



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 07:33 PM EST

PDB ID : 7JMF
EMDB ID : EMD-22392
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 42 - State 6 (S6)
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on : 2020-07-31
Resolution : 4.50 Å(reported)
Based on initial model : 5TB4

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

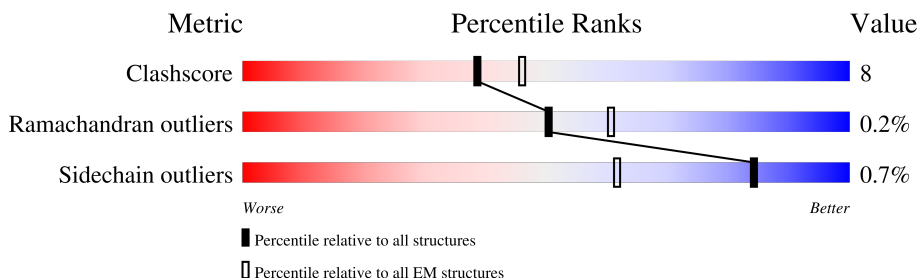
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	
1	F	108	
1	H	108	
1	J	108	
2	B	4687	
2	E	4687	
2	G	4687	
2	I	4687	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	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	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- Molecule 3 is ZINC ION (three-letter code: 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	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of

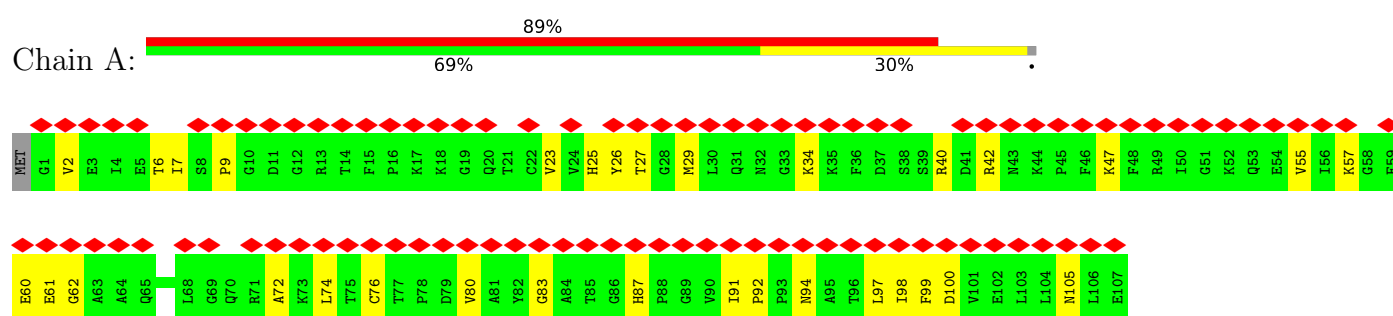
Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0

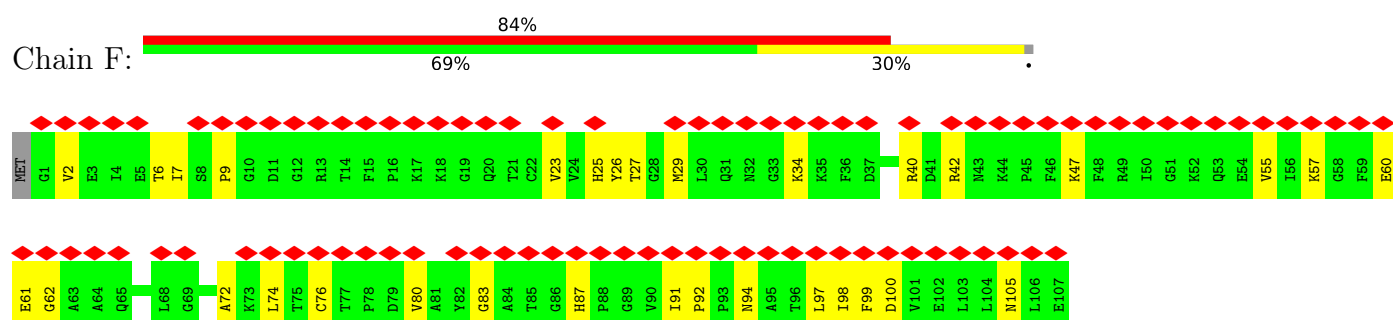
3 Residue-property plots [i](#)

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.

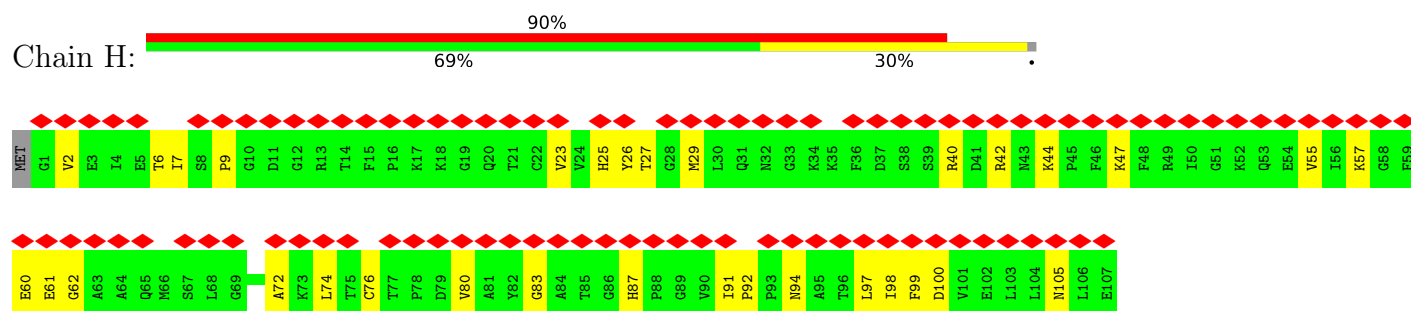
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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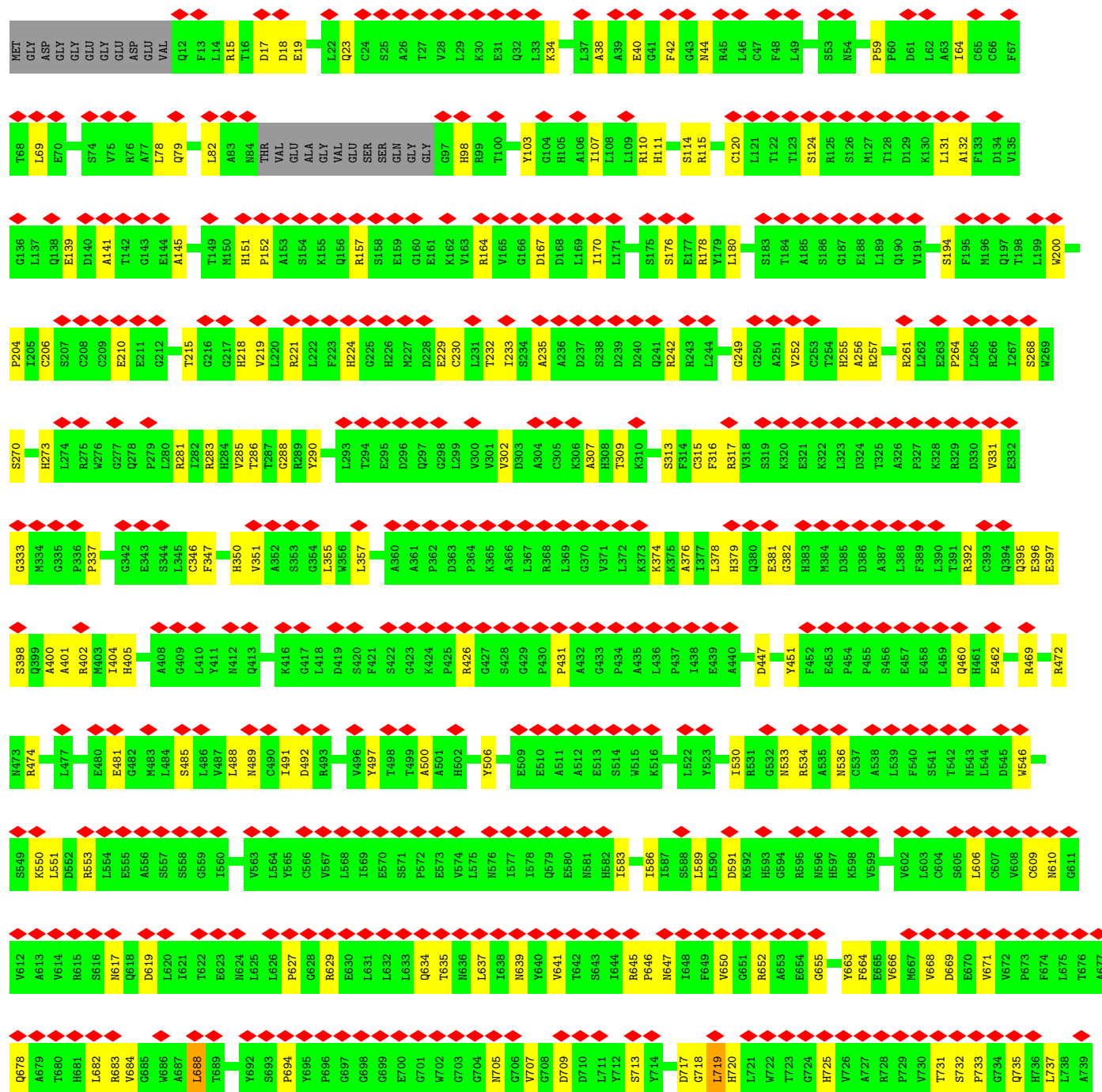
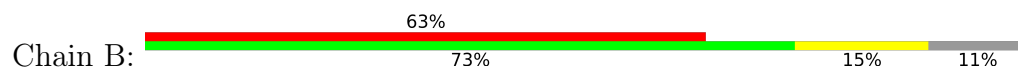


