wwPDB EM Validation Summary Report

Feb 22, 2025 – 03:41 PM EST

PDB ID	:	9BDT
EMDB ID	:	EMD-44469
Title	:	Apolipoprotein B 100 bound to LDL receptor and legobody
Authors	:	Dearborn, A.D.; Reimund, M.; Graziano, G.; Lei, H.; Kumar, A.; Neufeld, E.B.; Remaley, A.T.; Marcotrigiano, J.
Deposited on	:	2024-04-12
Resolution	:	5.40 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 ⓘ 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:

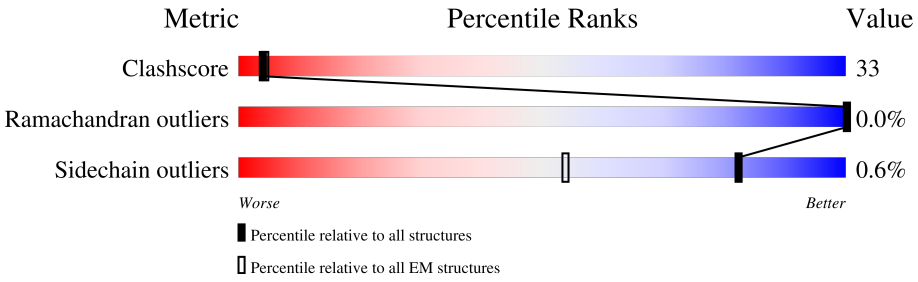
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 5.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4563	26% 33% 43% 24%
2	H	234	6% 35% 52% 13%
3	L	219	6% 50% 40% 10%
4	B	545	8% 41% 54% 6%
5	I	860	12% 11% 18% 70%
5	R	860	8% 17% 14% 68%
6	N	131	51% 47%
7	G	2	50% 50% 50%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 38899 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 Apolipoprotein B-100.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3476	Total	C	N	O	S	0	0
			27163	17244	4563	5277	79		

- Molecule 2 is a protein called Legobody 8D3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	203	Total	C	N	O	S	0	0
			1540	978	255	298	9		

- Molecule 3 is a protein called Legobody 8D3 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	198	Total	C	N	O	S	0	0
			1410	887	232	286	5		

- Molecule 4 is a protein called Maltodextrin-binding protein,Immunoglobulin G-binding protein A,Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	514	Total	C	N	O	S	0	0
			3948	2517	647	776	8		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP C3SHQ8
B	362	ALA	GLN	conflict	UNP P99134
B	363	LEU	ASN	conflict	UNP P99134
B	366	ALA	TYR	conflict	UNP P99134
B	368	ILE	VAL	conflict	UNP P99134
B	370	ILE	ASN	conflict	UNP P99134
B	375	THR	ASN	conflict	UNP P99134
B	376	GLU	ALA	conflict	UNP P99134

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Chain	Residue	Modelled	Actual	Comment	Reference
B	377	GLU	ASP	conflict	UNP P99134
B	392	VAL	GLN	conflict	UNP P99134
B	394	LYS	ALA	conflict	UNP P99134
B	395	GLU	ASN	conflict	UNP P99134
B	396	ILE	VAL	conflict	UNP P99134
B	398	ALA	GLY	conflict	UNP P99134
B	401	LYS	GLN	conflict	UNP P99134
B	405	GLU	ASP	conflict	UNP P99134
B	406	HIS	SER	conflict	UNP P99134
B	?	-	ALA	deletion	UNP P99134
B	411	GLY	ASP	conflict	UNP P99134
B	412	GLY	ALA	conflict	UNP P99134
B	413	SER	GLN	conflict	UNP P99134
B	414	GLY	GLN	conflict	UNP P99134
B	415	GLY	ASN	conflict	UNP P99134
B	416	ALA	ASN	conflict	UNP P99134
B	417	GLY	PHE	conflict	UNP P99134
B	418	SER	ASN	conflict	UNP P99134
B	419	GLY	LYS	conflict	UNP P99134
B	469	GLY	-	linker	UNP P99134
B	470	GLY	-	linker	UNP P99134
B	471	GLY	-	linker	UNP P99134
B	472	SER	-	linker	UNP P99134
B	473	GLY	-	linker	UNP P99134
B	474	GLY	-	linker	UNP P99134
B	475	GLY	-	linker	UNP P99134
B	476	SER	-	linker	UNP P99134
B	477	GLY	-	linker	UNP P99134
B	478	GLY	-	linker	UNP P99134
B	479	SER	-	linker	UNP P99134
B	538	GLY	-	expression tag	UNP P06654
B	539	SER	-	expression tag	UNP P06654
B	540	GLY	-	expression tag	UNP P06654
B	541	HIS	-	expression tag	UNP P06654
B	542	HIS	-	expression tag	UNP P06654
B	543	HIS	-	expression tag	UNP P06654
B	544	HIS	-	expression tag	UNP P06654
B	545	HIS	-	expression tag	UNP P06654
B	546	HIS	-	expression tag	UNP P06654

- Molecule 5 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	256	Total	C	N	O	S	0	0
			1925	1230	317	373	5		
5	R	273	Total	C	N	O	S	0	0
			1910	1133	324	409	44		

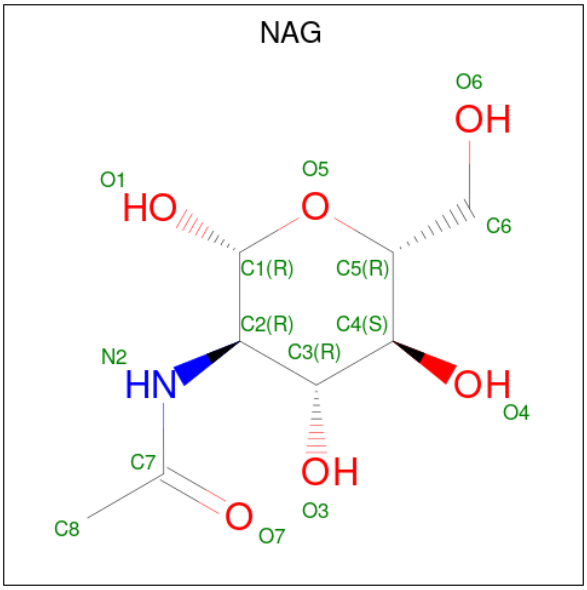
- Molecule 6 is a protein called ApoB100 nanobody 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	128	Total	C	N	O	S	0	0
			912	572	162	174	4		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

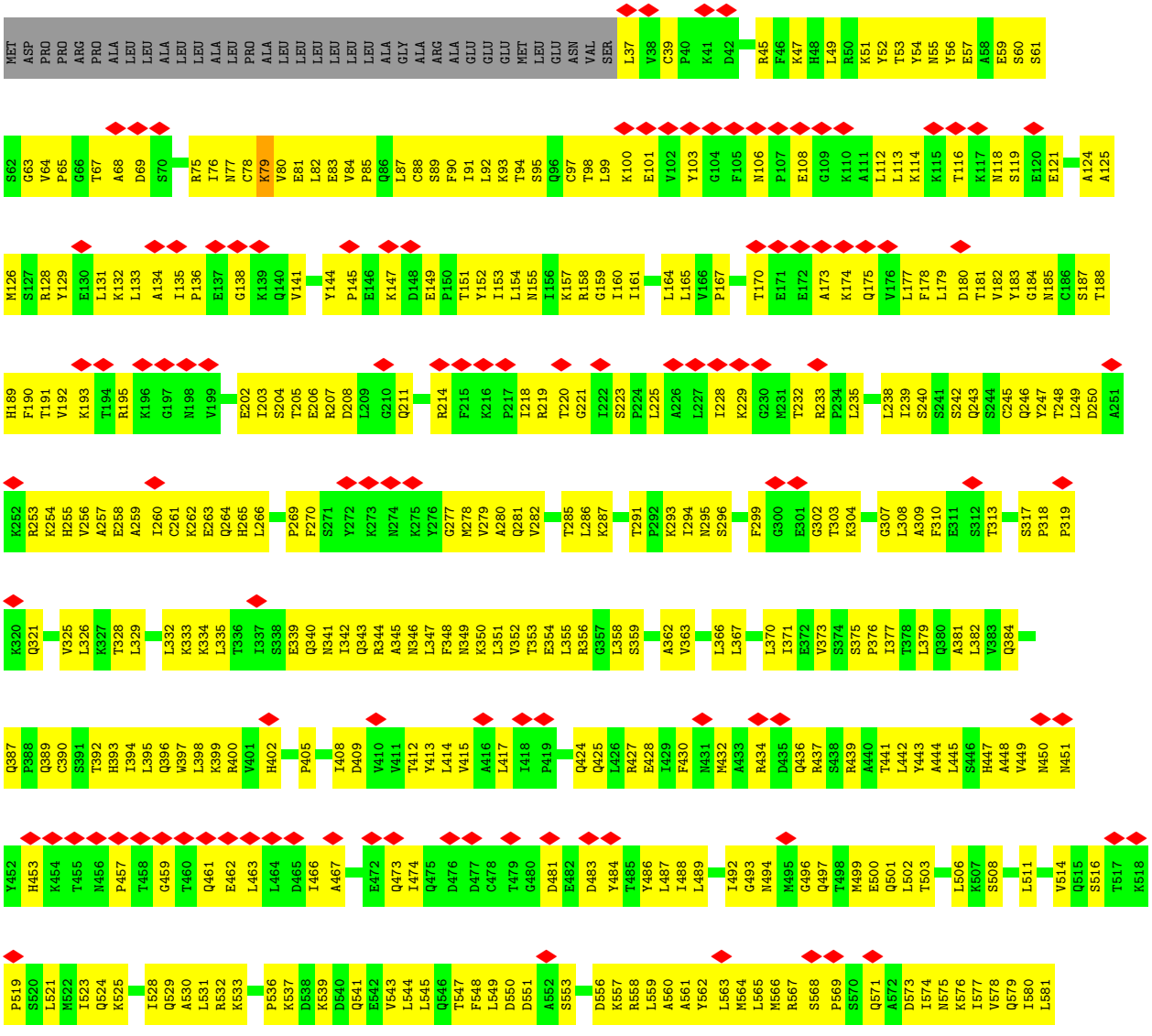
Mol	Chain	Residues	Atoms		AltConf
9	R	7	Total	Ca	0
			7	7	

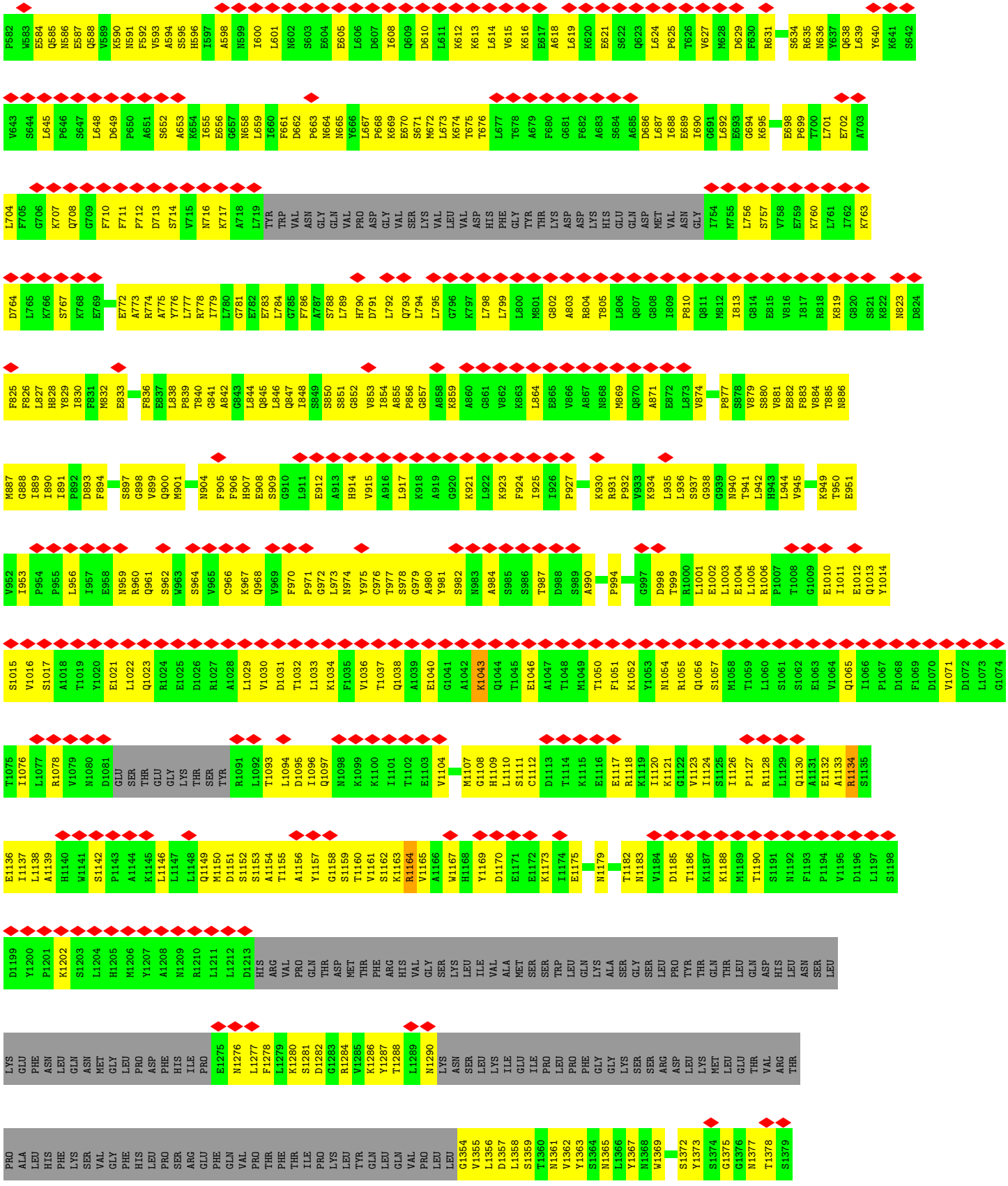
3 Residue-property plots (i)

