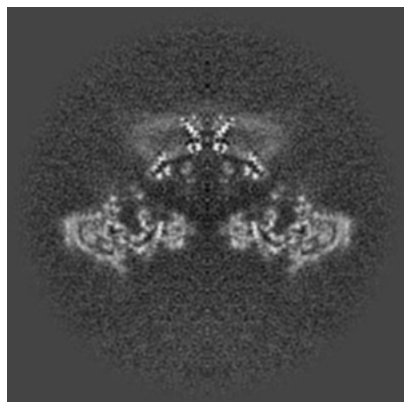


Z

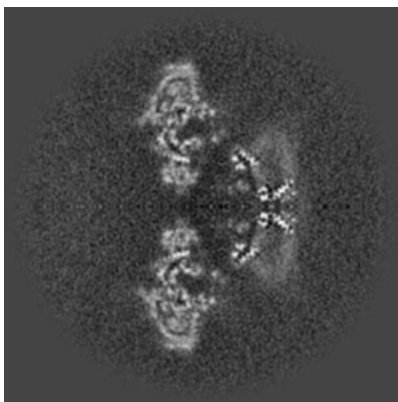
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

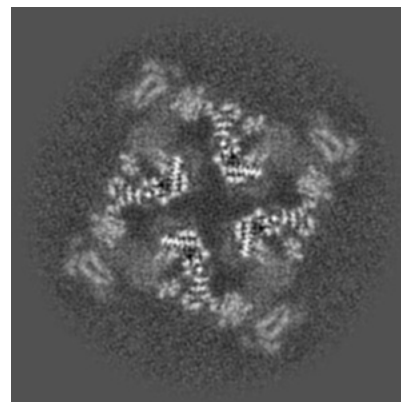
6.2.1 Primary map



X Index: 256

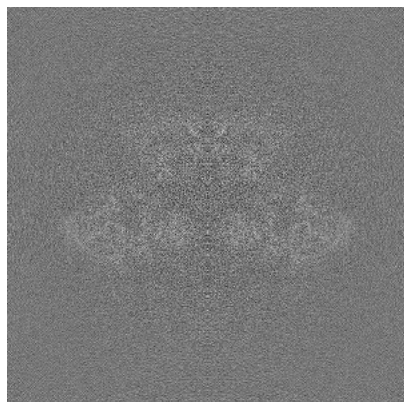


Y Index: 256

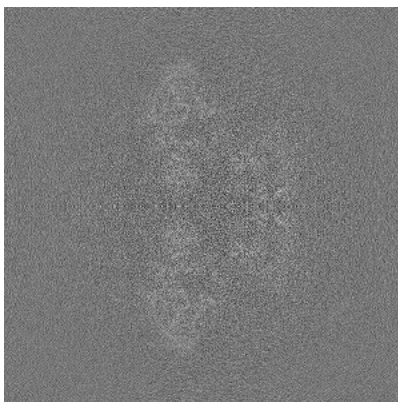


Z Index: 256

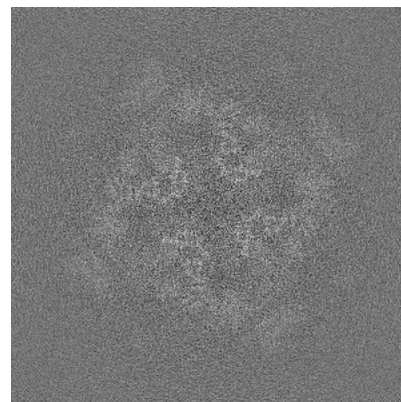
6.2.2 Raw map



X Index: 256



Y Index: 256

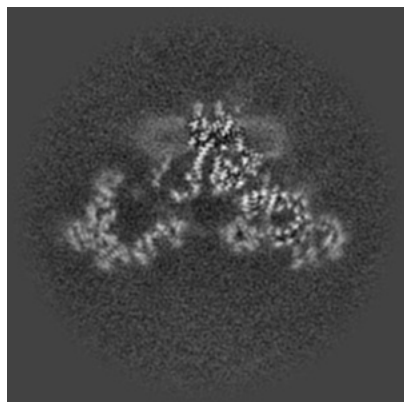


Z Index: 256

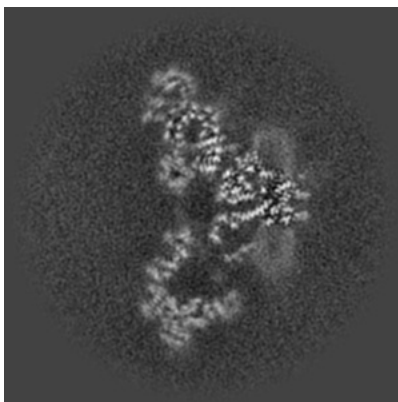
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

