



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:43 AM UTC

PDB ID : 5TB3 / pdb_00005tb3
EMDB ID : EMD-8394
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-11
Resolution : 4.70 Å(reported)

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

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

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:

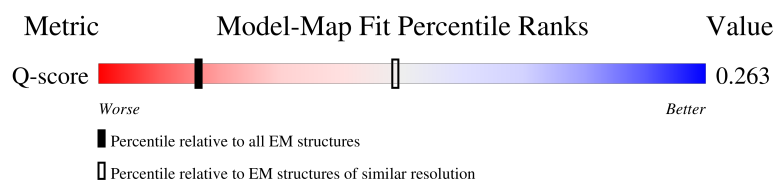
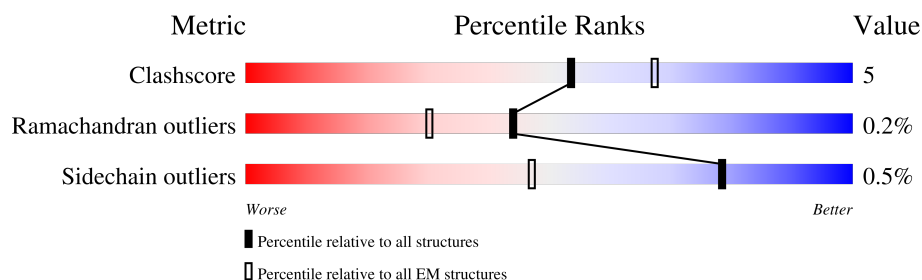
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 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	1989 (4.20 - 5.20)

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	108	80% 80% 19% .
1	F	108	80% 80% 19% .
1	H	108	80% 80% 19% .
1	J	108	81% 81% 18% .

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Mol	Chain	Length	Quality of chain
2	B	4416	66% 83% 12% 5%
2	E	4416	67% 84% 11% 5%
2	G	4416	66% 83% 12% 5%
2	I	4416	67% 83% 11% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121312 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	E	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	I	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	G	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		

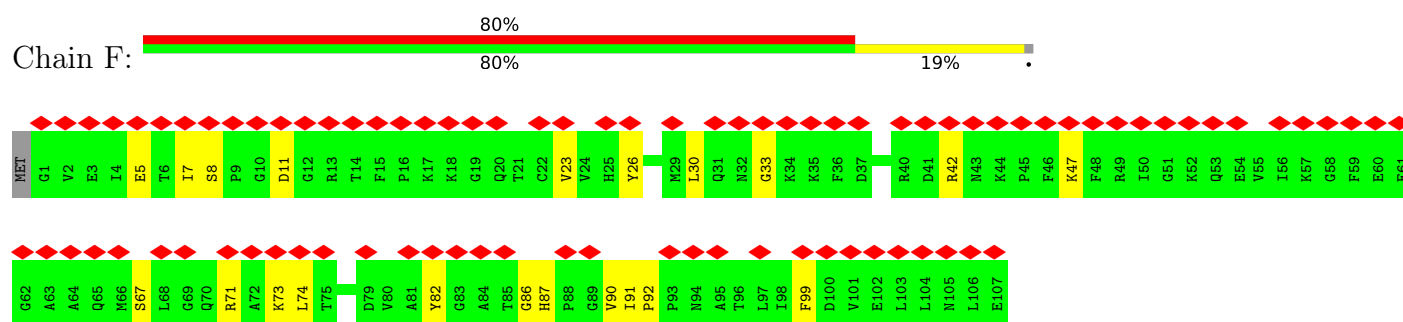
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

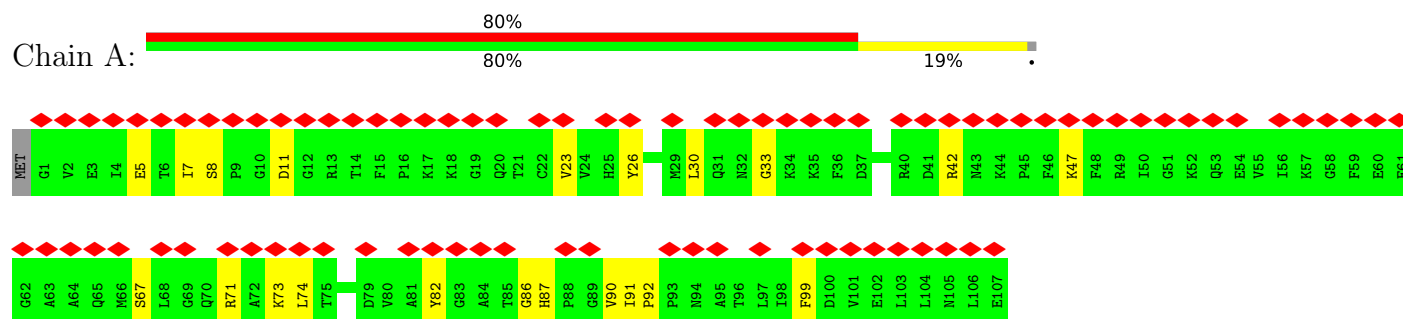
3 Residue-property plots [i](#)

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.

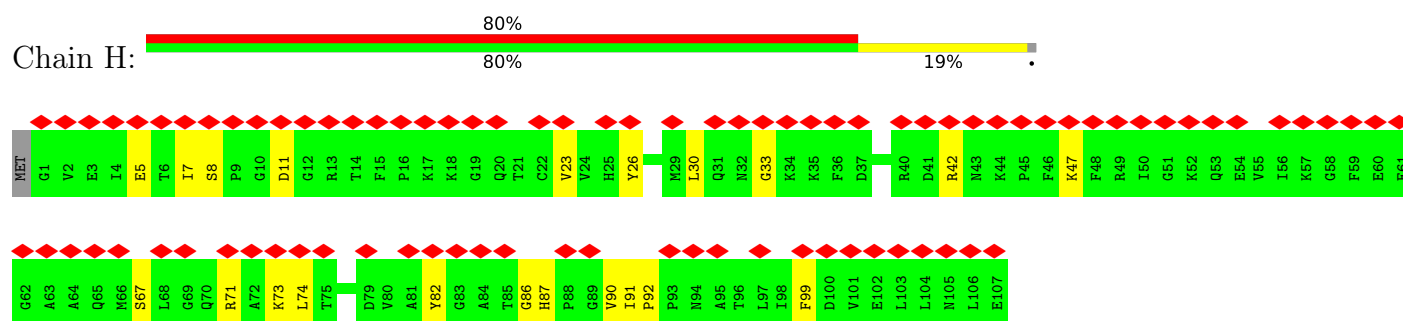
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



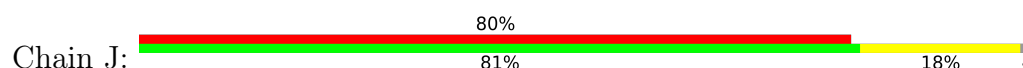
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

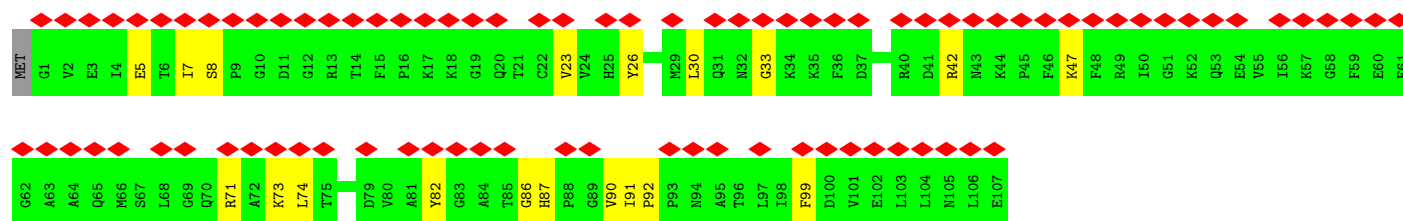


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

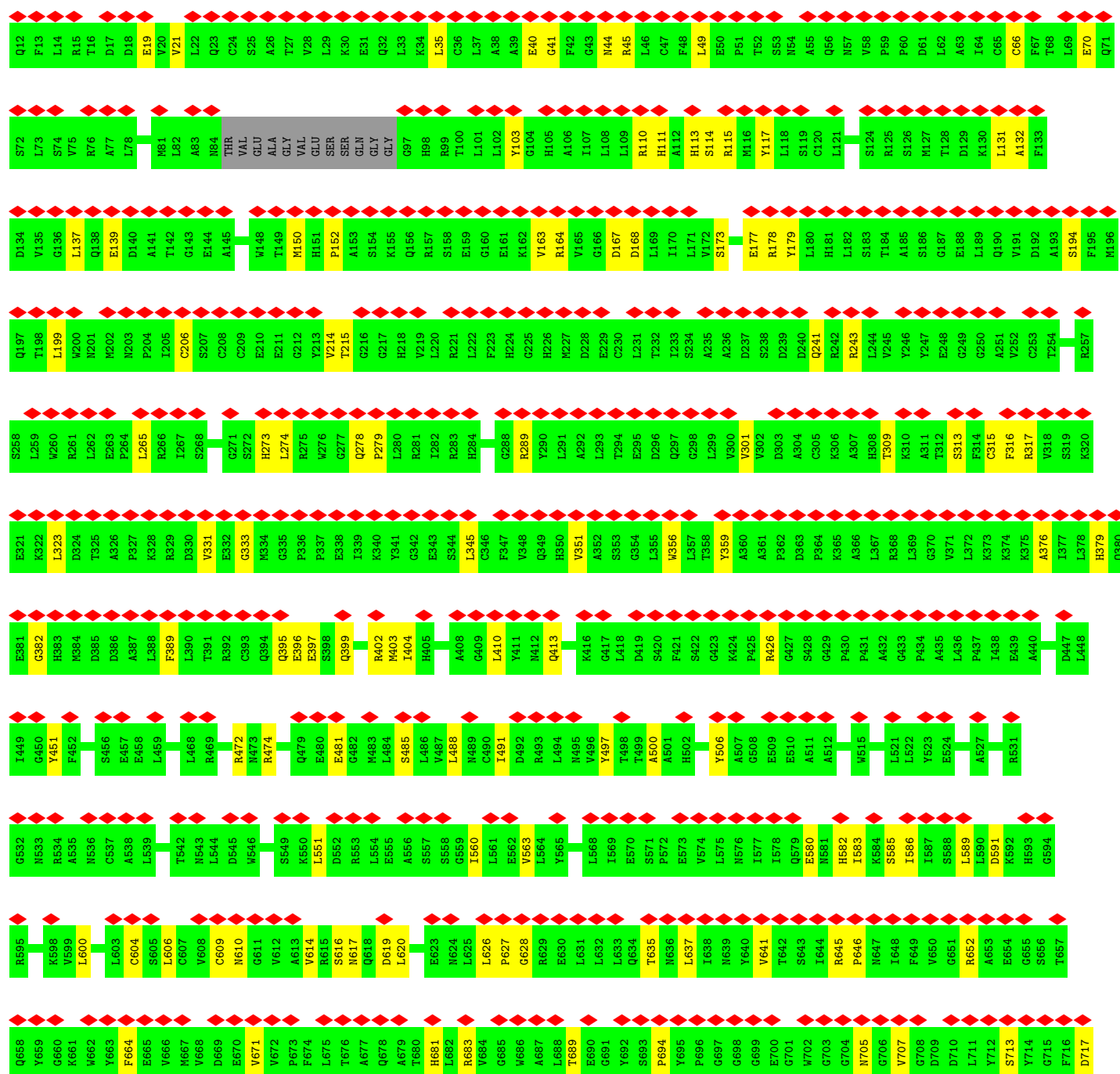
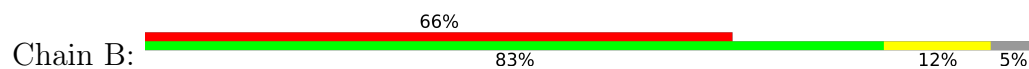