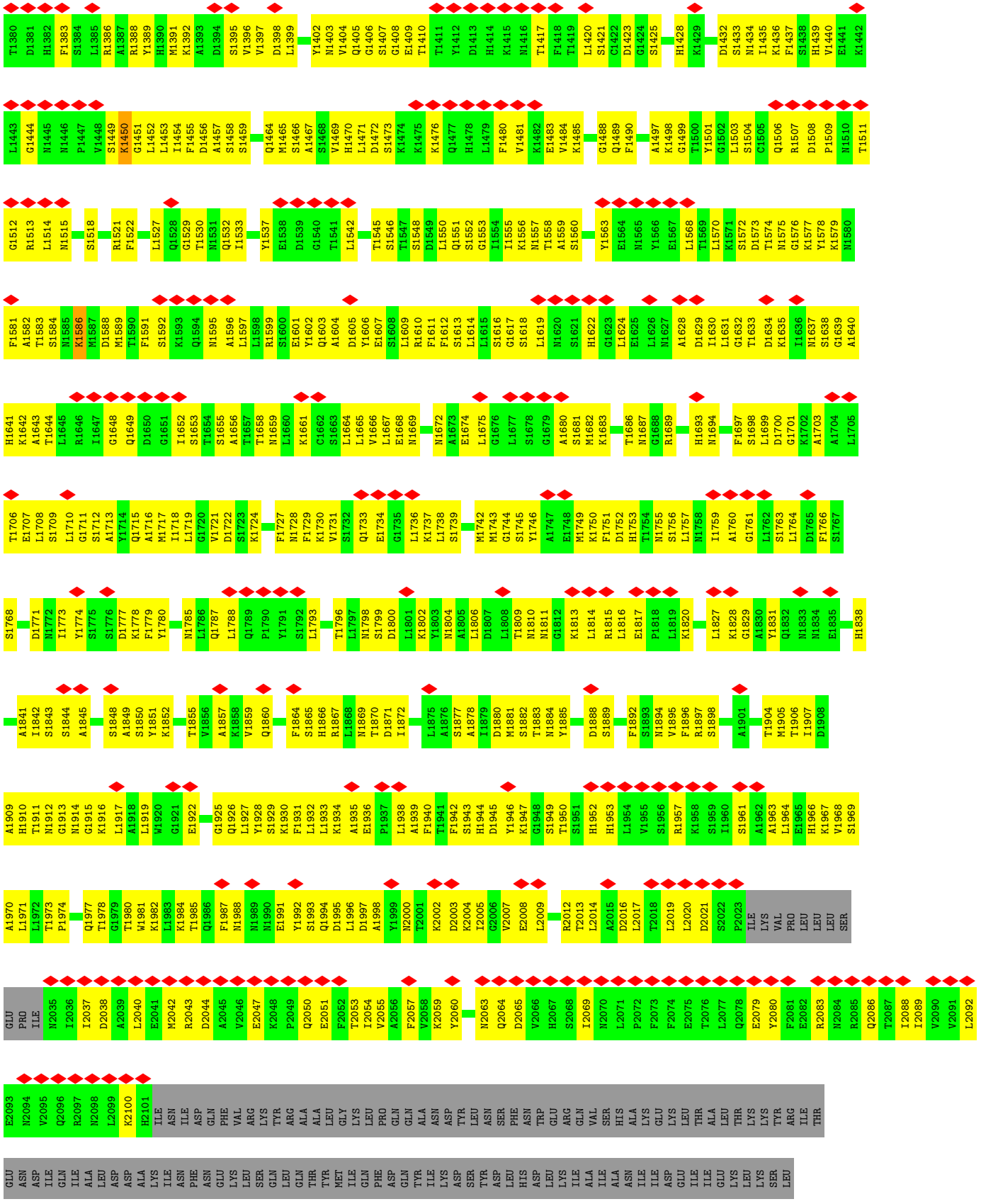
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Apolipoprotein B-100

Chain A:




P582 W583 E584 Q585 N586 E587 Q588 V589 K590 N591 F592 V593 A594 S595 H596 I597 A598 N599 I600 L601 N602 S603 E604 E605 L606 D607 I608 Q609 D610 L611 K612 K613 L614 V615 K616 E617 A618 L619 K620 E621 S622 Q623 L624 P625 T626 V627 M628 D629 F630 R631 S634 R635 N636 Y637 Q638 L639 Y640 K641 S642
V643 S644 L645 P646 S647 L648 D649 P650 A651 S652 A653 K654 I655 E656 G657 N658 L659 I660 F661 D662 P663 N664 N665 Y666 L667 P668 K669 E670 S671 M672 L673 K674 T675 T676 L677 T678 A679 F680 G681 F682 A683 S684 A685 D686 L687 I688 E689 I690 G691 L692 E693 G694 K695 E698 P699 T700 L701 E702 A703
L704 F705 G706 K707 Q708 G709 F710 F711 P712 D713 S714 V715 N716 K717 A718 L719 TYR TRP VAL ASN GLY GLN VAL PRO ASP GLY VAL SER LYS VAL LEU VAL ASP HIS PHE GLY TYR THR LYS ASP ASP LYS HIS GLU GLN ASP MET VAL ASN GLY I754 M755 L756 S757 V758 E759 K760 L761 I762 K763
D764 L765 K766 S767 K768 E769 E772 A773 R774 A775 Y776 L777 R778 I779 L780 G781 E782 E783 L784 G785 F786 A787 S788 L789 H790 D791 L792 Q793 L794 L795 G796 K797 L798 L799 L800 M801 G802 A803 R804 T805 L806 Q807 G808 I809 P810 Q811 M812 I813 G814 E815 V816 I817 R818 K819 G820 S821 K822 N823 D824
F825 F826 L827 H828 Y829 I830 F831 M832 E833 F836 E837 L838 P839 T840 G841 A842 G843 L844 Q845 L846 Q847 I848 S849 S850 S851 G852 V853 I854 A855 P856 G857 A858 K859 A860 G861 V862 K863 L864 E865 V866 A867 N868 M869 Q870 A871 E872 L873 V874 P877 S878 V879 S880 V881 E882 F883 V884 T885 N886
M887 G888 I889 I890 I891 P892 D893 F894 S897 G898 V899 Q900 M901 N904 F905 F906 H907 E908 S909 G910 L911 E912 A913 H914 V915 A916 L917 K918 A919 G920 K921 L922 K923 F924 I925 I926 P927 K930 R931 P932 V933 K934 L935 L936 S937 G938 G939 N940 T941 L942 H943 L944 V945 K949 T950 E951
V952 I953 P954 P955 L956 I957 E958 N959 R960 Q961 S962 W963 S964 V965 C966 K967 Q968 V969 F970 P971 G972 L973 N974 Y975 C976 T977 S978 G979 A980 Y981 S982 N983 A984 S985 S986 T987 D988 S989 A990 P994 G997 D998 T999 R1000 L1001 E1002 L1003 E1004 L1005 R1006 P1007 T1008 G1009 E1010 I1011 E1012 Q1013 Y1014
S1015 V1016 S1017 A1018 T1019 Y1020 E1021 L1022 Q1023 R1024 E1025 D1026 R1027 A1028 L1029 V1030 D1031 T1032 L1033 K1034 F1035 V1036 T1037 Q1038 A1039 E1040 G1041 A1042 K1043 Q1044 T1045 E1046 A1047 T1048 M1049 T1050 F1051 K1052 Y1053 N1054 R1055 Q1056 S1057 M1058 T1059 L1060 S1061 S1062 E1063 V1064 Q1065 I1066 P1067 D1068 F1069 D1070 V1071 D1072 L1073 G1074
T1075 I1076 L1077 R1078 V1079 N1080 D1081 GLU SER THR GLU GLY LYS THR SER TYR R1091 L1092 T1093 L1094 D1095 I1096 Q1097 N1098 K1099 K1100 I1101 T1102 E1103 V1104 M1107 G1108 H1109 L1110 S1111 C1112 D1113 T1114 K1115 E1116 E1117 R1118 K1119 I1120 K1121 G1122 V1123 I1124 S1125 I1126 P1127 R1128 L1129 Q1130 A1131 E1132 A1133 R1134 S1135
E1136 I1137 L1138 A1139 H1140 W1141 S1142 P1143 A1144 K1145 L1146 L1147 L1148 Q1149 M1150 D1151 S1152 S1153 A1154 T1155 A1156 Y1157 G1158 S1159 T1160 V1161 S1162 K1163 R1164 V1165 A1166 W1167 H1168 Y1169 D1170 E1171 E1172 K1173 I1174 E1175 N1179 T1182 N1183 V1184 D1185 T1186 K1187 K1188 M1189 T1190 S1191 N1192 F1193 P1194 V1195 D1196 L1197 S1198
D1199 Y1200 P1201 K1202 S1203 L1204 H1205 M1206 Y1207 A1208 N1209 R1210 L1211 L1212 D1213 HIS ARG VAL PRO GLN THR ASP MET THR PHE ARG HIS VAL GLY SER LYS LEU ILE VAL ALA MET SER SER TRP LEU GLN LYS ALA SER GLY SER LEU PRO TYR THR GLN THR LEU GLN ASP HIS LEU ASN SER LEU
LYS GLU PHE ASN LEU GLN ASN MET GLY LEU PRO ASP PHE HIS ILE PRO E1275 N1276 L1277 F1278 L1279 K1280 S1281 D1282 G1283 R1284 V1285 K1286 Y1287 T1288 L1289 N1290 LYS ASN SER LEU LYS ILE GLU ILE PRO LEU PRO PHE GLY GLY LYS SER SER ARG ASP LEU LYS MET LEU GLU THR VAL ARG THR
PRO ALA LEU HIS PHE LYS SER VAL GLY PHE HIS LEU PRO SER ARG GLU PHE GLN VAL PRO THR PHE THR ILE PRO LYS LEU TYR GLN LEU GLN VAL PRO LEU LEU G1354 V1355 L1356 D1357 L1358 S1359 T1360 N1361 V1362 Y1363 S1364 N1365 L1366 Y1367 N1368 W1369 S1372 Y1373 S1374 G1375 G1376 N1377 T1378 S1379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G1512 R1513 L1514 N1515 S1518 R1521 F1522 L1527 Q1528 G1529 T1530 N1531 Q1532 I1533 Y1537 E1538 D1539 G1540 T1541 L1542 T1545 S1546 T1547 S1548 D1549 L1550 Q1551 S1552 G1553 I1554 I1555 K1556 N1557 T1558 A1559 S1560 Y1563 E1564 N1565 Y1566 E1567 L1568 T1569 L1570 K1571 S1572 D1573 T1574 N1575 G1576 K1577 Y1578 K1579 N1580
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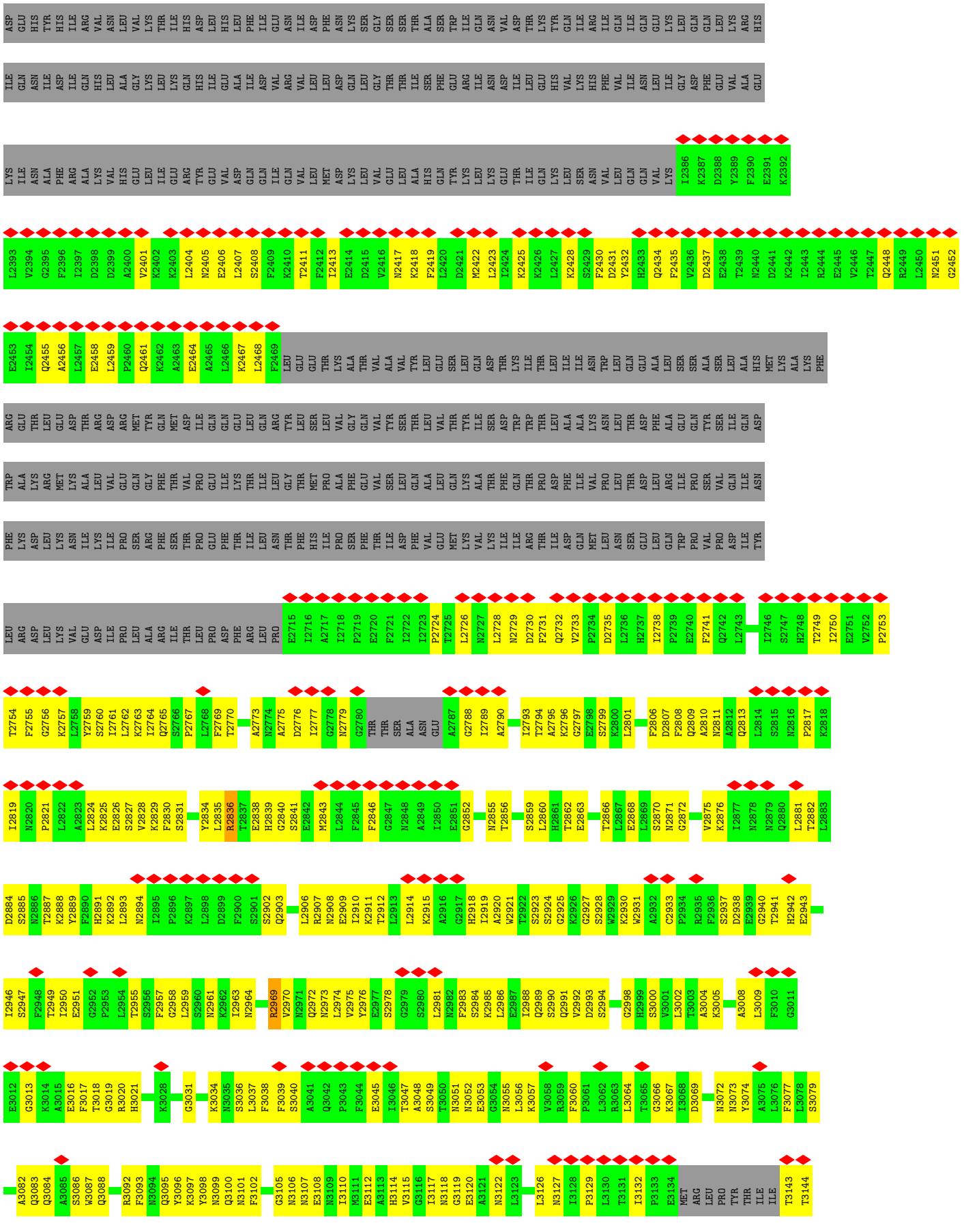
GLU PRO ILE N2035 I2036 I2037 D2038 A2039 L2040 E2041 M2042 R2043 D2044 A2045 V2046 E2047 K2048 P2049 Q2050 E2051 F2052 T2053 I2054 V2055 A2056 F2057 V2058 K2059 Y2060 N2063 Q2064 D2065 V2066 H2067 S2068 I2069 N2070 L2071 P2072 F2073 F2074 E2075 T2076 L2077 Q2078 E2079 Y2080 F2081 E2082 R2083 N2084 R2085 Q2086 T2087 I2088 I2089 V2090 V2091 L2092
E2093 N2094 V2095 Q2096 R2097 N2098 L2099 K2100 H2101 ILE ASN ILE ASP GLN PHE VAL ARG LYS TYR ARG ALA ALA LEU GLY LYS LEU PRO GLN GLN ALA ASN ASP TYR LEU ASN SER ASP TYR ASP LEU HIS ASP LEU LYS ILE ALA ILE ALA ASN ILE ILE ASP GLU ILE ILE GLU LYS LEU LYS LYS SER LEU
GLU ASN ASP ILE GLN ILE ALA LEU ASP ASP ALA LYS ILE ILE ASN PHE ASN GLU LYS LEU SER GLN LEU GLN THR TYR MET ILE LEU GLN PHE ASP GLN TYR ILE LYS ASP SER TYR ASP LEU HIS ASP LEU LYS ILE LEU ALA ILE ALA ASN ILE ILE ASP GLU ILE ILE GLU LYS LEU LYS LYS SER LEU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ILE GLN ASN ILE ASP ILE GLN HIS LEU ALA GLY LYS LEU LYS GLN HIS ILE GLU ALA ILE ASP VAL ARG VAL LEU LEU ASP GLN LEU GLY THR THR ILE SER PHE GLU ARG ILE ASN ASP ILE LEU GLU HIS VAL LYS HIS PHE VAL ILE ASN LEU ILE GLY ASP PHE GLU VAL ALA GLU
LYS ILE ASN ALA PHE ARG ALA LYS VAL HIS GLU LEU ILE GLU ARG TYR GLU VAL ASP GLN GLN ILE GLN VAL LEU MET ASP LYS LEU VAL GLU LEU ALA HIS GLN TYR LYS LEU LYS GLU THR ILE GLN LYS LEU SER ASN VAL LEU GLN GLN VAL LYS I2386 K2387 D2388 Y2389 F2390 E2391 K2392
L2393 V2394 G2395 F2396 I2397 D2398 D2399 A2400 V2401 K2402 K2403 L2404 N2405 E2406 L2407 S2408 F2409 K2410 T2411 F2412 I2413 E2414 D2415 V2416 N2417 K2418 F2419 L2420 D2421 M2422 L2423 I2424 K2425 K2426 L2427 K2428 S2429 F2430 D2431 Y2432 H2433 Q2434 F2435 V2436 D2437 E2438 T2439 N2440 D2441 K2442 I2443 R2444 E2445 V2446 T2447 Q2448 R2449 L2450 N2451 G2452
E2453 I2454 Q2455 A2456 L2457 E2458 L2459 P2460 Q2461 K2462 A2463 E2464 A2465 L2466 K2467 L2468 F2469 LEU GLU GLU THR LYS ALA THR VAL ALA VAL TYR LEU GLU SER LEU GLN ASP THR LYS ILE THR LEU ILE ILE ASN TRP LEU GLN GLU ALA LEU SER SER ALA SER LEU ALA HIS MET LYS ALA LYS PHE
ARG GLU THR LEU GLU ASP THR ARG ASP ARG MET TYR GLN MET ASP ILE GLN GLN GLU LEU GLN ARG TYR LEU SER LEU VAL GLY GLN VAL TYR SER THR LEU GLU VAL THR TYR ILE SER ASP TRP THR LEU LEU ALA ALA LYS ASN LEU THR ASP PHE ALA GLU GLN TYR SER ILE GLN ASP
TRP ALA LYS ARG MET LYS ALA LEU VAL GLU GLN GLY PHE THR VAL PRO GLU GLN ILE LYS THR ILE LEU GLY THR MET PRO ALA PHE GLU GLN VAL SER LEU GLN LEU ALA LEU GLN LYS ALA THR PHE GLN THR PRO ASP PHE ILE VAL PRO LEU THR THR ASP LEU ARG ILE PRO SER VAL GLN ILE ASN
PHE LYS ASP LEU LYS ASN ILE LYS ILE PRO SER PHE PHE THR ILE ASP PHE VAL GLU MET LYS VAL LYS ILE ILE ARG THR ILE ASP GLN MET LEU ASN SER GLU LEU GLN TRP PRO VAL PRO ASP ILE TYR
LEU ARG ASP LEU LYS VAL GLU ASP ILE PRO LEU ALA ARG ILE THR LEU PRO PRO ASP PHE ARG LEU PRO E2715 I2716 A2717 I2718 P2719 E2720 F2721 I2722 I2723 P2724 T2725 L2726 N2727 L2728 N2729 D2730 F2731 Q2732 V2733 P2734 D2735 L2736 H2737 I2738 P2739 E2740 F2741 Q2742 L2743 I2746 S2747 H2748 T2749 I2750 E2751 V2752 P2753
T2754 F2755 G2756 K2757 L2758 Y2759 S2760 I2761 L2762 K2763 I2764 Q2765 S2766 P2767 L2768 F2769 T2770 A2773 N2774 A2775 D2776 I2777 G2778 N2779 G2780 THR THR SER ALA ASN GLU A2787 G2788 I2789 A2790 I2793 T2794 A2795 K2796 G2797 E2798 S2799 K2800 L2801 F2806 D2807 F2808 Q2809 A2810 N2811 A2812 Q2813 L2814 S2815 N2816 P2817 K2818
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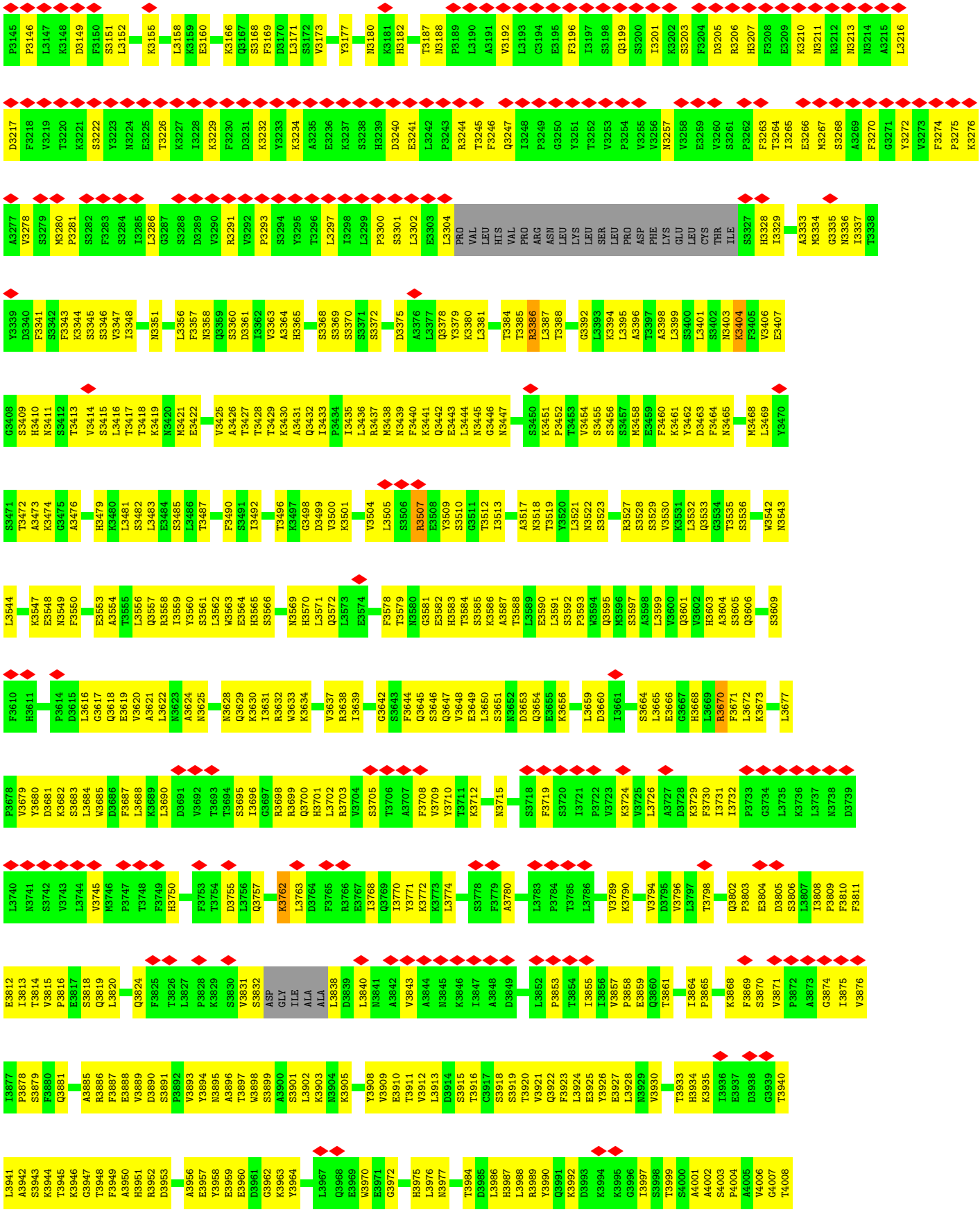
E3012 G3013 K3014 A3015 E3016 F3017 T3018 G3019 R3020 H3021 K3028 G3031 K3034 N3035 S3036 L3037 F3038 F3039 S3040 A3041 Q3042 P3043 F3044 E3045 I3046 T3047 A3048 S3049 T3050 N3051 N3052 E3053 G3054 N3055 L3056 K3057 V3058 R3059 F3060 P3061 L3062 R3063 L3064 T3065 G3066 K3067 I3068 D3069 N3072 N3073 Y3074 A3075 L3076 F3077 L3078 S3079
A3082 Q3083 Q3084 A3085 S3086 W3087 Q3088 R3092 F3093 N3094 Q3095 Y3096 K3097 Y3098 N3099 Q3100 N3101 F3102 G3105 N3106 N3107 E3108 N3109 I3110 M3111 E3112 A3113 H3114 V3115 G3116 I3117 N3118 G3119 E3120 A3121 N3122 L3123 L3126 N3127 I3128 P3129 L3130 T3131 I3132 P3133 E3134 MET ARG LEU PRO TYR THR ILE ILE T3143 T3144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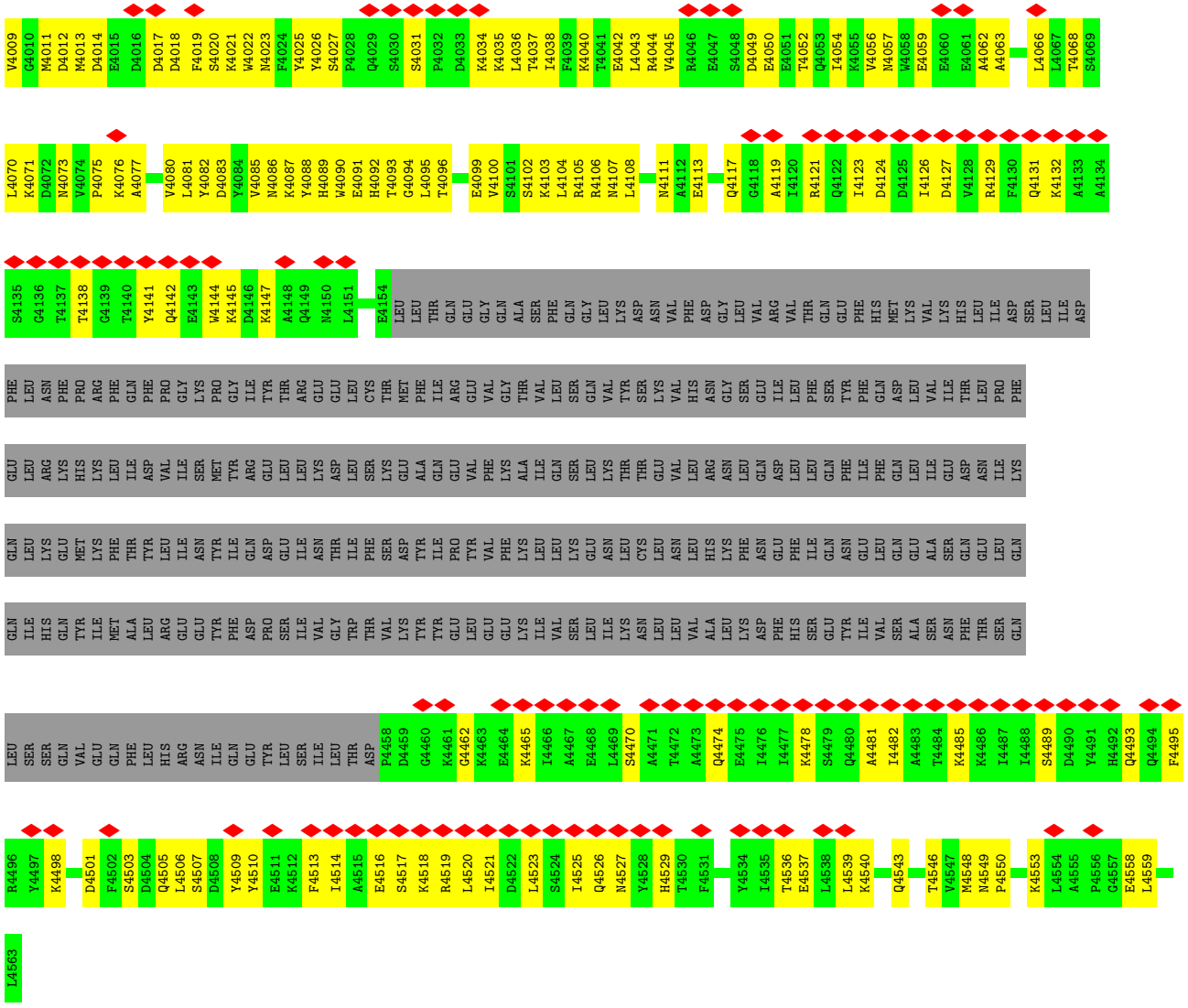
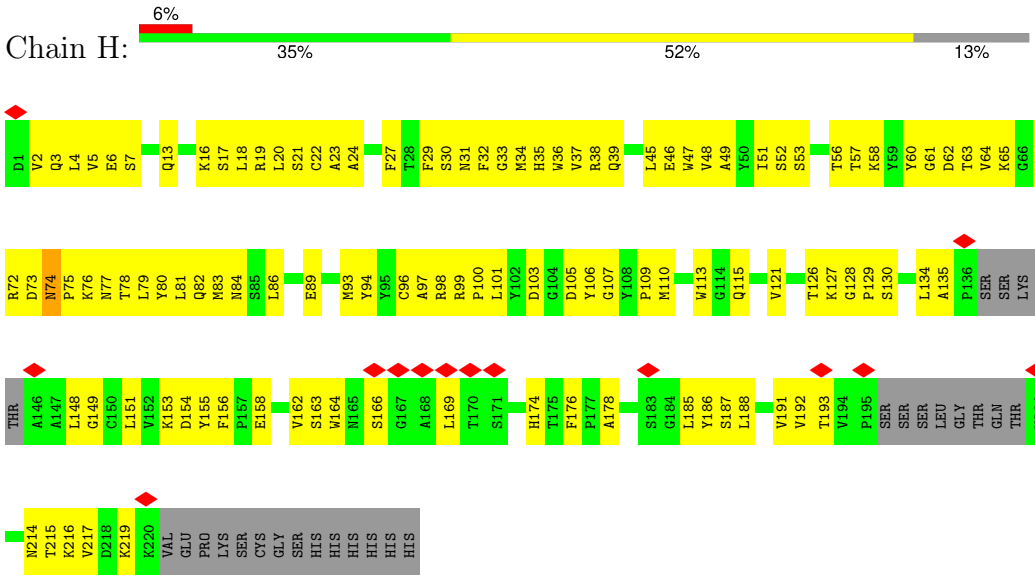
L3941 A3942 S3943 K3944 T3945 K3946 G3947 T3948 F3949 A3950 H3951 R3952 D3953 A3956 E3957 Y3958 E3959 E3960 D3961 G3962 K3963 Y3964 L3967 Q3968 E3969 W3970 E3971 G3972 H3975 L3976 N3977 T3984 D3985 L3986 H3987 L3988 R3989 Y3990 Q3991 K3992 D3993 K3994 K3995 G3996 I3997 S3998 T3999 S4000 A4001 A4002 S4003 P4004 A4005 V4006 G4007 T4008