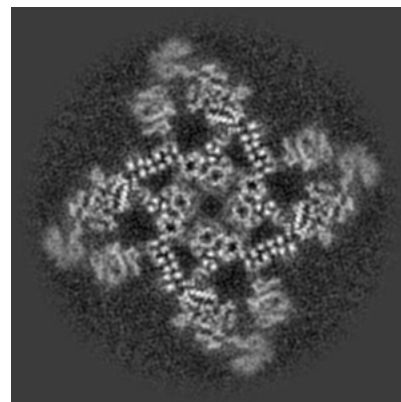
6.3.1 Primary map



X Index: 269

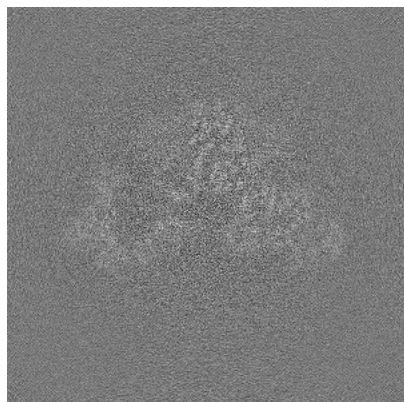


Y Index: 243

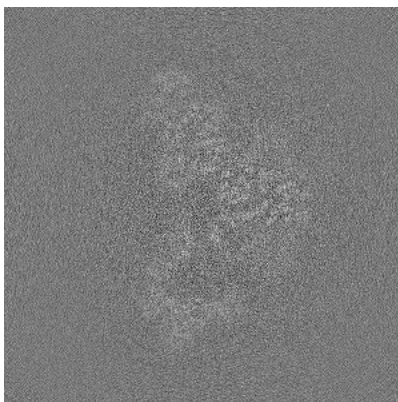


Z Index: 229

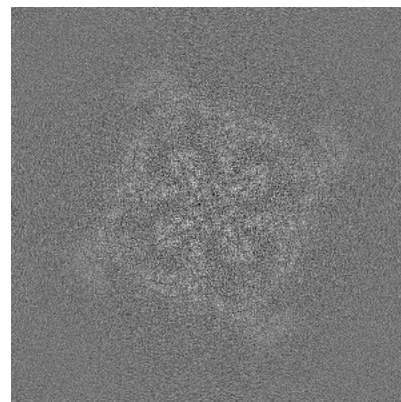
6.3.2 Raw map



X Index: 270



Y Index: 242

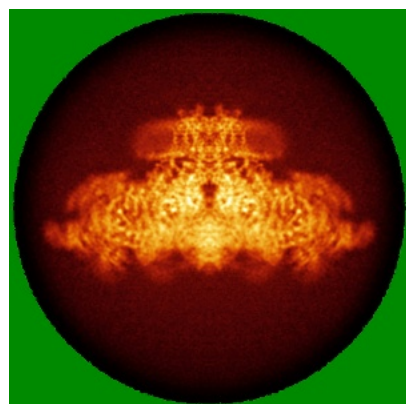


Z Index: 275

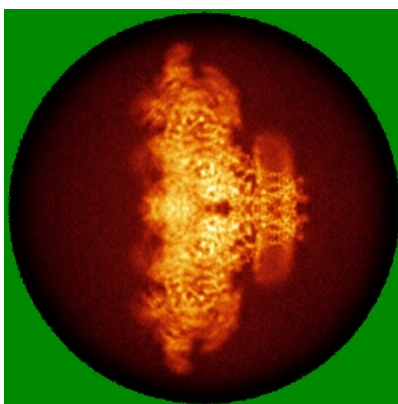
The images above show the largest variance slices of the map in three orthogonal directions.