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: ryanodine receptor 1



M1648	D1649	I1650	L1651	E1652	L1653	R1656	L1657	D1658	L1659	Q1660	R1661	F1662	H1663	S1664	H1665	T1666	L1667	R1668	L1669	Y1670	R1671	A1672	A1675	L1676	G1677	M1678	Q1614	N1679	L1680	V1681	A1682	H1683	A1684	S1687	H1688	L1689	D1690	Q1691	Q1692	L1693	L1694	L1695	H1696	A1697	L1698	E1699	D1700	A1701	H1702	L1703	P1704	G1705	P1706	L1707	A1708	R1709	G1710																										
X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1459	X1460	X1467	X1468	X1469	X1470	X1471	X1472	X1475	X1476	X1485	X1486	X1487	X1488	X1489	X1490	X1491	X1492	X1493	X1494	X1497	X1498	X1499	X1500	X1501	X1502	X1503	X1504	X1505	X1506	X1507	X1508	X1509	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	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1563	X1564	M1566	M1567	L1568	P1569	E1643	E1644	N1645	R1646	C1647																													
P1587	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	E1596	Q1597	Q1598	M1599	L1600	V1603	S1604	W1605	S1606	R1607	M1608	P1609	M1610	H1611	F1612	L1613	Q1614	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	L1633	L1634	T1635	M1636	M1637	A1638	L1639	H1640	I1641	P1642	E1643	E1644	N1645	R1646	C1647																										
G807	Y808	A809	P810	C811	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824	P825	I826	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	G841	P842	S843	R844	C845	L846	S847	H848	T849	D850	F851	V852	P853	C854	P855	V856	D857	THR	VAL	GLN	I861	V862	L863	P864	P865	H866	L867																									
E868	R869	I870	R871	E872	K873	L874	A875	E876	N877	I878	H879	E880	L881	Q882	A883	L884	T885	R886	I887	E888	Q889	G890	W891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927																								
T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	D958	Y959	M960	N961	S962	N963	G964	A968	P969	L970	D971	S972	L973	H974	V975	R976	T978	P979	A980	Q981	T982	T983	L984	V985	D986	L988	A989																											
G992	V1001	A1002	Q1003	G1004	W1005	S1006	Y1007	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	Q1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU																											
PRO	SER	GLN	GLU	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	L1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	T1082	V1083	Q1084	S1085	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120																										
A1121	Y1122	V1123	F1124	N1125	G1126	H1127	R1128	G1129	Q1130	R1131	W1132	H1133	L1134	G1135	S1136	F1139	G1140	R1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148	Y1149	G1150	C1151	M1152	L1155	T1156	E1157	N1158	I1161	F1162	L1163	L1164	M1165	G1166	E1167	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	L1182	E1183																											
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X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1459	X1460	X1467	X1468	X1469	X1470	X1471	X1472	X1475	X1476	X1485	X1486	X1487	X1488	X1489	X1490	X1491	X1492	X1493	X1494	X1497	X1498	X1499	X1500	X1501	X1502	X1503	X1504	X1505	X1506	X1507	X1508	X1509	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	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1563	X1564	M1566	M1567	L1568	P1569	E1643	E1644	N1645	R1646	C1647																													
P1587	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	E1596	Q1597	Q1598	M1599	L1600	V1603	S1604	W1605	S1606	R1607	M1608	P1609	M1610	H1611	F1612	L1613	Q1614	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	L1633	L1634	T1635	M1636	M1637	A1638	L1639	H1640	I1641	P1642	E1643	E1644	N1645	R1646	C1647																										
M1648	D1649	I1650	L1651	E1652	L1653	R1656	L1657	D1658	L1659	Q1660	R1661	F1662	H1663	S1664	H1665	T1666	L1667	R1668	L1669	Y1670	R1671	A1672	A1675	L1676	G1677	M1678	Q1614	N1679	L1680	V1681	A1682	H1683	A1684	S1687	H1688	L1689	D1690	Q1691	Q1692	L1693	L1694	L1695	H1696	A1697	L1698	E1699	D1700	A1701	H1702	L1703	P1704	G1705	P1706	L1707	A1708	R1709	G1710																										



WORLD WIDE
PDB
PROTEIN DATA BANK

X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3451	X3452	X3453	X3454	X3455	X3456	X3459	X3460	X3461	X3462	X3463	X3464	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535							
X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431				
X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3293	X3294	X3295	X3296	X3297	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311
X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371				
X3178	X3179	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243						
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	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3153	X3156	X3157	X3160	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177								
X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2973	X2974	X2975	X2976	X2979	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3034	X3035	X3036						
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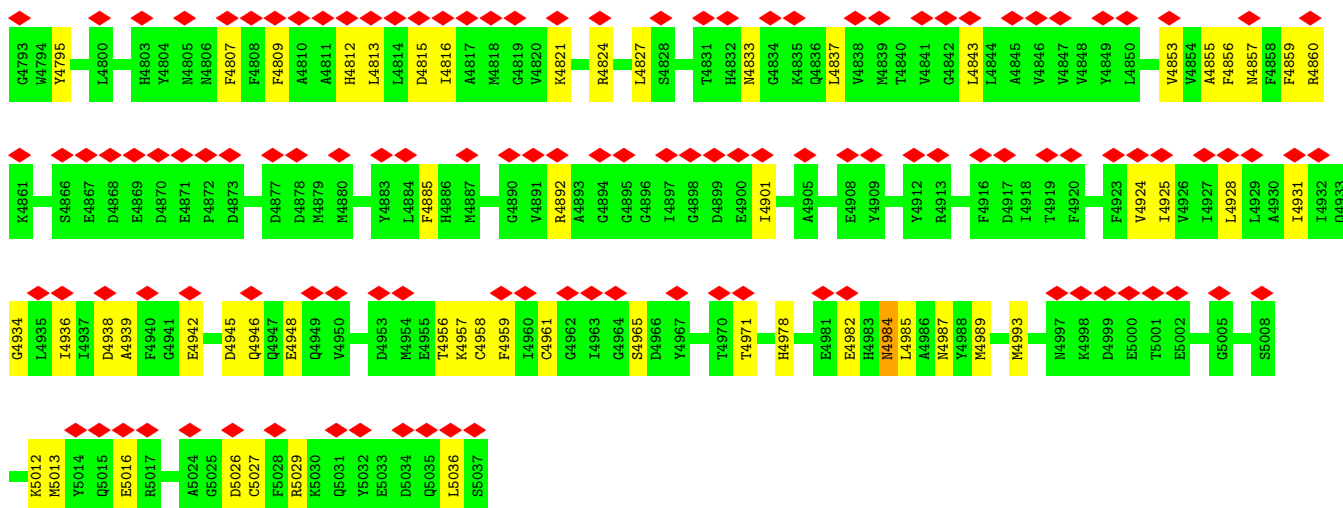
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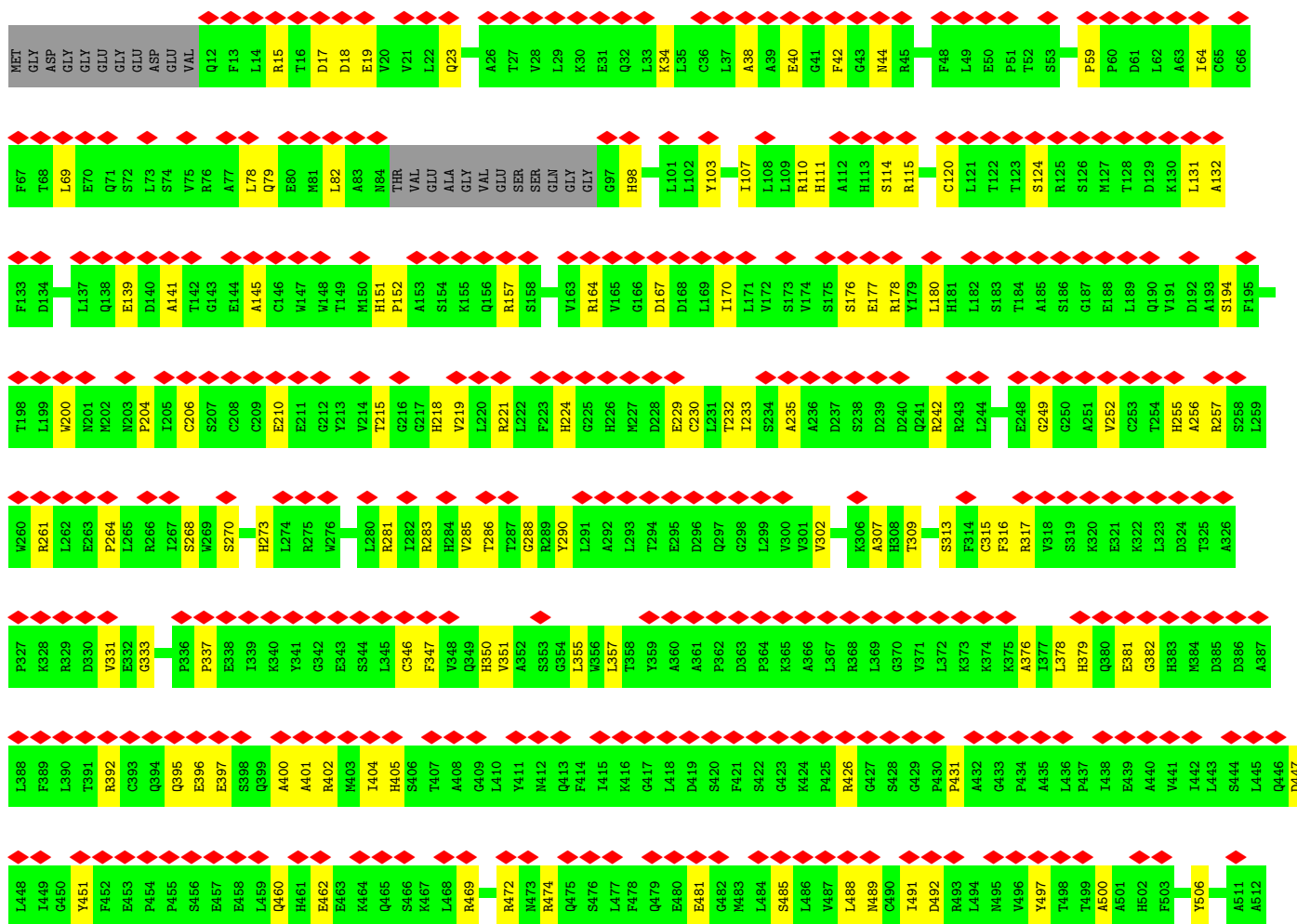
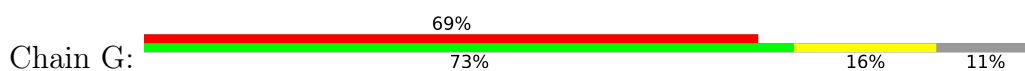








• Molecule 2: ryanodine receptor 1



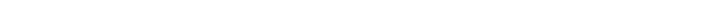
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M1260	G1200	P1138	E1078	ASN	N948	E888	E828	V767	G704	Y640	I578	K516
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G1265	G1205	W1143	Y1083	T953	K954	Y893	G833	N773	D709	R645	I583	L521
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P1267	D1207	S1145	S1085	L956	L1027	P895	R835	D774	L711	N647	S585	Y523
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L1270	S1210	V1148	W1088	A1030	T958	D898	H838	F777	Y714	V650	S588	L526
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X2542	X2543	X2544	X2545	X2546	X2547	X2548	X2549	X2550	X2551	X2552	X2555	X2556	X2557	X2558	X2559	X2560	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2573	X2574	X2575	X2576	X2577	X2578	X2579	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2591	X2592	X2593	X2594	X2595	X2598	X2599	X2602	X2603	X2604	X2605	X2606			
L2474	Q2475	L2476	P2477	L2478	L2479	X2487	X2488	X2489	X2490	X2491	X2492	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2503	X2504	X2505	X2506	X2507	X2508	X2509	X2510	X2511	X2512	X2513	X2514	X2515	X2516	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538		
A2350	N2351	V2352	V2353	V2354	L2355	L2356	L2357	L2358	R2359	K2360	P2361	E2362	C2363	F2364	G2365	P2366	A2367	L2368	R2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	A2379	L2380	E2381	E2382	A2383	L2384	R2385	L2386	S2387	E2388	D2389	P2390	A2391	G2394	P2395	GLY	VAL	ARG	ASP	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO		
PRO	GLU	GLU	M2414	M2415	G2419	I2422	M2423	S2424	F2425	Y2426	A2428	L2429	I2430	D2431	L2432	L2433	G2434	R2435	C2436	A2437	P2438	E2439	M2440	H2441	L2442	I2443	Q2444	A2445	G2446	K2447	G2448	E2449	A2450	L2451	R2452	I2453	A2454	R2455	I2456	L2457	S2458	L2460	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	I2469	L2470	S2471	L2472	P2473				