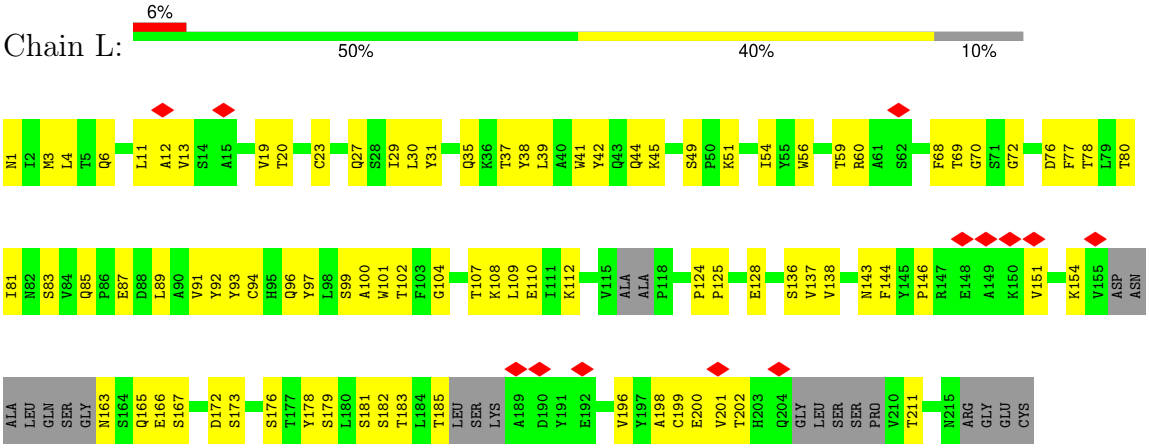
• Molecule 2: Legobody 8D3 Fab Heavy Chain

Chain H:



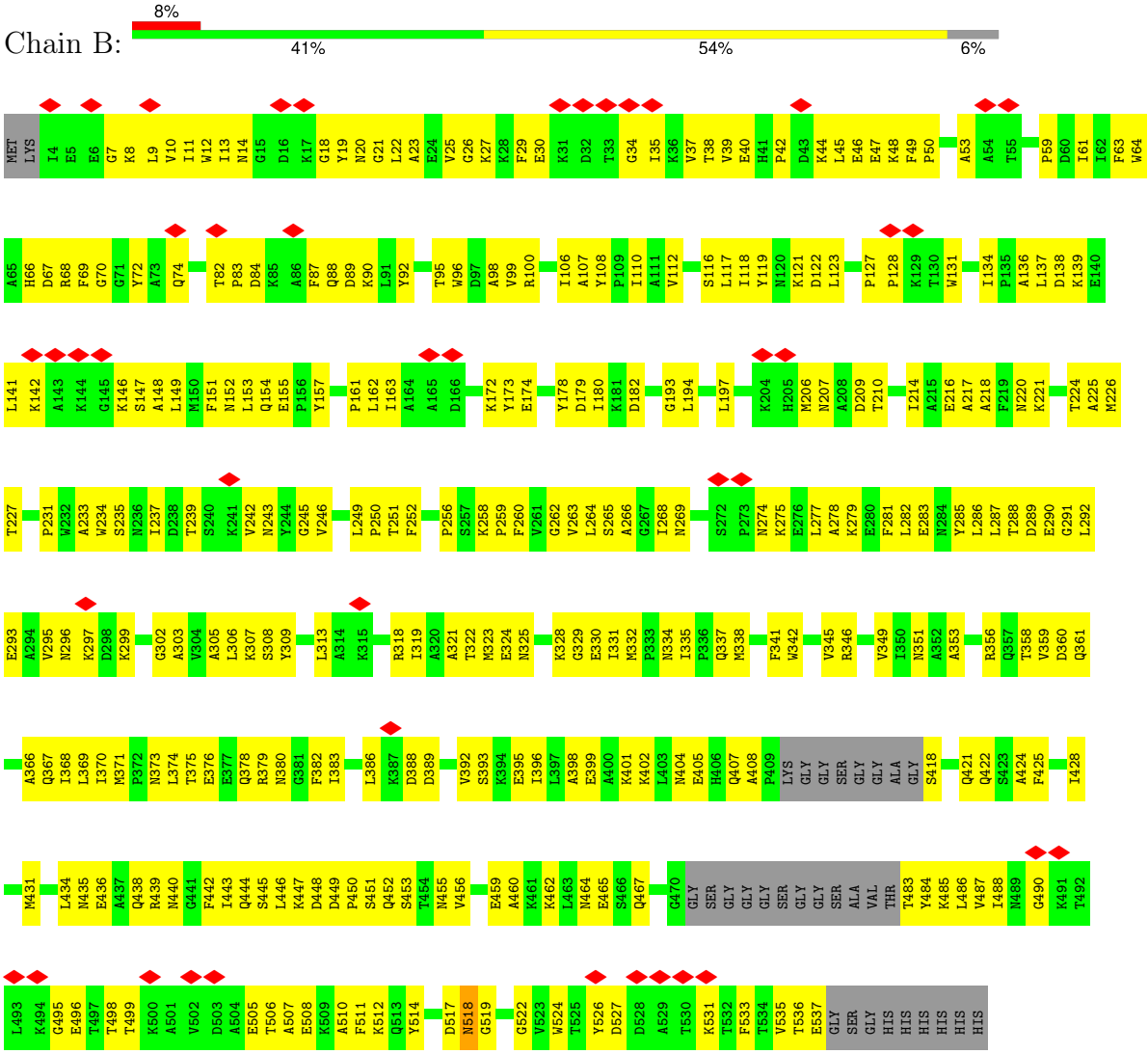
• Molecule 3: Legobody 8D3 Fab Light Chain

Chain L:



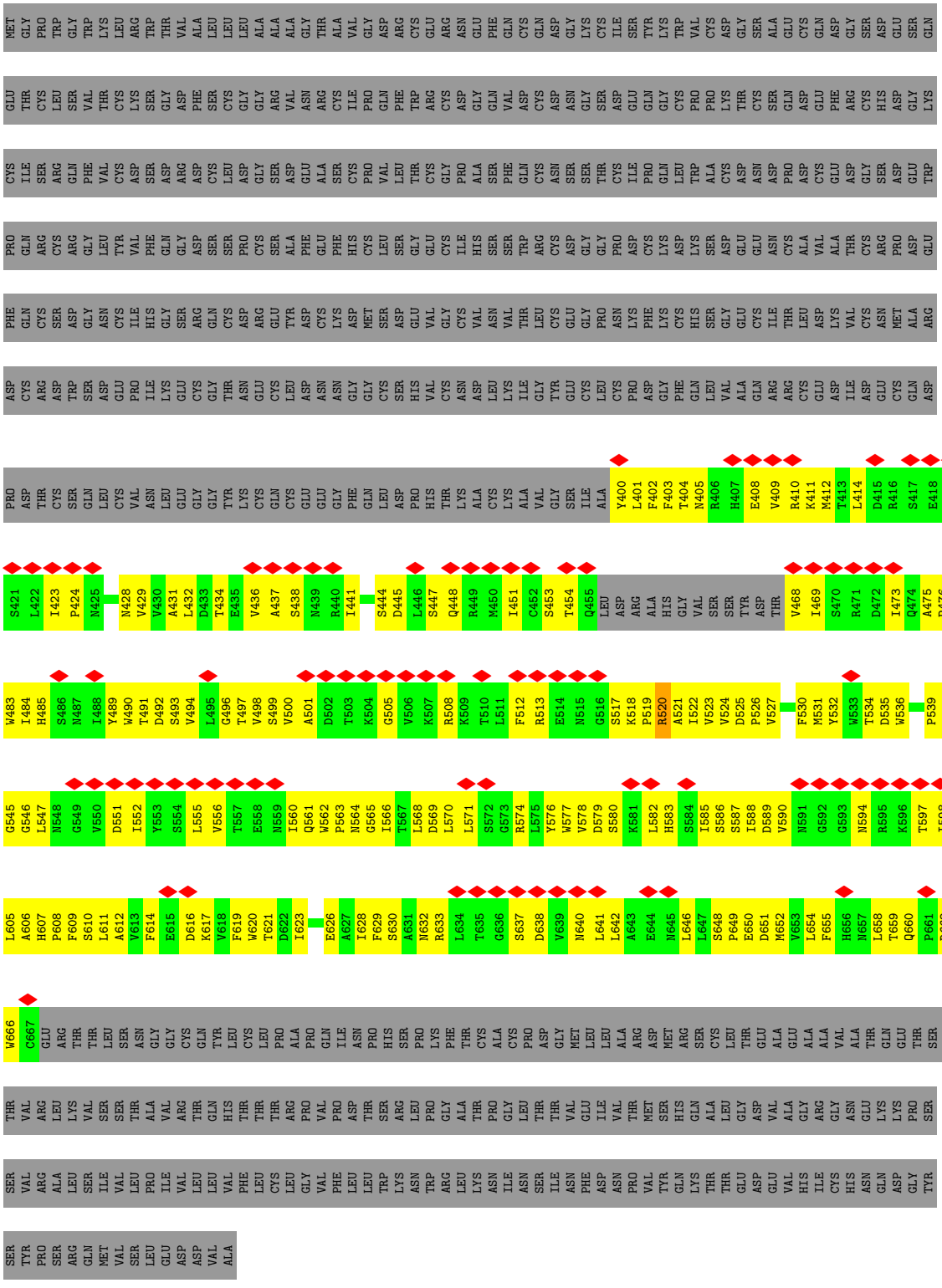
• Molecule 4: Maltodextrin-binding protein,Immunoglobulin G-binding protein A,Immunoglobulin G-binding protein G