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

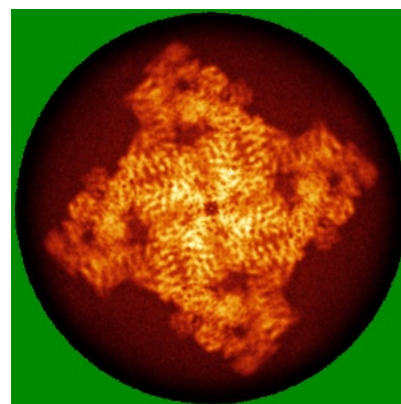
6.4.1 Primary map



X

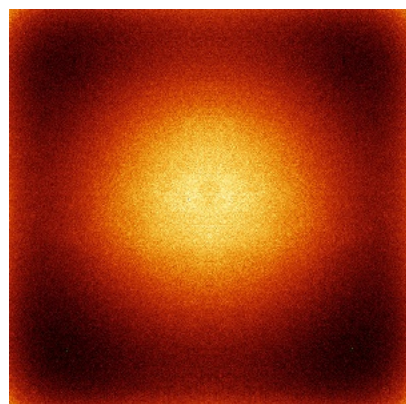


Y

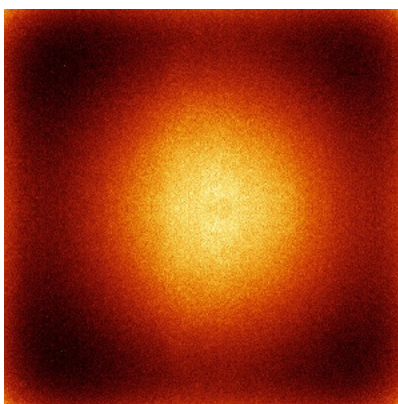


Z

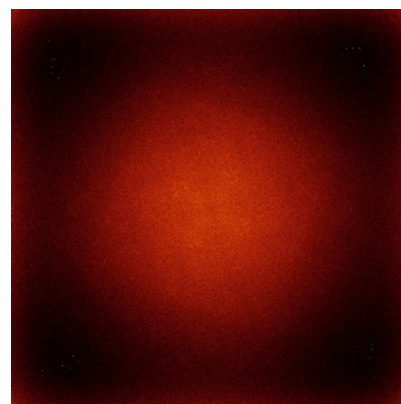
6.4.2 Raw map



X



Y

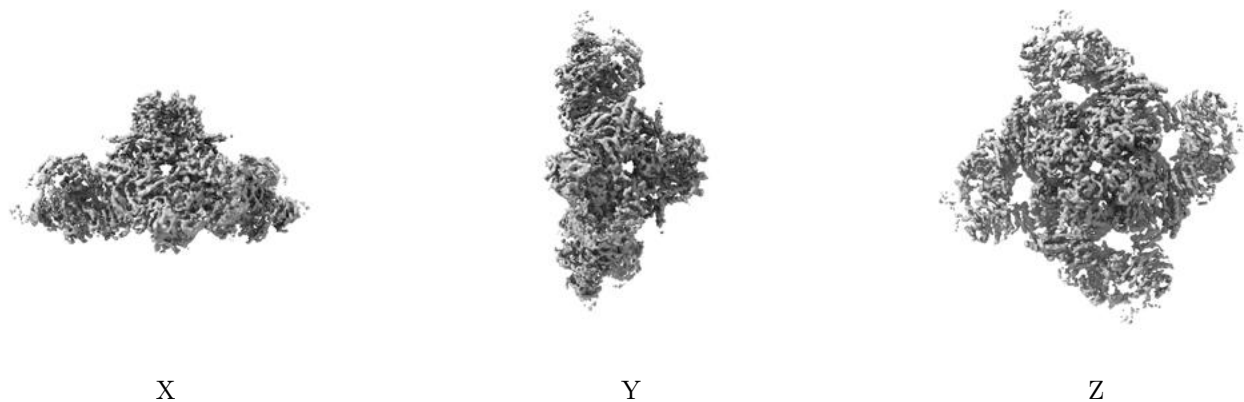


Z

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

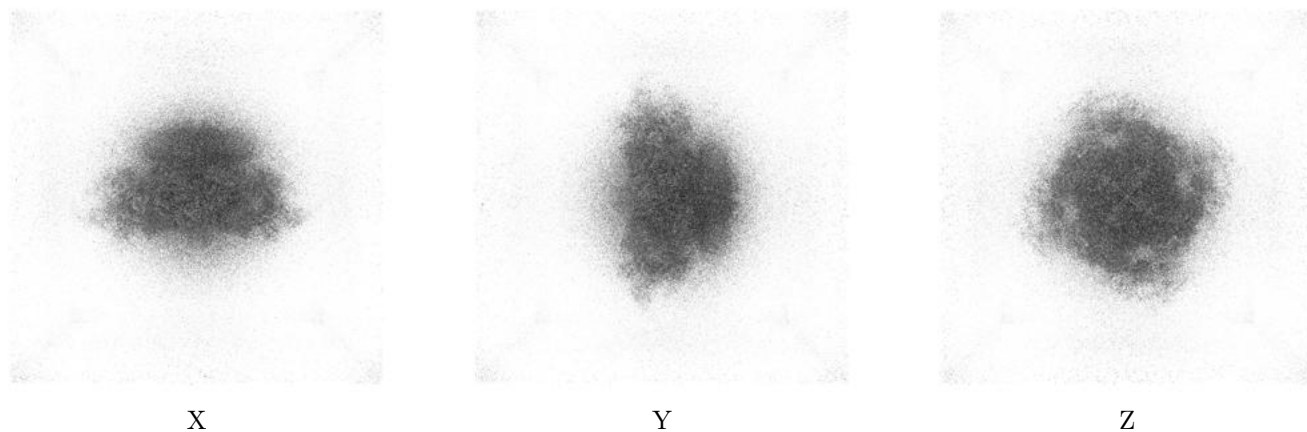
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

