wwPDB EM Validation Summary Report (i)

Feb 12, 2024 – 05:44 PM EST

PDB ID	:	3IZN
EMDB ID	:	EMD-5250
Title	:	Mm-cpn deltalid with ATP
Authors	:	Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.; Chiu, W.; Frydman, J.
Deposited on	:	2010-10-30
Resolution	:	6.40 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 (i) 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 (i)) were used in the production of this report:

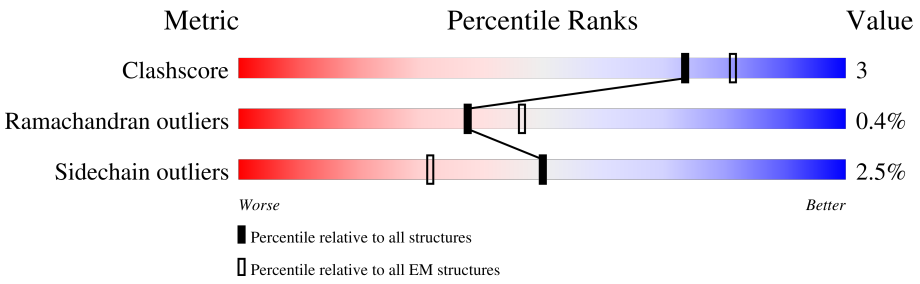
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.40 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 <=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	491	40% 90% 9% •
1	B	491	40% 90% 9% •
1	C	491	40% 89% 10% •
1	D	491	40% 90% 9% •
1	E	491	40% 90% 9% •
1	F	491	40% 90% 9% •
1	G	491	40% 90% 9% •
1	H	491	40% 90% 9% •

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Mol	Chain	Length	Quality of chain
1	I	491	41% 90% 9%
1	J	491	40% 90% 9%
1	K	491	41% 90% 10%
1	L	491	40% 90% 10%
1	M	491	41% 90% 9%
1	N	491	40% 90% 9%
1	O	491	41% 90% 9%
1	P	491	40% 90% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 58640 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 Chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	491	3665	2272	635	734	24	0	0
1	B	491	3665	2272	635	734	24	0	0
1	C	491	3665	2272	635	734	24	0	0
1	D	491	3665	2272	635	734	24	0	0
1	E	491	3665	2272	635	734	24	0	0
1	F	491	3665	2272	635	734	24	0	0
1	G	491	3665	2272	635	734	24	0	0
1	H	491	3665	2272	635	734	24	0	0
1	I	491	3665	2272	635	734	24	0	0
1	J	491	3665	2272	635	734	24	0	0
1	K	491	3665	2272	635	734	24	0	0
1	L	491	3665	2272	635	734	24	0	0
1	M	491	3665	2272	635	734	24	0	0
1	N	491	3665	2272	635	734	24	0	0
1	O	491	3665	2272	635	734	24	0	0
1	P	491	3665	2272	635	734	24	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP Q877G8
A	236	THR	-	expression tag	UNP Q877G8
A	237	ALA	-	expression tag	UNP Q877G8
A	238	SER	-	expression tag	UNP Q877G8
A	239	GLU	-	expression tag	UNP Q877G8
B	726	GLU	-	expression tag	UNP Q877G8
B	727	THR	-	expression tag	UNP Q877G8
B	728	ALA	-	expression tag	UNP Q877G8
B	729	SER	-	expression tag	UNP Q877G8
B	730	GLU	-	expression tag	UNP Q877G8
C	1217	GLU	-	expression tag	UNP Q877G8
C	1218	THR	-	expression tag	UNP Q877G8
C	1219	ALA	-	expression tag	UNP Q877G8
C	1220	SER	-	expression tag	UNP Q877G8
C	1221	GLU	-	expression tag	UNP Q877G8
D	1708	GLU	-	expression tag	UNP Q877G8
D	1709	THR	-	expression tag	UNP Q877G8
D	1710	ALA	-	expression tag	UNP Q877G8
D	1711	SER	-	expression tag	UNP Q877G8
D	1712	GLU	-	expression tag	UNP Q877G8
E	2199	GLU	-	expression tag	UNP Q877G8
E	2200	THR	-	expression tag	UNP Q877G8
E	2201	ALA	-	expression tag	UNP Q877G8
E	2202	SER	-	expression tag	UNP Q877G8
E	2203	GLU	-	expression tag	UNP Q877G8
F	2690	GLU	-	expression tag	UNP Q877G8
F	2691	THR	-	expression tag	UNP Q877G8
F	2692	ALA	-	expression tag	UNP Q877G8
F	2693	SER	-	expression tag	UNP Q877G8
F	2694	GLU	-	expression tag	UNP Q877G8
G	3181	GLU	-	expression tag	UNP Q877G8
G	3182	THR	-	expression tag	UNP Q877G8
G	3183	ALA	-	expression tag	UNP Q877G8
G	3184	SER	-	expression tag	UNP Q877G8
G	3185	GLU	-	expression tag	UNP Q877G8
H	3672	GLU	-	expression tag	UNP Q877G8
H	3673	THR	-	expression tag	UNP Q877G8
H	3674	ALA	-	expression tag	UNP Q877G8
H	3675	SER	-	expression tag	UNP Q877G8
H	3676	GLU	-	expression tag	UNP Q877G8
I	4163	GLU	-	expression tag	UNP Q877G8
I	4164	THR	-	expression tag	UNP Q877G8
I	4165	ALA	-	expression tag	UNP Q877G8

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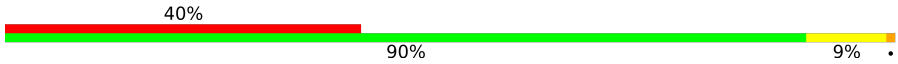
Chain	Residue	Modelled	Actual	Comment	Reference
I	4166	SER	-	expression tag	UNP Q877G8
I	4167	GLU	-	expression tag	UNP Q877G8
J	4654	GLU	-	expression tag	UNP Q877G8
J	4655	THR	-	expression tag	UNP Q877G8
J	4656	ALA	-	expression tag	UNP Q877G8
J	4657	SER	-	expression tag	UNP Q877G8
J	4658	GLU	-	expression tag	UNP Q877G8
K	5145	GLU	-	expression tag	UNP Q877G8
K	5146	THR	-	expression tag	UNP Q877G8
K	5147	ALA	-	expression tag	UNP Q877G8
K	5148	SER	-	expression tag	UNP Q877G8
K	5149	GLU	-	expression tag	UNP Q877G8
L	5636	GLU	-	expression tag	UNP Q877G8
L	5637	THR	-	expression tag	UNP Q877G8
L	5638	ALA	-	expression tag	UNP Q877G8
L	5639	SER	-	expression tag	UNP Q877G8
L	5640	GLU	-	expression tag	UNP Q877G8
M	6127	GLU	-	expression tag	UNP Q877G8
M	6128	THR	-	expression tag	UNP Q877G8
M	6129	ALA	-	expression tag	UNP Q877G8
M	6130	SER	-	expression tag	UNP Q877G8
M	6131	GLU	-	expression tag	UNP Q877G8
N	6618	GLU	-	expression tag	UNP Q877G8
N	6619	THR	-	expression tag	UNP Q877G8
N	6620	ALA	-	expression tag	UNP Q877G8
N	6621	SER	-	expression tag	UNP Q877G8
N	6622	GLU	-	expression tag	UNP Q877G8
O	7109	GLU	-	expression tag	UNP Q877G8
O	7110	THR	-	expression tag	UNP Q877G8
O	7111	ALA	-	expression tag	UNP Q877G8
O	7112	SER	-	expression tag	UNP Q877G8
O	7113	GLU	-	expression tag	UNP Q877G8
P	7600	GLU	-	expression tag	UNP Q877G8
P	7601	THR	-	expression tag	UNP Q877G8
P	7602	ALA	-	expression tag	UNP Q877G8
P	7603	SER	-	expression tag	UNP Q877G8
P	7604	GLU	-	expression tag	UNP Q877G8

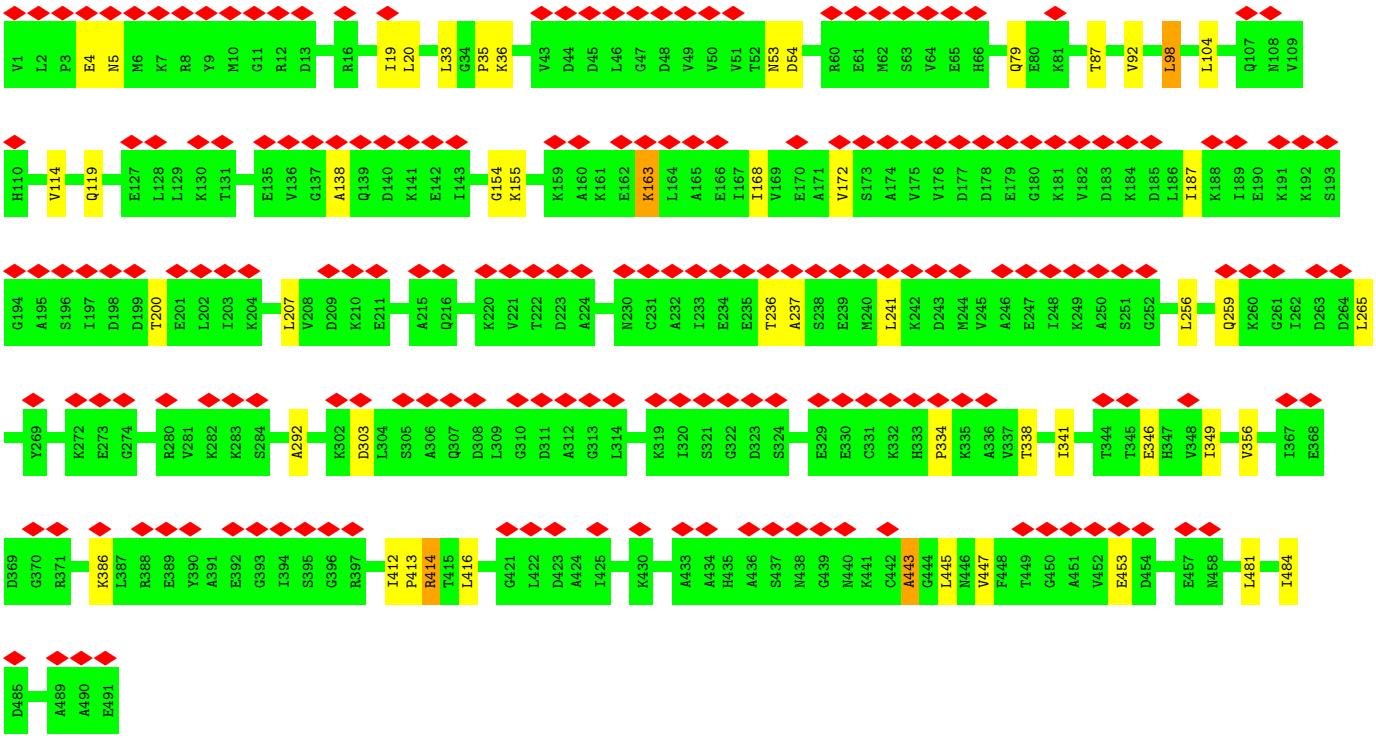
3 Residue-property plots (i)

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: Chaperonin

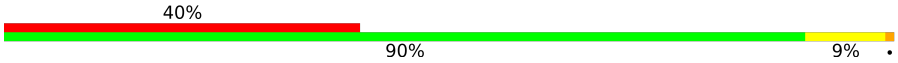
Chain A:

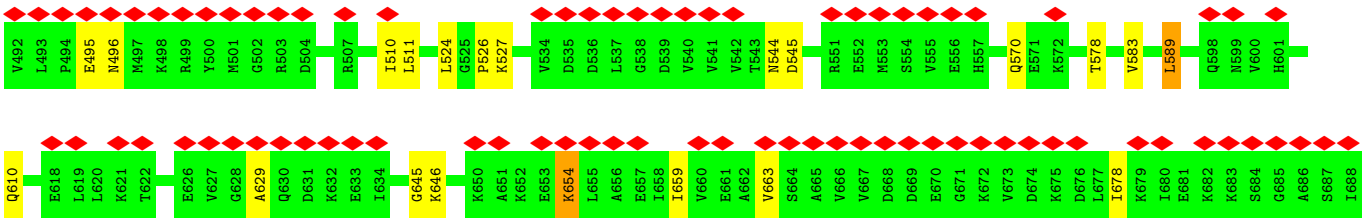




- Molecule 1: Chaperonin

Chain B:





D689 D690 T691 E692 L693 I694 K695 L698 V699 D700 K701 E702 A706 Q707 K711 V712 T713 D714 A715 N721 C722 A723 I724 E725 E726 T727 A728 S729 E730 M731 L732 K733 D734 M735 V736 A737 E738 I739 K740 A741 S742 G743 L747 Q750 K751 G752 I753 D754 D755 L756 Y760 K763

E764 G765 R771 V772 K773 K774 S775 A783 K793 D794 L795 S796 A797 Q798 D799 L800 G801 D802 A803 G804 L805 K810 I811 S812 G813 D814 S815 E820 E821 C822 K823 H824 P825 K826 A827 V828 T829 M830 L831 I832 T835 T836 E837 H838 V839 I840 V847 I858 E859 D860 G861 R862

K877 L878 R879 E880 Y881 A882 E883 G884 I885 S886 G887 R888 I903 P904 R905 T906 L907 G912 L913 D914 A915 I916 K921 A924 A925 H926 A927 S928 N929 G930 N931 K932 C933 A934 G935 L936 N937 V938 F939 T940 G941 A942 V943 E944 D945 E948 N949 L972 I975 D976 A980

A981 E982

- Molecule 1: Chaperonin

Chain C:

V983 L984 P985 E986 N987 M988 K989 R990 Y991 M992 G993 R994 D995 R998 I1001 L1002 L1015 G1016 P1017 K1018 V1025 D1026 D1027 L1028 G1029 D1030 V1031 V1032 V1033 T1034 N1035 D1036 R1042 E1043 M1044 S1045 V1046 E1047 H1048 Q1061 E1062 K1063 T1069 V1074 L1080 L1086 Q1089 N1090 V1091

H1092 V1096 Q1101 E1109 L1110 L1111 K1112 T1113 E1117 V1118 G1119 A1120 Q1121 D1122 K1123 E1124 I1125 G1136 K1137 K1141 A1142 K1143 E1144 K1145 L1146 A1147 E1148 I1149 I1150 V1151 E1152 A1153 V1154 V1155 A1156 V1157 V1158 D1159 D1160 E1161 G1162 K1163 V1164 D1165 K1166 D1167 L1168 I1169 K1170 I1171 E1172 K1173 K1174 S1175

G1176 A1177 S1178 I1179 D1180 D1181 T1182 E1183 L1184 I1185 K1186 L1189 V1190 D1191 K1192 E1193 A1197 Q1198 K1202 V1203 T1204 D1205 A1206 N1212 C1213 A1214 I1215 E1216 E1217 T1218 A1219 S1220 E1221 M1222 L1223 K1224 D1225 M1226 V1227 A1228 E1229 I1230 K1231 A1232 S1233 G1234 L1238 Q1241 K1242 G1243 I1244 D1245 D1246 L1247

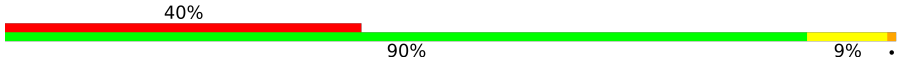
Y1251 K1254 E1255 G1256 R1262 V1263 K1264 K1265 S1266 A1274 K1284 D1285 L1286 S1287 A1288 Q1289 D1290 L1291 G1292 D1293 A1294 G1295 L1296 K1301 I1302 S1303 G1304 D1305 S1306 E1311 E1312 C1313 K1314 H1315 P1316 K1317 A1318 V1319 T1320 I1323 T1326 T1327 E1328 H1329 V1330 I1331 V1338 I1349 E1350

D1351 G1352 R1353 K1368 L1369 R1370 E1371 Y1372 A1373 E1374 G1375 I1376 S1377 G1378 R1379 I1394 P1395 R1396 T1397 L1398 G1403 L1404 D1405 A1406 I1407 K1412 A1415 A1416 H1417 A1418 S1419 N1420 G1421 N1422 K1423 C1424 A1425 G1426 L1427 N1428 V1429 F1430 T1431 G1432 A1433 V1434 E1435 D1436 E1439 N1440 L1463 I1466

D1467 A1471 A1472 E1473

- Molecule 1: Chaperonin

Chain D:



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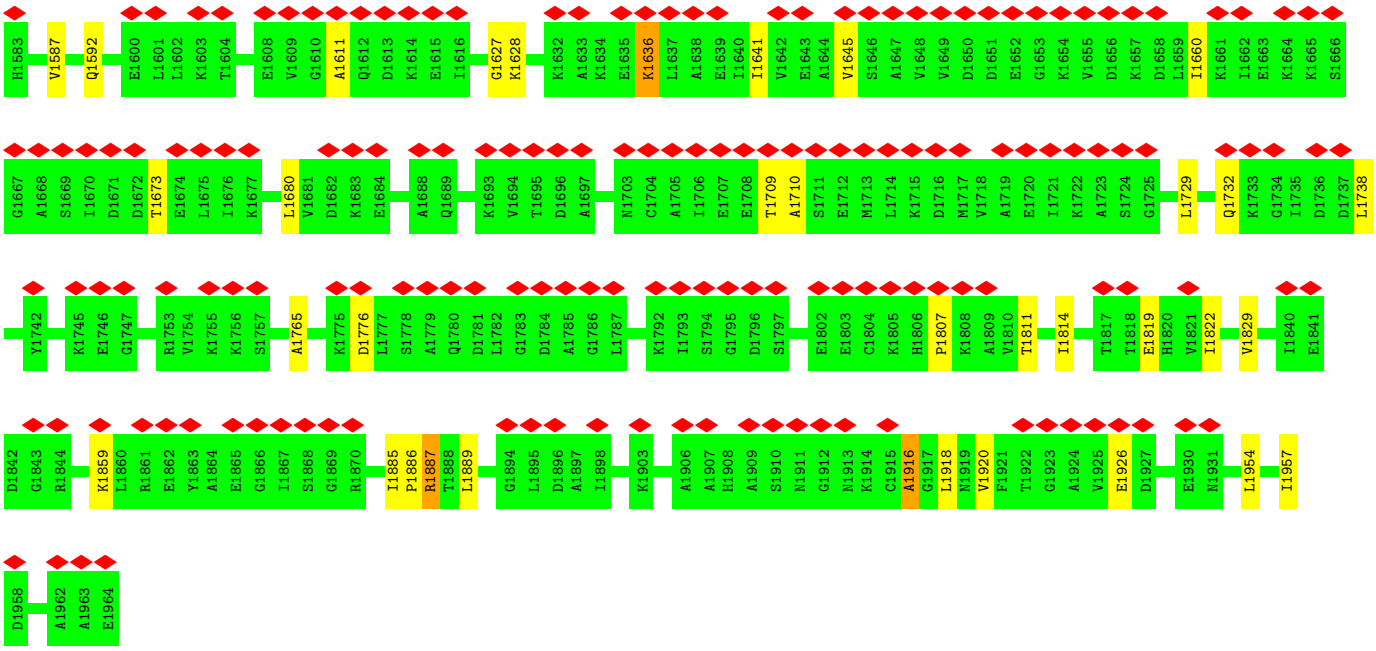
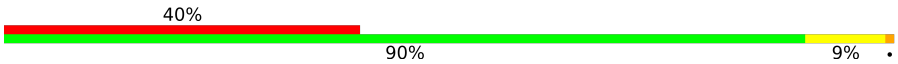
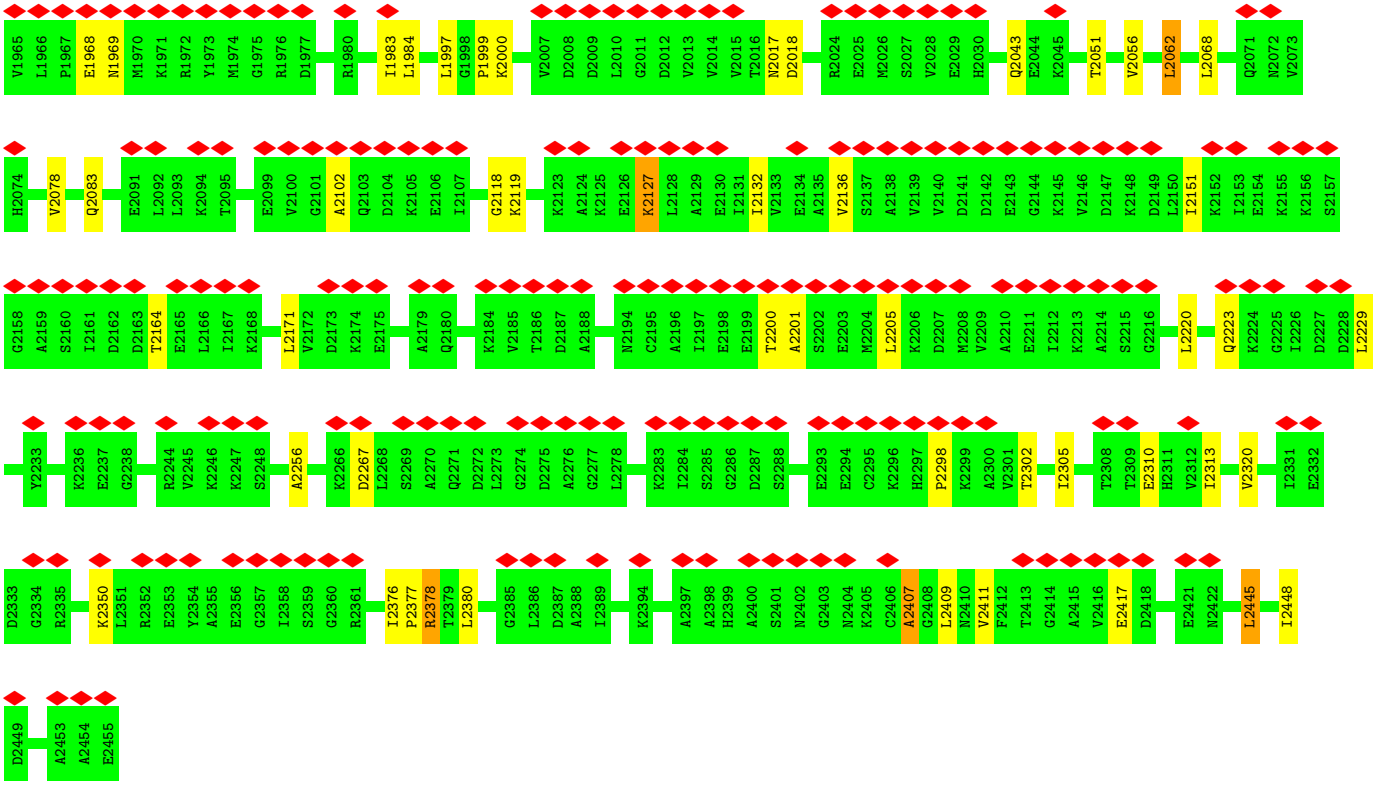