S4052	L3985	L3856	T3790	K3730	F3669	X3583	X3622	X3415	X3355	X3293	X3223
S4053	V3986	Q3857	G3791	K3731	E3670	X3584	X3623	X3416	X3356	X3294	X3224
N4054	D3987	M3858	A3792	S3732	D3671	X3585	X3624	X3417	X3357	X3295	X3225
V4055	V3989	V3859	M3793	C3733	R3672	X3586	X3625	X3418	X3358	X3296	X3226
E4056	N3960	N3860	V3794	H3734	M3673	X3587	X3626	X3419	X3359	X3297	X3227
M4057	G3991	E3861	S3795	L3735	I3674	X3588	X3627	X3420	X3360	X3298	X3228
	F3992	D3862	S3796	E3736	D3675	X3589	X3628	X3421	X3361	X3299	X3229
K4060	E3928	Q3863	T3797	E3737	D3676	X3590	X3629	X3422	X3362	X3300	X3230
F4061	S3929	L3798	L3797	G3738	L3677	X3591	X3630	X3423	X3363	X3301	X3231
F4062	L3930	L3798	G3738	S3678	S3678	X3592	X3631	X3424	X3364	X3302	X3232
F4063	S3931	V3865	K3799	G3739	K3679	X3593	X3632	X3425	X3365	X3303	X3233
D4063	D3932	I3866	L3800	E3740	A3680	X3594	X3633	X3426	X3366		X3234
M4064	F3997	N3867	N3741	GLY	G3681	X3594	X3634	X3427	X3367	X3307	X3235
F4065	H3998	Q3868	S3803	GLU	E3682	X3595	X3635	X3428	X3368	X3308	X3236
L4066	M3999	Q3869	T3804	ALA	Q3683	X3596	X3636	X3429	X3369	X3309	X3241
L4067	M4000	N3870	L3805	GLU	E3684	X3597	X3637	X3430	X3370	X3310	X3242
L4068	M4001	Q3871	N3806	GLU	E3685	X3598	X3638	X3431	X3371	X3311	X3243
L4069	K4002	E3872	G3807	E3747	E3686	X3599	X3639	X3432	X3372	X3312	X3244
D4070	L4003	K3873	G3808	E3748	E3687	X3600	X3640	X3433	X3373	X3313	X3245
I4071	A4004	V3874	N3809	V3749	E3688	X3601	X3641	X3434	X3374	X3314	X3246
V4072	Q4005	M3875		E3750	E3689	X3603	X3642	X3435	X3375	X3315	X3247
G4073	D4006	A3876	V3812	V3751	V3690	X3604	X3643	X3436	X3376	X3316	X3248
S4074	S4007	D3877	Q3813	S3752	E3691	X3605	X3644	X3437	X3377	X3317	X3249
E4075	S4008	E3878	Q3814	F3753	E3692	X3606	X3645	X3438	X3378	X3318	X3250
A4076	Q4009	D3878	K3815	E3754	E3693	X3607	X3646	X3439	X3379	X3319	X3251
F4077	Q3946	E3879	N3816	E3755	K3693	X3608	X3647	X3440	X3380	X3320	X3252
Q4078	F3947	F3880	L3817	K3756	K3694	X3609	X3648	X3441	X3381	X3321	X3253
D4079	K3948	T3881	D3818	E3757	P3697	X3610	X3649	X3442	X3382	X3322	X3254
V4080	N3949	Q3882	Y3819	M3758	L3698	X3611	X3650	X3443	X3383	X3323	X3255
L4013	N3950	D3883	L3820	E3759	H3699	X3612	X3651	X3444	X3384	X3324	X3256
K4014	E4015	L3884	K3821	K3760	Q3700	X3613	X3652	X3445	X3385	X3325	X3257
E4015	S3952	F3885	K3822	K3761	L3701	T3639	X3653	X3446	X3386	X3326	X3258
L4016	K3953	F3886	K3823	R3762	V3702	P3640	X3654	X3447	X3387	X3327	X3259
L4017	A3954			L3763	L3703	L3641	X3655	X3448	X3388	X3328	X3260
L4018	N3955	Q3889	F3829	L3764	H3704	Y3642	X3656	X3449	X3389	X3329	X3261
S3956	S3956	L3890	Q3830	Y3765	F3705	N3643	X3657	X3450	X3390	X3330	X3262
V3957	V3957	C3892	S3831	Q3766	S3706	L3644	X3658	X3451	X3391	X3331	X3263
A3958	A3958	E3893	L3832	Q3767	R3707	P3645	X3659	X3452	X3392	X3332	X3264
S3959	S3959	G3894	Q3833	S3768	T3708	T3646	X3660	X3453	X3393	X3333	X3265
					A3709	H3647	X3661	X3454	X3394	X3334	X3266
					L3710	R3648	X3662	X3455	X3395	X3335	X3267
					T3711	A3649	X3663	X3456	X3396	X3336	X3268
					E3712	C3650	X3664	X3457	X3397	X3337	X3269
					K3713	N3651	X3665	X3458	X3398	X3338	X3270
					S3714	K3652	X3666	X3459	X3399	X3339	X3271
					K3715	F3653	X3667	X3460	X3400	X3340	X3272
					L3716	L3654	X3668	X3461	X3401	X3341	X3273
					D3717	E3655	X3669	X3462	X3402	X3342	X3274
					T3718	S3656	X3670	X3463	X3403	X3343	X3275
					V3779	Y3657	X3671	X3464	X3404	X3344	X3276
					L3780	K3658	X3672	X3465	X3405	X3345	X3277
					D3719	E3659	X3673	X3466	X3406	X3346	X3278
					Q3781	A3659	X3674	X3467	X3407	X3347	X3279
					M3782	L3660	X3675	X3468	X3408	X3348	X3280
					L3783	A3660	X3676	X3469	X3409	X3349	X3281
					S3784	L3663	X3677	X3470	X3410	X3350	X3282
					A3785	T3664	X3678	X3471	X3411	X3351	X3283
					C3786	E3665	X3679	X3472	X3412	X3352	X3284
					K3787	D3666	X3680	X3473	X3413	X3353	X3285
					G3788	H3667	X3681	X3474	X3414	X3354	X3286
					E3789	S3668	X3682	X3475	X3415	X3355	X3287
								X3476	X3416	X3356	X3288
								X3477	X3417	X3357	X3289
								X3478	X3418	X3358	X3290
								X3479	X3419	X3359	X3291
								X3480	X3420	X3360	X3292

E4948	D4877	A4811	A4746	K4690	GLY	Y4554	GLU	GLY	LYS	SER	E4182	C4114
Q4949	D4878	H4812	S4747	L4681	ALA	Y4554	PRO	GLY	LYS	LEU	S4115	S4115
V4950	M4879	L4813	L4748	E4682	GLY	R4557	GLU	GLU	VAL	ARG	E4116	E4116
K4951	M4880	L4814	E4749	D4683	GLU	N4558	PRO	VAL	THR	ARG	A4117	A4117
E4952	Y4883	D4815	T4750	F4685	GLU	F4559	GLU	VAL	THR	ARG	D4118	D4118
D4953	L4884	L4816	T4751	G4686	GLY	Y4560	PRO	VAL	GLU	ARG	E4119	E4119
E4955	F4885	A4817	A4752	Y4687	ASP	T4561	PRO	VAL	LEU	ARG	M4120	M4120
T4956	H4886	M4818	H4753	I4688	GLU	L4562	LYS	VAL	LEU	ALA	E4121	E4121
C4957	M4887	G4819	M4754	T4689	ASP	R4563	ALA	VAL	ALA	ALA	E4122	E4122
F4959	G4890	A4821	R4756	K4692	GLU	Y4564	ASP	GLY	PRO	THR	I4123	I4123
I4960	L4822	T4822	K4757	G4693	M4627	L4565	GLU	PRO	ASP	ALA	M4124	M4124
G4962	L4823	L4823	K4758	D4694	GLY	A4566	ASN	PHE	PRO	GLU	F4125	F4125
L4963	A4893	R4824	P4758	F4695	GLY	L4567	GLY	ARG	THR	GLU	E4126	E4126
C4964	G4894	T4826	D4759	L4696	GLY	F4568	GLY	PRO	ASP	ALA	E4127	E4127
S4965	G4896	L4827	P4760	V4697	GLU	L4569	LYS	GLY	ASP	ALA	F4128	F4128
D4967	I4897	S4828	P4761	K4698	VAL	A4570	GLU	ALA	THR	GLU	A4129	A4129
F4968	G4898	S4829	F4762	Y4701	PRO	A4572	VAL	HIS	VAL	ALA	M4130	M4130
D4969	T4831	V4830	L4764	D4702	GLU	I4573	PRO	GLY	ALA	ALA	R4131	R4131
T4970	H4832	H4833	L4765	L4703	GLU	N4574	ALA	GLY	GLY	ALA	T4200	T4200
T4971	A4833	Q4834	L4766	V4704	PRO	F4575	PRO	GLY	PRO	GLY	N4201	N4201
T4977	K4835	Q4836	W4767	V4705	GLY	I4576	ALA	GLY	ALA	GLY	R4202	R4202
A4905	Q4837	L4837	L4768	P4709	ALA	L4578	ALA	LEU	LEU	GLY	E4134	E4134
E4908	L4837	Y4837	M4769	S4710	PRO	Y4580	PRO	GLN	LEU	ALA	P4135	P4135
Y4909	V4838	F4838	S4770	F4711	PRO	K4581	PRO	GLY	LEU	GLY	A4136	A4136
E4982	M4839	N4839	D4772	L4646	SER	V4582	PRO	ALA	ALA	ALA	Q4203	Q4203
Y4912	T4840	T4840	V4773	S4647	PRO	S4583	GLY	THR	GLY	GLY	Q4204	Q4204
F4916	V4841	V4841	K4774	L4648	PRO	D4584	LYS	THR	GLY	ALA	E4206	E4206
F4920	G4842	G4842	Y4775	L4649	ALA	S4585	PRO	ASP	ALA	GLY	M4207	M4207
F4924	L4843	L4843	Q4776	L4652	ALA	P4586	ALA	GLY	GLY	THR	P4208	P4208
V4926	A4845	A4845	I4777	V4653	LYS	P4587	LYS	GLY	GLY	VAL	K4211	K4211
I4927	V4846	V4846	W4778	V4654	GLU	GLY	GLY	ILE	GLY	ALA	R4215	R4215
L4928	V4847	V4847	K4779	P4655	ASP	GLY	LEU	ASP	ALA	THR	L4147	L4147
L4929	V4848	V4848	F4780	L4656	MET	GLY	GLY	ASP	ALA	ALA	I4150	I4150
I4930	F4857	F4857	G4781	C4657	GLY	GLY	GLY	GLY	ARG	ALA	S4151	S4151
I4931	F4858	F4858	V4782	I4658	GLY	GLY	ALA	GLY	GLY	GLY	D4220	D4220
I4932	Q4933	Q4933	Y4783	I4659	SER	GLY	ALA	GLY	GLY	THR	V4221	V4221
E5000	G4934	G4934	I4784	V4724	ALA	GLY	GLY	ASP	ALA	THR	E4154	E4154
T5001	L4935	L4935	F4785	L4725	GLY	GLY	GLY	ASP	ALA	ALA	P4155	P4155
E5002	I4936	I4936	T4786	D4726	ASP	GLY	GLY	ASP	ALA	ALA	H4156	H4156
H5003	I4937	I4937	D4786	K4727	LEU	ASP	GLY	GLY	GLY	GLY	D4157	D4157
T5004	D4938	D4938	Y4795	K4728	ALA	GLY	GLY	GLY	GLY	GLY	G4225	G4225
E5007	A4939	A4939	L4800	G4729	ALA	GLY	GLY	GLY	GLY	GLY	G4226	G4226
H5011	F4940	F4940	H4803	L4790	GLY	E4541	GLY	GLY	GLY	GLY	E4227	E4227
K5012	G4941	G4941	Y4804	D4791	ALA	G4542	GLY	GLY	GLY	GLY	E4228	E4228
Y5014	E4942	E4942	N4805	K4730	GLY	E4543	GLY	GLY	GLY	GLY	E4229	E4229
Q5015	R4944	R4944	N4806	K4665	ALA	L4544	GLY	GLY	GLY	GLY	K4230	K4230
	D4945	D4945	F4807	V4566	SER	L4545	GLY	GLY	GLY	GLY	M4231	M4231
	Q4946	Q4946	M4872	P4667	GLY	V4546	VAL	VAL	GLY	GLY	V4235	V4235
	Q4947	Q4947	D4873	L4568	GLY	Q4547	PRO	PRO	GLY	GLY	S4236	S4236
					GLY		PRO	PRO	GLY	GLY	F4237	F4237
					GLY		PRO	PRO	GLY	GLY	E4168	E4168
					GLY		PRO	PRO	GLY	GLY	S4169	S4169
					GLY		PRO	PRO	GLY	GLY	I4170	I4170
					GLY		PRO	PRO	GLY	GLY	L4171	L4171
					GLY		PRO	PRO	GLY	GLY	E4172	E4172
					GLY		PRO	PRO	GLY	GLY	Y4173	Y4173
					GLY		PRO	PRO	GLY	GLY	F4174	F4174
					GLY		PRO	PRO	GLY	GLY	R4175	R4175
					GLY		PRO	PRO	GLY	GLY	P4176	P4176
					GLY		PRO	PRO	GLY	GLY		
					GLY		PRO	PRO	GLY	GLY	R4180	R4180
					GLY		PRO	PRO	GLY	GLY	I4181	I4181
					GLY		PRO	PRO	GLY	GLY	Q4246	Q4246
					GLY		PRO	PRO	GLY	GLY	I4247	I4247
					GLY		PRO	PRO	GLY	GLY	A4248	A4248
					GLY		PRO	PRO	GLY	GLY	A4249	A4249
					GLY		PRO	PRO	GLY	GLY	Q4250	Q4250