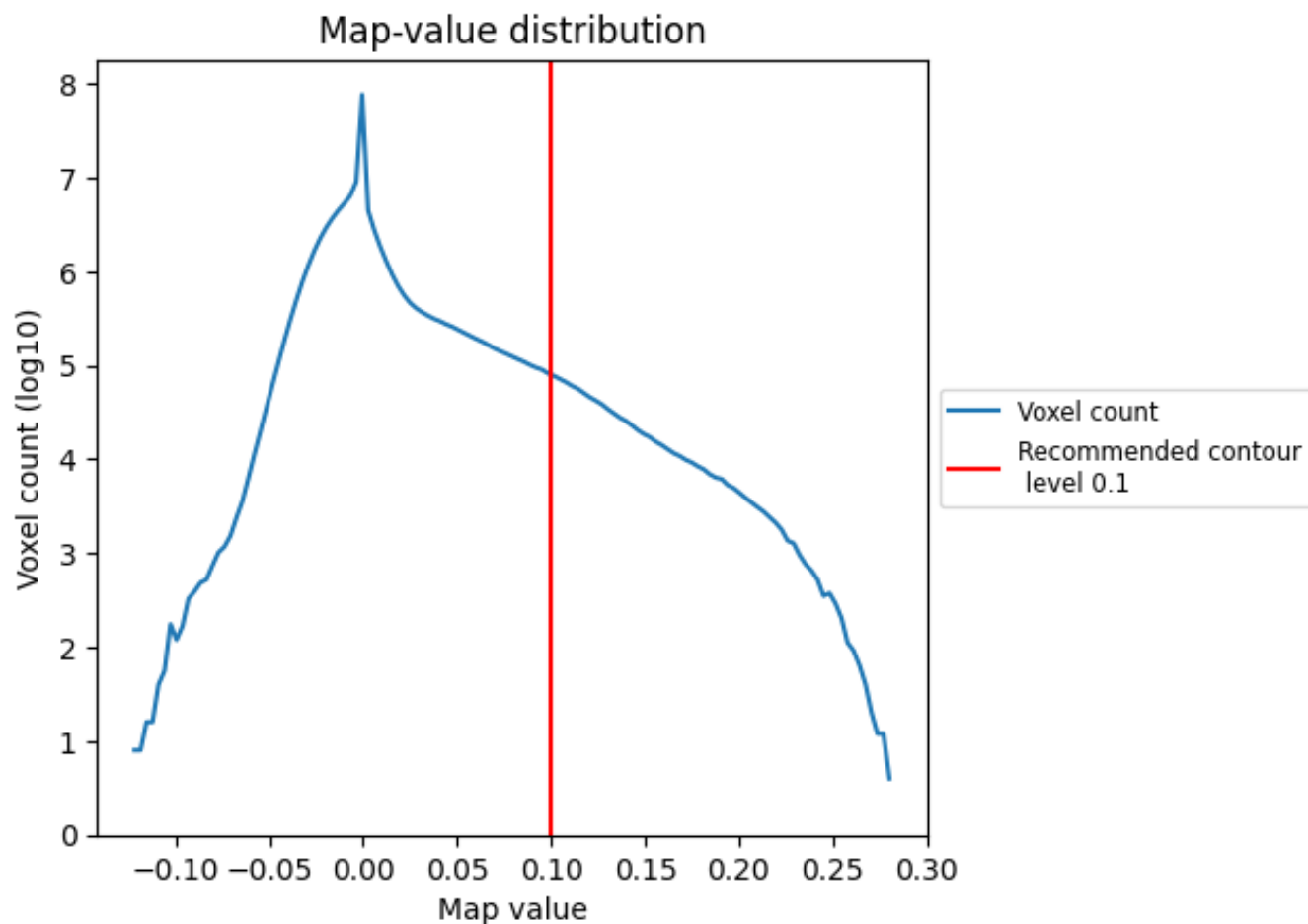
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