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

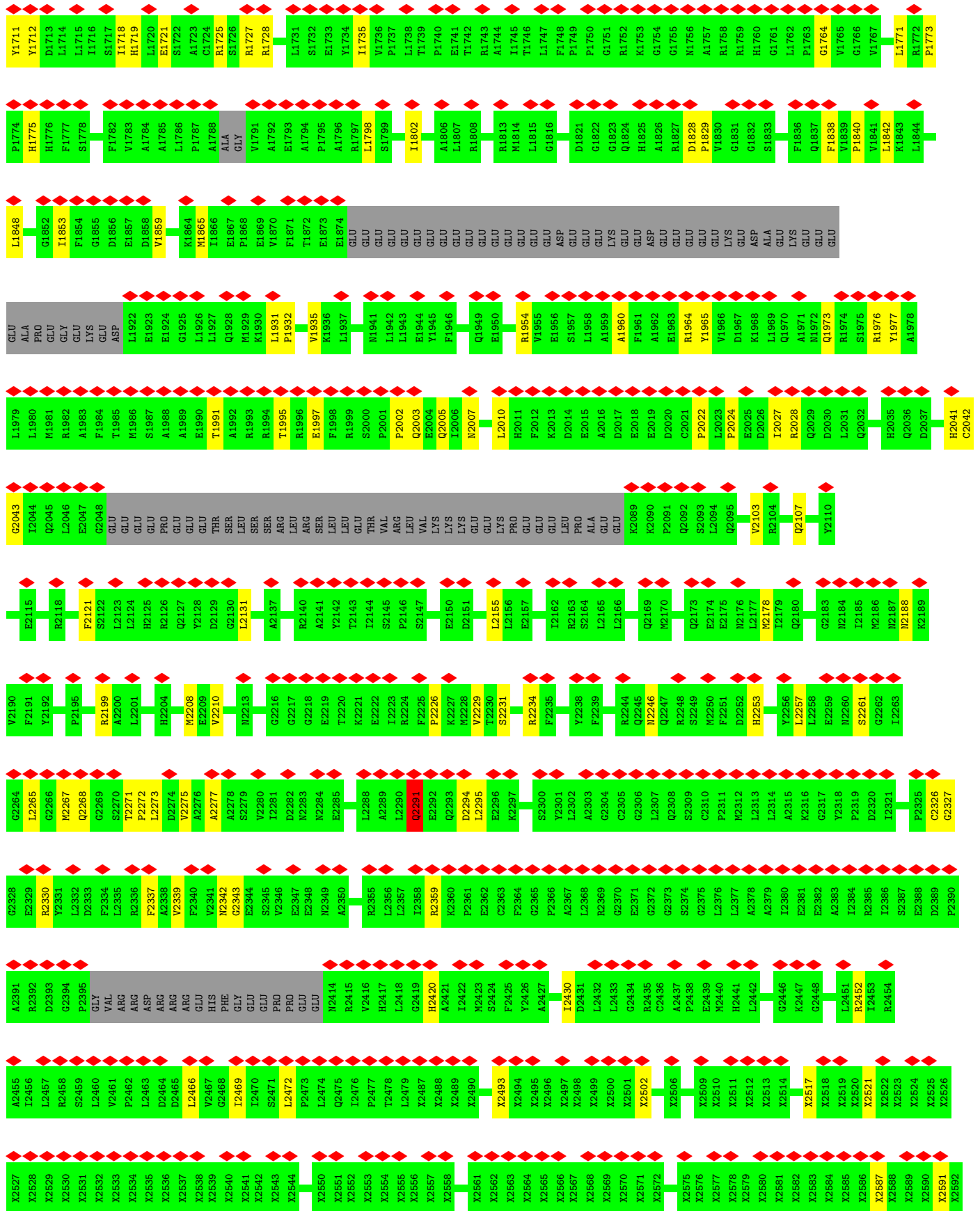




• Molecule 2: Ryanodine receptor 1



M1637	E1643	L1657	L1575	X1497	C1217	D1154	E1093	T1031	M961	K901	G841	V781	G718
A1638	E1644	L1658	S1576	X1504	G1218	L1155	A1094	K1032	S962	R902	P842	S782	L719
L1639	E1645	L1659	A1577	X1505	L1219	T1156	V1095	L1033	N963	L903	S843	S783	H720
H1640	R1646	Q1647	A1578	X1506	Q1220	E1157	T1096	S1034	G964	H904	R844	S784	L721
E1643	C1647	M1648	M1579	X1510	E1221	T1159	T1097	N1035	P965	P905	C845	A785	G724
E1644	E1648	D1649	F1580	X1511	F1222	I1160	E1099	R1036	K966	C906	R846	G786	H725
S1582	E1648	L1652	X1291	X1512	E1223	I1161	M1100	L1037	P967	L907	S847	G787	V726
R1583	E1648	L1653	X1292	X1513	E1224	F1162	R1101	S1038	A968	V908	H848	K788	V727
E1584	E1648	L1654	X1293	X1514	A1227	T1163	R1102	L1039	P969	N909	T849	V789	A727
K1585	E1648	L1655	X1294	X1515	I1228	L1164	V1103	G1040	L970	F910	D850	R790	R728
L1586	E1648	L1656	X1430	X1516	I1228	L1164	G1103	Q1041	D971	H911	F851	F791	P729
P1587	E1648	L1657	X1431	X1517	Q1231	V1168	W1104	A1042	L972	S912	V852	L792	V730
A1588	E1648	L1658	X1434	X1518	R1232	L1169	A1105	V1043	L972	L913	P853	G794	T731
P1589	E1648	L1659	X1437	X1519	T1235	M1170	R1106	R1044	H974	P914	C854	G795	S732
Q1590	E1648	L1660	X1438	X1520	W1236	S1171	E1108	T1045	V975	E915	P855	R796	P733
P1591	E1648	L1661	X1439	X1521	W1237	D1172	L1109	L1046	R976	P916	V856	G797	Q735
P1592	E1648	L1662	X1440	X1522	F1238	G1174	R1110	L1047	L977	E917	D857	G798	Q736
R1593	E1648	L1663	X1441	X1523	S1239	S1175	P1111	G1048	T978	R918	THR	E799	H736
R1594	E1648	L1664	X1442	X1524	K1240	E1176	D1112	Y1049	P979	N919	V800	F800	L737
E1595	E1648	L1665	X1443	X1525	S1241	T1177	V1113	G1050	A980	Y920	I861	K801	L738
V1597	E1648	L1666	X1444	X1526	F1245	A1178	L1114	Y1051	Q981	N921	V862	F802	L739
Q1598	E1648	L1667	X1445	X1527	E1246	F1179	L1115	I1052	T982	L922	L863	P804	P740
M1599	E1648	L1668	X1446	X1528	E1251	R1180	G1116	I1053	T983	Q923	P864	P805	E741
P1600	E1648	L1669	X1447	X1529	E1254	E1181	A1117	E1054	L984	M924	P865	P806	S745
M1601	E1648	L1670	X1448	X1530	H1254	I1182	E1119	PRO	P986	S925	H866	G807	C746
P1602	E1648	L1671	X1449	X1531	Y1255	E1184	L1120	ASP	R987	E927	L867	Y808	C747
V1603	E1648	L1672	X1450	X1532	E1256	I1185	A1121	GLU	L988	T928	E868	A809	L748
S1606	E1648	L1673	X1451	X1533	V1257	D1186	Y1122	PRO	L988	L929	R869	P810	D749
P1607	E1648	L1674	X1452	X1534	A1258	F1187	V1123	SER	A989	K930	I870	C811	L750
M1608	E1648	L1675	X1453	X1535	R1259	F1188	F1124	GLN	D999	T931	E871	E813	S751
H1611	E1648	L1676	X1456	X1537	M1260	L1189	N1125	VAL	Q1003	L932	K873	A814	V752
F1612	E1648	L1677	X1456	X1538	D1261	P1190	GLN	ASN	G1004	L933	K874	V815	P753
L1613	E1648	L1678	X1457	X1539	G1262	V1191	G1126	ASN	W1005	A934	L874	L816	S754
Q1614	E1648	L1679	X1458	X1540	T1263	C1192	H1127	SER	S1006	L935	A875	P817	I755
V1615	E1648	L1680	X1459	X1541	V1264	S1193	R1128	ARG	S1007	G936	E876	R818	F757
THR	E1648	L1681	X1460	X1542	D1265	L1194	G1130	TRP	S1008	C937	N877	E819	R758
ARG	E1648	L1682	X1464	X1543	T1266	G1195	R1131	R1071	A1009	H938	I878	R820	I759
ALA	E1648	L1683	X1473	X1544	P1267	Q1198	W1132	V1072	VAL	V939	H879	L821	N760
GLY	E1648	L1684	X1474	X1545	P1268	V1199	H1133	R1073	GLN	G940	E880	L822	G761
E1622	E1648	L1685	X1475	X1546	C1269	G1200	L1134	T1074	ASP	M941	L881	L823	C762
R1623	E1648	L1686	X1476	X1547	L1270	L1201	G1135	F1075	PRO	A942	W882	E824	P763
L1624	E1648	L1687	X1477	X1548	R1271	L1202	S1136	R1076	ALA	D943	A883	P825	V764
G1625	E1648	L1688	X1478	X1549	R1272	M1203	F1139	A1077	ARG	E944	L884	I826	Q765
W1626	E1648	L1689	X1479	X1550	A1273	L1204	G1140	E1078	ASN	K945	T885	K827	G766
A1627	E1648	L1690	X1480	X1551	H1274	G1205	R1141	S1080	PRO	A946	R886	E828	V767
V1628	E1648	L1691	X1481	X1552	Q1206	Q1206	R1142	R1020	GLN	E947	I887	E829	F768
Q1629	E1648	L1692	X1482	X1553	D1207	Q1207	P1142	L1021	ILE	D948	E888	Y829	E769
C1630	E1648	L1693	X1483	X1554	V1208	V1208	W1143	V1022	PRO	Q889	A770	R830	A770
Q1631	E1648	L1694	X1484	X1555	S1209	S1209	W1145	V1023	ARG	N949	F771	R831	F771
D1632	E1648	L1695	X1485	X1556	S1210	S1210	S1146	Y1024	ALA	G890	N772	E832	N772
P1633	E1648	L1696	X1486	X1557	L1211	L1211	G1146	R1025	ASN	K951	W891	G833	L773
L1634	E1648	L1697	X1487	X1558	L1212	L1212	D1147	L1026	ASN	K952	T892	P834	D774
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	E1648	L1700	X1492	X1561	A1215	A1215	E1091	E1029	GLN	L955	P895	P837	F777
	E1648	L1701	X1492	X1562	I1216	I1216	F1092	A1030	VAL	P956	V896	H838	F778
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	E1648	L1705	X1492	X1566					ASP				
	E1648	L1706	X1492	X1567					ASP				
	E1648	L1707	X1492	X1568					ASP				
	E1648	L1708	X1492	X1569					ASP				
	E1648	L1709	X1492	X1570					ASP				
	E1648	L1710	X1492	X1571					ASP				





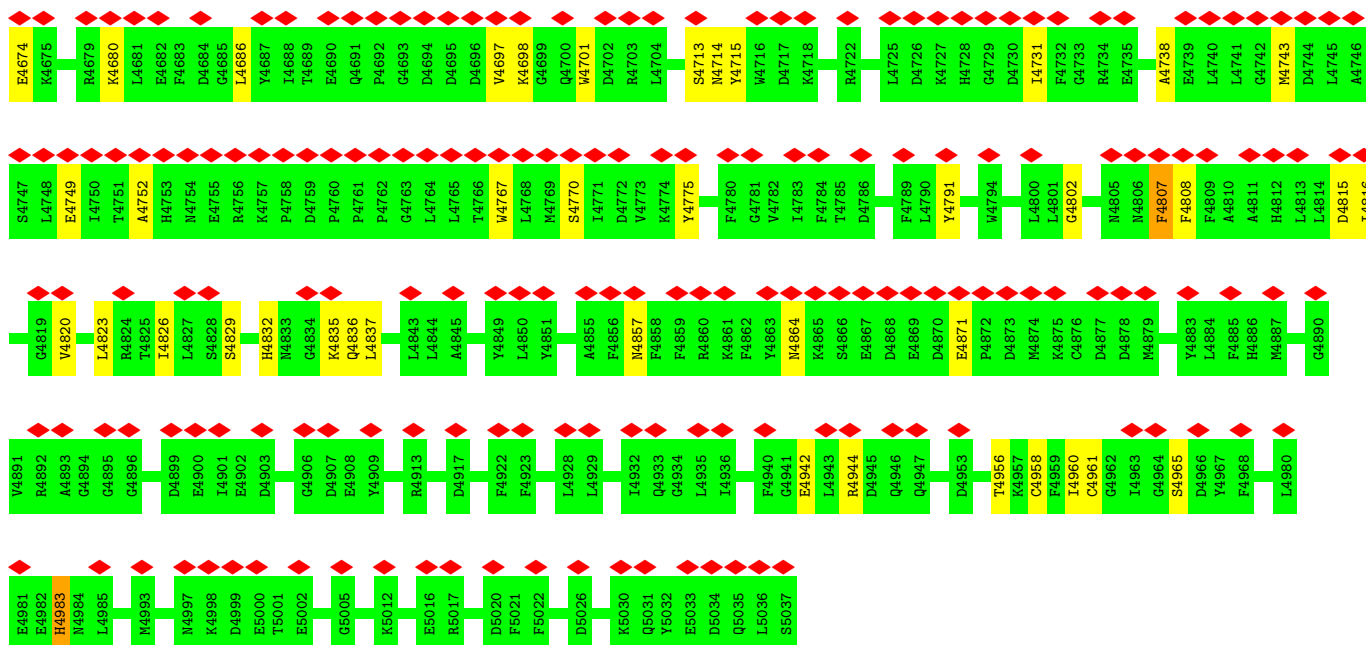
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E4739	S4252	G4033	G4033	A3954	L3721	A3649	X3563
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G4742	X4322	Q4102	Q4102	K3959	Y3726	M3652	X3566
M4743	X4325	F4103	F4103	Q3960	A3726	F3653	X3567
D4744	X4325	T4104	T4104	Y3961	L3805	L3654	X3568
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A4746	X4334	P4106	P4106	S3963	N3809	S3657	X3570
S4747	X4340	E4107	E4107	L3890	M3729	K3658	X3571
E4748	X4341	L4108	L4108	L3891	A3730	A3659	X3572
L4749	X4342	Q4109	Q4109	L3892	L3731	A3660	X3573
I4750	X4343	F4110	F4110	E3967	H3734	W3661	X3574
T4751	X4344	L4111	L4111	Y3968	L3735	I3662	X3575
A4752	X4345	L4112	L4112	T3969	E3736	L3663	X3576
H4753	X4346	S4113	S4113	E3970	E3737	T3664	X3577
D4754	X4347	E4114	E4114	Q3971	Q3738	E3665	X3578
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L4756	X4349	E4116	E4116	Q3978	E3740	H3667	X3580
R4757	X4352	A4117	A4117	R3984	N3741	S3668	X3581
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D4764	X4359	M4124	M4124	L3994	V3749	X3588	X3588
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L4768	X4363	F4128	F4128	H3998	F3753	X3593	X3593
M4769	X4364	A4129	A4129	X3999	E3754	Q3683	X3594
D4770	X4365	N4130	N4130	M4001	E3755	E3684	X3595
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L4778	X4373	Q4140	Q4140	Q4009	L3763	E3692	X3605
L4779	X4374	F4141	F4141	E4011	L3764	K3693	X3606
L4780	X4375	M4142	M4142	L4012	Q3766	L3703	X3607
L4781	X4376	L4147	L4147	L4013	Q3767	H3704	X3608
L4782	X4377	E4152	E4152	K4014	S3768	F3705	X3609
L4783	X4378	H4156	H4156	E4015	R3769	S3706	X3610
L4784	X4379	R4159	R4159	L4016	L3770	R3707	X3611
L4785	X4380	L4160	L4160	L4017	H3771	T3711	X3612
L4786	X4381	F4161	F4161	D4018	T3772	E3712	X3613
L4787	X4382	E4239	E4239	K4090	G3774	Y3714	X3614
L4788	X4383	L4233	L4233	K4091	A3775	K3715	X3643
L4789	X4384	E4239	E4239	D4092	E3777		X3644
L4790	X4385	F4163	F4163	Q4021			X3645
L4791	X4386	L4164	L4164				X3646
L4792	X4387						X3647
L4793	GLY						X3648
L4794							X3649
L4795							X3650
L4796							X3651
L4797							X3652
L4798							X3653
L4799							X3654
L4800							X3655
L4801							X3656
G4802							X3657