Chain B:



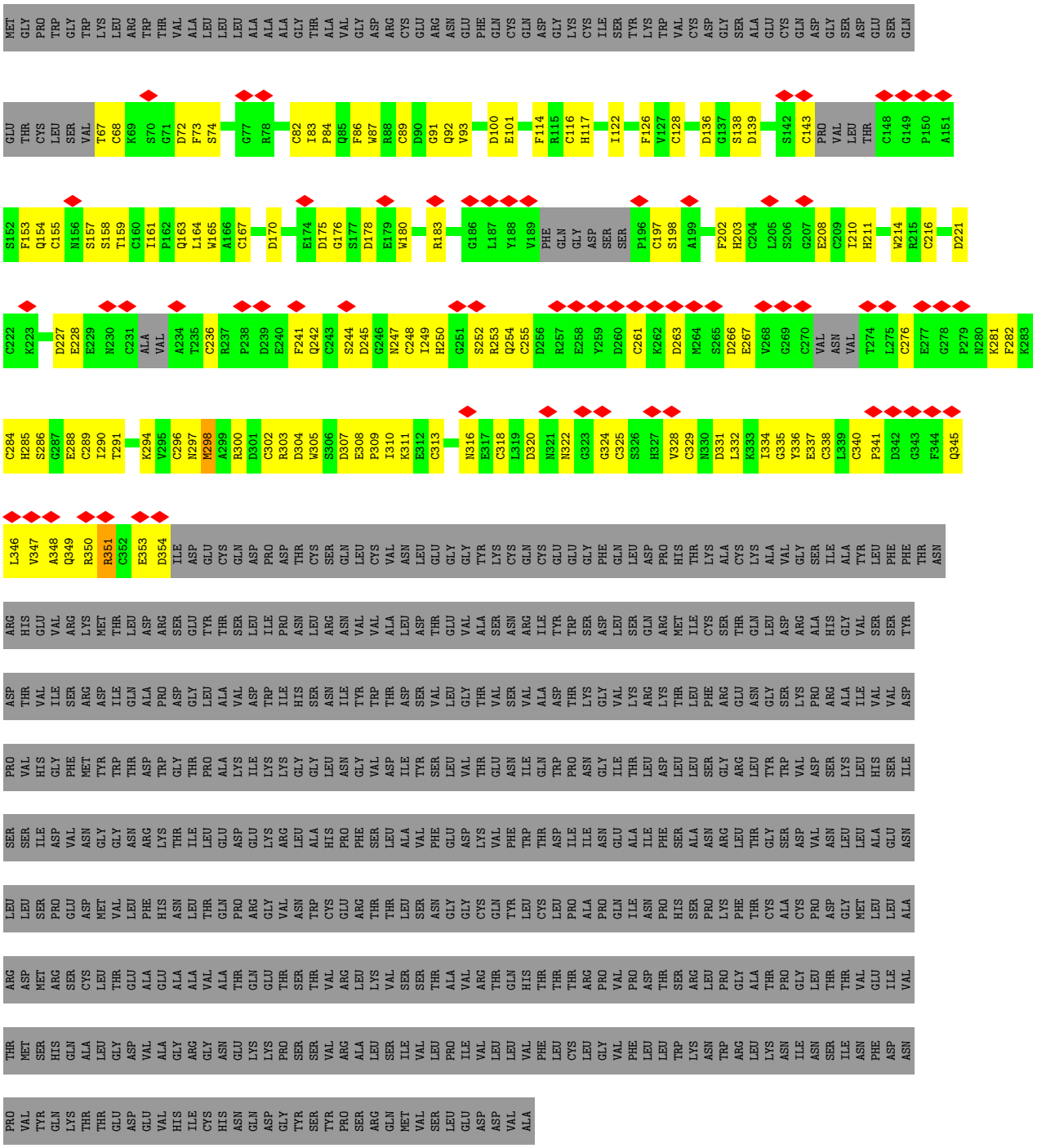
• Molecule 5: Low-density lipoprotein receptor

Chain I:



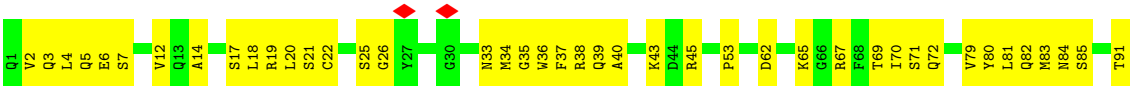
• Molecule 5: Low-density lipoprotein receptor

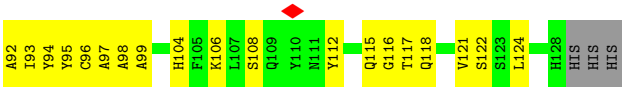
Chain R:



• Molecule 6: ApoB100 nanobody 4

Chain N:





• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	527598	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.38	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.376	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.76, 557.76, 557.76	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6600001, 1.6600001, 1.6600001	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.25	0/27687	0.51	0/37490
2	H	0.29	0/1581	0.56	0/2155
3	L	0.25	0/1438	0.50	0/1973
4	B	0.25	0/4032	0.45	0/5473
5	I	0.25	0/1969	0.53	0/2700
5	R	0.26	0/1944	0.53	0/2637
6	N	0.25	0/930	0.53	0/1258
All	All	0.25	0/39581	0.51	0/53686

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	27163	0	26925	1750	0
2	H	1540	0	1470	133	0
3	L	1410	0	1265	66	0
4	B	3948	0	3850	273	0
5	I	1925	0	1789	161	0
5	R	1910	0	1516	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	912	0	824	49	0
7	G	28	0	25	1	0
8	A	56	0	52	4	0
9	R	7	0	0	0	0
All	All	38899	0	37716	2498	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 33.

The worst 5 of 2498 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:H:83:MET:HB3	2:H:86:LEU:HD21	1.40	1.00
1:A:3549:ASN:HB3	1:A:3564:GLU:HB3	1.42	1.00
1:A:3590:GLU:HB2	1:A:3597:SER:HB2	1.48	0.95
5:I:534:THR:HB	5:I:565:GLY:HA2	1.50	0.94
4:B:456:VAL:HA	4:B:459:GLU:HB3	1.50	0.92

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	3450/4563 (76%)	3221 (93%)	229 (7%)	0	100	100
2	H	197/234 (84%)	182 (92%)	15 (8%)	0	100	100
3	L	188/219 (86%)	179 (95%)	9 (5%)	0	100	100
4	B	508/545 (93%)	479 (94%)	29 (6%)	0	100	100
5	I	252/860 (29%)	212 (84%)	40 (16%)	0	100	100
5	R	263/860 (31%)	225 (86%)	37 (14%)	1 (0%)	30	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	N	126/131 (96%)	112 (89%)	14 (11%)	0	100	100
All	All	4984/7412 (67%)	4610 (92%)	373 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	R	298	MET

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	3013/4080 (74%)	2993 (99%)	20 (1%)	81	87
2	H	169/199 (85%)	168 (99%)	1 (1%)	84	88
3	L	145/192 (76%)	145 (100%)	0	100	100
4	B	408/433 (94%)	407 (100%)	1 (0%)	92	94
5	I	201/755 (27%)	200 (100%)	1 (0%)	86	89
5	R	204/755 (27%)	203 (100%)	1 (0%)	86	89
6	N	80/103 (78%)	79 (99%)	1 (1%)	65	77
All	All	4220/6517 (65%)	4195 (99%)	25 (1%)	82	88

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3386	ARG
1	A	3670	ARG
5	R	351	ARG
1	A	3507	ARG
1	A	3762	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	66	HIS
4	B	296	ASN
5	I	564	ASN
1	A	886	ASN
1	A	828	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	G	1	1,7	14,14,15	1.25	2 (14%)	17,19,21	2.09	2 (11%)
7	NAG	G	2	7	14,14,15	0.41	0	17,19,21	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	NAG	O5-C1	4.01	1.50	1.43
7	G	1	NAG	C1-C2	2.05	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	1	NAG	C1-O5-C5	7.75	122.58	112.19
7	G	1	NAG	C1-C2-N2	2.41	114.23	110.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	2	NAG	C4-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	G	1	NAG	C4-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6

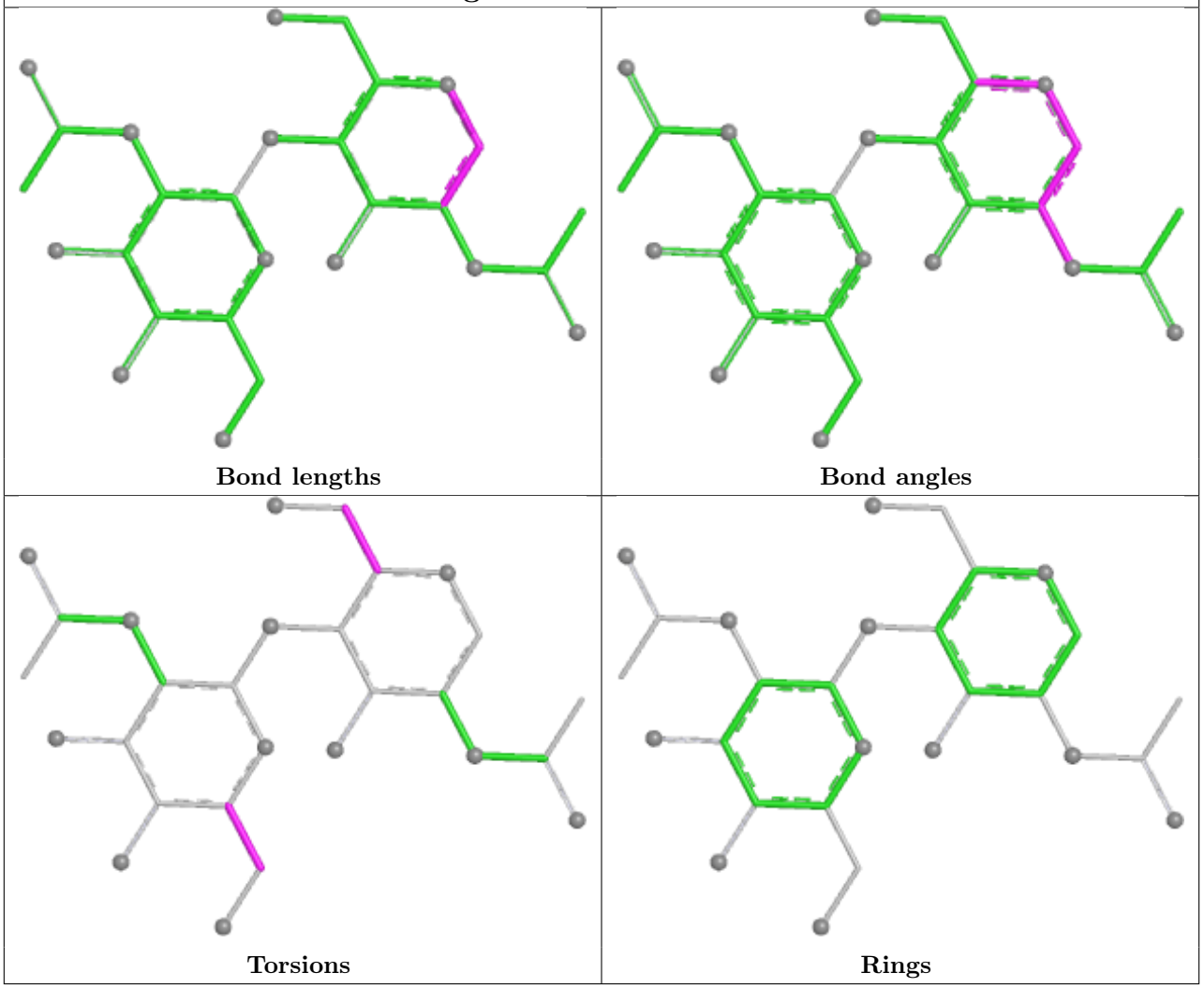
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	A	4603	1	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	A	4601	1	14,14,15	0.27	0	17,19,21	0.46	0
8	NAG	A	4602	1	14,14,15	0.31	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	A	4604	1	14,14,15	0.37	0	17,19,21	1.33	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	4603	1	-	4/6/23/26	0/1/1/1
8	NAG	A	4601	1	-	2/6/23/26	0/1/1/1
8	NAG	A	4602	1	-	0/6/23/26	0/1/1/1
8	NAG	A	4604	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	4604	NAG	C2-N2-C7	4.62	129.09	122.90
8	A	4604	NAG	C1-C2-N2	2.03	113.64	110.43

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	4603	NAG	C4-C5-C6-O6
8	A	4601	NAG	C4-C5-C6-O6
8	A	4603	NAG	O5-C5-C6-O6
8	A	4601	NAG	O5-C5-C6-O6
8	A	4603	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	4601	NAG	1	0
8	A	4602	NAG	2	0
8	A	4604	NAG	1	0

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.