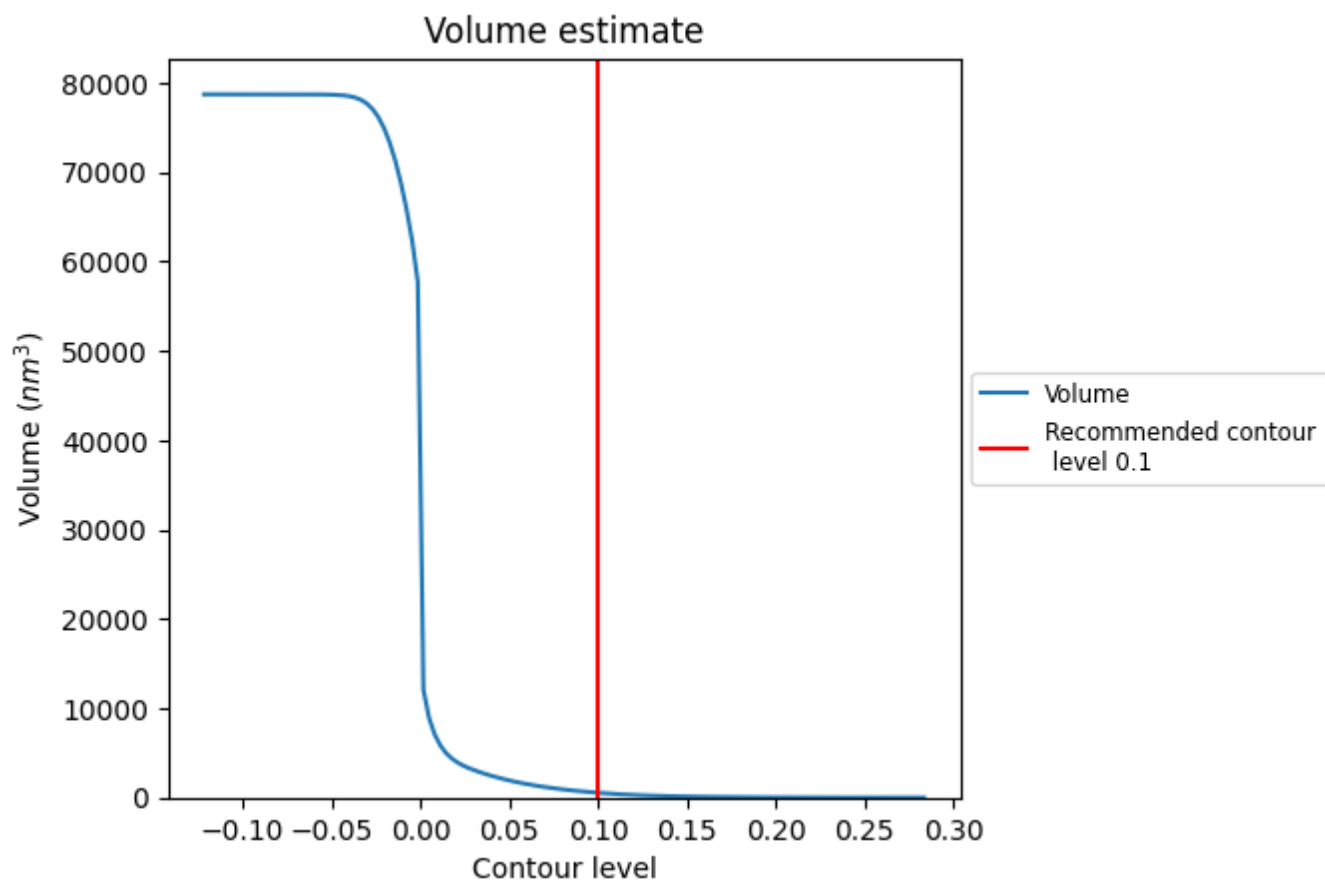
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

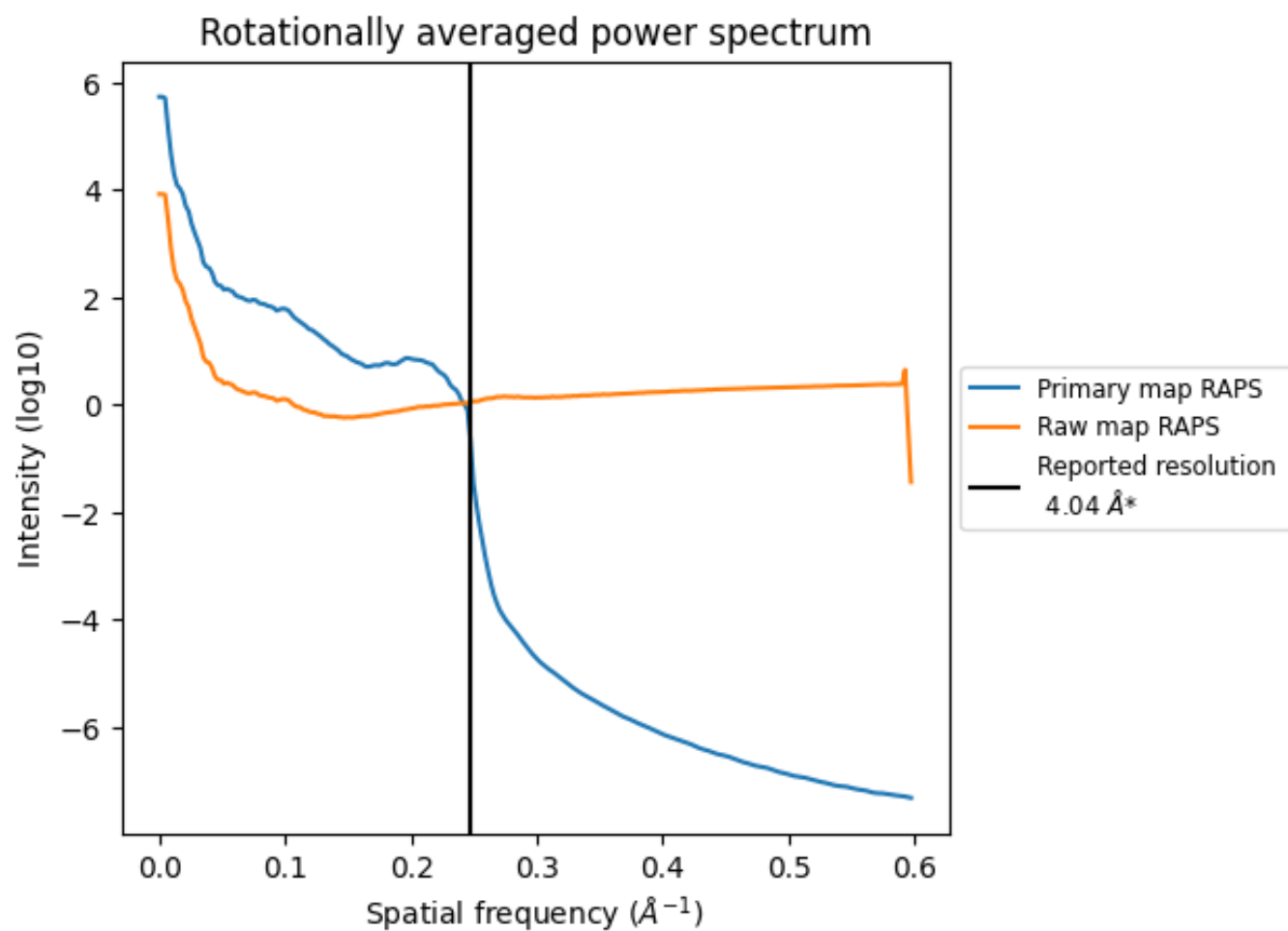
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 534 nm^3 ; this corresponds to an approximate mass of 482 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](#)