- Molecule 1: Chaperonin

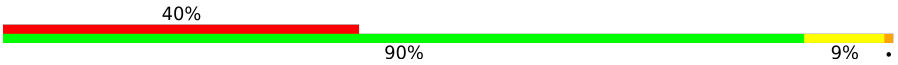
Chain E:





- Molecule 1: Chaperonin

Chain F:



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H2565 V2569 Q2574 E2582 L2583 L2584 K2585 T2586 E2590 V2591 G2592 A2593 Q2594 D2595 K2596 E2597 I2598 G2609 K2610 K2614 A2615 K2616 E2617 K2618 L2619 A2620 E2621 I2622 I2623 V2624 E2625 A2626 V2627 S2628 A2629 V2630 V2631 D2632 D2633 E2634 G2635 K2636 V2637 D2638 K2639 D2640 L2641 I2642 K2643 I2644 E2645 K2646 K2647 S2648

G2649 A2650 S2651 I2652 D2653 D2654 T2655 E2656 L2657 I2658 K2659 L2662 V2663 D2664 K2665 E2666 A2670 Q2671 K2675 V2676 T2677 D2678 A2679 N2685 C2686 A2687 I2688 E2689 E2690 T2691 A2692 S2693 E2694 M2695 L2696 K2697 D2698 M2699 V2700 A2701 E2702 I2703 K2704 A2705 S2706 G2707 L2711 Q2714 K2715 G2716 I2717 D2718 D2719 L2720

Y2724 K2727 E2728 G2729 R2735 V2736 K2737 K2738 S2739 A2747 K2757 D2758 L2759 S2760 A2761 Q2762 D2763 L2764 G2765 D2766 A2767 G2768 L2769 K2774 I2775 S2776 G2777 D2778 S2779 E2784 E2785 C2786 K2787 H2788 P2789 K2790 A2791 V2792 T2793 I2796 T2799 T2800 E2801 H2802 V2803 I2804 V2811 I2822 E2823

D2824 G2825 R2826 K2841 L2842 R2843 E2844 Y2845 A2846 E2847 G2848 I2849 S2850 G2851 R2852 I2867 P2868 R2869 T2870 L2871 G2876 L2877 D2878 A2879 I2880 K2885 A2888 A2889 H2890 A2891 S2892 N2893 G2894 N2895 K2896 C2897 A2898 G2899 L2900 N2901 V2902 F2903 T2904 G2905 A2906 V2907 E2908 D2909 E2912 N2913 L2936 I2939

D2940 A2944 A2945 E2946

- Molecule 1: Chaperonin

Chain G: 40% 90% 9%

V2947 L2948 P2949 E2950 N2951 M2952 K2953 R2954 Y2955 M2956 G2957 R2958 D2959 R2962 I2965 L2966 L2979 G2980 P2981 K2982 V2989 D2990 D2991 L2992 G2993 D2994 V2995 V2996 V2997 T2998 N2999 D3000 R3006 E3007 M3008 S3009 V3010 E3011 H3012 Q3025 E3026 K3027 T3033 V3038 L3044 L3050 Q3053 N3054 V3055

H3056 V3060 Q3065 E3073 L3074 L3075 K3076 T3077 E3081 V3082 G3083 A3084 Q3085 D3086 K3087 E3088 I3089 G3100 K3101 K3105 A3106 K3107 E3108 K3109 L3110 A3111 E3112 I3113 I3114 V3115 E3116 A3117 V3118 S3119 A3120 V3121 V3122 D3123 D3124 E3125 G3126 K3127 V3128 D3129 K3130 D3131 L3132 I3133 K3134 I3135 E3136 K3137 K3138 S3139

G3140 A3141 S3142 I3143 D3144 D3145 T3146 E3147 L3148 I3149 K3150 L3153 V3154 D3155 K3156 E3157 A3161 Q3162 K3166 V3167 T3168 D3169 A3170 N3176 C3177 A3178 I3179 E3180 E3181 T3182 A3183 S3184 E3185 M3186 L3187 K3188 D3189 M3190 V3191 A3192 E3193 I3194 K3195 A3196 S3197 G3198 L3202 Q3205 K3206 G3207 I3208 D3209 D3210 L3211

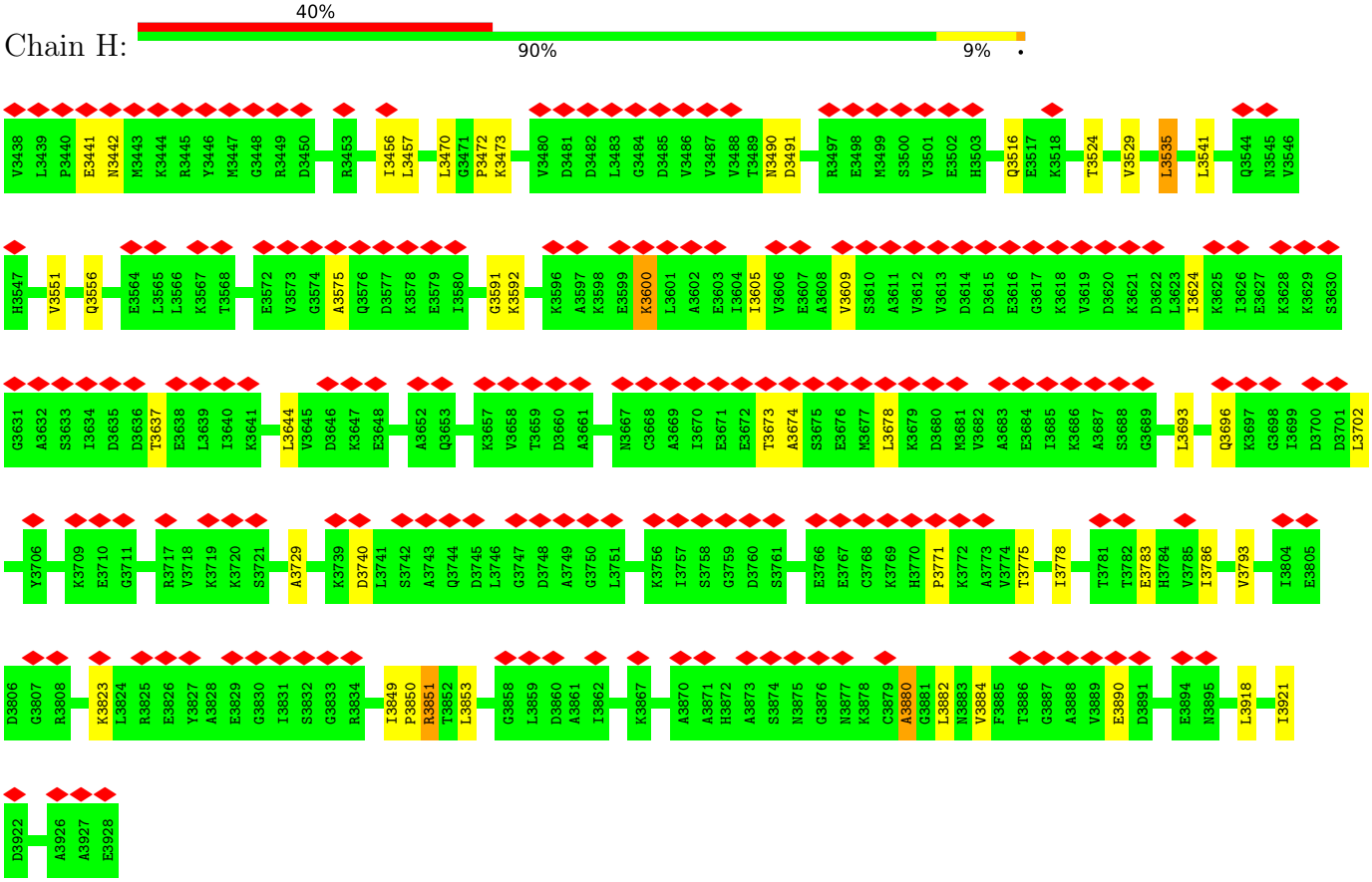
Y3215 K3218 E3219 G3220 R3226 V3227 K3228 K3229 S3230 A3238 K3248 D3249 L3250 S3251 A3252 Q3253 D3254 L3255 G3256 D3257 A3258 G3259 L3260 K3265 I3266 S3267 G3268 D3269 S3270 E3275 E3276 C3277 K3278 H3279 P3280 K3281 A3282 V3283 T3284 I3287 T3290 T3291 E3292 H3293 V3294 I3295 V3302 I3313 E3314

D3315 G3316 R3317 K3332 L3333 R3334 E3335 Y3336 A3337 E3338 G3339 I3340 S3341 G3342 R3343 I3358 P3359 R3360 T3361 L3362 G3367 L3368 D3369 A3370 I3371 K3376 A3379 A3380 H3381 A3382 S3383 N3384 G3385 N3386 K3387 C3388 A3389 G3390 L3391 N3392 V3393 F3394 T3395 G3396 A3397 V3398 E3399 D3400 E3403 N3404 L3427 I3430

D3431 A3435 A3436 E3437

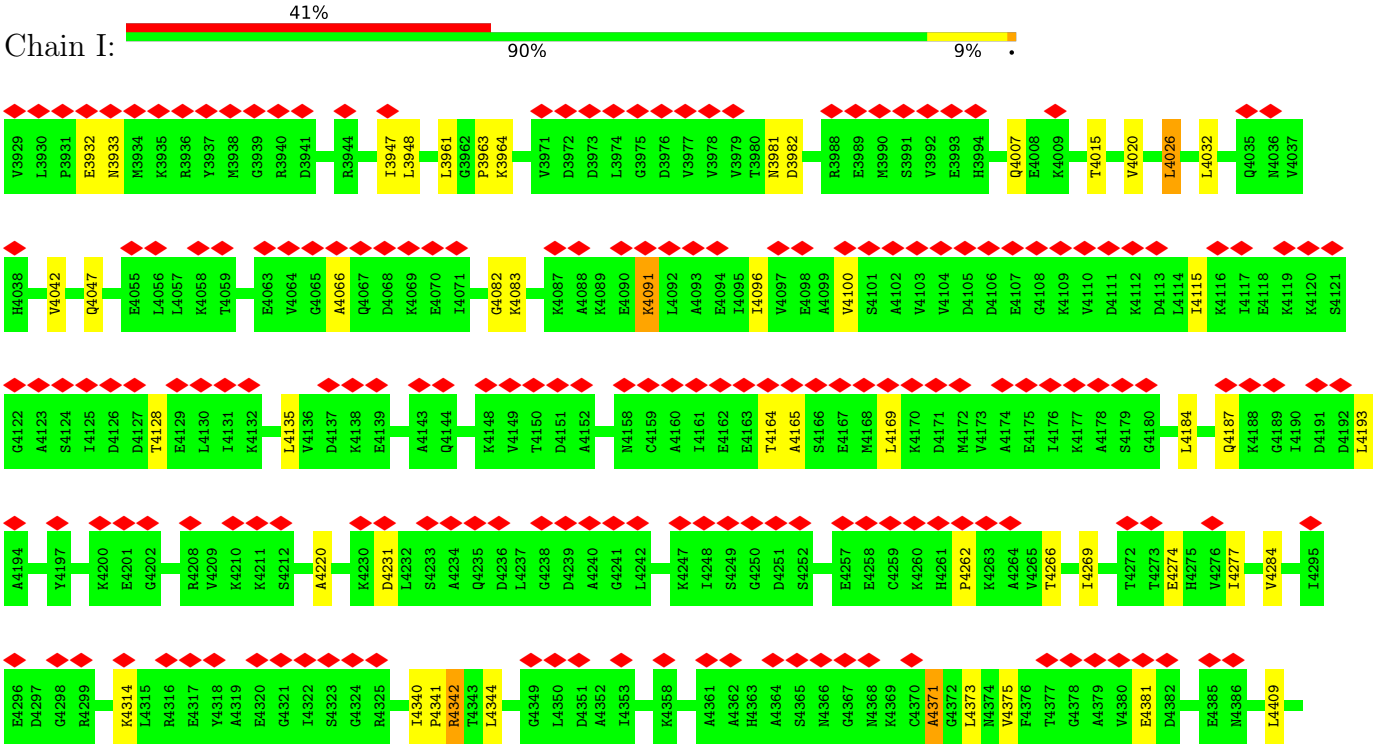
- Molecule 1: Chaperonin

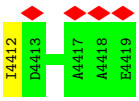
Chain H:



- Molecule 1: Chaperonin

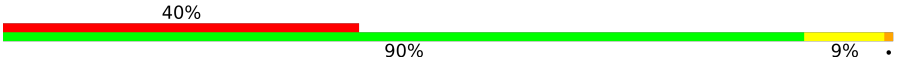
Chain I:

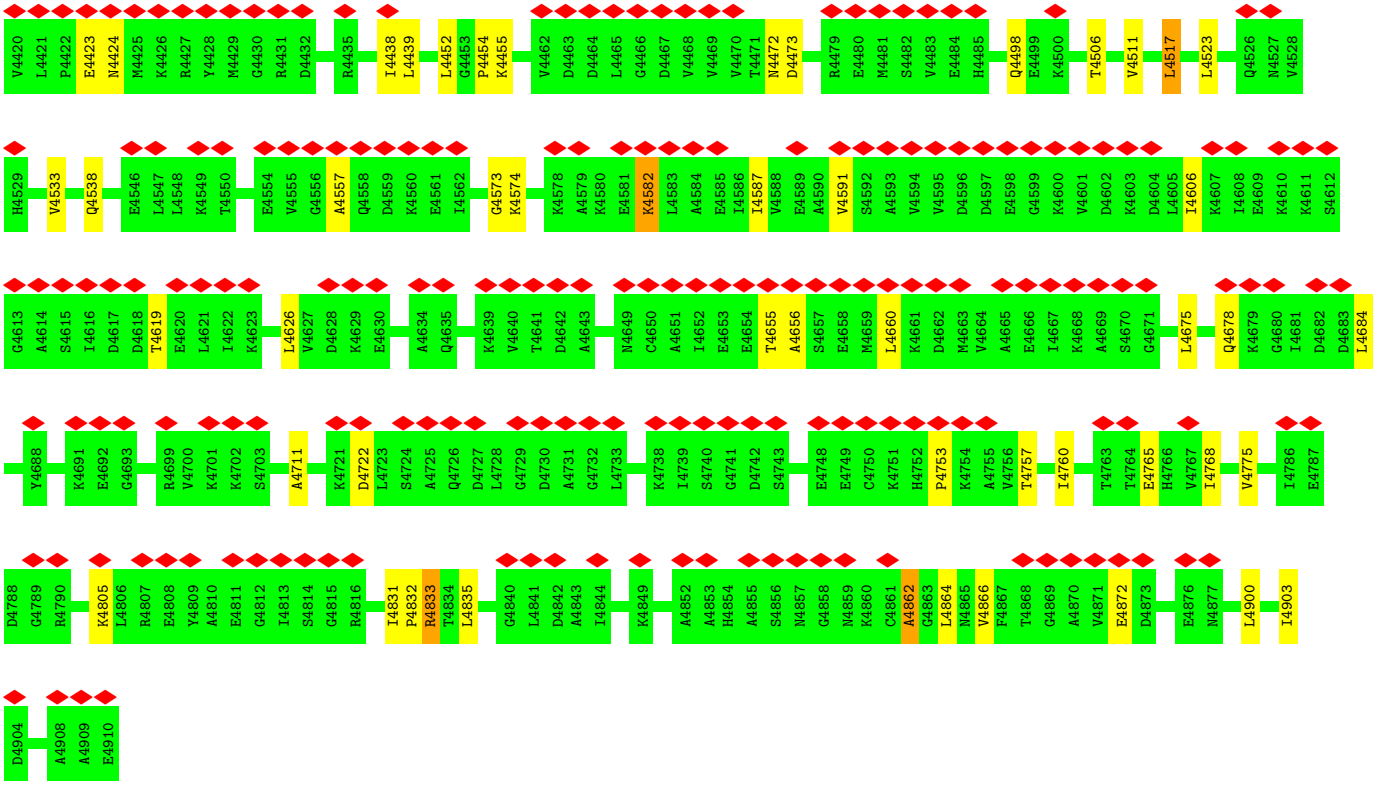




- Molecule 1: Chaperonin

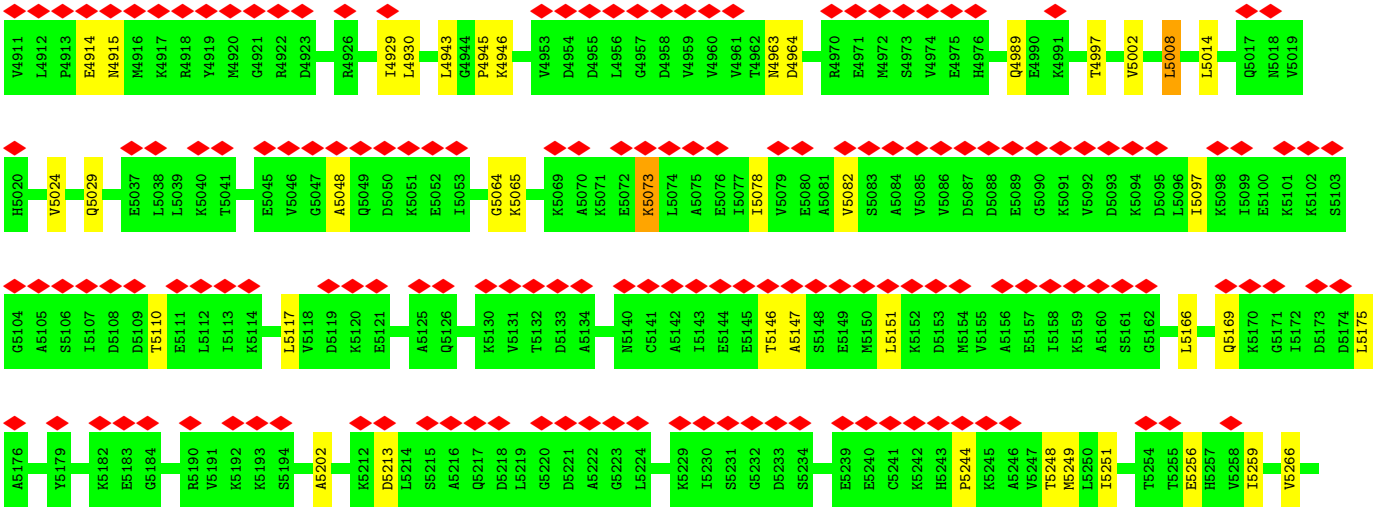
Chain J:

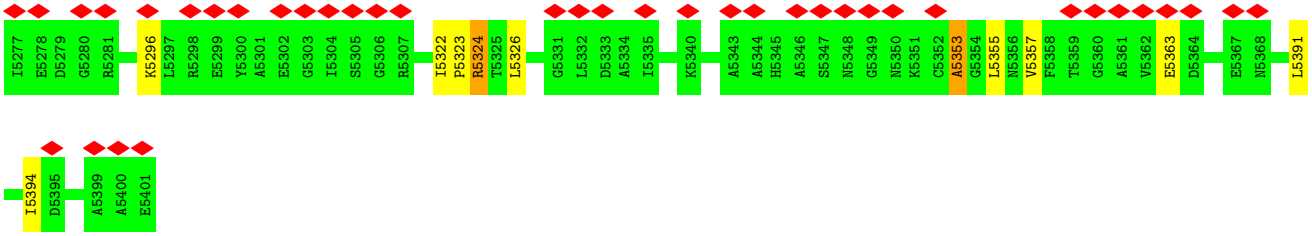




- Molecule 1: Chaperonin

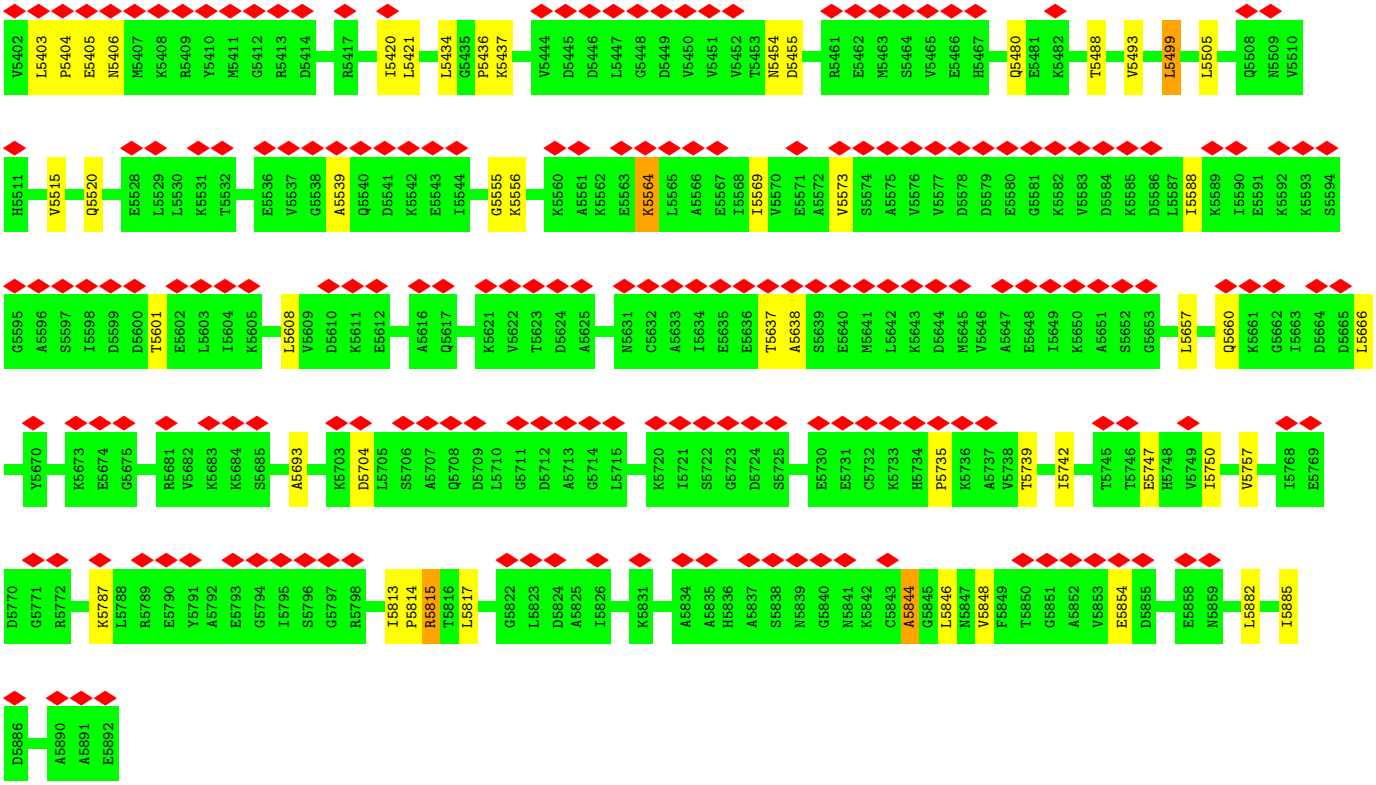
Chain K:





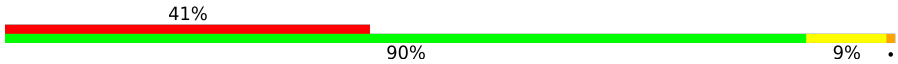
• Molecule 1: Chaperonin

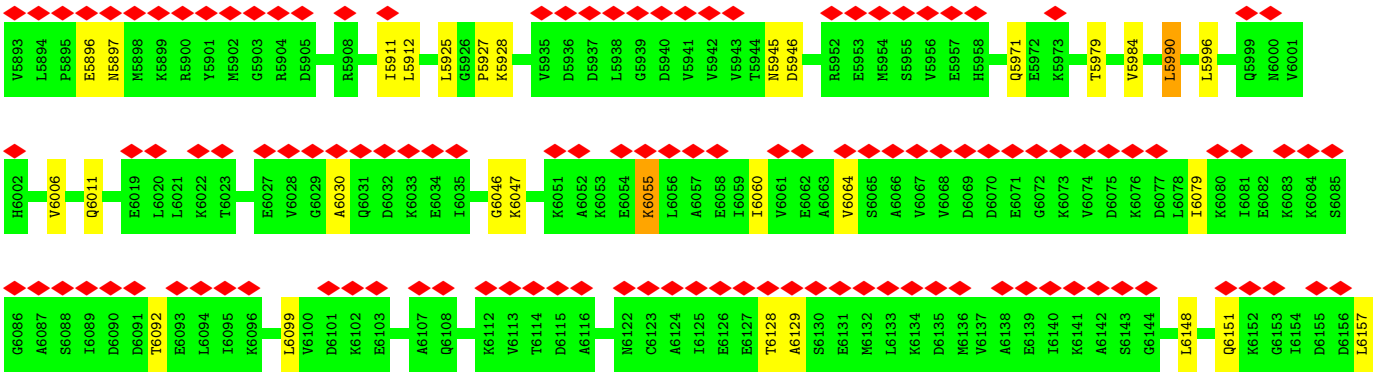
Chain L:

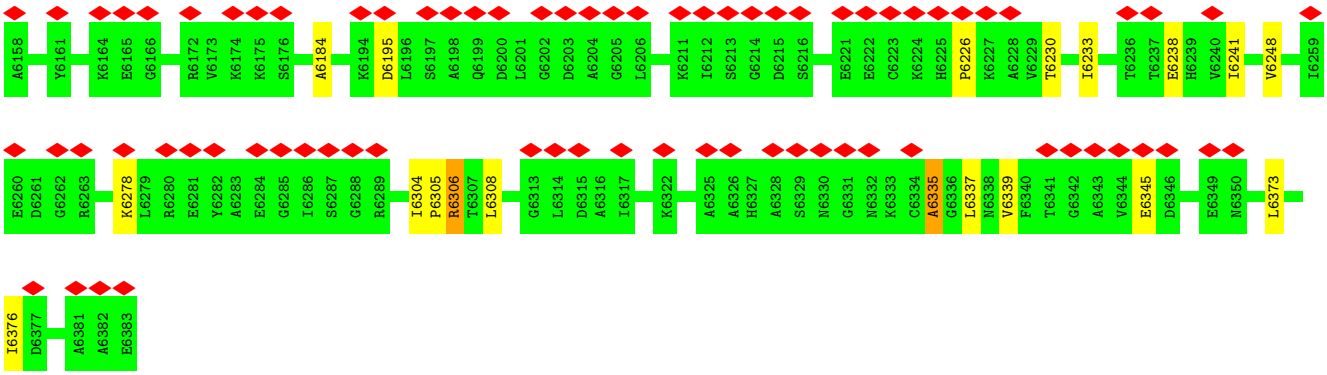


• Molecule 1: Chaperonin

Chain M:

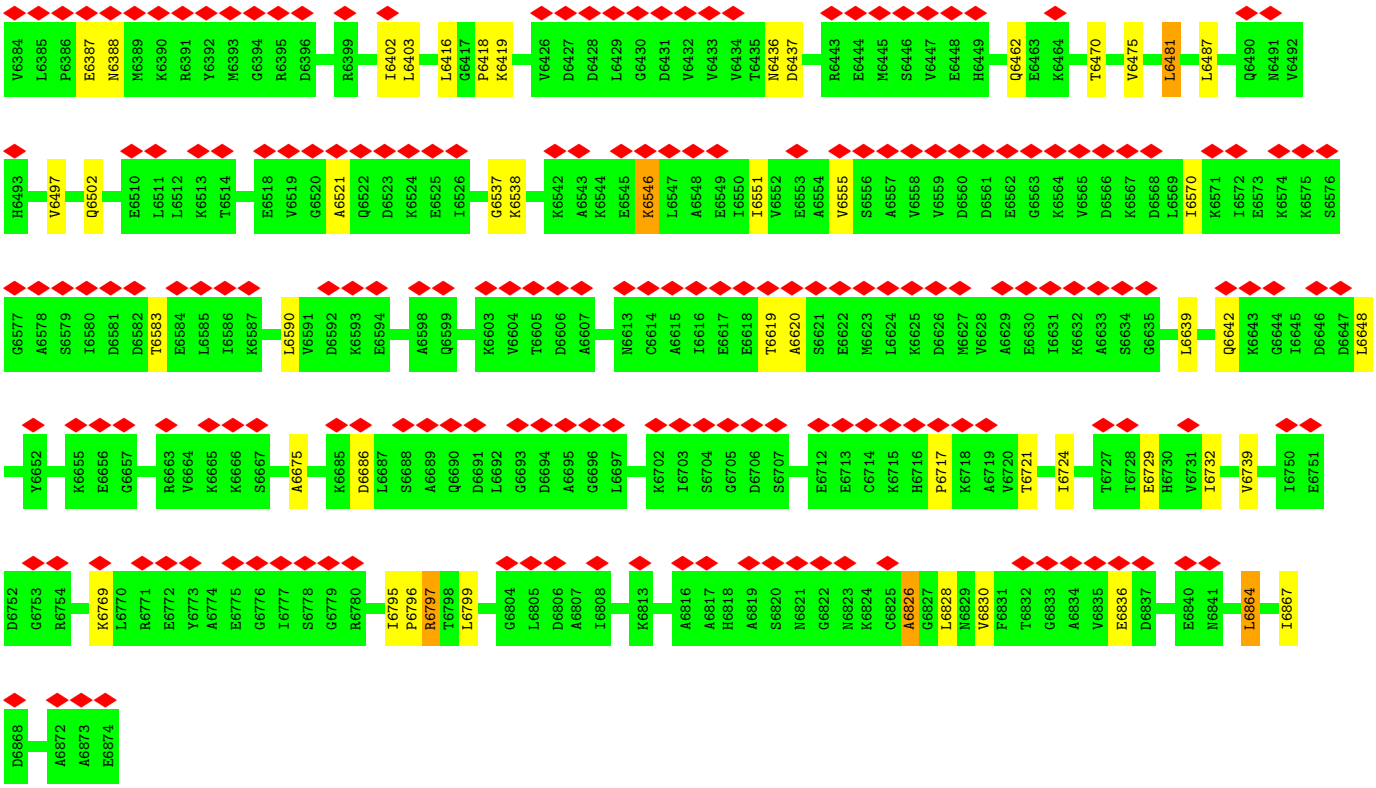






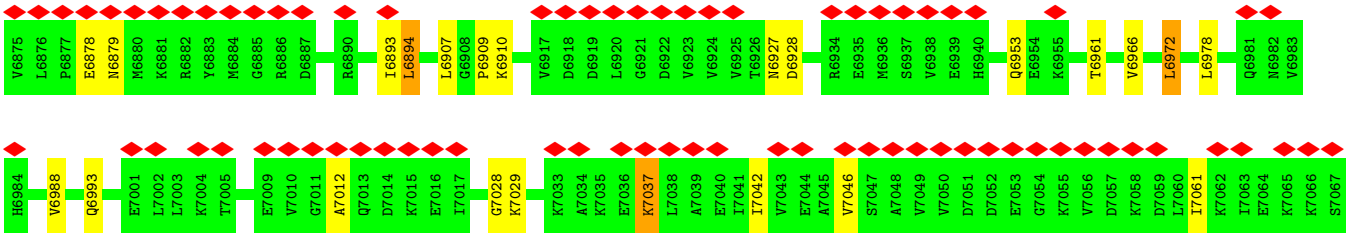
- Molecule 1: Chaperonin

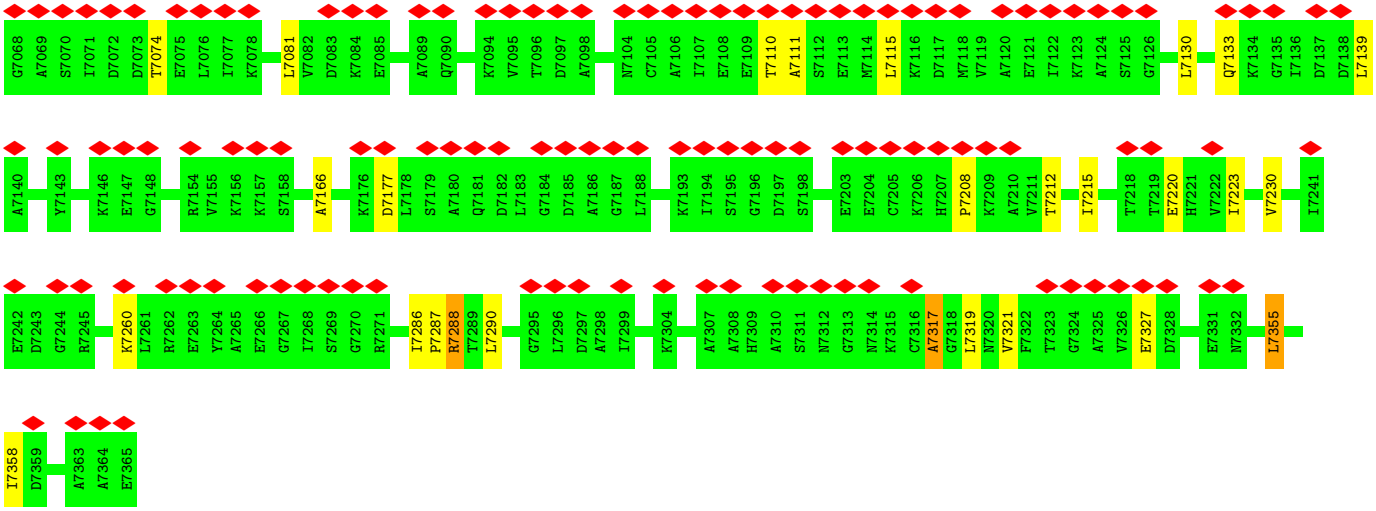
Chain N: 40% 90% 9%



- Molecule 1: Chaperonin

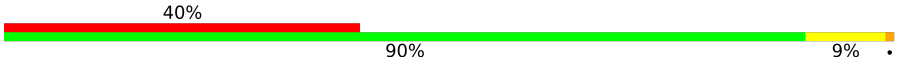
Chain O: 41% 90% 9%

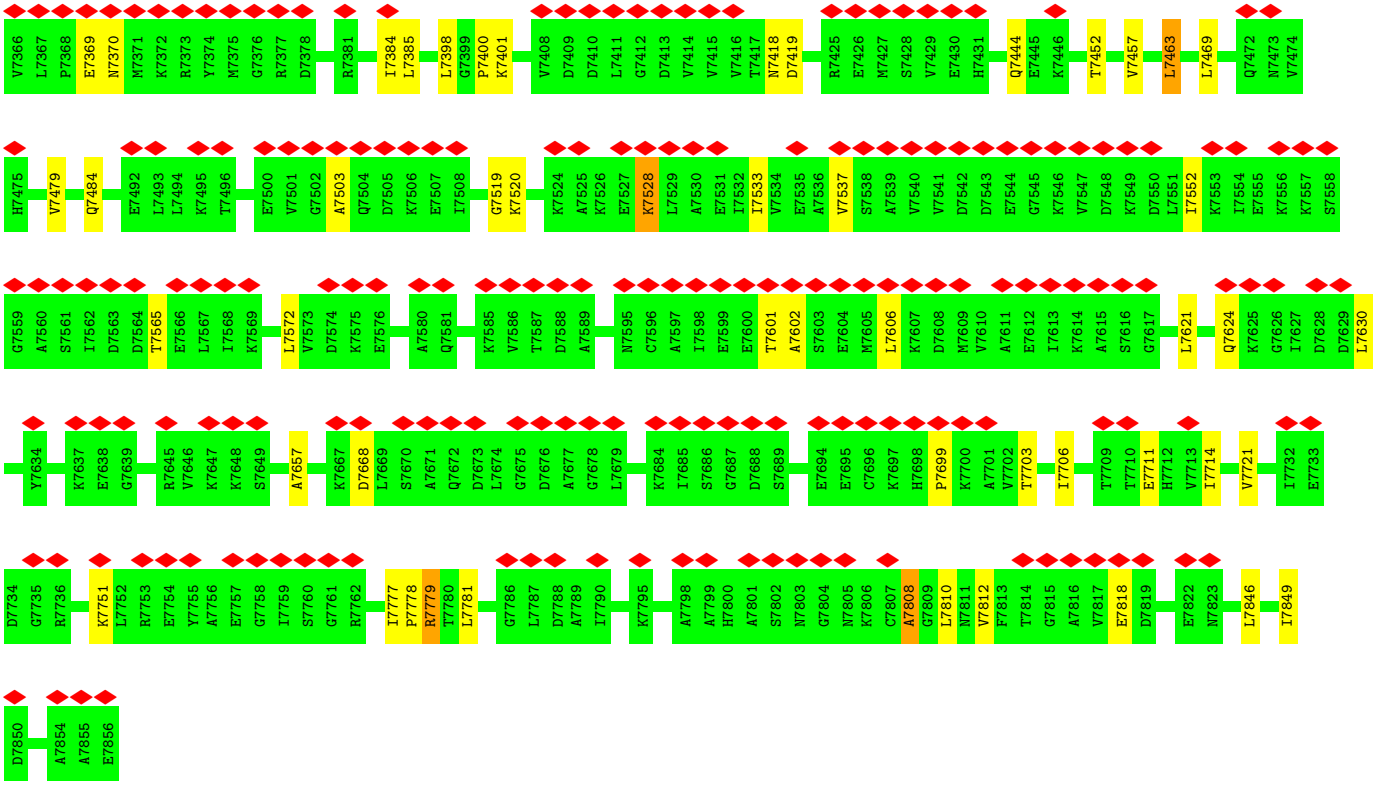




- Molecule 1: Chaperonin

Chain P:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D8	Depositor
Number of particles used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 10000 (10k x 10k)	Depositor
Maximum map value	2.733	Depositor
Minimum map value	-0.479	Depositor
Average map value	0.087	Depositor
Map value standard deviation	0.353	Depositor
Recommended contour level	1.58	Depositor
Map size (Å)	289.44, 289.44, 289.44	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.01, 2.01, 2.01	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	B	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	C	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	D	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	E	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	F	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	G	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	H	0.88	1/3686 (0.0%)	0.75	1/4961 (0.0%)
1	I	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	J	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	K	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	L	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	M	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	N	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	O	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	P	0.88	1/3686 (0.0%)	0.75	1/4961 (0.0%)
All	All	0.88	16/58976 (0.0%)	0.76	16/79376 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	3
1	P	0	3
All	All	0	48

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1916	ALA	C-O	5.10	1.33	1.23
1	F	2898	ALA	C-O	5.07	1.32	1.23
1	H	3880	ALA	C-O	5.07	1.32	1.23
1	K	5353	ALA	C-O	5.07	1.32	1.23
1	N	6826	ALA	C-O	5.07	1.32	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1477	GLU	CA-C-O	-6.63	106.17	120.10
1	O	6878	GLU	CA-C-O	-6.63	106.17	120.10
1	A	4	GLU	CA-C-O	-6.62	106.20	120.10
1	B	495	GLU	CA-C-O	-6.62	106.20	120.10
1	I	3932	GLU	CA-C-O	-6.62	106.20	120.10

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLN	Mainchain
1	A	138	ALA	Mainchain
1	A	453	GLU	Mainchain
1	B	610	GLN	Mainchain
1	B	629	ALA	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3665	0	3804	24	0
1	B	3665	0	3801	24	0
1	C	3665	0	3801	25	0
1	D	3665	0	3801	24	0
1	E	3665	0	3801	25	0
1	F	3665	0	3801	26	0
1	G	3665	0	3801	24	0
1	H	3665	0	3801	24	0
1	I	3665	0	3801	24	0
1	J	3665	0	3801	24	0
1	K	3665	0	3801	25	0
1	L	3665	0	3801	24	0
1	M	3665	0	3801	23	0
1	N	3665	0	3801	24	0
1	O	3665	0	3801	26	0
1	P	3665	0	3801	24	0
All	All	58640	0	60819	390	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 3.

The worst 5 of 390 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1247:LEU:HD23	1:C:1247:LEU:C	2.17	0.65
1:J:4684:LEU:C	1:J:4684:LEU:HD23	2.17	0.65
1:P:7630:LEU:C	1:P:7630:LEU:HD23	2.17	0.65
1:A:265:LEU:C	1:A:265:LEU:HD23	2.17	0.65
1:G:3211:LEU:C	1:G:3211:LEU:HD23	2.17	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	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	B	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	C	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	D	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	E	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	F	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	G	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	H	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	I	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	J	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	K	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	L	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	M	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	N	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	O	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	P	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
All	All	7824/7856 (100%)	7488 (96%)	304 (4%)	32 (0%)	38	72

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	496	ASN
1	C	987	ASN
1	D	1478	ASN
1	E	1969	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	B	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	C	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	D	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	E	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	F	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	G	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	H	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	I	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	J	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	K	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	L	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	M	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	N	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	O	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	P	393/393 (100%)	383 (98%)	10 (2%)	47	68
All	All	6288/6288 (100%)	6128 (98%)	160 (2%)	50	68

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5704	ASP
1	O	7037	LYS
1	L	5882	LEU
1	N	6403	LEU
1	P	7385	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	4888	GLN
1	K	5379	GLN
1	P	7834	GLN
1	L	5870	GLN
1	D	1942	GLN

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

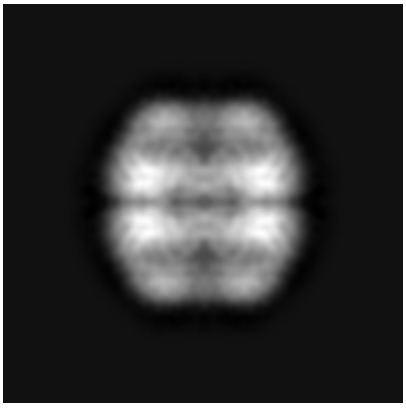
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5250. These allow visual inspection of the internal detail of the map and identification of artifacts.

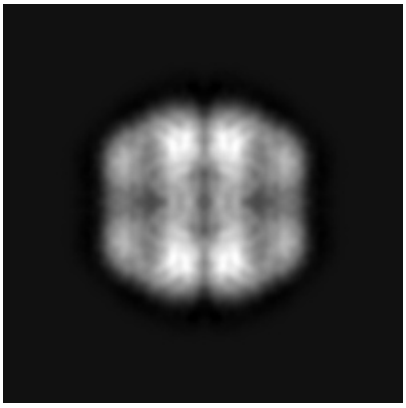
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



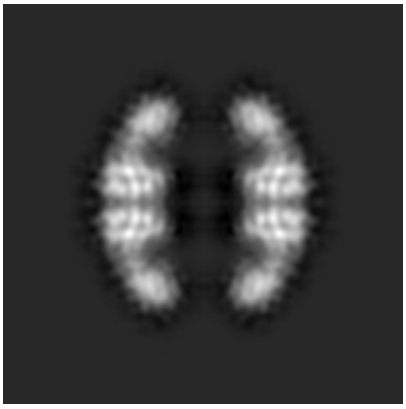
Y

Z

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

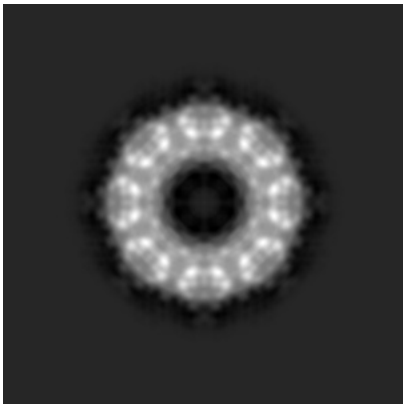
6.2 Central slices (i)

6.2.1 Primary map



X Index: 72

Y Index: 72

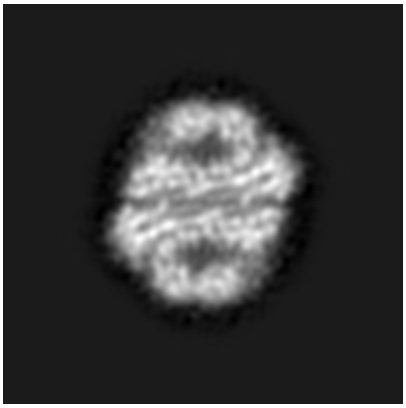


Z Index: 72

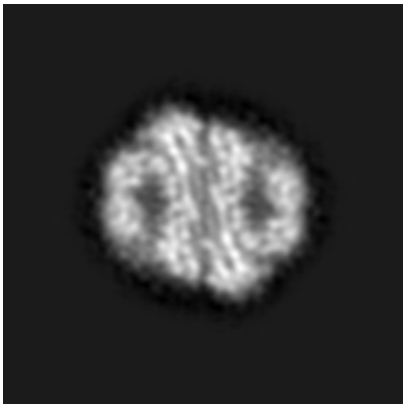
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 92



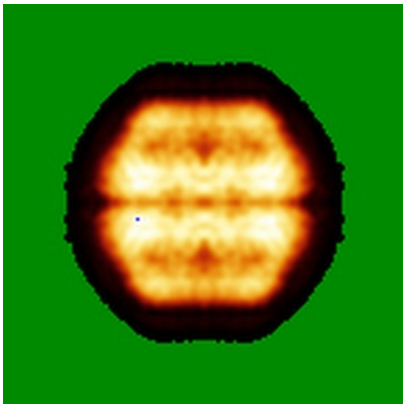
Y Index: 92

Z Index: 61

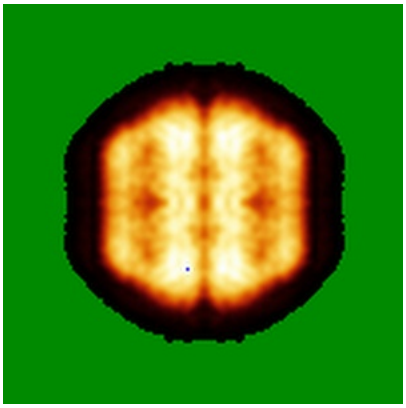
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