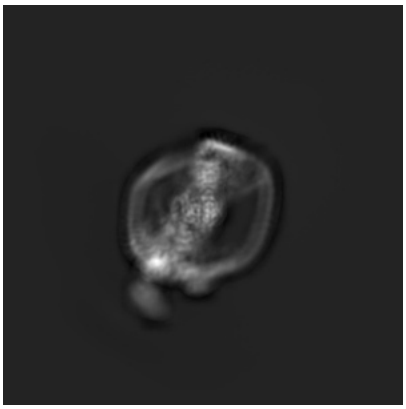
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44469. These allow visual inspection of the internal detail of the map and identification of artifacts.

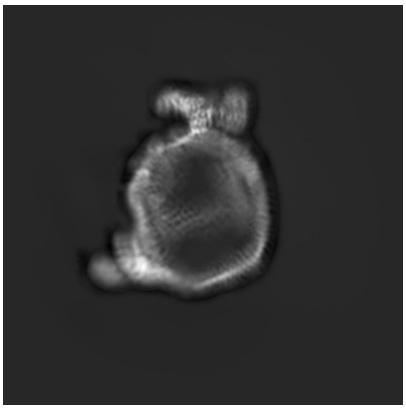
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

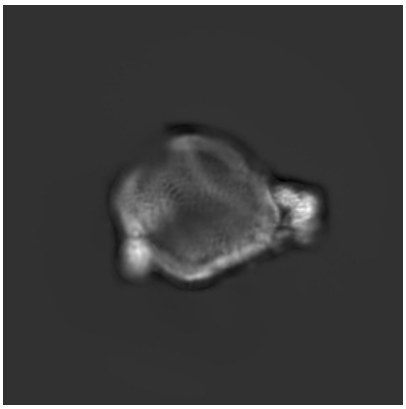
6.1.1 Primary map



X

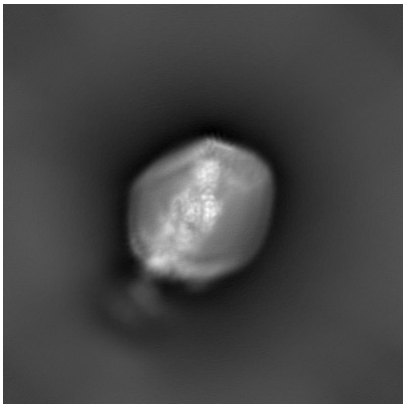


Y

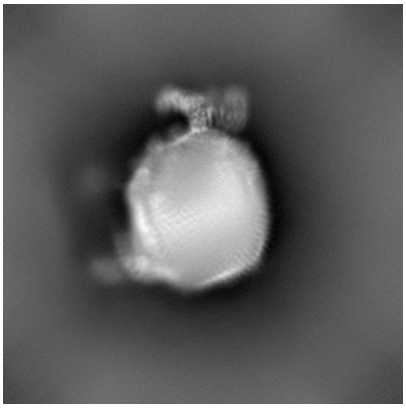


Z

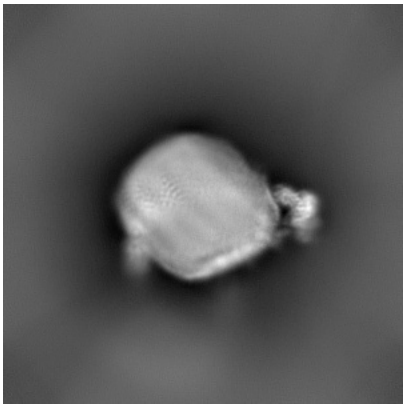
6.1.2 Raw map



X



Y



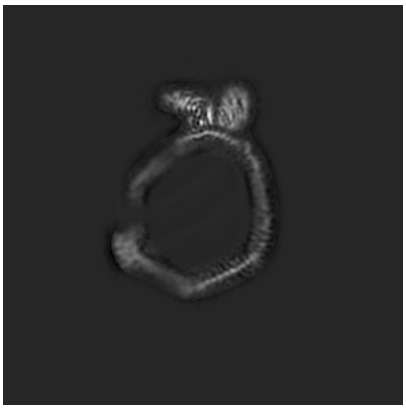
Z

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

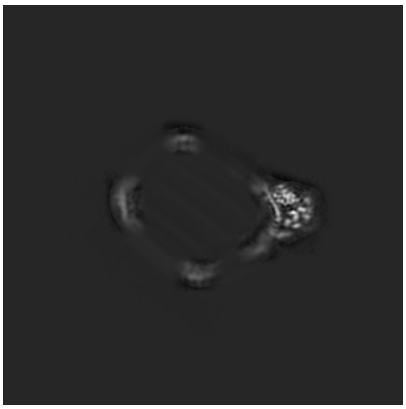
6.2 Central slices (i)

6.2.1 Primary map

X Index: 168

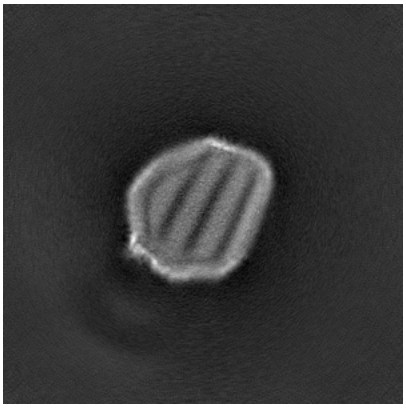


Y Index: 168

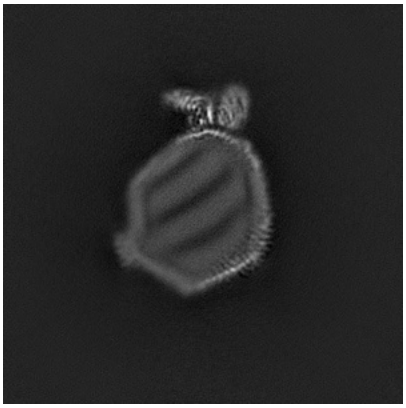


Z Index: 168

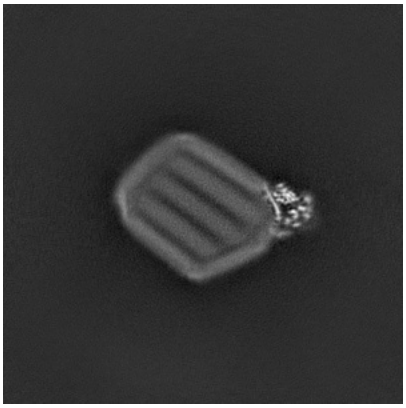
6.2.2 Raw map



X Index: 168



Y Index: 168

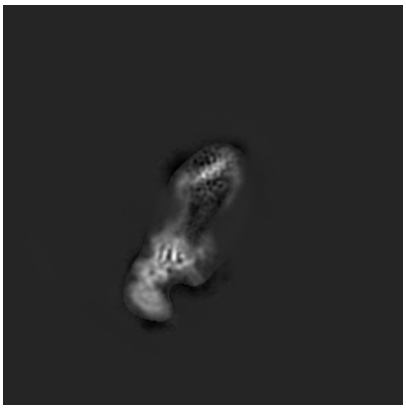


Z Index: 168

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

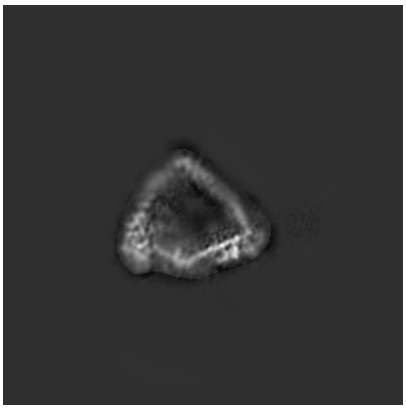
6.3 Largest variance slices (i)

6.3.1 Primary map



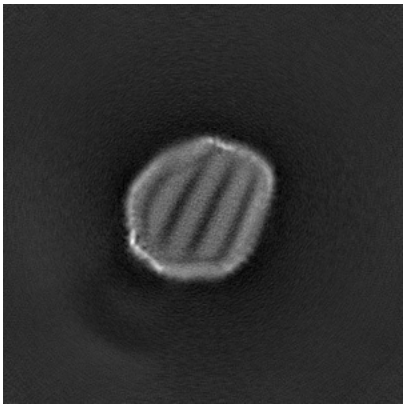
X Index: 112

Y Index: 171

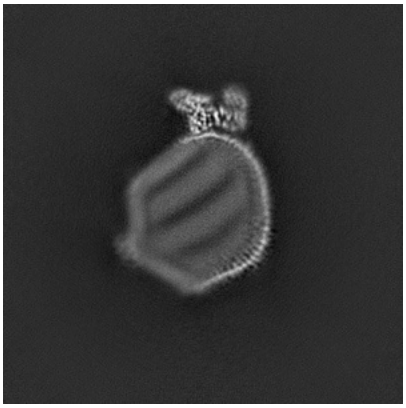


Z Index: 120

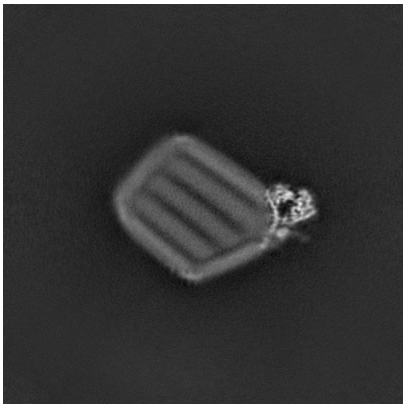
6.3.2 Raw map



X Index: 164



Y Index: 172

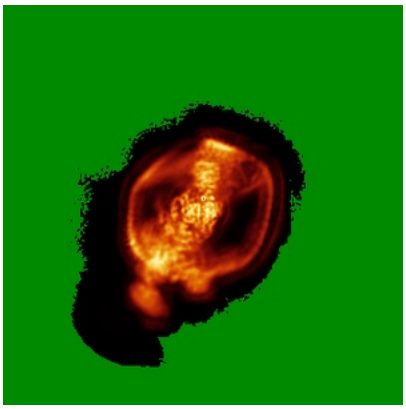


Z Index: 160

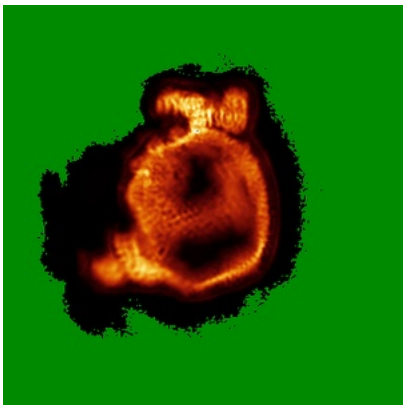
The images above show the largest variance slices of the map in three orthogonal directions.