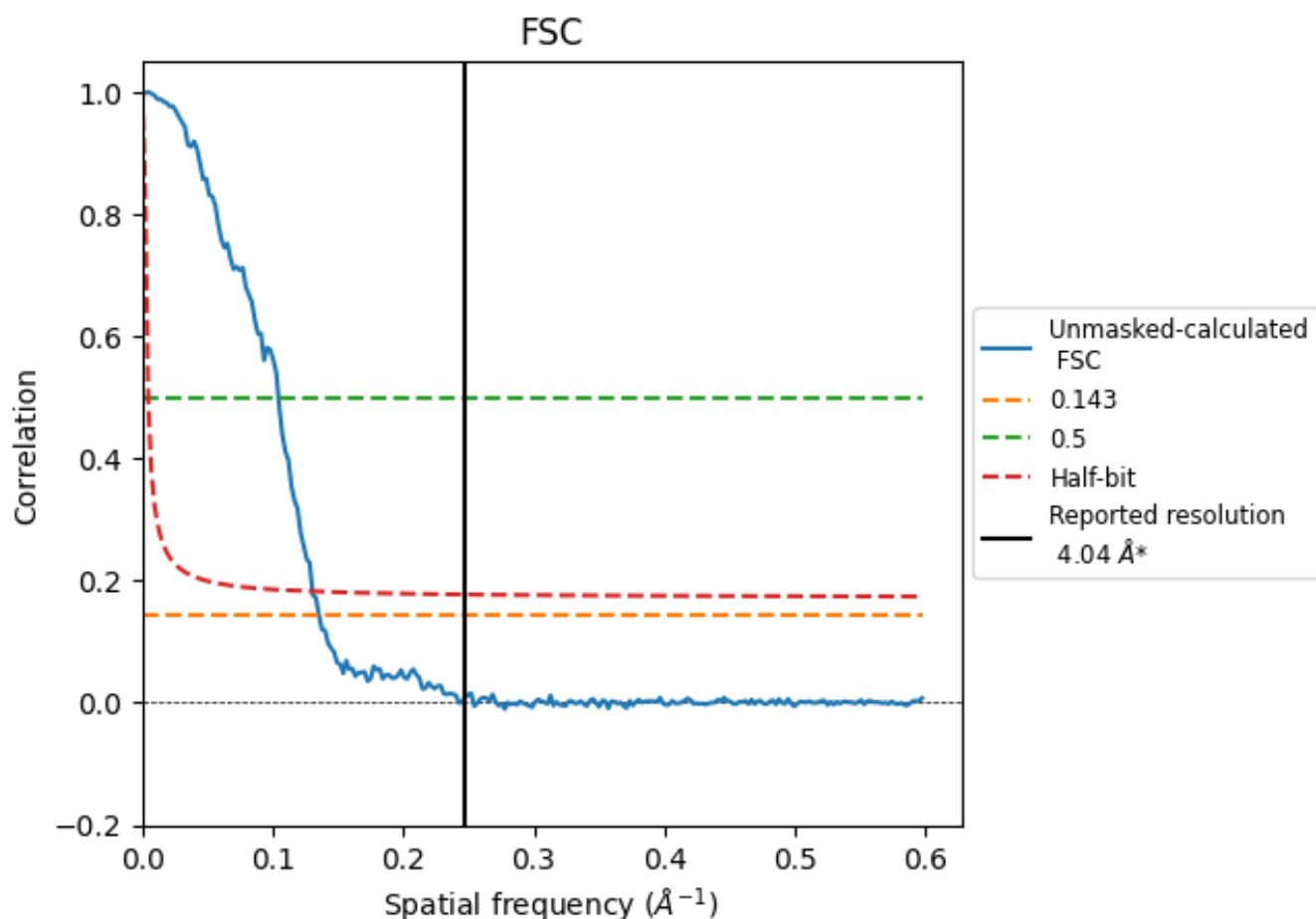


*Reported resolution corresponds to spatial frequency of 0.248 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.248 Å⁻¹