X1504	X1505	X1506	X1510	X1511	X1512	X1513	X1514	X1515	X1516	X1517	X1518	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1537	X1538	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1561	X1562	X1563	X1564	X1573	X1574	X1575	X1576	A1577				
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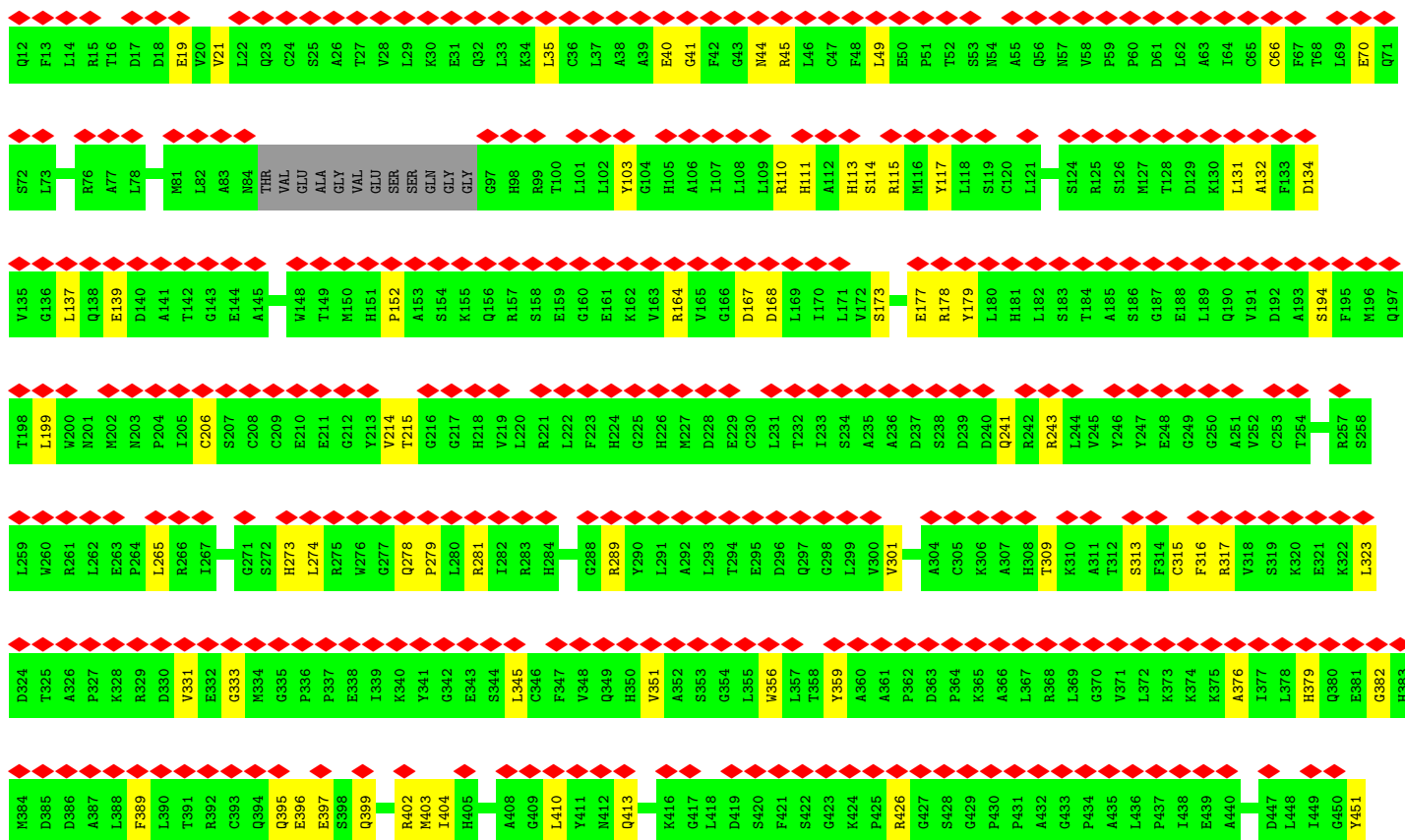
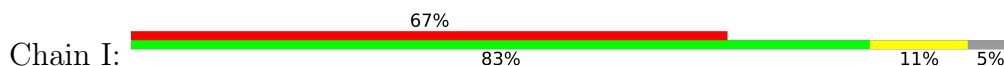


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X3346	X3285	X3215	X3149	X3018	T2938	L2878	A2818	F2758	X2668	X2606	X2538	D2464
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X3348	X3287	X3217	X3151	X3020	X2942	E2880	X2820	E2760	X2670	X2608	X2540	L2466
X3349	X3288	X3218	X3152	X3021	X2943	M2881	W2821	Y2761	X2671	X2609	X2541	V2467
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X3353	X3292	X3222	X3156	X3025	X2947	T2885	K2825	K2765	X2675	X2613		S2471
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X3363	X3302	X3232	X3172	X3035	X2957	E2895	LYS	W2775	X2685	X2624	X2561	X2488
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X3366	X3305	X3235	X3175	X3038	X2960	G2898	ARG	D2778	X2688	X2627	X2564	
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	X3341	X3280	X3211	X3144	X3013	X3013	W2933	L2813	S2753			

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GLY	X3405	X3512	W3661	H3734	X3821	C3892	X3968	S4051	L4112	R4189	R4188	X4342	GLY
SER	X3406	X3513	I3662	L3735	D3822	E3893	T3969	M4054	S4113	T4190	S4118	X4343	SER
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TRP	X3408	X3515	T3664	E3737	X3826	N3897	G3978	M4057	S4117	E4191	A4117	X4345	TRP
GLY	X3409	X3516	E3665	G3738	X3825	N3898	Q3979	L4058	E4118	E4192	D4118	F4540	GLY
GLY	X3410	X3517	D3666	G3739	E3826	F3899	Q3980	L4059	E4119	E4193	E4119	W4541	GLY
ALA	X3411	X3518	H3667	G3740	G3827	Q3901	X3984	K4060	E4120	E4194	E4120	G4542	ALA
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GLY	X3419	X3526	E3750	E3750	X3846	T3912	V3995	L4066	K4067	Q4204	A4203	W4582	GLY
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GLY	X3441	X3546	X3546	L3770	V3865	D3941	K4014	I4087	I4087	E4232	E4232	W4582	GLY
GLY	X3442	X3547	X3547	H3771	X3866	V3942	E4015	S4089	S4089	E4233	E4233	S4583	GLY
GLY	X3443	X3548	X3548	T3772	N3867	I3943	L4016	L4089	L4089	E4234	E4234	S4584	GLY
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GLY	X3451	X3554	X3554	M3778	E3873	F3949	D4022	K4095	K4095	S4252	S4252	GLY	GLY
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GLY	X3453	X3556	X3556	L3715	L3716	X3875	E3876	M4097	M4097	X4320	X4320	GLY	GLY
GLY	X3454	X3557	X3557	D3717	D3718	X3876	E3877	S4098	S4098	X4321	X4321	SER	SER
GLY	X3455	X3558	X3558	E3719	E3718	D3877	E3878	Q4100	Q4100	X4322	X4322	ALA	ALA
GLY	X3456	X3559	X3559	V3720	V3721	X3878	E3879	F4103	F4103	X4323	X4323	GLY	GLY
GLY	X3457	X3560	X3560	L3721	L3722	F3880	Q3960	G4038	G4038	X4324	X4324	ASP	ASP
GLY	X3458	X3561	X3561	Y3722	Y3723	T3881	V3961	M4039	M4039	X4325	X4325	LEU	LEU
GLY	X3459	X3562	X3562	X3725	X3726	Q3882	F3962	A4041	A4041	X4330	X4330	GLY	GLY
GLY	X3460	X3563	X3563	N3729	N3730	D3883	X3886						
GLY	X3464	X3565	X3565										
GLY	X3465	X3566	X3566										
GLY	X3466	X3567	X3567										



• Molecule 2: Ryanodine receptor 1

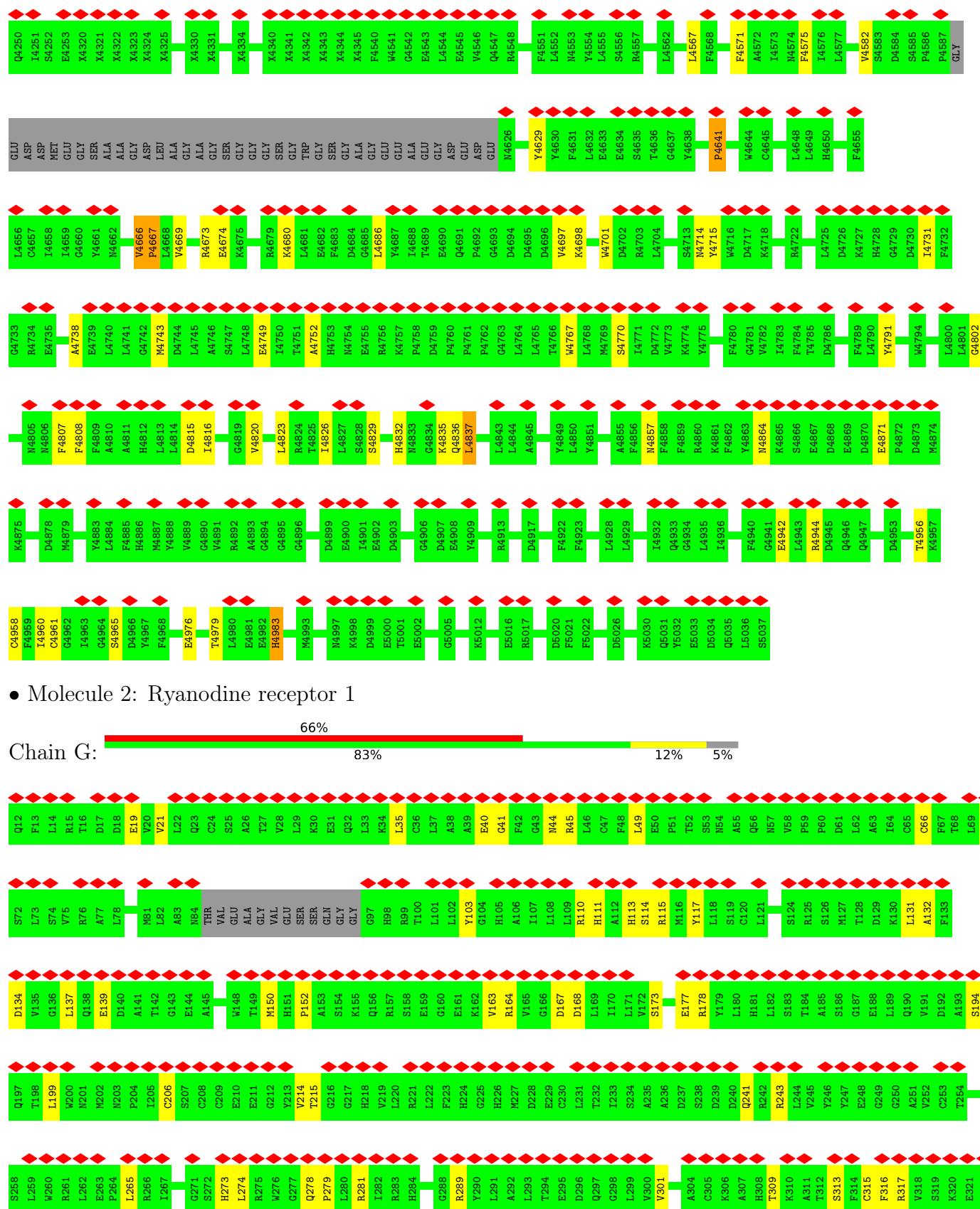






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X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	