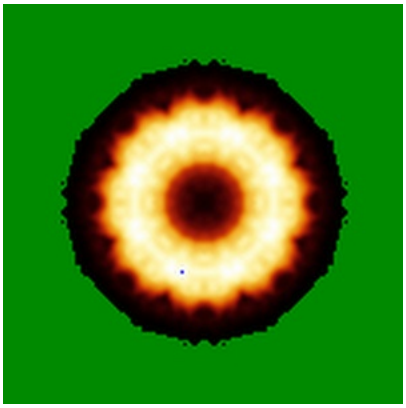
6.4.1 Primary map



X



Y

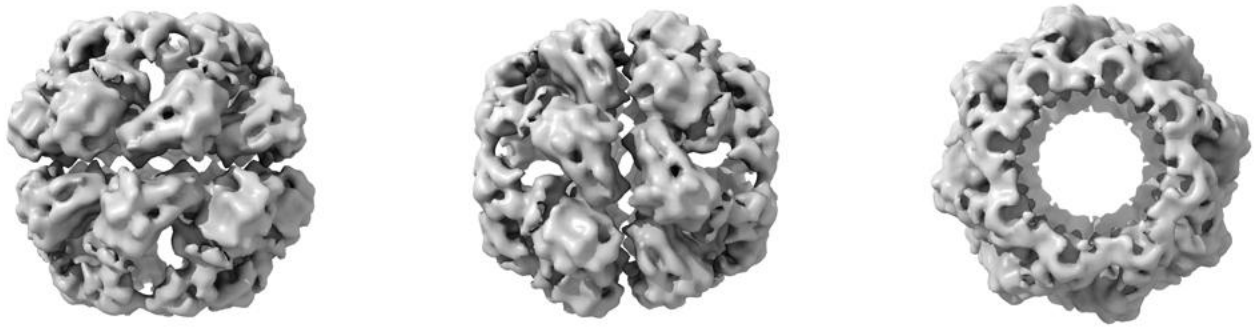


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.58. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

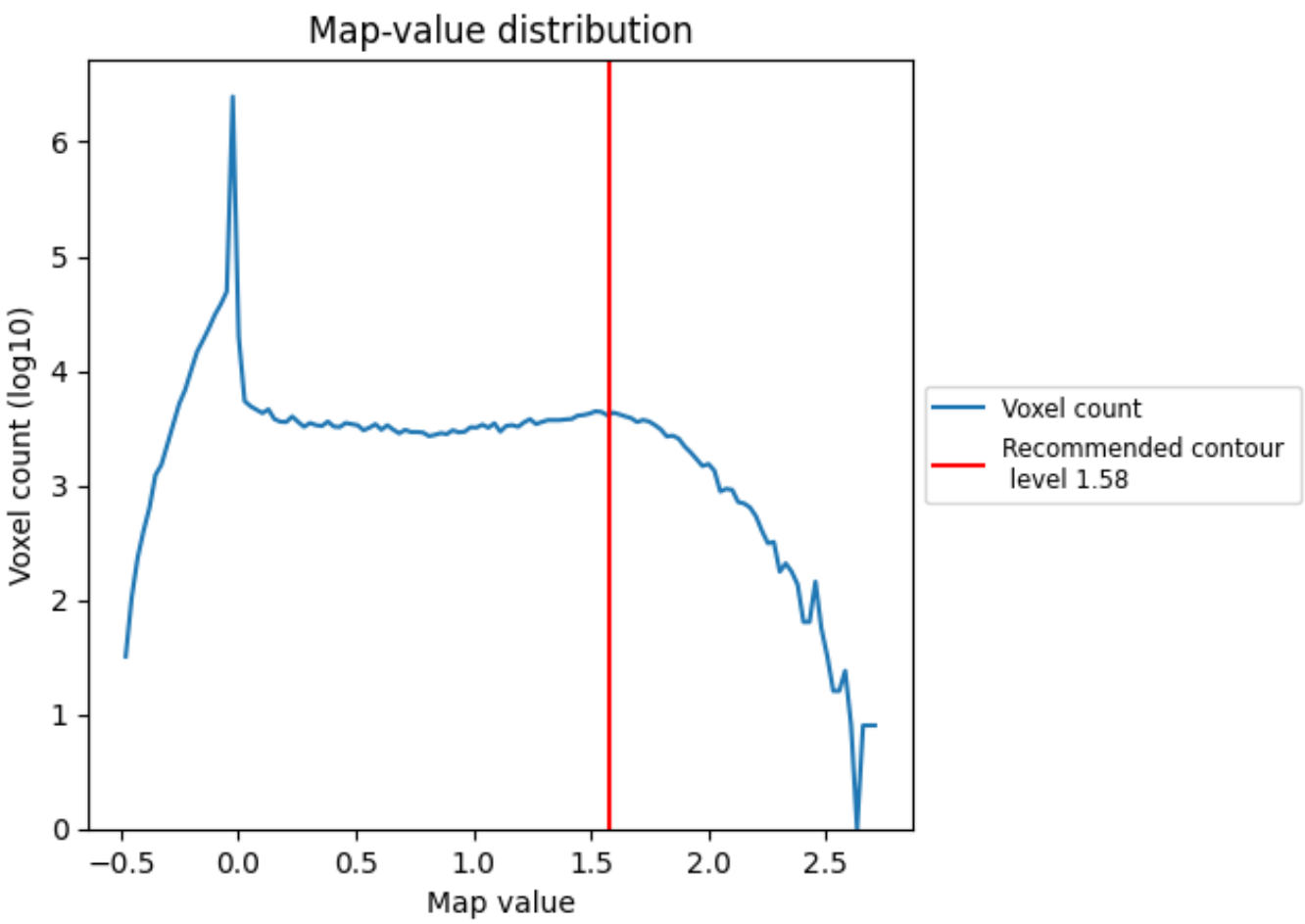
6.6 Mask visualisation (i)

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

7 Map analysis (i)

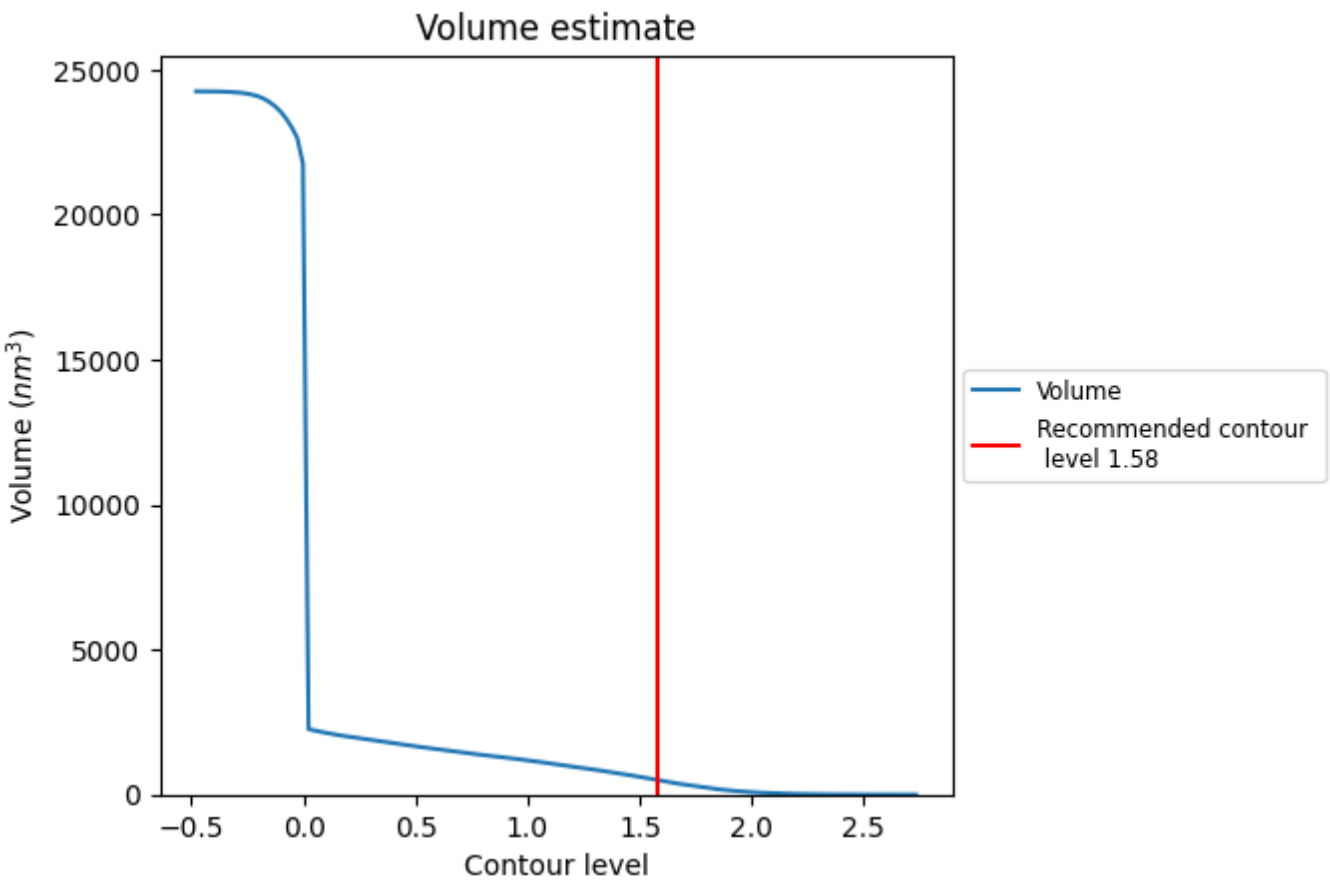
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