Chain I:  70% 73% 16% 11%



R1584	K1585	N1586	P1587	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	E1596	V1597	Q1598	M1599	L1600	M1601	P1602	V1603	S1604	S1605	S1606	R1607	M1608	P1609	M1610	H1611	F1612	Q1614	V1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	P1633	L1634	T1635	M1636	M1637	A1638	L1639	H1640	I1641	P1642	E1643																																																																																																																																							
X1512	X1513	X1514	X1515	X1516	X1517	X1518	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554											X1559	X1560	X1561	X1562	X1563	X1564	X1565	X1566	X1567	X1568	X1569	X1570	X1571	X1572	X1573	X1574	X1575	X1576	X1577	X1578	X1579	F1580	L1581	X1582	E1583																																																																																																																			
X1445	X1446	X1449			X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462	X1463	X1464	X1465	X1466	X1467	X1468	X1469	X1470	X1471	X1472	X1473	X1474	X1475	X1476	X1477	X1484			X1485	X1486	X1487	X1488	X1489	X1490	X1491	X1492	X1493	X1494	X1495	X1496	X1497	X1498	X1499	X1500	X1503			X1504	X1505	X1506	X1507	X1508	X1509	X1510	X1511																																																																																																																																		
P1253	H1254	Y1255	E1256	V1257	A1258	R1259	M1260	G1261	T1262	T1263	V1264	D1265	T1266	P1267	P1268	C1269	L1270	R1271	L1272	A1273	L1274	H1274	R1275	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1283	X1284	X1285	X1286	X1287	X1288	X1289	X1290	X1291	X1292	X1293	X1294	X1295	X1296	X1297	X1298	X1299	X1300	X1301	X1302	X1303	X1304	X1305	X1306	X1307	X1308	X1309	X1310	X1311	X1312	X1313	X1314	X1315	X1316	X1317	X1318	X1319	X1320	X1321	X1322	X1323	X1324	X1325	X1326	X1327	X1328	X1329	X1330	X1331	X1332	X1333	X1334	X1335	X1336	X1337	X1338	X1339	X1340	X1341	X1342	X1343	X1344	X1345	X1346	X1347	X1348	X1349	X1350	X1351	X1352	X1353	X1354	X1355	X1356	X1357	X1358	X1359	X1360	X1361	X1362	X1363	X1364	X1365	X1366	X1367	X1368	X1369	X1370	X1371	X1372	X1373	X1374	X1375	X1376	X1377	X1378	X1379	X1380	X1381	X1382	X1383	X1384	X1385	X1386	X1387	X1388	X1389	X1390	X1391	X1392	X1393	X1394	X1395	X1396	X1397	X1398	X1399	X1400	X1401	X1402	X1403	X1404	X1405	X1406	X1407	X1408	X1409	X1410	X1411	X1412	X1413	X1414	X1415	X1416	X1417	X1418	X1419	X1420	X1421	X1422	X1423	X1424	X1425	X1426	X1427	X1428	X1429	X1430	X1431	X1432	X1433	X1434	X1435	X1436	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444
P763	V764	Q765	G766	V767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780	W781	S782	F783	S784	A785	G786	V787	K788	W789	R790	S791	L792	L793				H797	G798	E799	F800	K801	F802	L803	P804	P805	P806	G807	Y808	A809	P810	C811	H812	A813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824																																																																																																																																			
P825	I826	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	V840	G841	P842	S843	R844	C845	L846	S847	H848	T849	D850	F851	V852	P853	C854	P855	V856	D857	THR	VAL	G861	V862	L863	P864	P865	H866	L867	E868	R869	I870	R871	E872	K873	L874	A875	E876	N877	I878	H879	E880	L881	W882	A883	L884																																																																																																																																						
T885	R886	I887	E888	Q889	G890	K891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	G926	E927	T928	L929	K930	T931	L932	L933	L935	G936	C937	H938	V939	G940	N941	A942	D943	E944																																																																																																																																						
K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	N960	N961	S962	N963	G964	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	G992			A997	R998	D999	R0000	V0001	A0002	Q0003	G0004	W0005	S0006	I0007	S0008	A0009	VAL																																																																																																																																						
GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R01020	L01021	V01022	P01023	Y01024	R01025	L01026	L01027	D01028	E01029	A01030	T01031	K01032	R01033	S01034	N01035	R01036	D01037	S01038	L01039	C01040	Q01041	V01042	V01043	R01044	T01045	L01046	L01047	G01048	Y01049	G01050	Y01051	N01052	T01053	E01054	PRO	PRO	ASP	GLN	GLU	PRO	PRO	SER	GLN	VAL	ASN	GLN	SER	ARG	THR	D01070																																																																																																																																					
R01071	V01072	R01073	F01074	R01075	R01076	A01077	E01078	K01079	S01080	Y01081	T01082	V01083	Q01084	S01085	Q01086	R01087	W01088	Y01089	F01090	E01091	F01092	E01093	A01094	V01095	T01096				E01099	M01100	V01102	G01103	W01104	A01105	R01106	P01107	E01108	L01109	R01110	P01111	D01112	V01113	E01114	L01115	G01116	A01117	D01118	E01119	L01120	A01121	Y01122	L01182	E01183	L01184	G01185	D01186	G01187	F01188	L01189	P01190	V01191	C01192	Q1130	R1131																																																																																																																																
W01132	H01133	L01134	G01135	S01136	F01139			G01140	R01141	P01142	W01143	Q01144	S01145	G01146	D01147	V01148	V01149	G01150	C01151	M01152	I01153	D01154	L01155	T01156	E01157	N01158	T01159	I01160	I01161	F01162	T01163	L01164	N01165	G01166	E01167	V01168	L01169	M01170	S01171	D01172	S01173	G01174	S01175	E01176	T01177	A01178	F01179	R01180	E01181	L01182	E01183	L01184	G01185	D01186	G01187	F01188	L01189	P01190	V01191	C01192																																																																																																																																				
S01193	L01194	G01195	P01196	Q01197	Q01198	V01199	G01200	H01201	L01202	N01203	L01204	G01205	Q01206	D01207	V01208	S01209	S01210	L01211	R01212	F01213	F01214	A01215	I01216	C01217	G01218	L01219	Q01220	E01221	G01222	F01223	E01224	P01225	F01226	A01227	I01228	N01229	M01230	Q01231	R01232	P01233	V01234	T01235	T01236	W01237	F01238	S01239	K01240	S01241	L01242	P01243	Q01244	F01245	E01246	P01247	V01248	P01249	P01250	E01251	H01252																																																																																																																																					
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E2381	E2382	A2383	T2384	T2385	T2386	S2387	E2388	E2389	P2390	A2391	R2392	D2393	F2394	L2395	R2396	F2397	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	L2352	V2353	V2354	R2355	L2356	L2357	L2358	R2359	R2360	P2361	E2362	C2363	F2364	G2365	P2366	G2367	L2368	R2369	Q2370	E2371	E2439	M2440	H2441	T2442	L2443	Q2444																																																																																																																																																																																																																																										
P2319	D2320	I2321	G2322	W2323	G2327	G2328	E2329	R2330	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	A2338	V2339	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	L2288	A2289	L2290	Q2291	E2292	Q2293	L2294	L2295	E2296	K2297	F2298	C2299	R2240	R2241	L2242	S2243	R2244	Q2245	N2246	Q2247	R2248	G2249	Q2300	V2301	L2302	A2303	G2304	C2305	G2306	L2307	Q2308	S2309	C2310	P2311	M2312	L2313	L2314	L2376	L2377	A2378	A2379	T2380																																																																																																																																																																																																																															
E2259	M2260	S2261	G2262	G2264	L2265	G2266	M2267	Q2268	G2269	S2270	T2271	P2272	L2273	D2274	V2275	A2276	A2277	A2278	S2279	V2280	I2281	D2282	M2283	N2284	E2285	L2286	A2287	L2288	V2289	T2290	S2291	C2292	C2293	F2295	L2296	C2297	Y2298	F2299	C2240	R2241	I2242	S2243	R2244	Q2245	N2246	Q2247	R2248	S2249	M2250	F2251	L2252	H2253	L2254	S2255	L2256	L2257	L2258																																																																																																																																																																																																																																													
E2259	M2260	S2261	G2262	G2264	L2265	G2266	M2267	Q2268	G2269	S2270	T2271	P2272	L2273	D2274	V2275	A2276	A2277	A2278	S2279	V2280	I2281	D2282	M2283	N2284	E2285	L2286	A2287	L2288	V2289	T2290	S2291	C2292	C2293	F2295	L2296	C2297	Y2298	F2299	C2240	R2241	I2242	S2243	R2244	Q2245	N2246	Q2247	R2248	S2249	M2250	F2251	L2252	H2253	L2254	S2255	L2256	L2257	L2258																																																																																																																																																																																																																																													
P2319	D2320	I2321	G2322	W2323	G2327	G2328	E2329	R2330	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	A2338	V2339	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	L2352	V2353	V2354	R2355	L2356	L2357	L2358	R2359	R2360	P2361	E2362	C2363	F2364	G2365	P2366	G2367	L2368	R2369	Q2370	E2371	E2439	M2440	H2441	T2442	L2443	Q2444																																																																																																																																																																																																																																															
P2319	D2320	I2321	G2322	W2323	G2327	G2328	E2329	R2330	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	A2338	V2339	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	L2352	V2353	V2354	R2355	L2356	L2357	L2358	R2359	R2360	P2361	E2362	C2363	F2364	G2365	P2366	G2367	L2368	R2369	Q2370	E2371	E2439	M2440	H2441	T2442	L2443	Q2444																																																																																																																																																																																																																																															
P1706	L1707	A1708	R1709	G1710	Y1711	Y1712	D1713	L1714	L1715	I1716	S1717	L1718	H1719	L1720	E1721	S1722	A1723	C1724	R1725	S1726	H1727	R1728	S1729	M1730	L1731	S1732	E1733	Y1734	A1735	I1736	L1738	T1739	P1740	E1741	T1742	R1743	A1744	I1745	T1746	L1747	F1748	P1749	P1750	G1751	R1752	K1753	G1754	G1755	N1756	A1757	R1758	E1759	R1760	G1761	L1762	P1763	G1764	V1765	G1766																																																																																																																																																																																																																																											
V1767	T1768	T1769	S1770	L1771	R1772	P1773	P1774	H1775	H1776	F1777	S1778	P1779	P1780	C1781	F1782	V1783	A1784	A1785	T1786	P1787	A1788	ALA	GLY	VAL	ALA	E1793	A1794	P1795	A1796	R1797	L1798	S1799	I1802	P1803	L1804	E1805	A1806	L1807	R1808	D1809	K1810	G1811	A1812	R1813	M1814	L1815	G1816	A1817	A1818	V1819	R1820	D1821	G1822	L1823	Q1824	H1825	A1826	R1827																																																																																																																																																																																																																																												
D1828	P1829	V1830	G1831	G1832	S1833	V1834	E1835	F1836	Q1837	F1838	V1839	P1840	A1841	L1842	K1843	L1844	V1845	S1846	T1847	L1848	L1849	V1850	M1851	G1852	I1853	F1854	G1855	D1856	E1857	D1858	V1859	Q1860	I1861	T1862	L1863	K1864	M1865	I1866	E1869	V1870	F1871	T1872	E1873	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	R1827																																																																																																																																																																																																																																										
G1949	E1950	L1951	Q1952	H1953	R1954	V1955	E1956	S1957	L1958	A1959	A1960	F1961	A1962	A1963	R1964	V1965	V1966	L1969	Q1970	Q1973	R1976	Y1977	A1978	L1979	L1980	M1981	R1982	A1983	F1984	T1985	M1986	S1987	A1988	A1989	E1990	T1991	A1992	R1993	R1994	T1995	R1996	E1997	F1998	R1999	S2000	P2001	V2002	Q2003	E2004	Q2005	T2006	N2007	W2008	L2009	L2010	H2011																																																																																																																																																																																																																																														
F2012	K2013	D2014	E2015	A2016	D2017	E2018	E2019	D2020	C2021	P2022	L2023	P2024	R2027	Q2028	Q2029	D2030	L2031	F2034	L2038	L2039	A2040	H2041	C2042	G2043	I2044	Q2045	L2046	E2047	GLU	GLU	GLU	PRO	GLU	GLU	GLU	THR	SER	LEU	SER	SER	ARG	LEU	SER	ARG	LEU	VAL	LYS	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040	L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	L2077	L2078	L2079	L2080	L2081	L2082	L2083	L2084	L2085	L2086	L2087	L2088	L2089	L2090	L2091	L2092	L2093	L2094	L2095	L2096	L2097	L2098	L2099	L2100	L2101	L2102	L2103	L2104	L2105	L2106	L2107	L2108	L2109	L2110	L2111	L2112	L2113	L2114	L2115	L2116	L2117	L2118	L2119	L2120	L2121	L2122	L2123	L2124	L2125	L2126	L2127	L2128	L2129	L2130	L2131	L2132	L2133	L2134	L2135	L2136	L2137	L2138	L2139	L2140	L2141	L2142	L2143	L2144	L2145	L2146	L2147	L2148	L2149	L2150	L2151	L2152	L2153	L2154	L2155	L2156	L2157	L2158	L2159	L2160	L2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258
LYS	GLU	GLU	LYS	PRO	GLU	GLU	LEU	PRO	ALA	GLU	K2089	K2090	P2091	Q2092	S2093	L2094	Q2095	E2096	L2097	V2098	S2099	H2100	M2101	V2102	R2103	R2104	W2105	A2106	Q2107	E2108	D2109	V2110	V2111	Q2112	S2113	P2114	E2115	L2116	V2117	R2118	A2119	M2120	F2121	S2122	L2123	L2124	H2125	L2126	Q2127	Y2128	D2129	Q2130	L2131	G2132	L2135	R2136																																																																																																																																																																																																																																														
A2137	L2138	P2139	R2140	M2203	A2141	Y2142	T2143	I2144	S2145	P2146	S2147	S2148	V2149	E2150	D2151	T2152	L2155	L2156	E2157	C2158	L2159	G2160	Q2161	I2162	R2163	S2164	L2165	L2166	I2167	V2168	Q2169	M2170	G2171	F2172	E2175	N2176	L2177	M2178	I2179	Q2180	S2181	L2182	G2183	N2184	I2185	M2186	N2187	N2188	K2189	V2190	F2191	Y2192	Q2193	H2194	S2255	L2256	L2257	M2198																																																																																																																																																																																																																																												
R2199	A2200	L2201	G2202	M2203	H2204	E2205	T2206	V2207	M2208	E2209	V2210	M2211	V2212	M2213	L2214	L2215	G2216	G2217	G2218	E2219	T2220	K2221	E2222	L2223	R2224	F2225	P2226	K2227	M2228	V2229	T2230	S2231	C2232	C2233	F2235	L2236	C2237	Y2238	F2239	C2240	R2241	I2242	S2243	R2244	Q2245	N2246	Q2247	R2248	G2249	M2250	F2251	L2252	H2253	L2254	S2255	L2256	L2257	L2258																																																																																																																																																																																																																																												
E2259	M2260	S2261	G2262	G2264	L2265	G2266	M2267	Q2268	G2269	S2270	T2271	P2272	L2273	D2274	V2275	A2276	A2277	A2278	S2279	V2280	I2281	D2282	M2283	N2284	E2285	L2286	A2287	L2288	V2289	T2290	S2291	C2292	C2293	F2295	L2296	C2297	Y2298	F2299	C2240	R2241	I2242	S2243	R2244	Q2245	N2246	Q2247	R2248	G2249	M2250	F2251	L2252	H2253	L2254	S2255	L2256	L2257	L2258																																																																																																																																																																																																																																													
P2319	D2320	I2321	G2322	W2323	G2327	G2328	E2329	R2330	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	A2338	V2339	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	L2352	V2353	V2354	R2355	L2356	L2357	L2358	R2359	R2360	P2361	E2362	C2363	F2364	G2365	P2366	G2367	L2368	R2369	Q2370	E2371	E2439	M2440	H2441	T2442	L2443	Q2444																																																																																																																																																																																																																																															
E2381	E2382	A2383	T2384	T2385	T2386	S2387	E2388	E2389	P2390	A2391	R2392	D2393	F2394	L2395	R2396	F2397	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	L2352	V2353	V2354	R2355	L2356	L2357	L2358	R2359	R2360	P2361	E2362	C2363	F2364	G2365	P2366	G2367	L2368	R2369	Q2370	E2371	E2439	M2440	H2441	T2442	L2443	Q2444																																																																																																																																																																																																																																										