8.2 Resolution estimates [i](#)

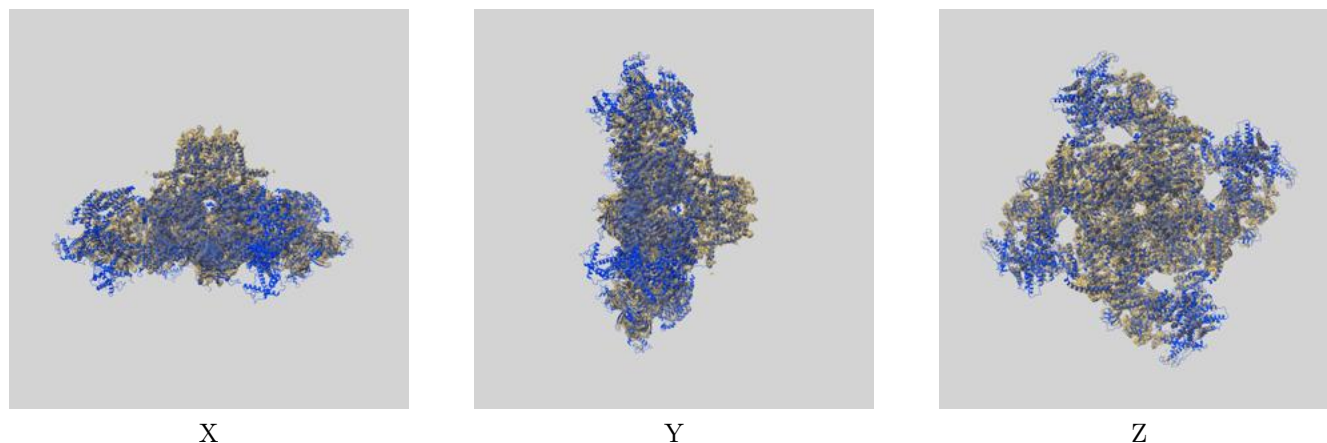
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.04	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.39	9.58	7.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.39 differs from the reported value 4.04 by more than 10 %

9 Map-model fit [i](#)

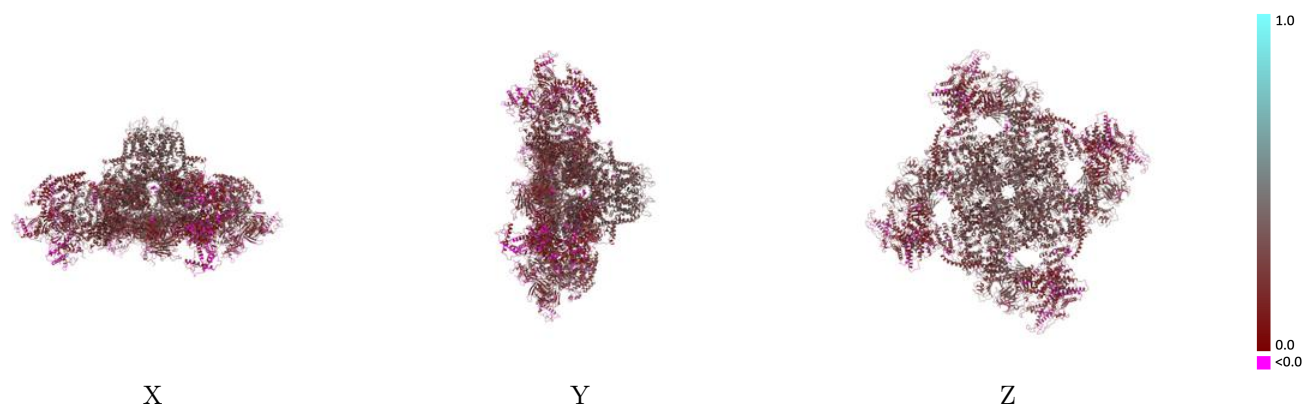
This section contains information regarding the fit between EMDB map EMD-47386 and PDB model 9E19. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



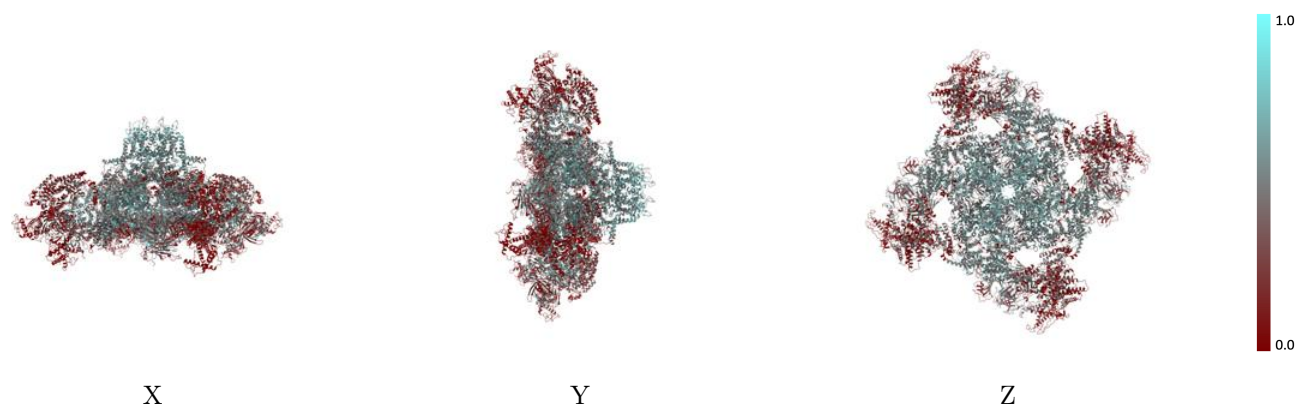
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