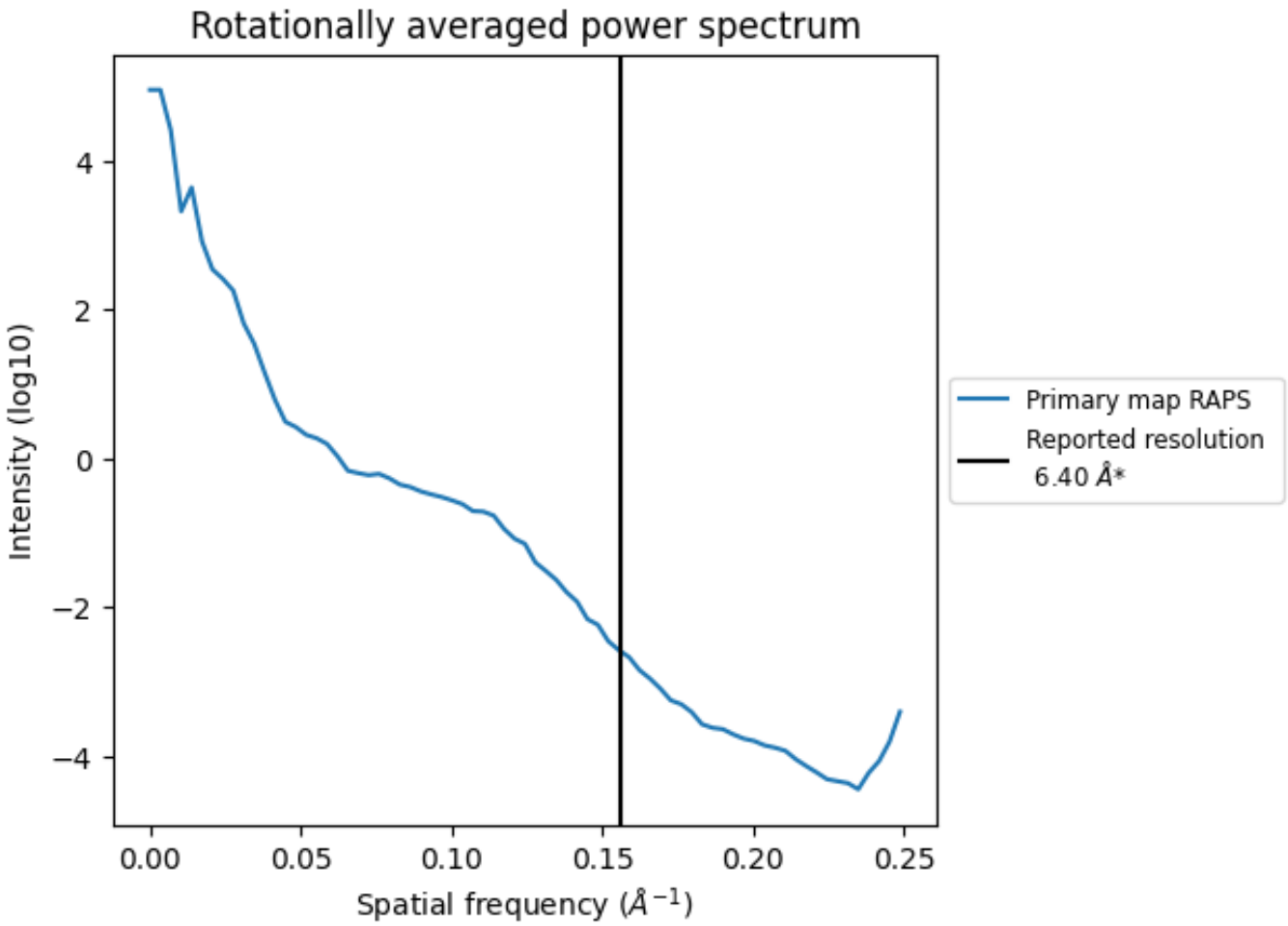
7.2 Volume estimate (i)



The volume at the recommended contour level is 500 nm^3; this corresponds to an approximate mass of 452 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.156 Å^{-1}

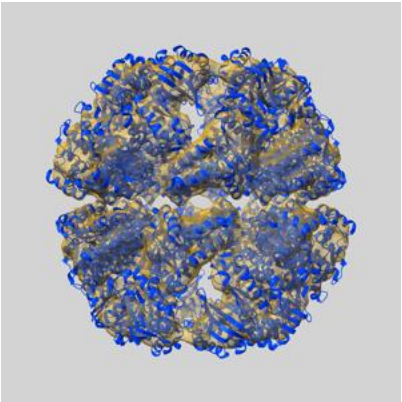
8 Fourier-Shell correlation (i)

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

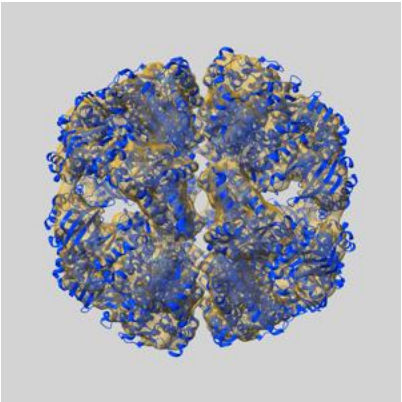
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5250 and PDB model 3IZN. Per-residue inclusion information can be found in section 3 on page 7.

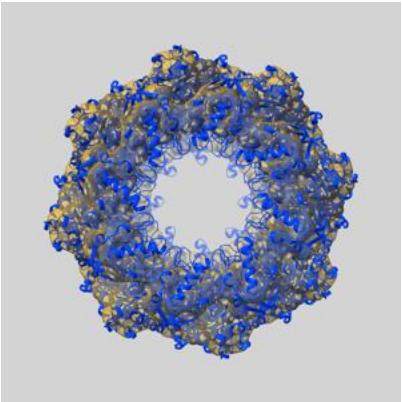
9.1 Map-model overlay (i)



X



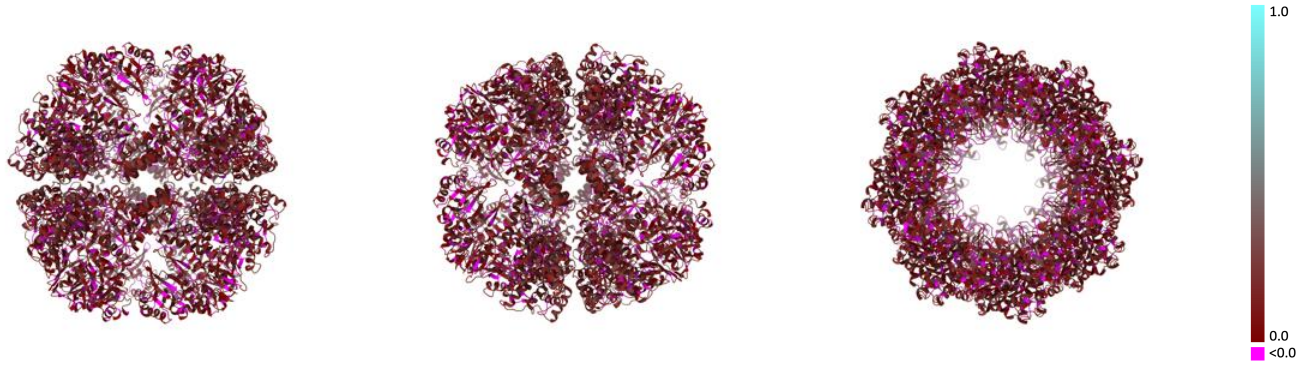
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.58 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.

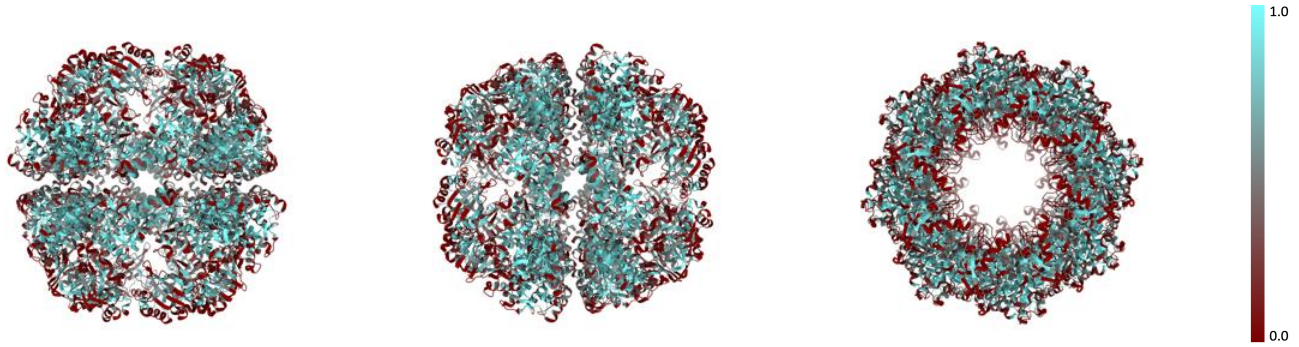
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

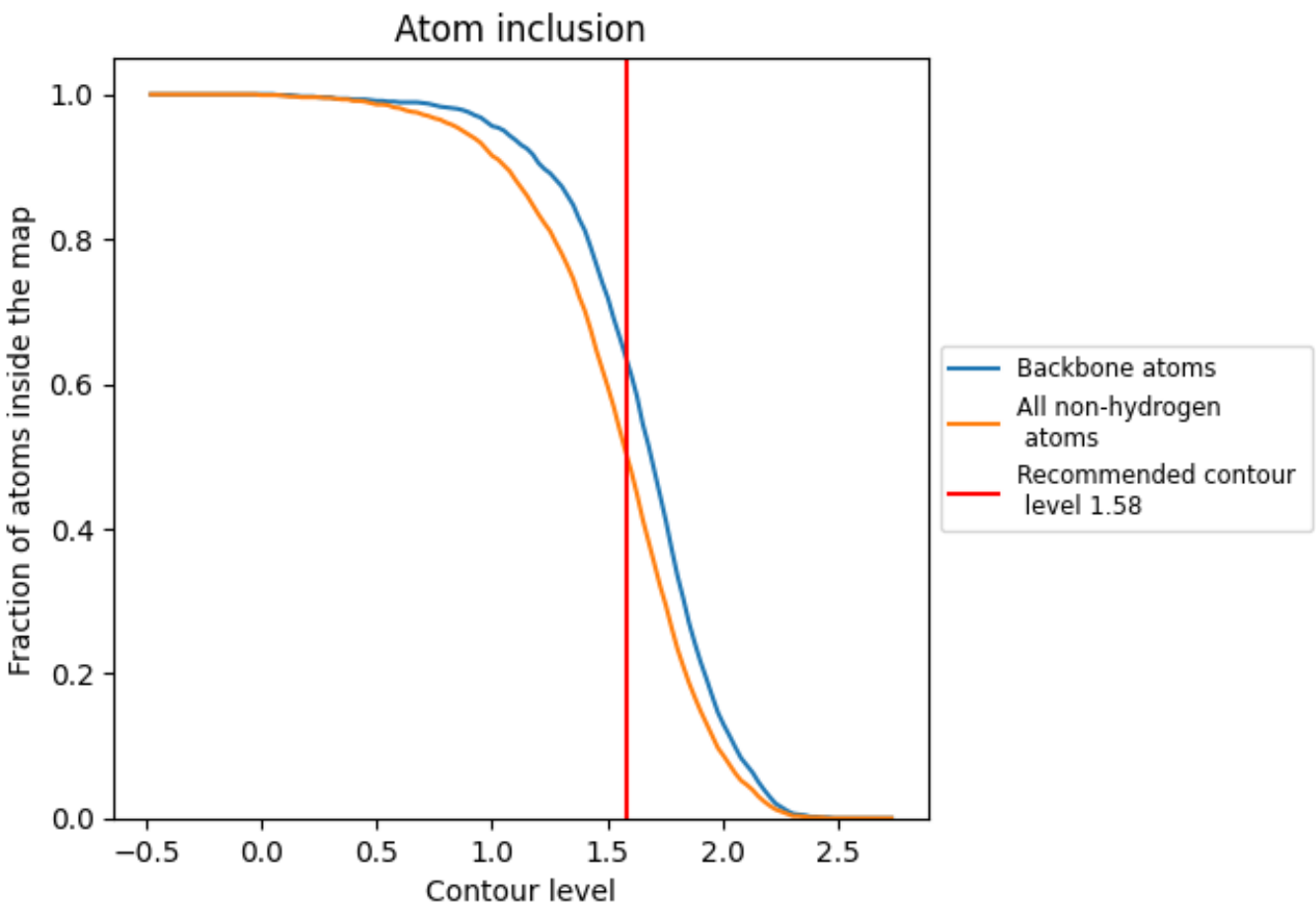
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1.58).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.58) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5060	0.1120
A	0.5070	0.1120
B	0.5070	0.1130
C	0.5070	0.1130
D	0.5070	0.1130
E	0.5070	0.1120
F	0.5070	0.1130
G	0.5070	0.1120
H	0.5070	0.1120
I	0.5060	0.1110
J	0.5060	0.1110
K	0.5060	0.1110
L	0.5060	0.1120
M	0.5060	0.1110
N	0.5060	0.1110
O	0.5060	0.1100
P	0.5060	0.1100