A4203	Q4204	W4205	E4206	W4207	P4208	K4211	K4214	R4215	L4218	F4219	D4220	V4221	N4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	F4234	F4237	C4238	E4239	D4240	T4241	L4242	F4243	E4244	M4245	Q4246	L4247	A4248	Q4249	Q4250	L4251	S4252	E4253	PRO	GLU	GLY	PRO	ALA	ASP	GLU	ASP	GLU	GLY	NET	GLY												
P4135	A4136	R4137	D4138	I4139	G4140	F4141	M4142	V4143	A4144	L4147	L4150	S4151	E4152	P4155	H4156	D4157	P4158	R4159	L4160	R4161	N4162	E4165	L4166	A4167	E4168	S4169	I4170	L4171	E4172	R4175	P4176	Y4177	L4178	G4179	R4180	I4181	E4182	S4187	R4188	R4189	I4190	E4191	R4192	I4193	Y4194	N4195	E4196	I4197	S4198	E4199	T4200	M4201	R4202										
G4073	S4074	E4075	A4076	F4077	Q4078	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	G4086	L4087	L4088	S4089	K4090	K4091	G4092	F4093	Q4094	K4095	A4096	M4097	D4098	Q4099	I4100	K4101	Q4102	F4103	T4104	Q4105	P4106	E4107	I4108	Q4109	L4112	S4113	E4116	A4117	D4118	E4119	N4120	E4121	M4122	I4123	N4124	F4125	E4126	E4127	F4128	E4129	A4130	R4131	Q4132	E4134							
E4011	L4012	L4013	K4014	E4015	L4016	L4017	D4018	L4019	Q4020	K4021	D4022	M4023	V4024	L4027	L4028	S4029	L4030	L4031	M4034	V4035	V4036	M4037	G4038	M4039	L4040	A4041	R4042	Q4043	M4044	V4045	D4046	M4047	L4048	V4049	E4050	S4051	S4052	S4053	M4054	V4055	E4056	M4057	L4058	L4059	K4060	F4061	F4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	V4072						
N3950	F3951	S3952	K3953	A3954	M3955	S3956	V3957	A3958	K3959	V3960	V3961	F3962	S3963	L3964	T3965	E3966	Y3968	I3969	Q3970	C3971	P3972	C3973	T3974	Q3975	N3976	Q3977	Q3978	A3981	H3982	S3983	R3984	V3986	D3987	A3988	V3989	V3990	G3991	F3992	L3993	H3994	V3995	F3996	A3997	H3998	M3999	M4000	M4001	K4002	L4003	A4004	Q4005	D4006	E3945	S4007	S4008	Q4009	I4010						
E4011	L4012	L4013	K4014	E4015	L4016	L4017	D4018	L4019	Q4020	K4021	D4022	M4023	V4024	L4027	L4028	S4029	L4030	L4031	M4034	V4035	V4036	M4037	G4038	M4039	L4040	A4041	R4042	Q4043	M4044	V4045	D4046	M4047	L4048	V4049	E4050	S4051	S4052	S4053	M4054	V4055	E4056	M4057	L4058	L4059	K4060	F4061	F4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	V4072						
G4073	S4074	E4075	A4076	F4077	Q4078	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	G4086	L4087	L4088	S4089	K4090	K4091	G4092	F4093	Q4094	K4095	A4096	M4097	D4098	Q4099	I4100	K4101	Q4102	F4103	T4104	Q4105	P4106	E4107	I4108	Q4109	L4112	S4113	E4116	A4117	D4118	E4119	N4120	E4121	M4122	I4123	N4124	F4125	E4126	E4127	F4128	E4129	A4130	R4131	Q4132	E4134							
P4135	A4136	R4137	D4138	I4139	G4140	F4141	M4142	V4143	A4144	L4147	L4150	S4151	E4152	P4155	H4156	D4157	P4158	R4159	L4160	R4161	N4162	E4165	L4166	A4167	E4168	S4169	I4170	L4171	E4172	R4175	P4176	Y4177	L4178	G4179	R4180	I4181	E4182	S4187	R4188	R4189	I4190	E4191	R4192	I4193	Y4194	N4195	E4196	I4197	S4198	E4199	T4200	M4201	R4202										
A4203	Q4204	W4205	E4206	W4207	P4208	K4211	K4214	R4215	L4218	F4219	D4220	V4221	N4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	F4234	F4237	C4238	E4239	D4240	T4241	L4242	F4243	E4244	M4245	Q4246	L4247	A4248	Q4249	Q4250	L4251	S4252	E4253	PRO	GLU	GLY	PRO	ALA	ASP	GLU	ASP	GLU	GLY	NET	GLY												
X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3449	X3450	X3451				
X3452	X3453	X3454		X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549		X3552	X3553	X3554	X3555	X3556	X3557				
X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3603	X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	T3639	P3640	L3641	Y3642				
N3643	L3644	P3645	T3646	H3647	R3648	A3649	C3650	N3651	N3652	P3653	L3654	E3655	S3656	Y3657	K3658	A3659	X3660	V3661	L3662	L3663	T3664	E3665	M3666	H3667	S3668	F3669	E3670	R3671	R3672	M3673	D3675	D3676	S3677	S3678	K3679	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693		L3698	H3699		V3702	F3705	S3706							
R3707	T3708	A3709	T3710	T3711	E3712	R3713	S3714	N3715	L3716	D3717	E3718	D3719	Y3720	L3721	Y3722	M3723	A3724	Y3725	C3726	K3727	G3728	E3729	T3730	G3731	A3732	M3733	V3734	R3735	E3736	E3737	G3738	G3739	E3740	N3741	GLU	GLU	ALA	G3681	E3682	Q3683	E3684	E3685	E3686	V3749	V3750	V3751	S3752	F3753	E3689	V3690	E3755	K3756	E3757	M3758		E3759	K3760	Q3761	R3762	L3763	Y3765	Q3766	
Q3767	S3768	R3769	L3770	H3771	T3772	R3773	G3774	A3775	A3776	E3777	M3778	V3779	L3780	Q3781	M3782	L3783	S3784	A3785	C3786	K3787	G3788	E3789	N3851	M3790	G3791	A3792	M3793	V3794	S3795	L3798	K3799	L3800	G3801	L3802	S3803	L3804	L3805	N3806	G3807	Q3808	N3809	A3810	E3811	Q3812	Q3813	Q3814	K3815	K3816	L3817	D3818	V3819	L3820	K3821	D3822	Q3823	K3824	E3825	V3826					
F3829	Q3830	S3831	L3832	H3833	A3834	L3835	M3836	Q3837	T3838	C3839	S3840	V3841	L3842	D3843	L3844	N3845	A3846	F3847	E3848	R3849	Q3850	N3851	K3852	A3853	E3854	G3855	L3856	G3857	M3858	V3859	L3860	E3861	D3862	G3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870	G3871	E3872	K3873	V3874	M3875	A3876	D3877	D3878	E3879	F3880	S3881	Q3882	D3883	L3884	F3885	R3886	F3887	L3888				
Q3889	L3890	L3891	C3892	E3893	G3894	H3895	N3896	N3897	D3898	F3899	Q3900	N3901	R3904	T3905	Q3906	T3907	G3908	N3909	T3910	T3911	T3912	L3913	N3914	L3915	T3916	G3917	C3918	T3919	V3920	D3921	F3922	L3923	L3924	R3925	L3926	Q3927	E3928	S3929	L3930	S3931	D3932	F3933	Y3934	W3935	Y3936	Y3937	S3938	Q3939	K3940	D3941	V3942	L3943	E3944	E3945	Q3946	G3947	K3948	R3949					
N3950	F3951	S3952	K3953	A3954	M3955	S3956	V3957	A3958	K3959	V3960	V3961	F3962	S3963	L3964	T3965	E3966	Y3968	I3969	Q3970	C3971	P3972	C3973	T3974	Q3975	N3976	Q3977	Q3978	A3981	H3982	S3983	R3984	V3986	D3987	A3988	V3989	V3990	G3991	F3992	L3993	H3994	V3995	F3996	A3997	H3998	M3999	M4000	M4001	K4002	L4003	A4004	Q4005	D4006	E3945	S4007	S4008	Q4009	I4010						
E4011	L4012	L4013	K4014	E4015	L4016	L4017	D4018	L4019	Q4020	K4021	D4022	M4023	V4024	L4027	L4028	S4029	L4030	L4031	M4034	V4035	V4036	M4037	G4038	M4039	L4040	A4041	R4042	Q4043	M4044	V4045	D4046	M4047	L4048	V4049	E4050	S4051	S4052	S4053	M4054	V4055	E4056	M4057	L4058	L4059	K4060	F4061	F4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	V4072						
G4073	S4074	E4075	A4076	F4077	Q4078	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	G4086	L4087	L4088	S4089	K4090	K4091	G4092	F4093	Q4094	K4095	A4096	M4097	D4098	Q4099	I4100	K4101	Q4102	F4103	T4104	Q4105	P4106	E4107	I4108	Q4109	L4112	S4113	E4116	A4117	D4118	E4119	N4120	E4121	M4122	I4123	N4124	F4125	E4126	E4127	F4128	E4129	A4130	R4131	Q4132	E4134							
P4135	A4136	R4137	D4138	I4139	G4140	F4141	M4142	V4143	A4144	L4147	L4150	S4151	E4152	P4155	H4156	D4157	P4158	R4159	L4160	R4161	N4162	E4165	L4166	A4167	E4168	S4169	I4170	L4171	E4172	R4175	P4176	Y4177	L4178	G4179	R4180	I4181	E4182	S4187	R4188	R4189	I4190	E4191	R4192	I4193	Y4194	N4195	E4196	I4197	S4198	E4199	T4200	M4201	R4202										
A4203	Q4204	W4205	E4206	W4207	P4208	K4211	K4214	R4215	L4218	F4219	D4220	V4221	N4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	M4231	F4234	F4237	C4238	E4239	D4240	T4241	L4242	F4243	E4244	M4245	Q4246	L4247	A4248	Q4249	Q4250	L4251	S4252	E4253	PRO	GLU	GLY	PRO	ALA	ASP	GLU	ASP	GLU	GLY	NET	GLY												