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

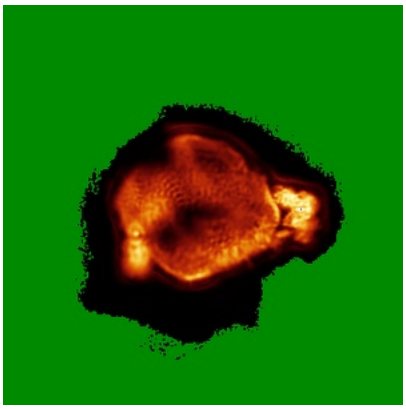
6.4.1 Primary map



X

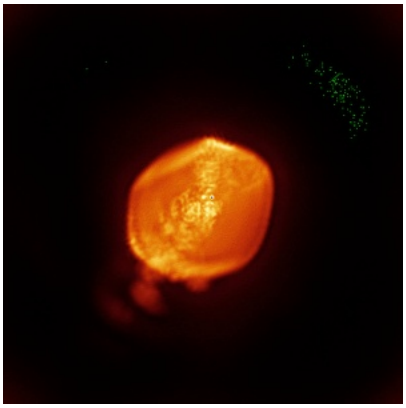


Y

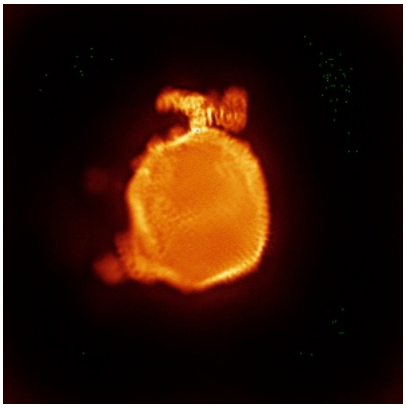


Z

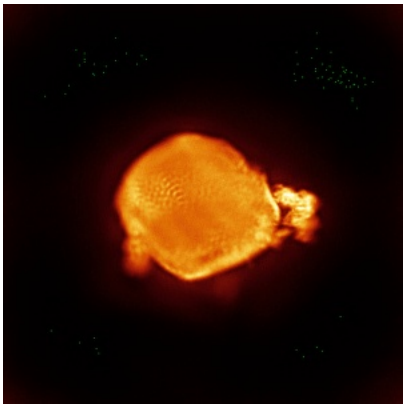
6.4.2 Raw map



X



Y



Z

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

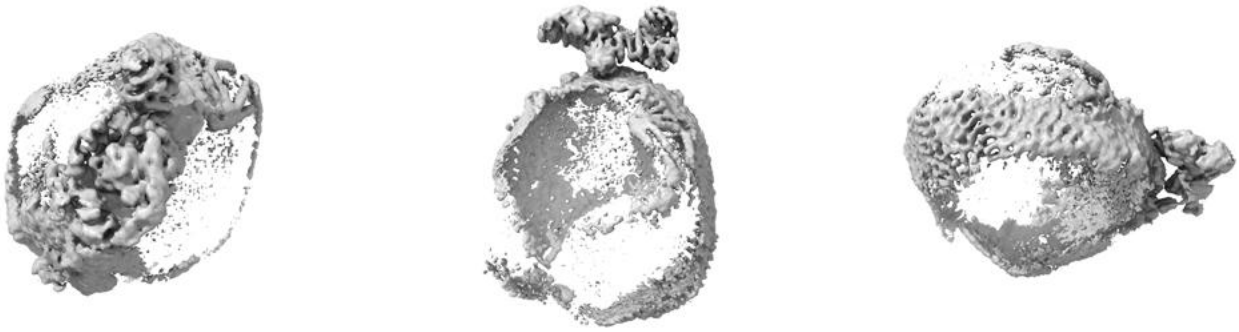
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map



X Y Z

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

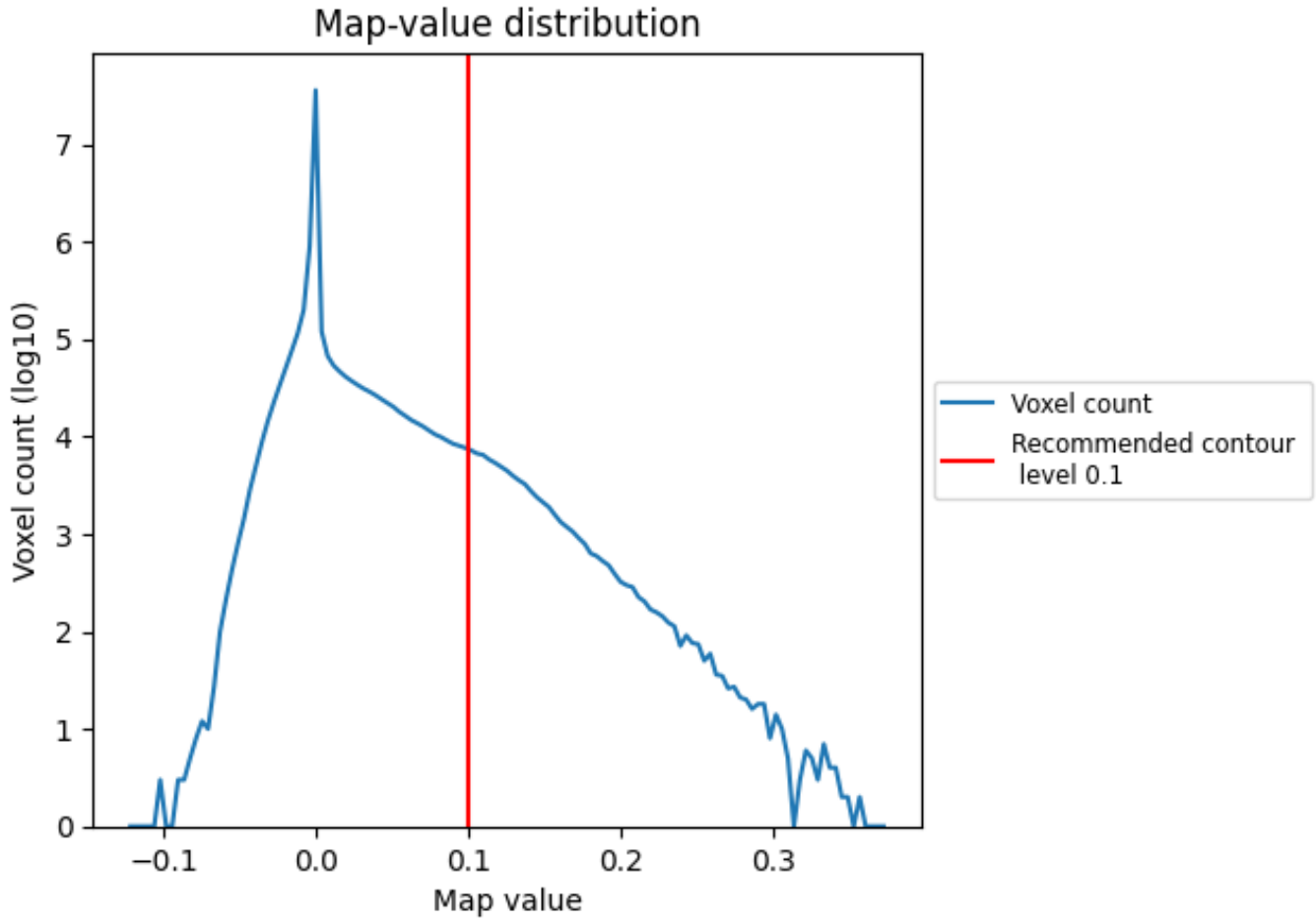
6.6 Mask visualisation (i)

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

7 Map analysis

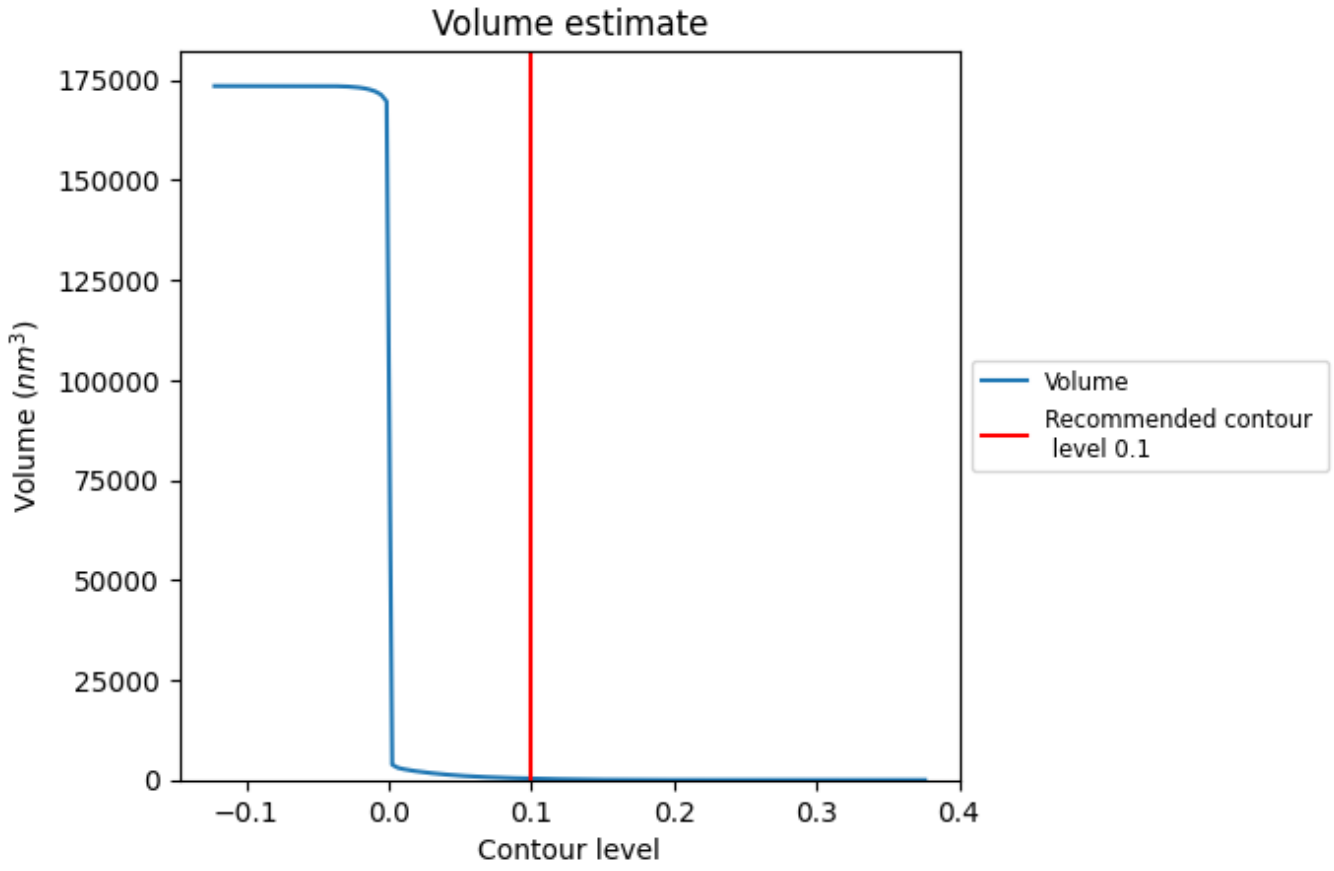
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

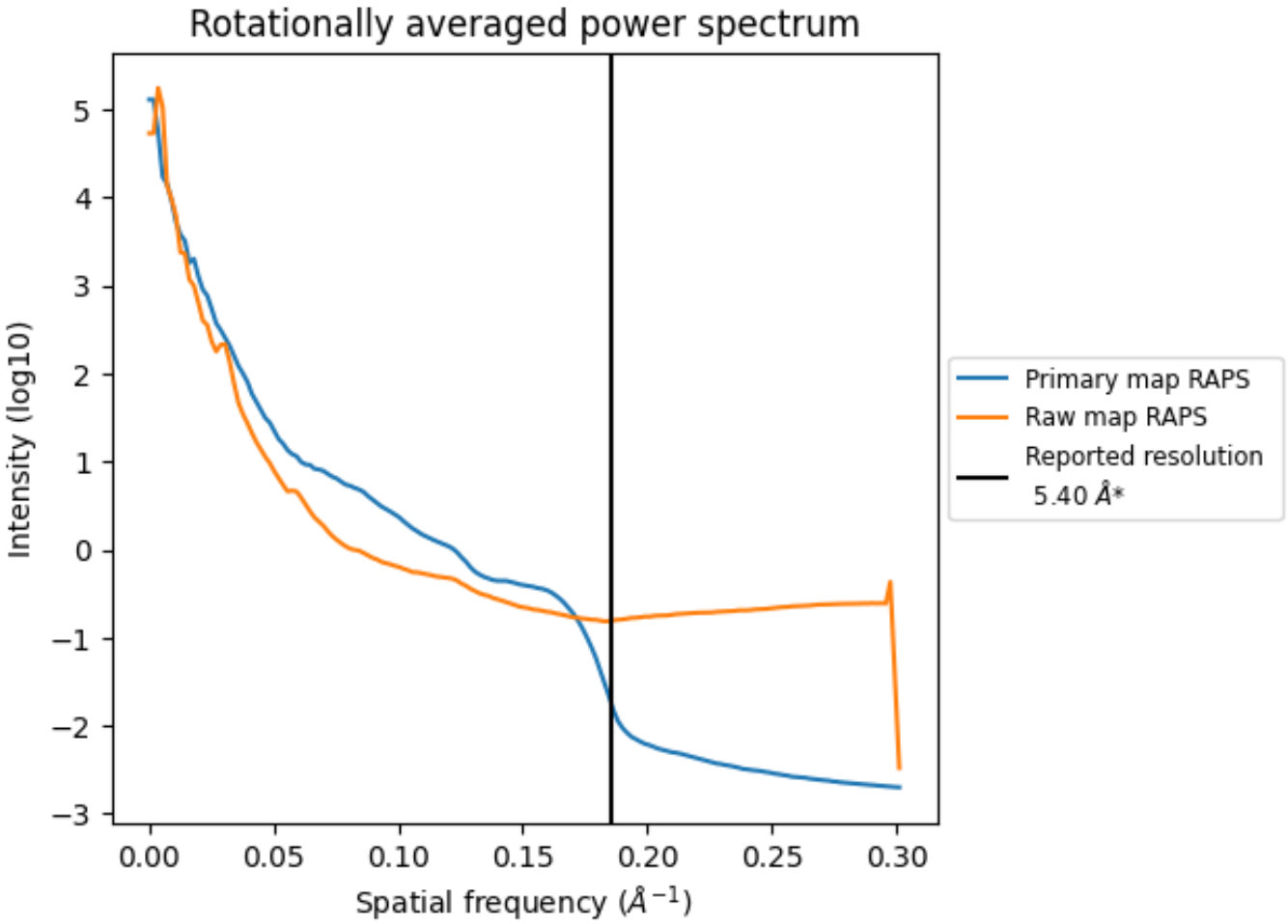
7.2 Volume estimate (i)