E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	W1104	A1105	R1106	E1107	E1108	L1109	P1110	P1111	D1112	V1113	E1114	G1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	M1125	G1126	H1127	R1128	S1006	G1129	Q1130	R1131	W1132	H1133	L1134	G1135	S1136	F1139	G1140	R1141	P1142	V1143	Q1144	S1145	G1146	D1147	V1148	V1149	G1150	G1151	M1152	
T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRD	PRD	PRD	ASP	GLN	GLU	PRD	SER	GLN	VAL	M1125	GIU	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	S1085	G1086	Y1089	F1090	E1091	F1092
M961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	D999	Q1003	G1004	W1005	Y1006	S1007	L1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030			
G841	P842	S843	R844	C845	L846	S847	H848	T849	D850	F851	W852	P853	C854	P855	W856	D857	THR	VAL	GLN	I861	W862	L863	P864	P865	H866	L867	E868	R869	L870	R871	E872	A873	L874	A875	E876	R877	R878	H879	E880	L881	W882	A883	L884	R885	R886	L887	E888	Q889	G890	W891	T892	Y893	G894	P895	W896	R897	D898	D899	Y959
V780	V781	S782	F783	S784	A785	G786	W787	K788	W789	R790	F791	L792	L793	G794	G795	R796	H797	G798	E799	F800	K801	F802	L803	P804	P805	P806	G807	Y808	A809	H812	E813	A814	W815	L816	P817	R818	E819	R820	L821	R822	L823	E824	P825	L826	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	W840	
D717	G718	L719	H720	L721	G724	H725	V726	A727	R728	F729	W730	T731	S732	F733	G734	Q735	H736	L737	A739	P740	E741	S745	C746	G747	L748	L750	S751	V752	F753	W754	I755	S756	F757	Y758	P759	G760	G761	G762	F763	V764	G765	G766	V767	F768	E769	A770	F771	W772	L773	D774	G775	L776	F777	F778	P779				
T657	Q658	Y659	G660	T661	W662	Y663	F664	E665	V666	W667	W668	D669	E670	V671	V672	P673	F674	L675	T676	A677	Q678	A679	T680	H681	L682	R683	W684	G685	W686	A687	L688	E690	G691	W692	Q693	T694	Y695	P696	G697	G698	G699	E700	G701	W702	G703	G704	W705	G706	W707	G708	D709	D710	L711	Y712	S713	Y714	G715	F716	
G594	R595	K598	G599	L600	L603	C604	S605	L606	C607	V608	C609	N610	G611	V612	A613	R615	S616	Q618	D619	L620	E623	N624	L625	L626	P627	G628	R629	E630	L631	L632	L633	Q634	T635	N636	L637	T638	N639	Y640	V641	T642	S643	T644	R645	P646	N647	T648	F649	V650	G651	R652	A653	E654	G655	S656					
R531	G532	N533	R534	A535	N536	C537	A538	L539	T542	N543	L544	D545	W546	S549	K550	L551	D552	R553	L554	E555	A556	S557	S558	G559	I560	L561	E562	V563	L564	L568	I569	E570	S571	P572	E573	V574	L575	N576	I577	I578	Q579	E580	N581	H582	I583	K584	S585	I586	I587	S588	L589	D591	K592	H593					
Y451	F452	S456	E457	E458	L459	E463	S466	L467	L468	R469	R472	M473	R474	Q479	E480	E481	S485	L486	V487	L488	M489	C490	I491	D492	R493	L494	Y497	T498	T499	A500	A501	H502	Y506	A507	G508	E509	E510	A511	A512	E513	S514	W515	L521	L522	Y523	E524	A527	L521	L522	Y523	E524	A527							
H383	K384	D385	D386	A387	L388	F389	L390	T391	R392	C393	Q394	Q395	E396	E397	S398	Q399	R402	M403	I404	H405	A408	G409	L410	Y411	M412	Q413	K416	G417	L418	D419	S420	F421	S422	G423	K424	P425	R426	G427	S428	G429	P430	P431	A432	G433	P434	A435	L436	P437	I438	E439	A440	D447	L448	I449	G450				
L323	D324	T325	A326	P327	K328	R329	D330	V331	E332	G333	M334	G335	P336	P337	E338	I339	K340	Y341	G342	E343	S344	L345	C346	F347	V348	Q349	H350	V351	A352	S353	G354	L355	W356	L357	T358	Y359	A360	A361	P362	D363	P364	K365	A366	L367	R368	L369	G370	V371	L372	K373	K374	K375	A376	I377	L378	H379	Q380	E381	G382



X3007	X3008	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3071	X3072	X3073	X3074	X3075	X3076	X3077	X3078	X3079	X3080	X3081	X3082	X3083	X3084	X3085	X3086	X3087	X3088	X3089	X3090	X3091	X3092	X3093	X3094	X3095	X3096	X3097	X3098	X3099	X3100	X3101	X3102	X3103	X3104	X3105	X3106	X3107	X3108	X3109	X3110	X3111	X3112	X3113	X3114	X3115	X3116	X3117	X3118	X3119	X3120	X3121	X3122	X3123	X3124	X3125	X3126	X3127	X3128	X3129	X3130	X3131	X3132	X3133	X3134	X3135	X3136	X3137
L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	N2935	A2936	V2937	T2938	R2939	E2940	X2941	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X2981	X2982	X2983	X2984	X2985	X2986	X2987	X2988	X2989	X2990	X2991	X2992	X2993	X2994	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006																																																	
L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	K2892	E2893	L2894	E2895	L2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	T2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	R2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926																																																																					
W2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	E2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	THR	ARG	LYS	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866																																																																						
L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	E2759	E2760	Y2761	T2762	H2763	E2764	K2765	V2766	F2767	E2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	L2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	R2800	D2801	K2802	E2803	Y2805	R2806																																																																						
X2594	X2595	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655																																																																						
X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2541	X2542	X2543	X2544	X2550	X2551	X2552	X2553	X2554	X2555	X2556	X2557	X2558	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2575	X2576	X2577	X2578	X2579	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2589	X2590	X2593																																																																									
T2453	R2454	A2455	L2456	R2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	I2469	S2471	L2472	P2473	L2474	Q2475	L2476	P2477	T2478	L2479	X2487	X2488	X2489	X2490	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2506	X2511	X2512	X2513	X2514	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526																																																																										
A2391	R2392	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HTS	PHE	GLY	GLU	PRO	PRO	GLU	N2414	R2415	L2416	H2417	L2418	G2419	H2420	A2421	L2422	N2423	S2424	L2425	V2426	A2427	T2430	D2431	L2432	L2433	G2434	R2435	C2436	A2437	P2438	E2439	M2440	H2441	L2442	A2445	G2446	G2447	G2448	E2449	L2451	R2452																																																																											
G2328	E2329	R2330	Y2331	L2332	D2333	P2334	L2335	R2336	P2337	A2338	V2339	P2340	N2341	G2342	E2343	S2345	E2346	E2347	E2348	N2349	A2350	R2355	L2356	L2357	L2358	R2359	K2360	P2361	E2362	C2363	P2364	G2365	P2366	A2367	L2368	R2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	A2379	L2380	E2381	E2382	L2383	L2384	R2385	L2386	S2387	E2388	D2389	P2390																																																																							
G2264	L2265	G2266	M2267	Q2268	D2269	S2270	T2271	P2272	L2273	D2274	E2275	A2276	A2277	A2278	S2279	V2280	L2281	D2282	N2283	N2284	E2285	L2288	A2289	L2290	Q2291	E2292	Q2293	D2294	L2295	E2296	K2297	S2300	Y2301	L2302	A2303	G2304	G2305	G2306	G2307	E2308	S2309	C2310	P2311	M2312	L2313	L2314	A2315	K2316	G2317	Y2318	P2319	D2320	L2321	P2325	C2326	G2327																																																																								
Y2192	P2195	N2196	R2199	A2200	L2201	H2204	M2208	E2209	V2210	N2213	G2216	G2217	G2218	E2219	T2220	K2221	E2222	L2223	R2224	F2225	P2226	H2228	V2229	T2230	S2231	R2234	F2235	V2238	F2239	S2243	R2244	Q2245	N2246	Q2247	R2248	S2249	M2250	F2251	D2252	H2253	Y2256	L2257	L2258	E2259	N2260	S2261	G2262	L2263																																																																																

Q4038	K3959	L3886	L3721	X3458	X3395	X3274	X3204	X3138
Q4039	Q3960	L3889	Y3722	X3459	X3396	X3275	X3205	X3139
Q4040	V3961	Q3889	M3729	X3460	X3397	X3276	X3206	X3140
	F3962	L3890	A3730	X3461	X3398	X3277	X3207	X3141
	N3963	L3891	K3731	X3462	X3399	X3278	X3208	X3142
	S3964	C3892	S3732	X3463	X3400	X3279	X3209	X3143
	L3965	C3733	K3658	X3464	X3401	X3280	X3210	X3144
	T3966	H3734	A3659	X3465	X3402	X3281	X3211	X3145
	E3967	D3022	A3660	X3466	X3403	X3282	X3212	X3146
	Y3968	E3825	V3735	X3467	X3404	X3283	X3213	X3147
	I3969	F3826	E3737	X3468	X3405	X3284	X3214	X3148
	Q3970	C3827	L3662	X3469	X3406	X3285	X3215	X3149
	G3971	Q3827	L3663	X3470	X3407	X3286	X3216	X3150
		Q3830	T3664	X3471	X3408	X3287	X3217	X3151
		Q3833	E3665	X3472	X3409	X3288	X3218	X3152
		A3834	D3666	X3473	X3410	X3289	X3219	X3153
		L3842	H3667	X3474	X3411	X3290	X3220	X3154
		D3843	S3668	X3475	X3412	X3291	X3221	X3155
		A3846	E3670	X3476	X3413	X3292	X3222	X3156
		E3949	D3671	X3477	X3414	X3293	X3223	X3157
		K3850	R3672	X3478	X3415	X3294	X3224	X3158
		N3851	M3673	X3479	X3416	X3295	X3225	X3159
		F3852	L3674	X3480	X3417	X3296	X3226	X3160
		A3853	D3676	X3481	X3418	X3297	X3227	X3161
		E3925	K3679	X3482	X3419	X3298	X3228	X3162
		S3926	A3680	X3483	X3420	X3299	X3229	X3163
		E3927	E3755	X3484	X3421	X3300	X3230	X3170
		L3856	Q3756	X3485	X3422	X3301	X3231	X3171
		Q3857	E3757	X3486	X3423	X3302	X3232	X3172
		N3858	Q3758	X3487	X3424	X3303	X3233	X3173
		F3933	E3759	X3488	X3425	X3304	X3234	X3174
		Y3934	K3760	X3489	X3426	X3305	X3235	X3175
		S4007	Q3761	X3490	X3427	X3306	X3236	X3176
		S4008	R3762	X3491	X3428	X3307	X3241	X3177
		Y4081	L3763	X3492	X3429	X3308	X3242	X3178
		Q4009	Y3765	X3493	X3430	X3309	X3243	X3179
		I4010	Q3766	X3494	X3431	X3310	X3244	X3180
		E4011	Q3767	X3495	X3432	X3311	X3245	X3181
		L4012	S3768	X3496	X3433	X3312	X3246	X3182
		L4013	L3770	X3497	X3434	X3313	X3247	X3183
		K4014	R3769	X3498	X3435	X3314	X3248	X3184
		E4015	L3771	X3499	X3436	X3315	X3249	X3185
		L4016	H3771	X3500	X3437	X3316	X3250	X3186
		E4017	Q3772	X3501	X3438	X3317	X3251	X3187
		S4089	R3773	X3502	X3439	X3318	X3252	X3188
		K4090	E3706	X3503	X3440	X3319	X3253	X3189
		D4091	R3707	X3504	X3441	X3320	X3254	X3190
		D4092	E3777	X3505	X3442	X3321	X3255	X3191
		F4093	Y3778	X3506	X3443	X3322	X3256	X3192
		Q4094	Y3779	X3507	X3444	X3323	X3257	X3193
		K4095	L3780	X3508	X3445	X3324	X3258	X3194
		E4032	E3712	X3509	X3446	X3325	X3259	X3195
		G4033	K3713	X3510	X3447	X3326	X3260	X3196
		N4034	P3640	X3511	X3448	X3327	X3261	X3197
			L3641	X3512	X3449	X3328	X3262	X3198
			K3714	X3513	X3450	X3329	X3263	X3199
			K3715	X3514	X3451	X3330	X3264	X3200
			L3716	X3515	X3452	X3331	X3265	X3201
			D3717	X3516	X3453	X3332	X3266	X3202
			E3718	X3517	X3454	X3333	X3267	X3203
			D3719	X3518	X3455	X3334	X3268	
			I3804	X3519	X3456	X3335	X3269	
				X3560	X3457	X3336	X3270	
				X3561		X3337	X3271	
						X3338	X3272	
						X3339	X3273	