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	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	0.404	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.16	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: CA, 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	0.32	0/834	0.58	0/1123
1	F	0.32	0/834	0.57	0/1123
1	H	0.32	0/834	0.58	0/1123
1	J	0.32	0/834	0.57	0/1123
2	B	0.32	0/25428	0.57	5/34534 (0.0%)
2	E	0.33	0/25428	0.57	5/34534 (0.0%)
2	G	0.33	0/25428	0.57	5/34534 (0.0%)
2	I	0.33	0/25428	0.57	5/34534 (0.0%)
All	All	0.33	0/105048	0.57	20/142628 (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
2	B	0	17
2	E	0	18
2	G	0	17
2	I	0	17
All	All	0	69

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	719	LEU	CA-CB-CG	6.48	130.21	115.30
2	E	719	LEU	CA-CB-CG	6.45	130.14	115.30
2	G	719	LEU	CA-CB-CG	6.45	130.13	115.30
2	B	719	LEU	CA-CB-CG	6.44	130.11	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	977	LEU	CA-CB-CG	6.06	129.24	115.30

There are no chirality outliers.

5 of 69 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	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	19	0
1	F	818	0	824	19	0
1	H	818	0	824	19	0
1	J	818	0	824	21	0
2	B	29369	0	24710	415	0
2	E	29369	0	24708	425	0
2	G	29369	0	24708	429	0
2	I	29369	0	24711	430	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
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102133	1756	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 8.

The worst 5 of 1756 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:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.65	0.78
2:G:177:GLU:HG3	2:I:2452:ARG:HH12	1.54	0.70
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.72	0.70
2:G:111:HIS:HD2	2:G:114:SER:H	1.38	0.70
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.72	0.70

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%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4687 (69%)	2862 (88%)	367 (11%)	6 (0%)	47	81
2	E	3235/4687 (69%)	2861 (88%)	367 (11%)	7 (0%)	47	81
2	G	3235/4687 (69%)	2863 (88%)	365 (11%)	7 (0%)	47	81
2	I	3235/4687 (69%)	2863 (88%)	365 (11%)	7 (0%)	47	81
All	All	13360/19180 (70%)	11833 (89%)	1500 (11%)	27 (0%)	50	81

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1829	PRO
2	B	1932	PRO
2	E	1829	PRO
2	G	1829	PRO

Continued on next page...

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Mol	Chain	Res	Type
2	I	1829	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	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
2	E	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
2	G	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
2	I	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
All	All	10324/13192 (78%)	10252 (99%)	72 (1%)	84	90

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	688	LEU
2	I	4984	ASN
2	I	1076	ARG
2	I	3805	LEU
2	E	1141	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	4886	HIS
2	I	3882	GLN
2	I	57	ASN
2	I	765	GLN

Continued on next page...

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Mol	Chain	Res	Type
2	I	4130	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	I	12
2	B	12

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
2	G	12
2	E	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3613:UNK	C	3639:THR	N	43.91
1	B	3613:UNK	C	3639:THR	N	43.68
1	G	3613:UNK	C	3639:THR	N	43.62
1	E	3613:UNK	C	3639:THR	N	43.61
1	I	3163:UNK	C	3170:UNK	N	16.30

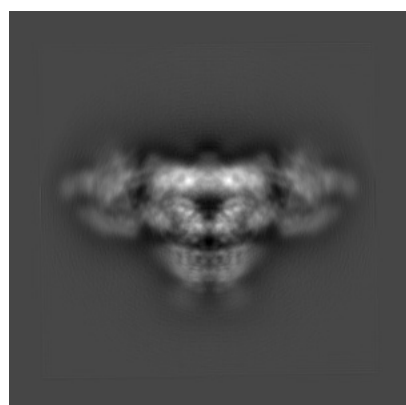
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22392. These allow visual inspection of the internal detail of the map and identification of artifacts.

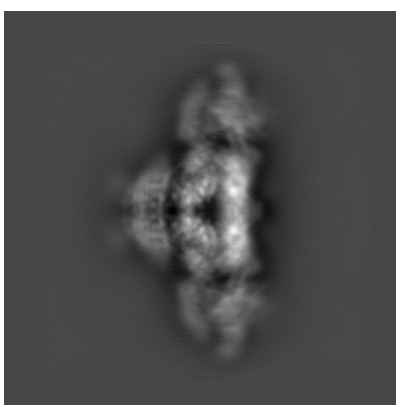
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

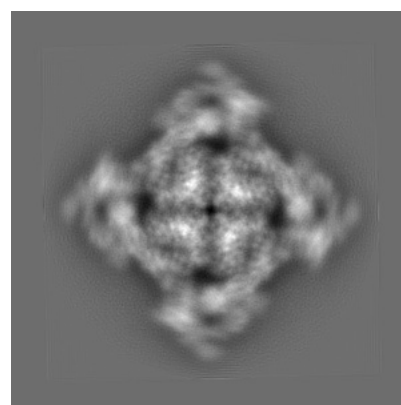
6.1.1 Primary map



X



Y

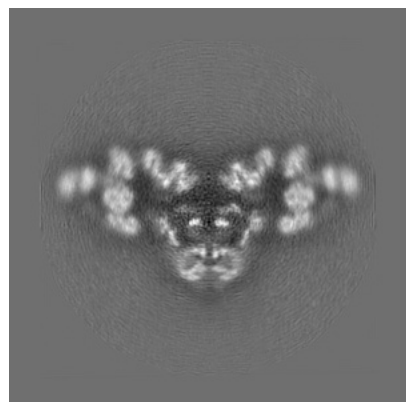


Z

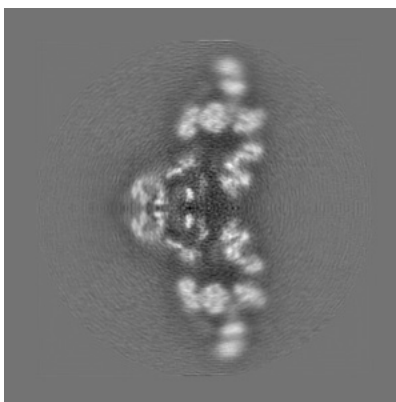
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