The volume at the recommended contour level is 346 nm^3; this corresponds to an approximate mass of 313 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)

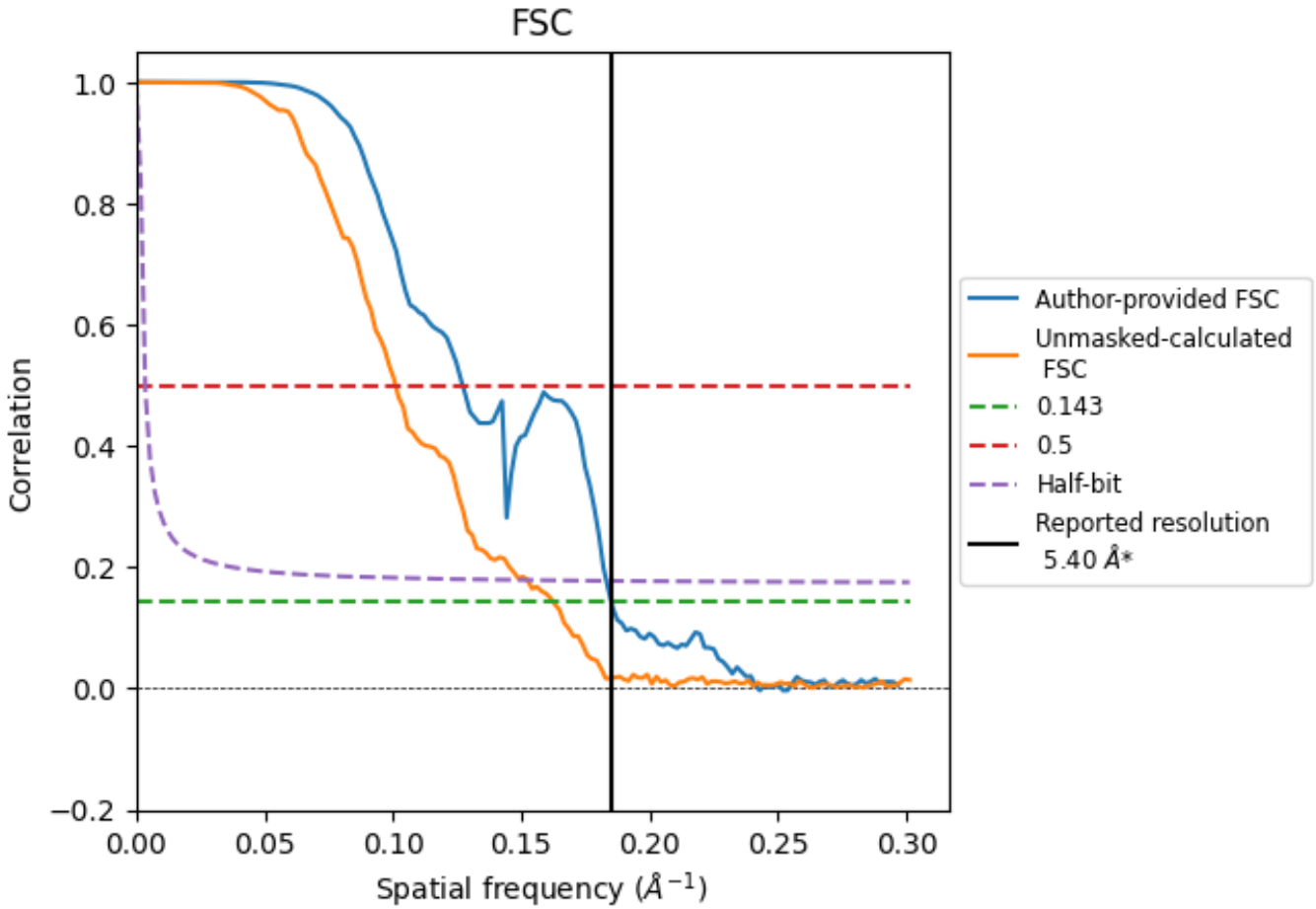


*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8.2 Resolution estimates (i)

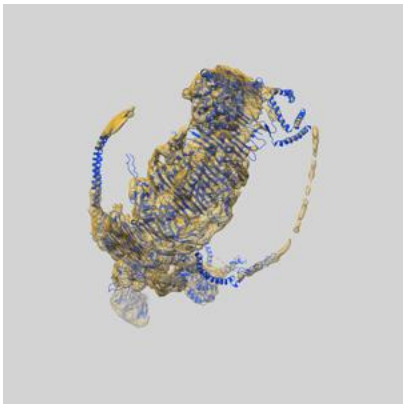
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	5.41	7.87	5.46
Unmasked-calculated*	6.16	9.90	6.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.16 differs from the reported value 5.4 by more than 10 %

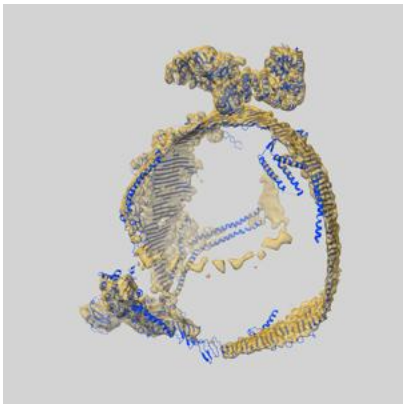
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44469 and PDB model 9BDT. Per-residue inclusion information can be found in section 3 on page 7.

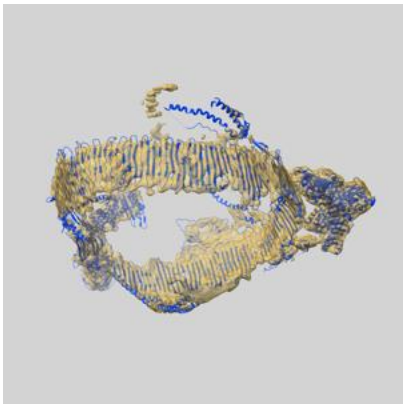
9.1 Map-model overlay



X



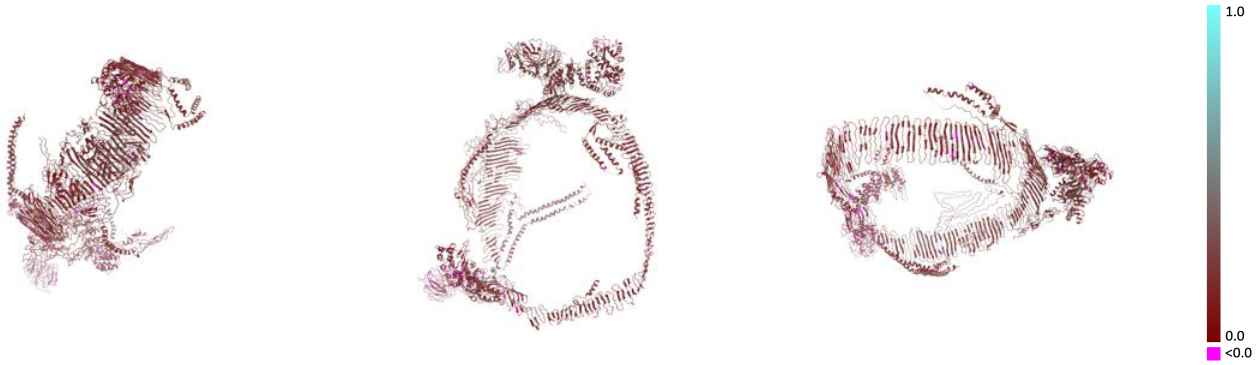
Y



Z

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

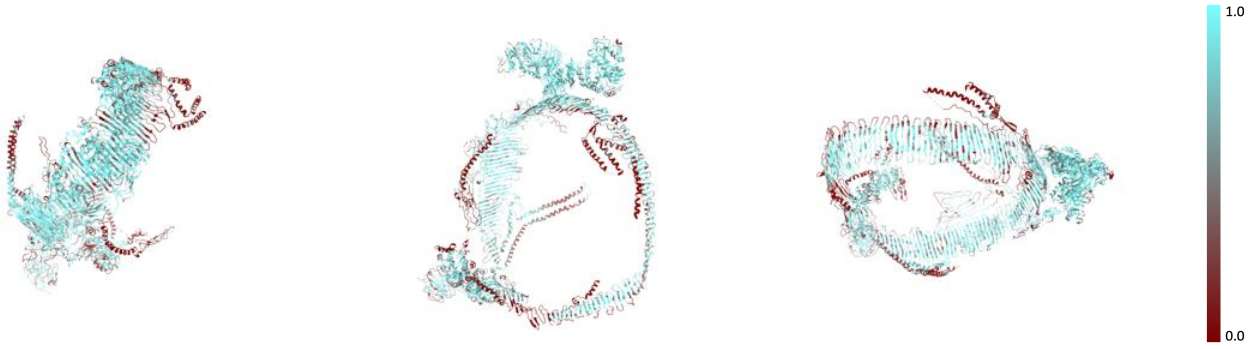
9.2 Q-score mapped to coordinate model (i)



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.

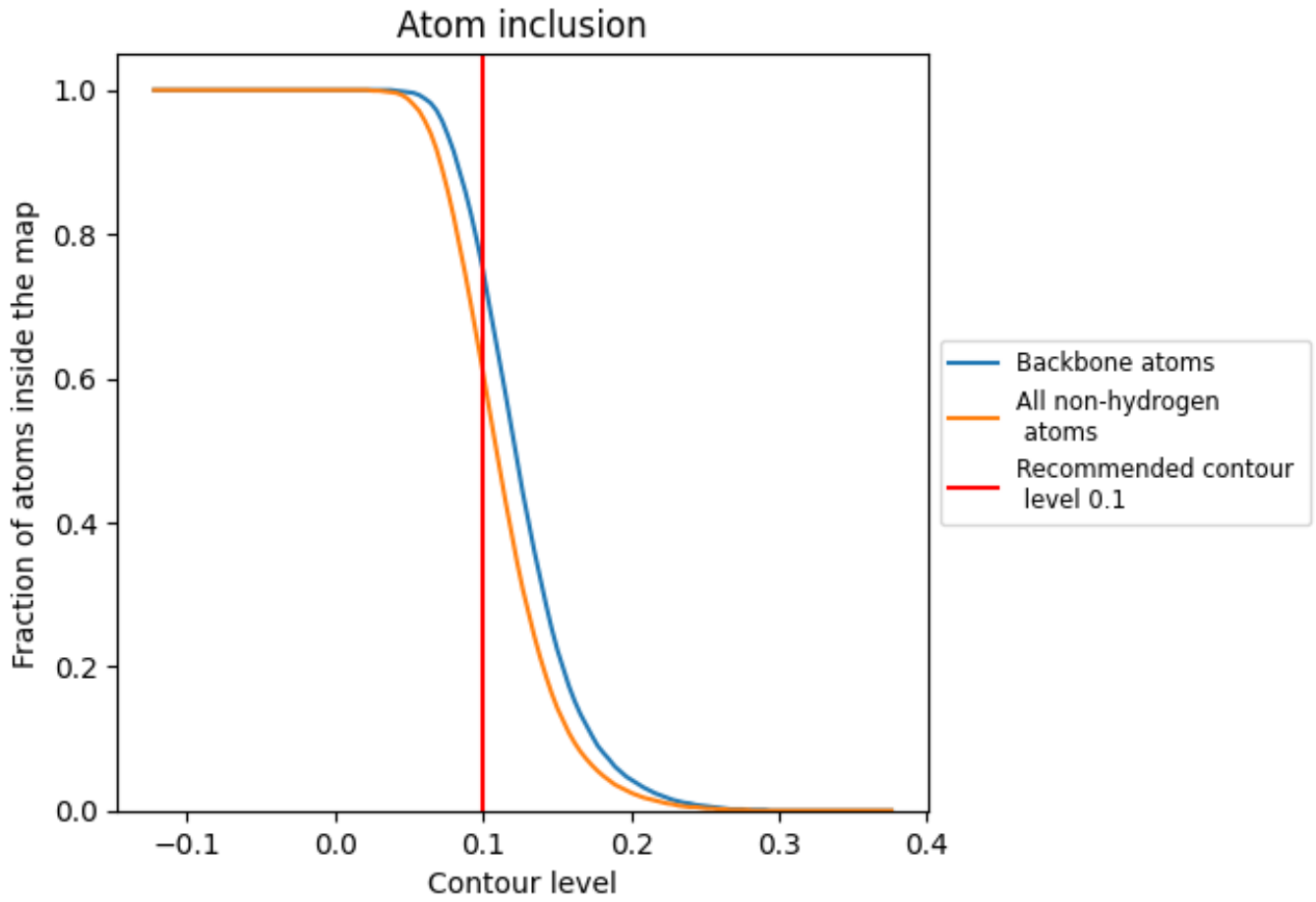
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6080	0.1980
A	0.5500	0.1950
B	0.7640	0.2050
G	0.5000	0.3120
H	0.8240	0.2450
I	0.5950	0.0930
L	0.8130	0.2580
N	0.8820	0.2910
R	0.6770	0.2090