G4962	I4963	G4964	S4965	D4966	Y4967	F4968	E4976	T4977	H4978	T4979	L4980	E4981	E4982	H4983	M4993	M4997	K4998	D4999	E5000	T5001	E5002	G5005	K5012	E5016	R5017	D5020	F5021	F5022	D5026	K5030	Q5031	Y5032	E5033	D5034	Q5035	L5036	S5037																	
F4809	A4810	A4811	H4812	L4813	L4814	D4815	I4816	G4819	V4820	L4823	R4824	T4825	I4826	L4827	S4828	S4829	H4832	M4833	G4834	K4835	Q4836	L4837	L4843	L4844	A4845	Y4849	L4850	Y4851	A4855	F4856	M4857	F4858	F4859	R4860	K4861	F4862	Y4863	M4864	K4865	S4866	E4867	D4868	E4869	D4870	E4871	P4872	D4873	M4874	K4875	C4876	D4877	D4878	M4879	
E4739	L4740	L4741	G4742	M4743	D4744	L4745	A4746	S4747	L4748	E4749	L4750	T4751	A4752	H4753	M4754	E4755	R4756	K4757	P4758	D4759	P4760	P4761	P4762	G4763	L4764	L4765	T4766	W4767	L4768	M4769	S4770	L4771	D4772	V4773	K4774	Y4775	F4780	G4781	V4782	L4783	F4784	T4785	D4786	F4789	L4790	Y4791	V4794	L4800	L4801	G4802	M4805	N4806	F4807	F4808
N4662	V4666	P4667	L4668	V4669	R4673	E4674	K4675	R4679	K4680	L4681	E4682	F4683	D4684	G4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	G4693	D4694	D4695	D4696	V4697	K4698	G4699	Q4700	W4701	D4702	R4703	L4704	S4713	N4714	Y4715	W4716	D4717	K4718	R4722	L4725	D4726	K4727	H4728	G4729	D4730	I4731	F4732	G4733	R4734	E4735	A4738		
SER	ALA	ALA	GLY	LEU	ALA	GLY	ALA	GLY	SER	SER	GLY	TSP	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	ASP	ASP	GLU	M4626	Y4629	Y4630	F4631	L4632	E4633	E4634	S4635	T4636	G4637	Y4638	P4641	V4644	C4645	L4648	L4649	H4650	F4655	L4656	C4657	I4658	I4659	G4660	Y4661							
F4174	R4175	P4176	R4180	M4184	G4185	A4186	S4187	R4188	R4189	I4190	E4191	R4192	E4196	I4197	S4198	E4199	T4200	N4201	R4202	A4203	Q4204	M4205	E4206	M4207	P4208	Q4209	V4210	K4211	E4212	R4215	F4219	N4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	L4233	S4236	Q4250	I4251	S4252	L4166	A4253	A4167	E4168	S4169			
F4103	T4104	G4105	P4106	E4107	I4108	Q4109	F4110	L4111	L4112	S4113	C4114	S4115	E4116	A4117	D4118	E4119	M4120	E4121	M4122	I4123	M4124	F4125	E4126	E4127	F4128	A4129	M4130	R4131	F4132	Q4133	E4134	R4137	D4138	I4139	G4140	F4141	M4142	L4147	E4152	H4153	H4156	R4159	L4160	R4161	L4164	E4165	L4166	A4167	E4168	S4169				
F4174	R4175	P4176	R4180	M4184	G4185	A4186	S4187	R4188	R4189	I4190	E4191	R4192	E4196	I4197	S4198	E4199	T4200	N4201	R4202	A4203	Q4204	M4205	E4206	M4207	P4208	Q4209	V4210	K4211	E4212	R4215	F4219	N4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	L4233	S4236	Q4250	I4251	S4252	L4166	A4253	A4167	E4168	S4169			
X4322	X4323	X4324	X4325	X4330	X4331	X4334	X4340	X4341	X4342	X4343	X4344	X4345	F4340	F4341	W4341	G4342	E4343	L4344	E4345	W4346	Q4347	R4348	F4351	L4352	M4353	Y4354	L4355	S4356	R4357	L4362	L4363	F4367	F4368	F4371	A4372	I4373	M4374	F4375	I4376	L4377	V4382	S4383	D4384	S4385	P4386	P4387	GLY	GLU	ASP	ASP	MET	GLU	GLY	
F4103	T4104	G4105	P4106	E4107	I4108	Q4109	F4110	L4111	L4112	S4113	C4114	S4115	E4116	A4117	D4118	E4119	M4120	E4121	M4122	I4123	M4124	F4125	E4126	E4127	F4128	A4129	M4130	R4131	F4132	Q4133	E4134	R4137	D4138	I4139	G4140	F4141	M4142	L4147	E4152	H4153	H4156	R4159	L4160	R4161	L4164	E4165	L4166	A4167	E4168	S4169				
F4174	R4175	P4176	R4180	M4184	G4185	A4186	S4187	R4188	R4189	I4190	E4191	R4192	E4196	I4197	S4198	E4199	T4200	N4201	R4202	A4203	Q4204	M4205	E4206	M4207	P4208	Q4209	V4210	K4211	E4212	R4215	F4219	N4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	L4233	S4236	Q4250	I4251	S4252	L4166	A4253	A4167	E4168	S4169			
X4322	X4323	X4324	X4325	X4330	X4331	X4334	X4340	X4341	X4342	X4343	X4344	X4345	F4340	F4341	W4341	G4342	E4343	L4344	E4345	W4346	Q4347	R4348	F4351	L4352	M4353	Y4354	L4355	S4356	R4357	L4362	L4363	F4367	F4368	F4371	A4372	I4373	M4374	F4375	I4376	L4377	V4382	S4383	D4384	S4385	P4386	P4387	GLY	GLU	ASP	ASP	MET	GLU	GLY	
SER	ALA	ALA	GLY	LEU	ALA	GLY	ALA	GLY	SER	SER	GLY	TSP	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	ASP	ASP	GLU	M4626	Y4629	Y4630	F4631	L4632	E4633	E4634	S4635	T4636	G4637	Y4638	P4641	V4644	C4645	L4648	L4649	H4650	F4655	L4656	C4657	I4658	I4659	G4660	Y4661							
N4662	V4666	P4667	L4668	V4669	R4673	E4674	K4675	R4679	K4680	L4681	E4682	F4683	D4684	G4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	G4693	D4694	D4695	D4696	V4697	K4698	G4699	Q4700	W4701	D4702	R4703	L4704	S4713	N4714	Y4715	W4716	D4717	K4718	R4722	L4725	D4726	K4727	H4728	G4729	D4730	I4731	F4732	G4733	R4734	E4735	A4738		
E4739	L4740	L4741	G4742	M4743	D4744	L4745	A4746	S4747	L4748	E4749	L4750	T4751	A4752	H4753	M4754	E4755	R4756	K4757	P4758	D4759	P4760	P4761	P4762	G4763	L4764	L4765	T4766	W4767	L4768	M4769	S4770	L4771	D4772	V4773	K4774	Y4775	F4780	G4781	V4782	L4783	F4784	T4785	D4786	F4789	L4790	Y4791	V4794	L4800	L4801	G4802	M4805	N4806	F4807	F4808
F4809	A4810	A4811	H4812	L4813	L4814	D4815	I4816	G4819	V4820	L4823	R4824	T4825	I4826	L4827	S4828	S4829	H4832	M4833	G4834	K4835	Q4836	L4837	L4843	L4844	A4845	Y4849	L4850	Y4851	A4855	F4856	M4857	F4858	F4859	R4860	K4861	F4862	Y4863	M4864	K4865	S4866	E4867	D4868	E4869	D4870	E4871	P4872	D4873	M4874	K4875	C4876	D4877	D4878	M4879	
Y4883	L4884	F4885	H4886	M4887	Y4888	V4889	G4890	V4891	R4892	A4893	G4894	G4895	G4896	D4899	E4900	I4901	E4902	D4903	G4906	D4907	E4908	Y4909	R4913	D4917	F4922	F4923	L4928	L4929	I4932	Q4933	G4934	L4935	L4936	F4940	G4941	E4942	L4943	R4944	D4945	Q4946	Q4947	D4953	T4956	K4957	C4958	F4959	I4960	C4961						
G4962	I4963	G4964	S4965	D4966	Y4967	F4968	E4976	T4977	H4978	T4979	L4980	E4981	E4982	H4983	M4993	M4997	K4998	D4999	E5000	T5001	E5002	G5005	K5012	E5016	R5017	D5020	F5021	F5022	D5026	K5030	Q5031	Y5032	E5033	D5034	Q5035	L5036	S5037																	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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

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	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.46	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.22	0/25438	0.53	6/34548 (0.0%)
2	E	0.22	0/25438	0.53	6/34548 (0.0%)
2	G	0.22	0/25438	0.53	6/34548 (0.0%)
2	I	0.22	0/25438	0.53	6/34548 (0.0%)
All	All	0.22	0/105088	0.53	24/142684 (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	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	56

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2807	TRP	CA-C-N	-6.65	113.36	120.94
2	E	2807	TRP	C-N-CA	-6.65	113.36	120.94
2	B	2807	TRP	CA-C-N	-6.62	113.40	120.94
2	B	2807	TRP	C-N-CA	-6.62	113.40	120.94
2	I	2807	TRP	CA-C-N	-6.61	113.40	120.94

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	12	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	11	0
2	B	29509	0	24752	291	0
2	E	29509	0	24753	281	0
2	G	29509	0	24753	286	0
2	I	29509	0	24753	287	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121312	0	102307	1168	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 5.

The worst 5 of 1168 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)
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.10	0.70
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.10	0.70
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.10	0.69
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.10	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.61	0.65

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	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	43	78
2	E	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	43	78
2	G	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	43	78
2	I	3237/4416 (73%)	2890 (89%)	341 (10%)	6 (0%)	43	78
All	All	13368/18096 (74%)	11931 (89%)	1413 (11%)	24 (0%)	44	78

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2481 (100%)	12 (0%)	81	82
2	E	2493/3022 (82%)	2481 (100%)	12 (0%)	81	82
2	G	2493/3022 (82%)	2481 (100%)	12 (0%)	81	82
2	I	2493/3022 (82%)	2481 (100%)	12 (0%)	81	82
All	All	10324/12444 (83%)	10276 (100%)	48 (0%)	78	82

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	1657	LEU
2	I	4983	HIS
2	I	1676	LEU
2	I	3663	LEU
2	G	719	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 186 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	1691	GLN
2	G	113	HIS
2	I	1970	GLN
2	I	3950	ASN
2	G	461	HIS

5.3.3 RNA ⓘ

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 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.38
1	E	4345:UNK	C	4540:PHE	N	73.38
1	I	4345:UNK	C	4540:PHE	N	73.38
1	G	4345:UNK	C	4540:PHE	N	73.38

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	48.21

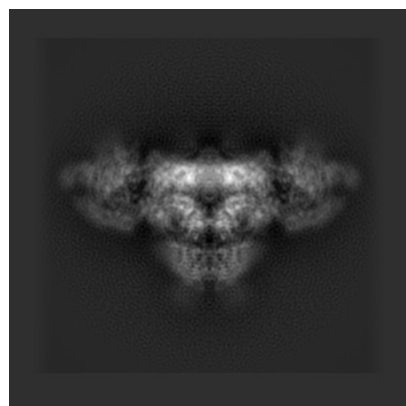
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8394. These allow visual inspection of the internal detail of the map and identification of artifacts.