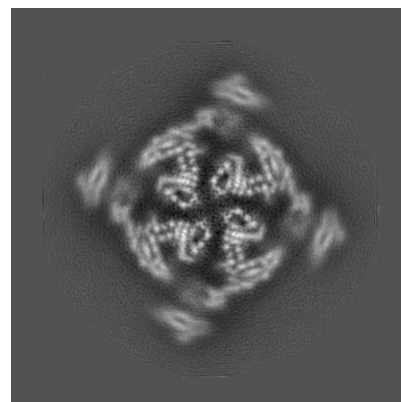
6.2.1 Primary map



X Index: 200



Y Index: 200

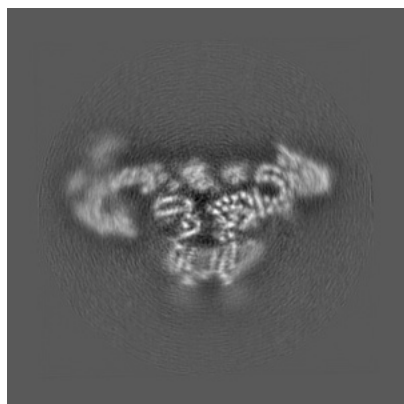


Z Index: 200

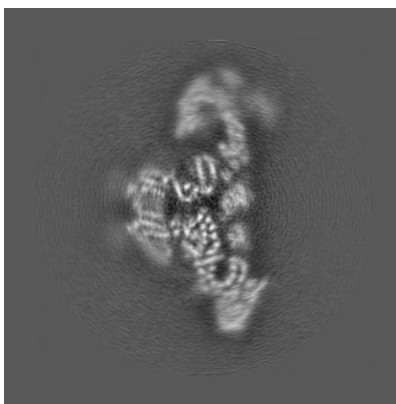
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

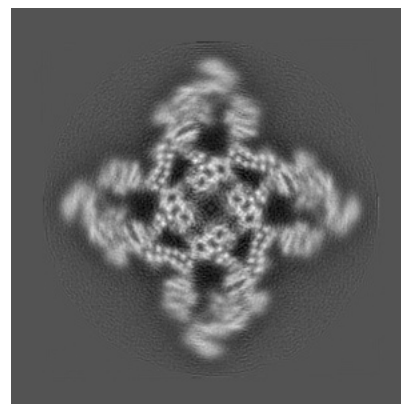
6.3.1 Primary map



X Index: 177



Y Index: 177



Z Index: 226

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

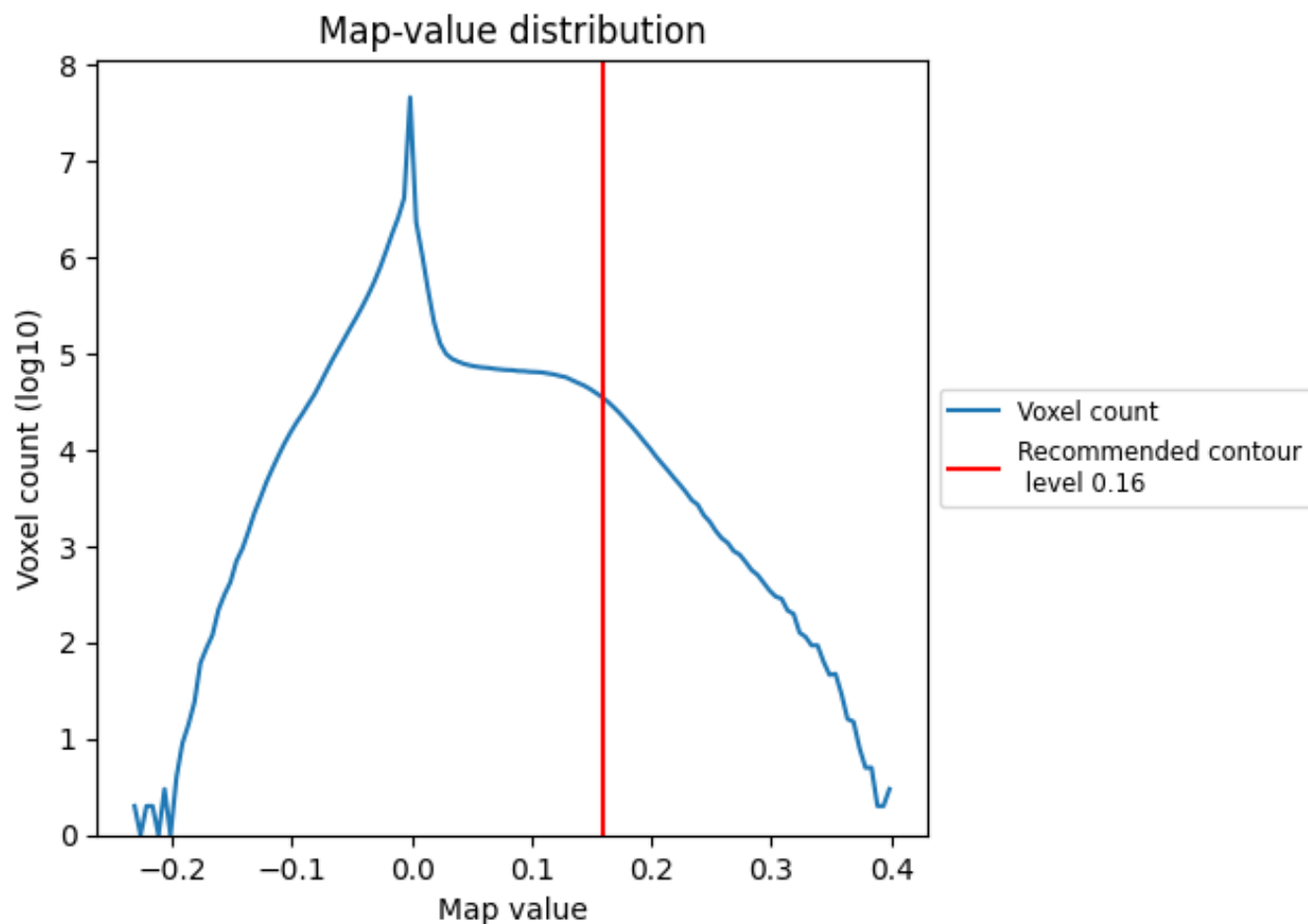
6.5 Mask visualisation

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

7 Map analysis [i](#)

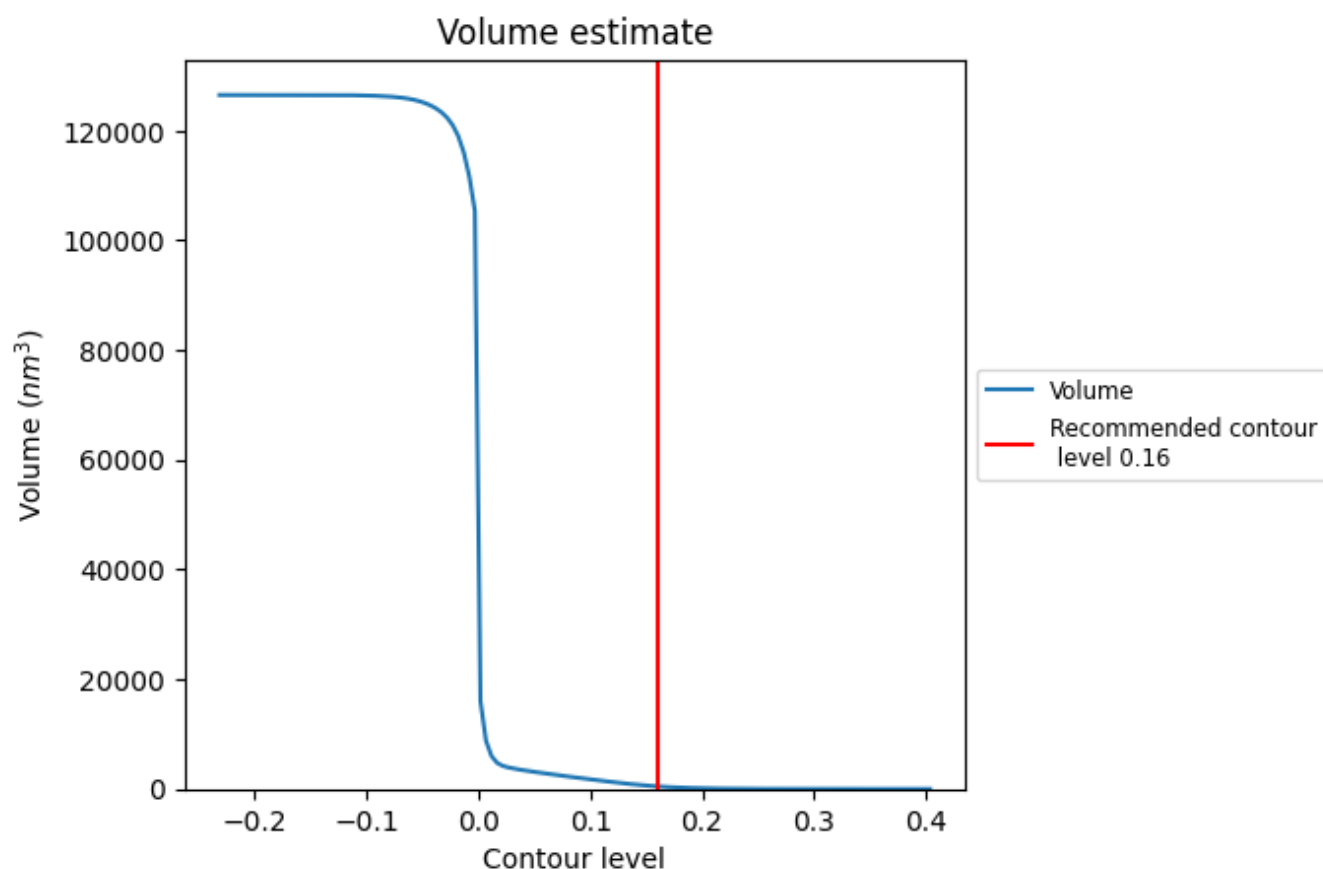
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

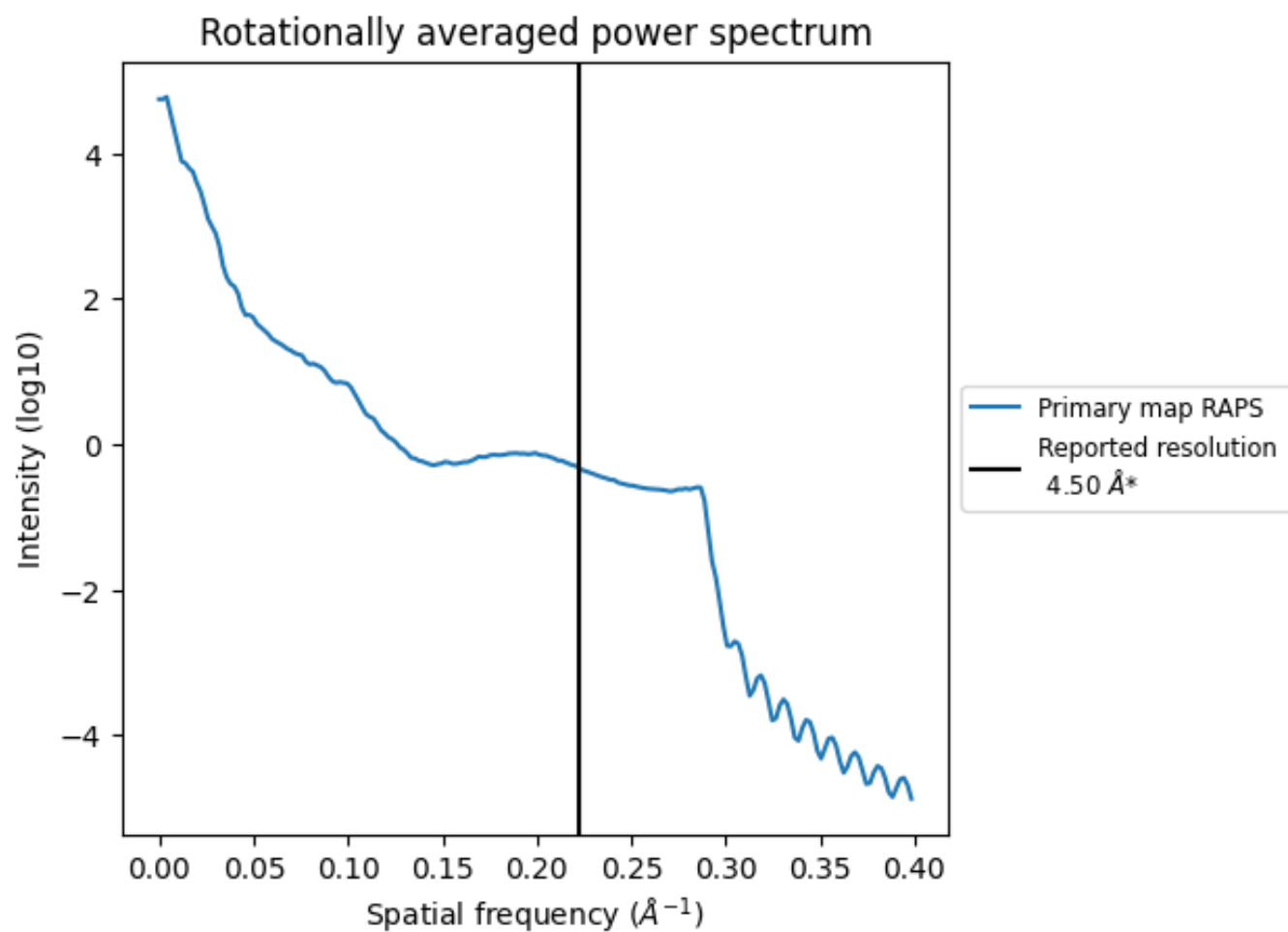
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 469 nm^3 ; this corresponds to an approximate mass of 423 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 0.222 Å⁻¹