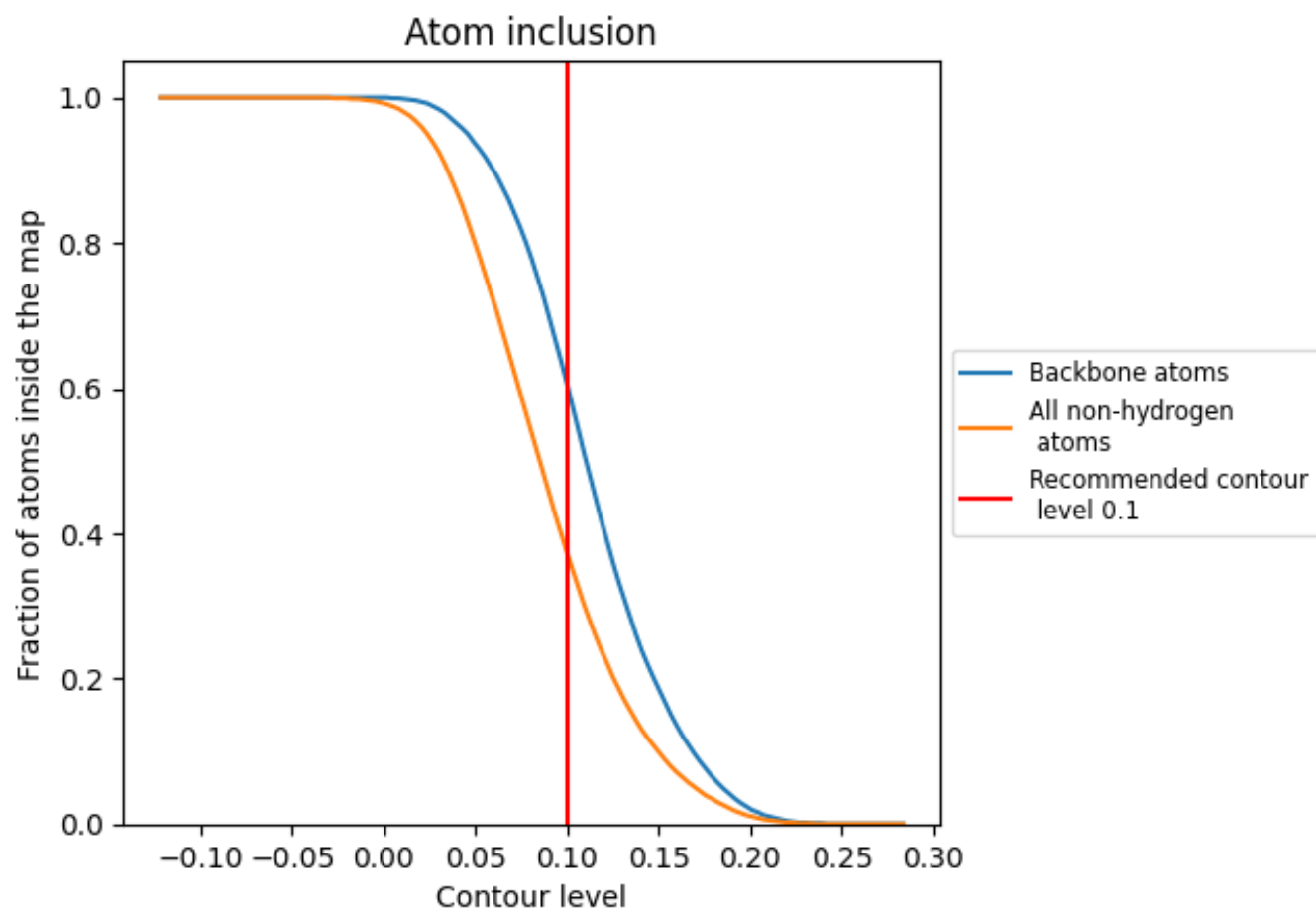
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 37% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3740	0.2250
A	0.3800	0.2270
B	0.3770	0.2240
C	0.3780	0.2240
D	0.3790	0.2250
E	0.1930	0.2270
F	0.1950	0.2210
G	0.1980	0.2260
H	0.1910	0.2270

1.0

0.0

<0.0