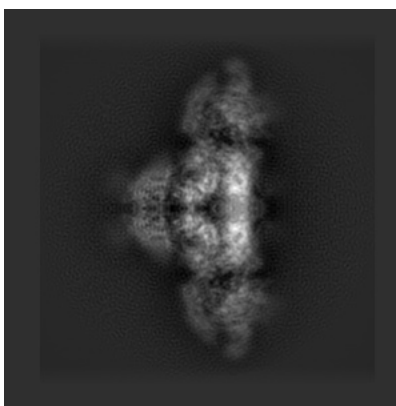
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

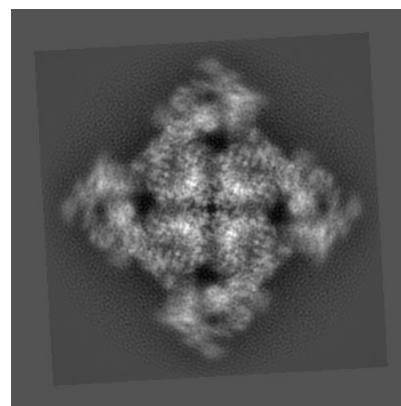
6.1.1 Primary map



X

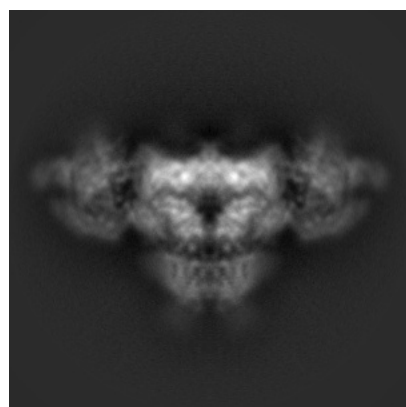


Y

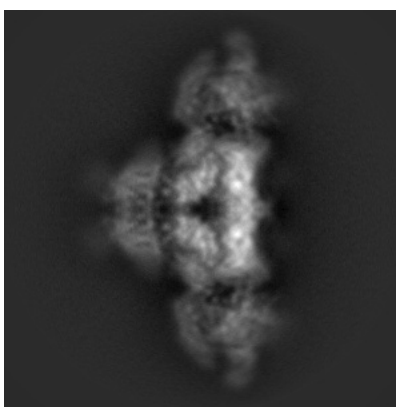


Z

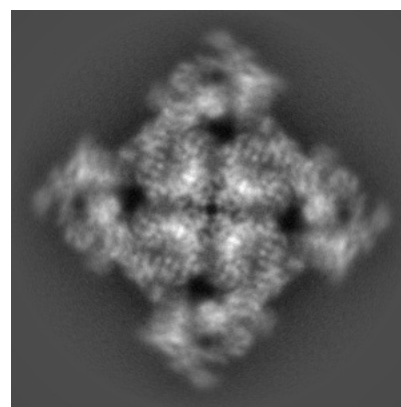
6.1.2 Raw map



X



Y

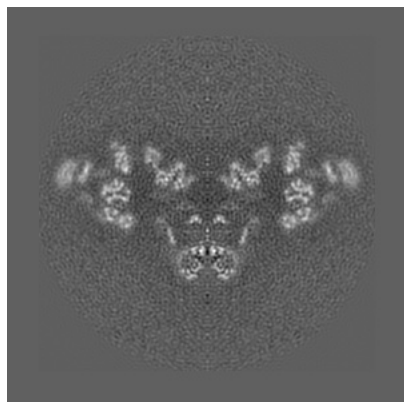


Z

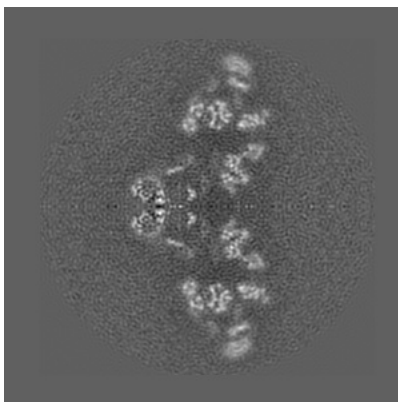
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

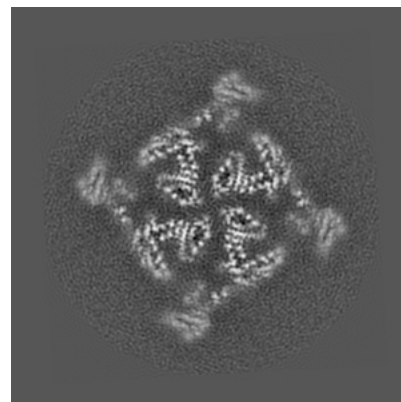
6.2.1 Primary map



X Index: 200

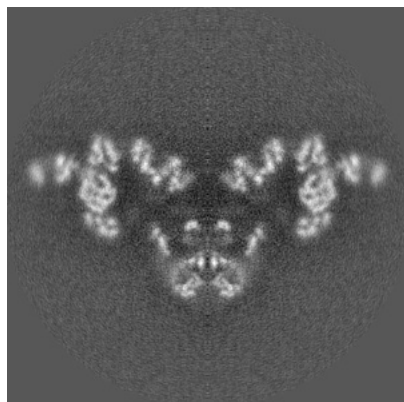


Y Index: 200

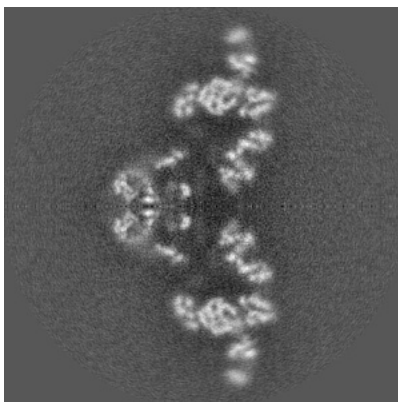


Z Index: 200

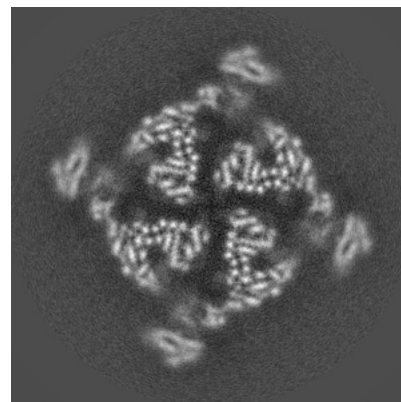
6.2.2 Raw map



X Index: 168



Y Index: 168

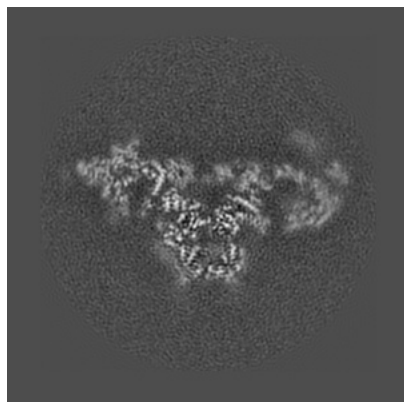


Z Index: 168

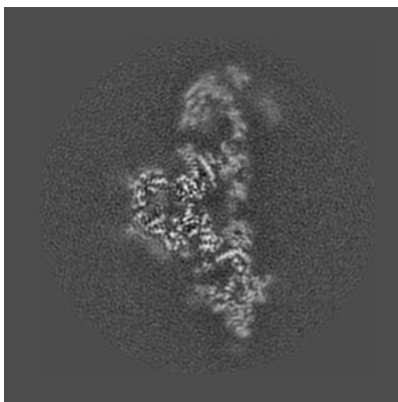
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

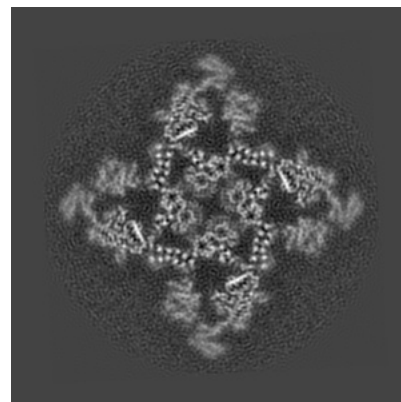
6.3.1 Primary map



X Index: 217

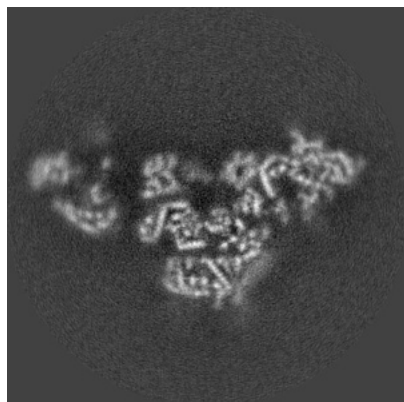


Y Index: 183

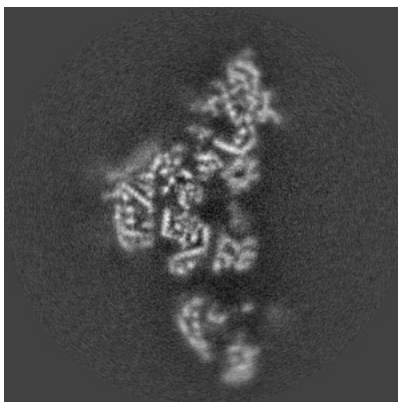


Z Index: 227

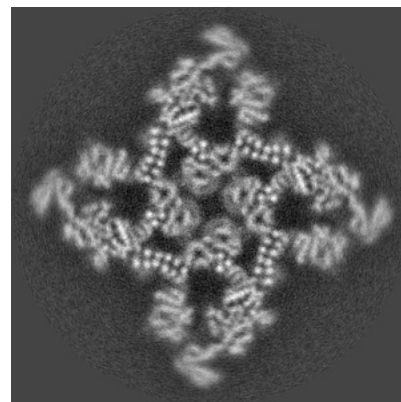
6.3.2 Raw map



X Index: 154



Y Index: 182

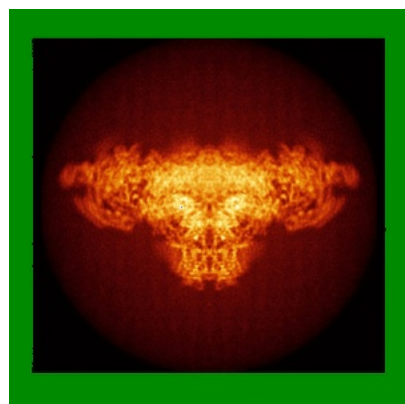


Z Index: 193

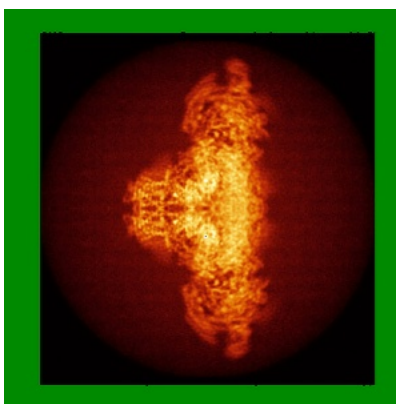
The images above show the largest variance slices of the map in three orthogonal directions.

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

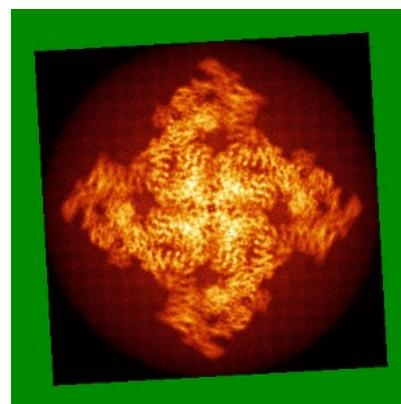
6.4.1 Primary map



X



Y

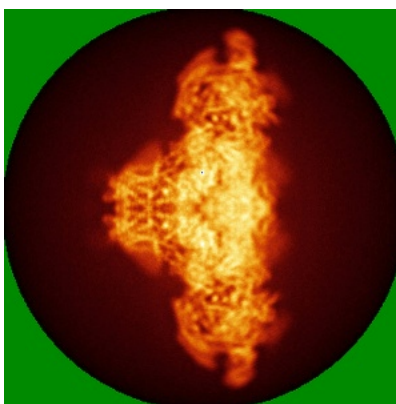


Z

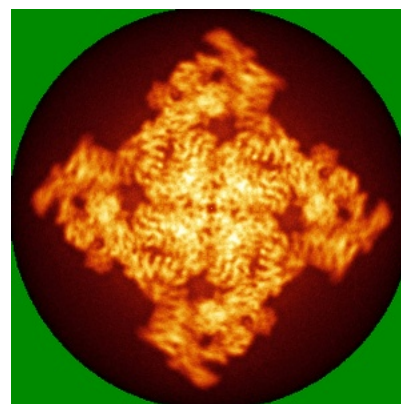
6.4.2 Raw map



X



Y

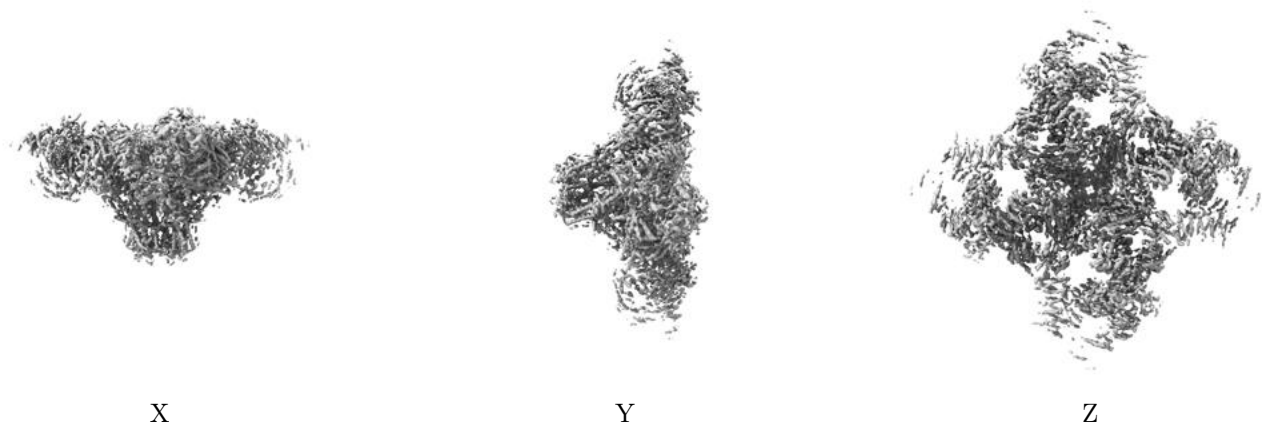


Z

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.