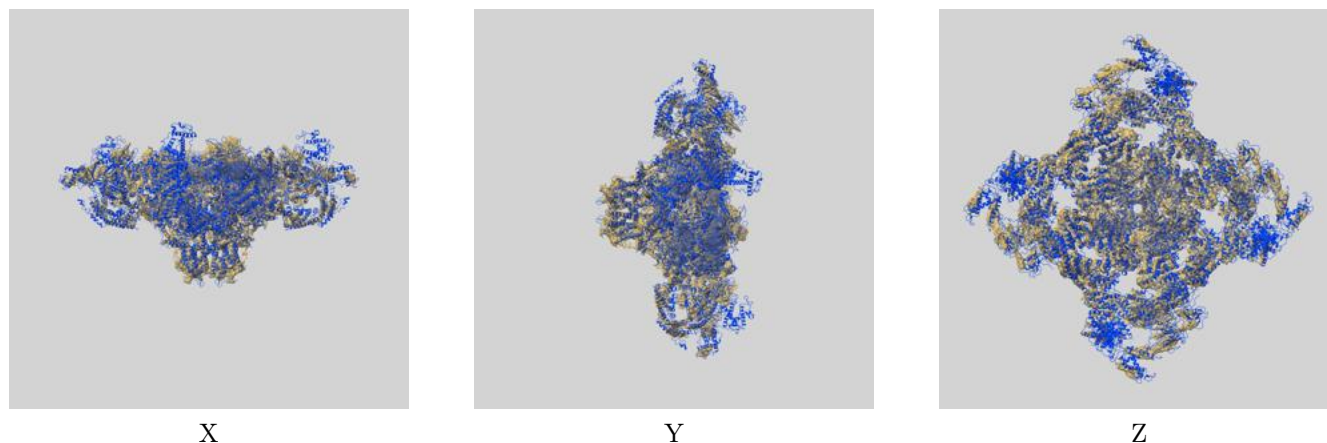
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

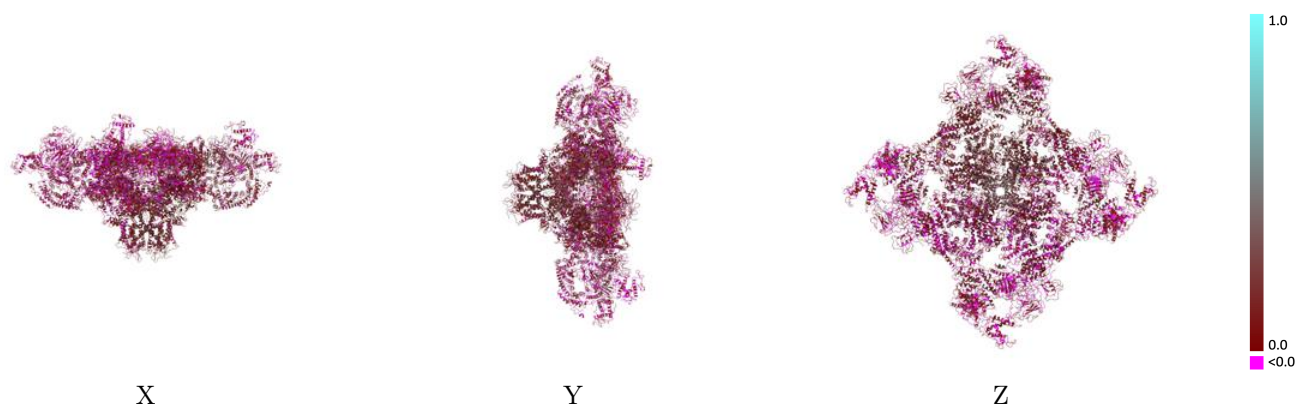
This section contains information regarding the fit between EMDB map EMD-22392 and PDB model 7JMF. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



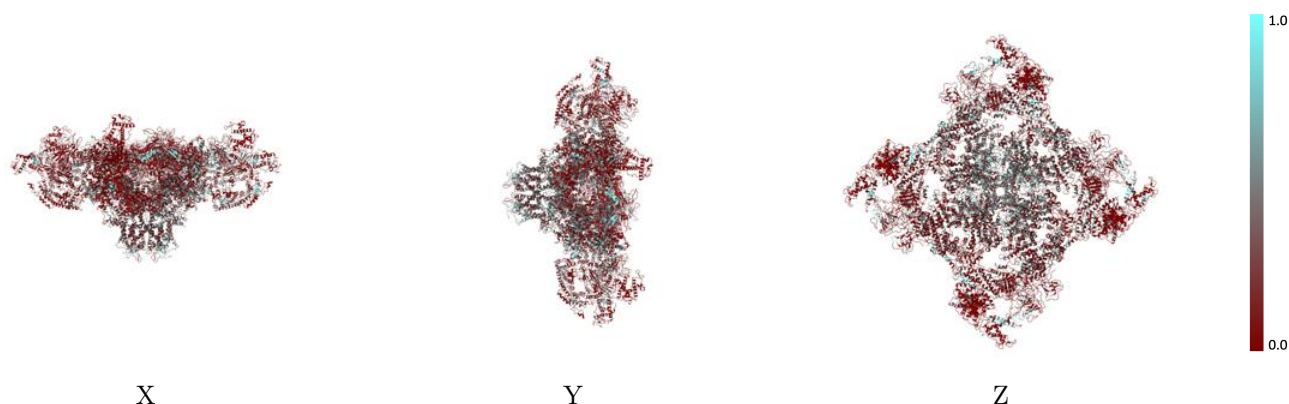
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



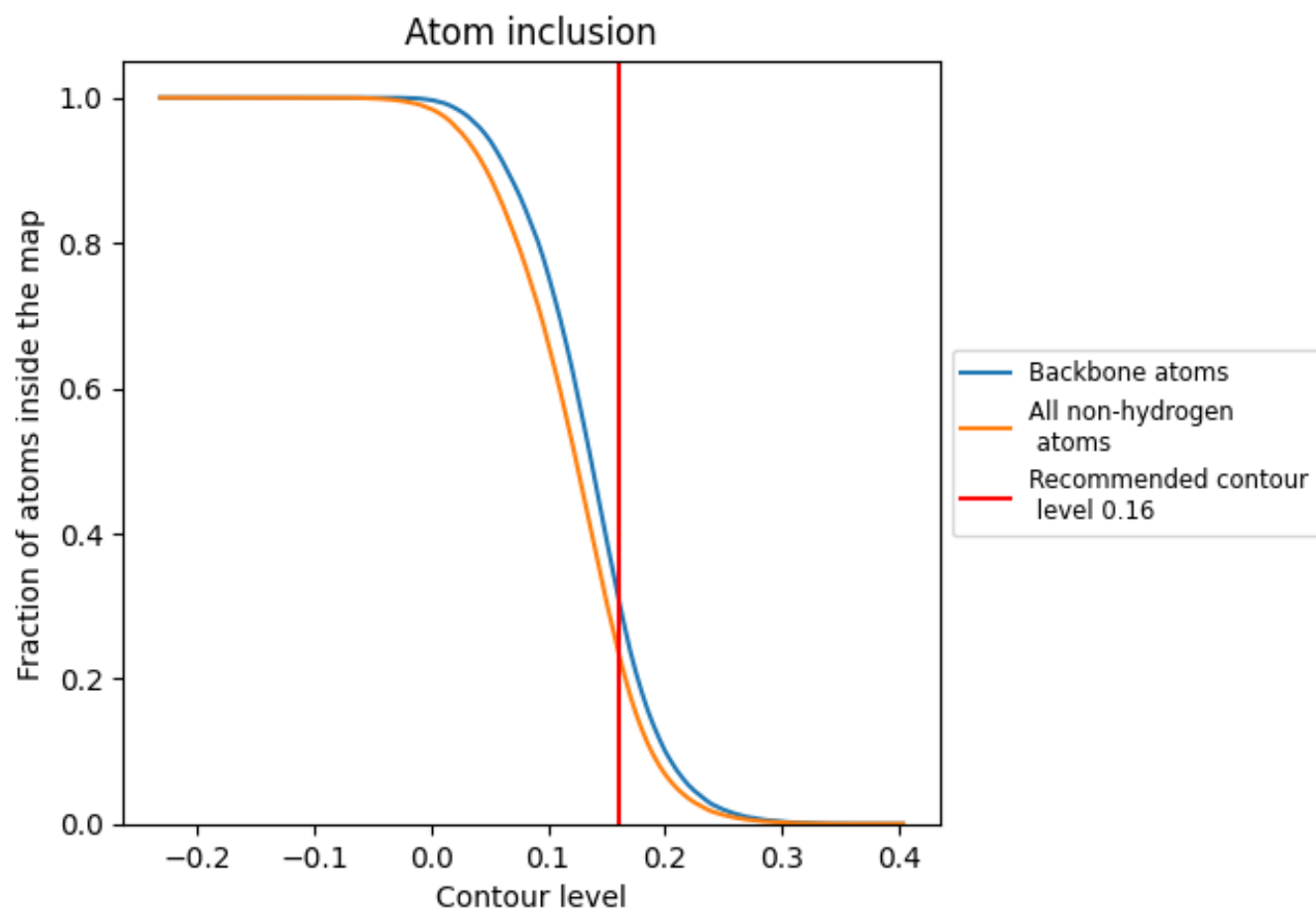
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 31% of all backbone atoms, 24% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2382	<div></div> 0.1100
A	<div></div> 0.1452	<div></div> 0.1330
B	<div></div> 0.2722	<div></div> 0.1490
E	<div></div> 0.2580	<div></div> 0.1200
F	<div></div> 0.1427	<div></div> 0.0750
G	<div></div> 0.2199	<div></div> 0.0820
H	<div></div> 0.1092	<div></div> 0.0850
I	<div></div> 0.2146	<div></div> 0.0890
J	<div></div> 0.1253	<div></div> 0.0820