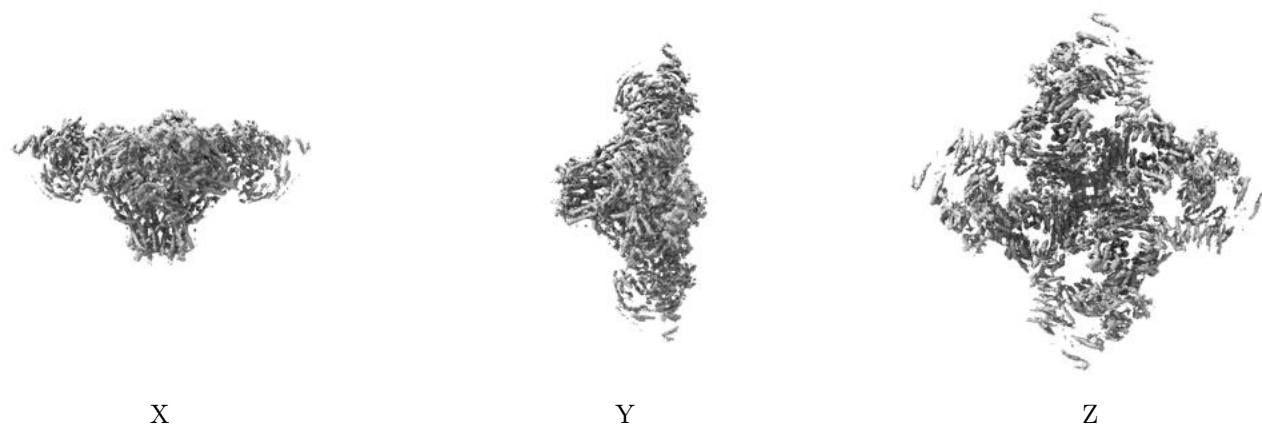
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

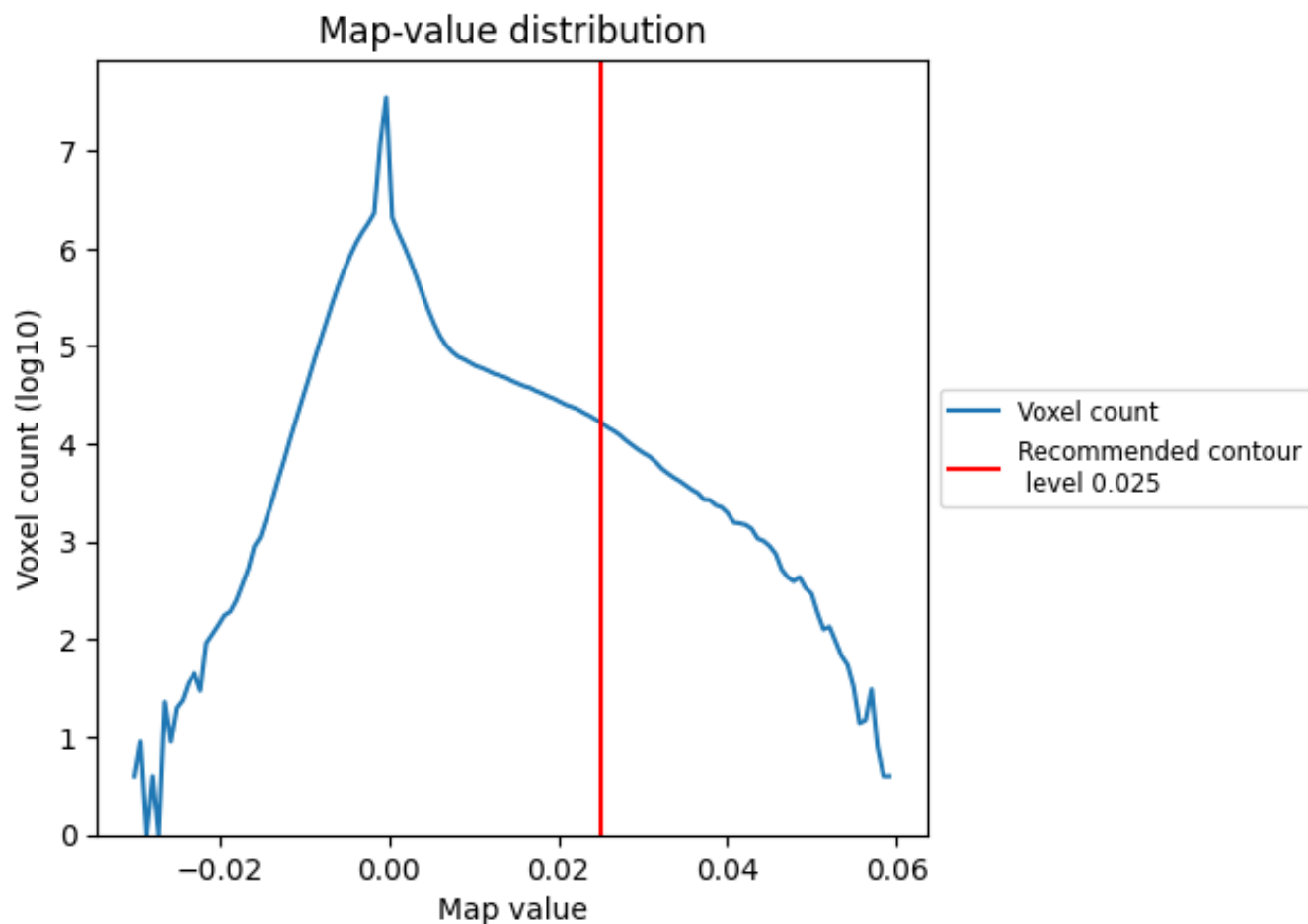
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

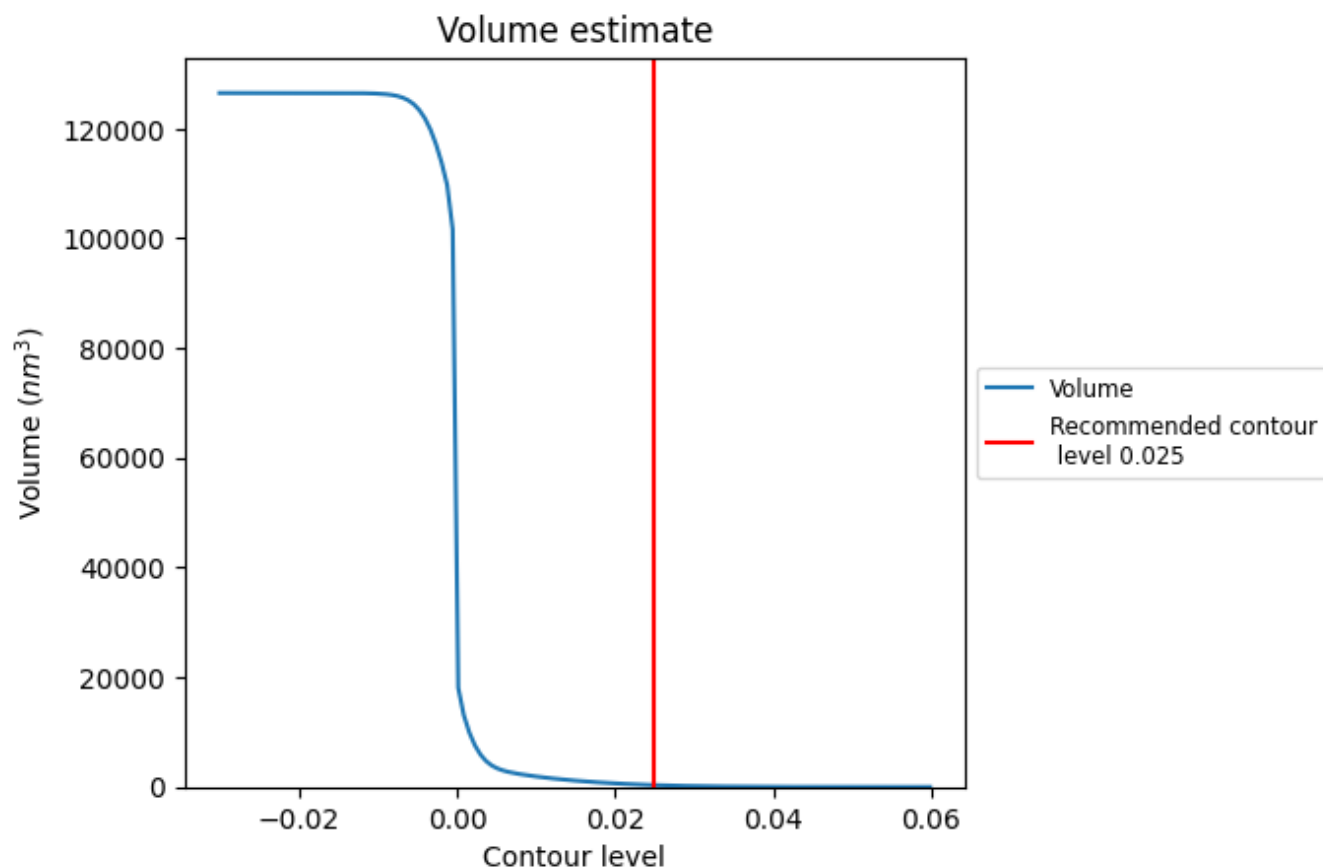
This section contains the results of statistical analysis of the map.

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.

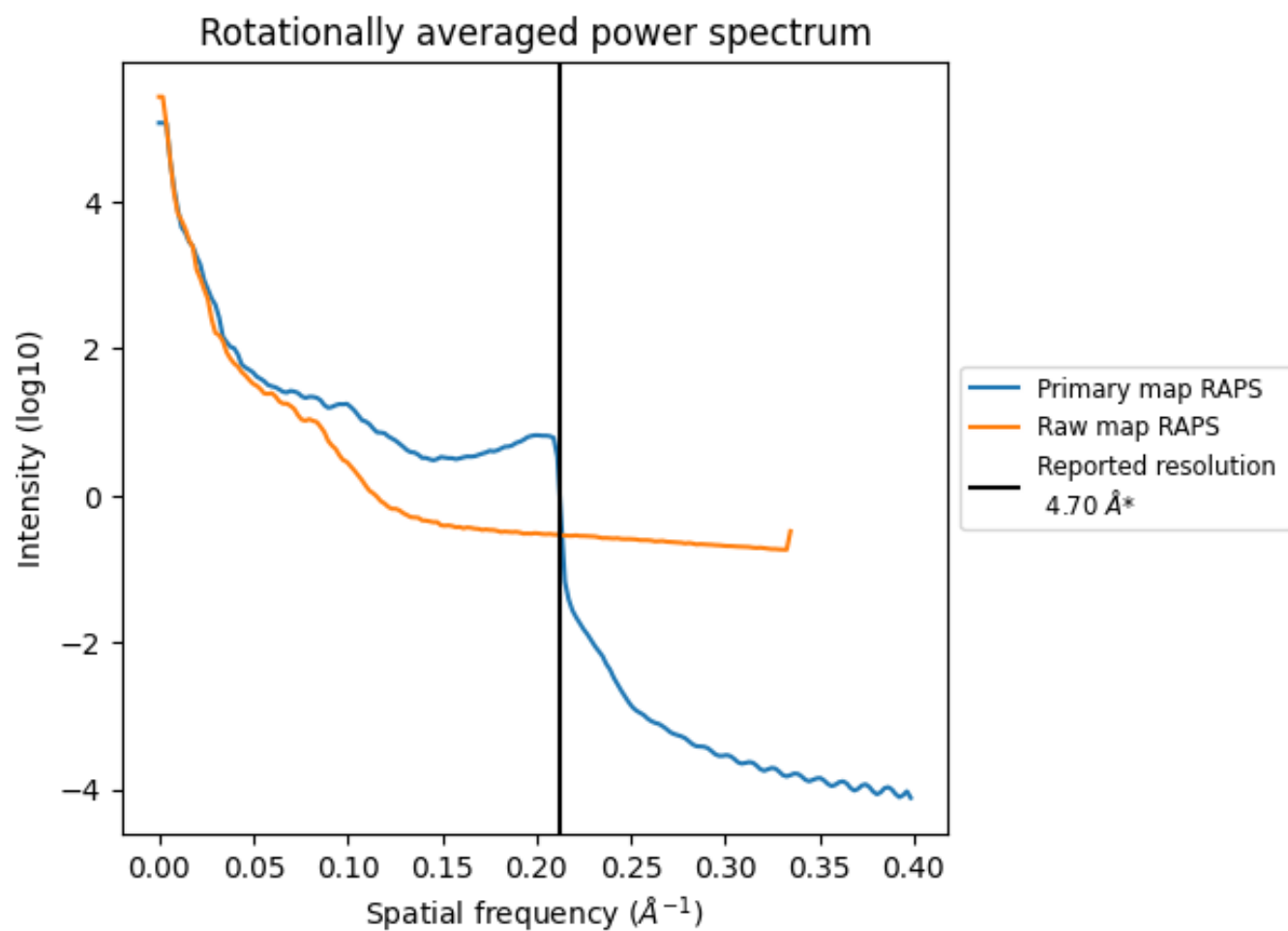
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm^3 ; this corresponds to an approximate mass of 299 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

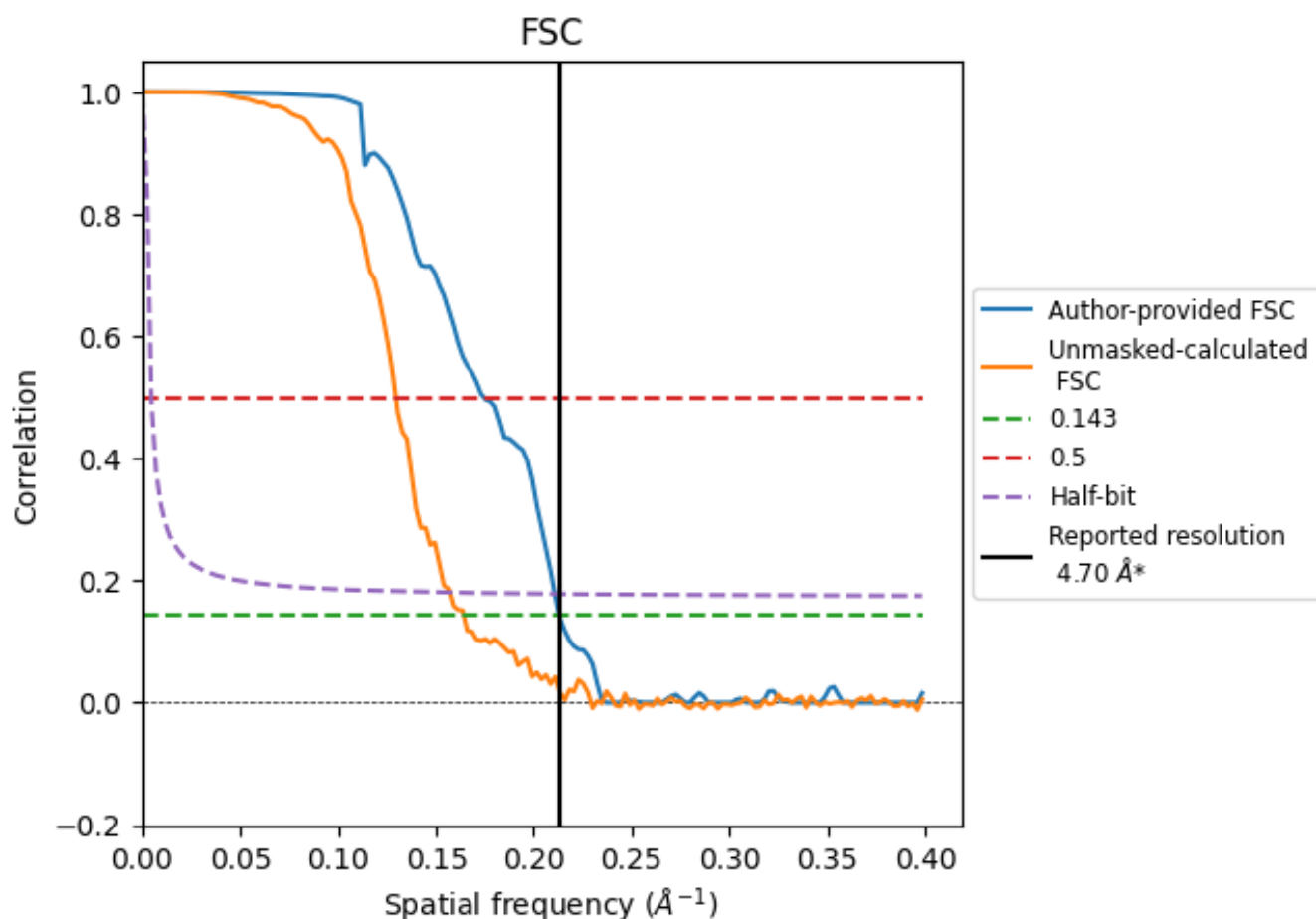


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

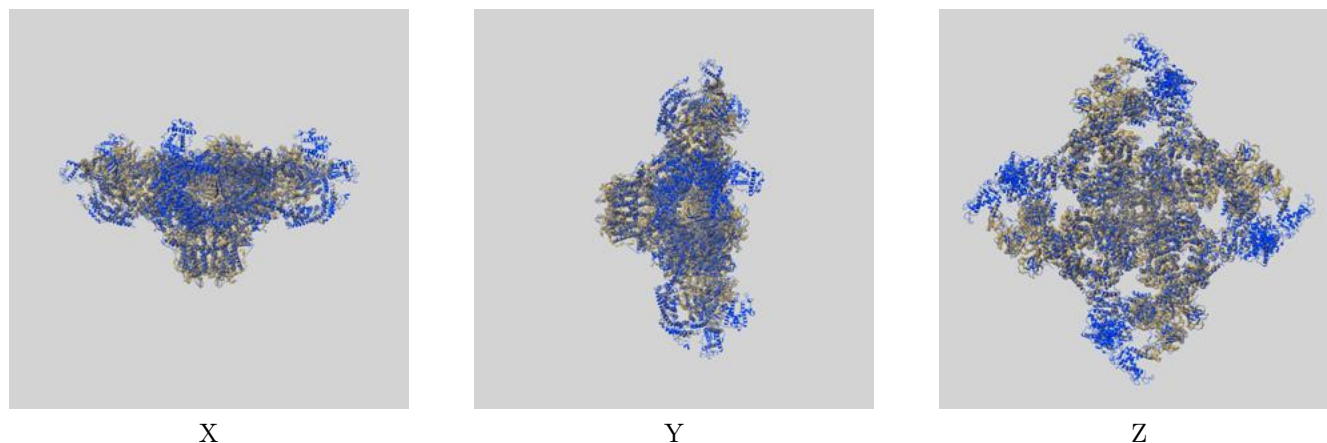
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.69	5.73	4.74
Unmasked-calculated*	6.09	7.73	6.37

*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 6.09 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

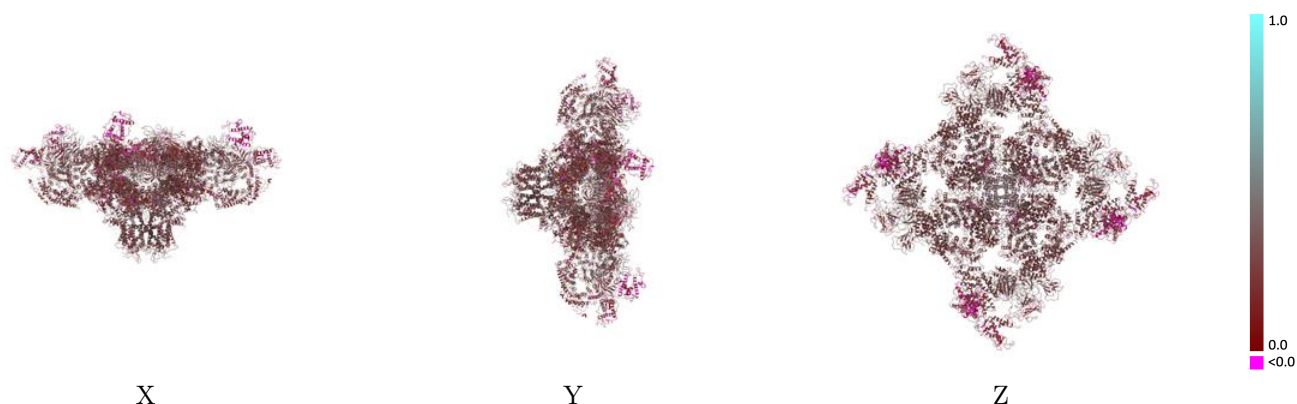
This section contains information regarding the fit between EMDB map EMD-8394 and PDB model 5TB3. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



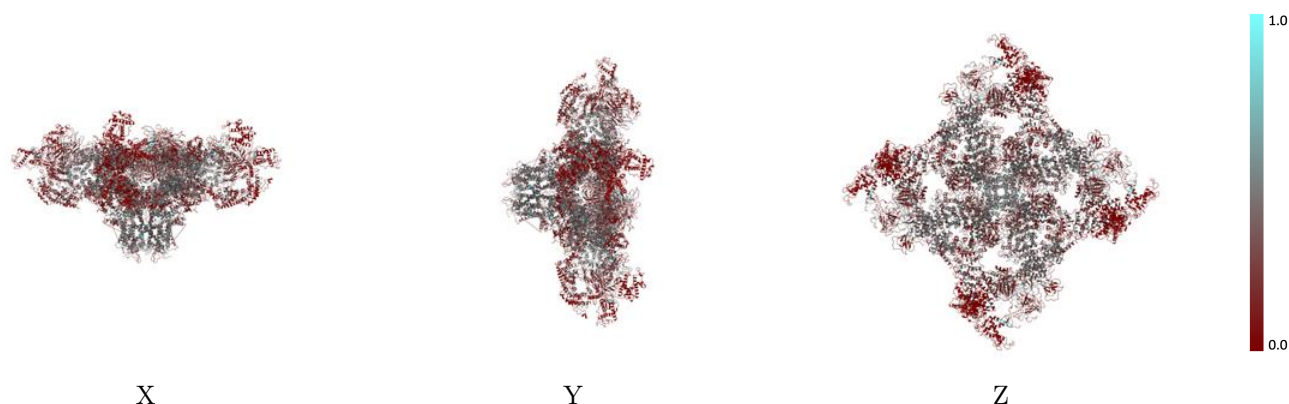
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



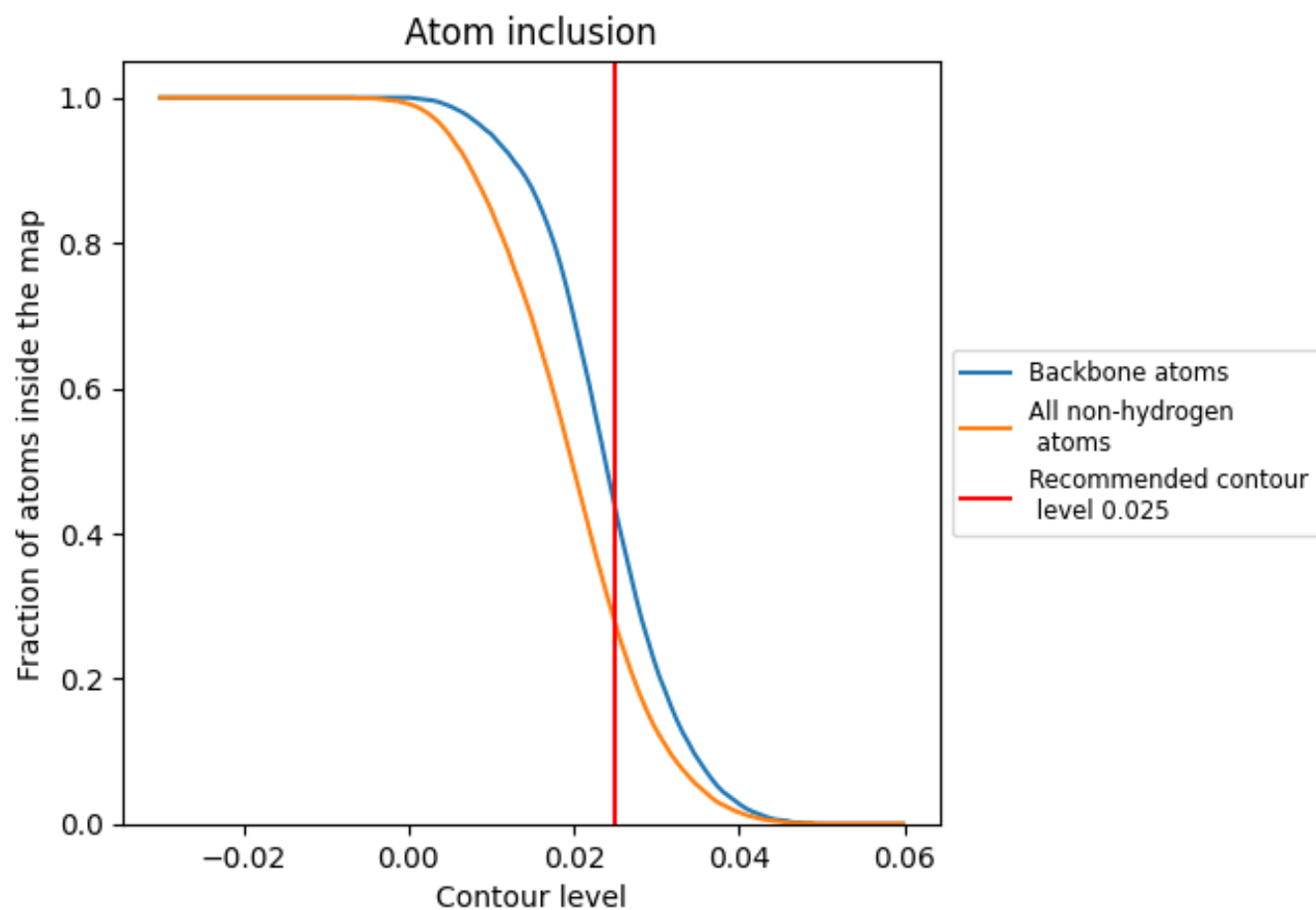
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 28% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2760	0.2630
A	0.2390	0.2880
B	0.2780	0.2620
E	0.2770	0.2620
F	0.2380	0.2900
G	0.2770	0.2620
H	0.2390	0.2920
I	0.2770	0.2620
J	0.2390	0.2900

