wwPDB EM Validation Summary Report (i)

Apr 5, 2022 – 01:17 pm BST

PDB ID	:	7O7M
EMDB ID	:	EMD-12748
Title	:	(h-alpha2M)4 native II
Authors	:	Luque, D.; Goulas, T.; Mata, C.P.; Mendes, S.R.; Gomis-Ruth, F.X.; Caston, J.R.
Deposited on	:	2021-04-13
Resolution	:	6.60 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 following versions of software and data (see references (i)) were used in the production of this report:

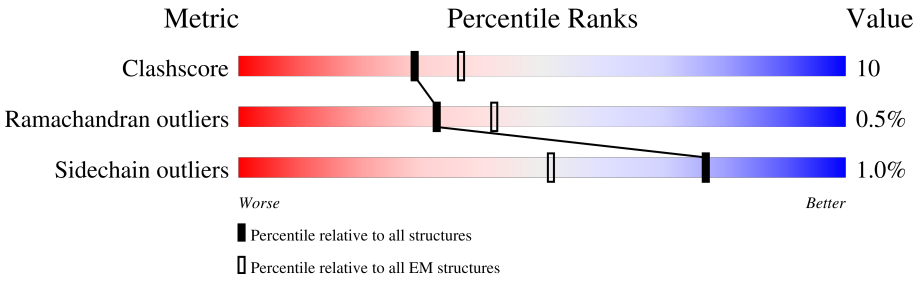
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 6.60 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	1474	73% 77% 19% .
1	B	1474	29% 69% 26% . .
1	C	1474	73% 76% 19% .
1	D	1474	29% 69% 26% . .
2	E	4	25% 25% 50% 25%
2	H	4	25% 25% 50% 25%
3	F	3	33% 33% 67%
3	I	3	33% 33% 67%

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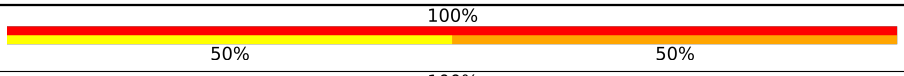
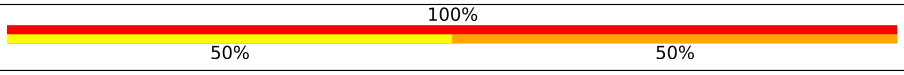
Mol	Chain	Length	Quality of chain
4	G	2	
4	J	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 44614 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.

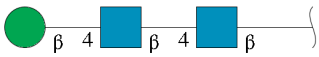
- Molecule 1 is a protein called Alpha-2-macroglobulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	B	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	C	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	D	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	4	Total	C	N	O	0	0
			50	28	2	20		
2	H	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		

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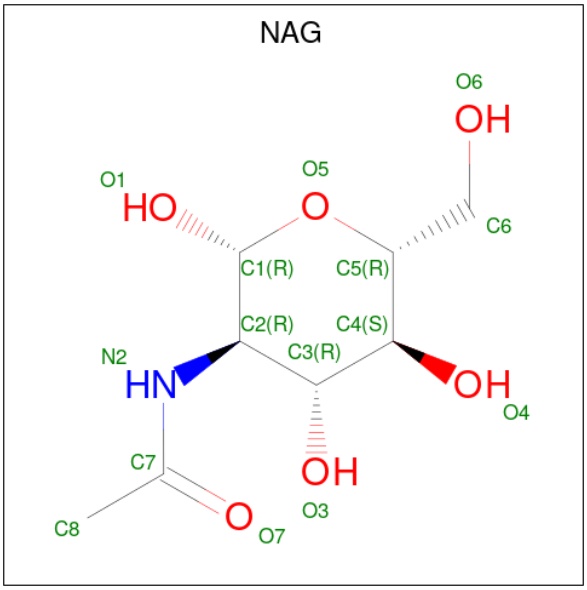
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 4 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
4	G	2	Total 28	C 16	N 2	O 10	0	0
4	J	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 112	C 64	N 8	O 40	0
5	A	1	Total 112	C 64	N 8	O 40	0
5	A	1	Total 112	C 64	N 8	O 40	0

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Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	A	1	Total C N O 112 64 8 40	0
5	B	1	Total C N O 70 40 5 25	0
5	B	1	Total C N O 70 40 5 25	0
5	B	1	Total C N O 70 40 5 25	0
5	B	1	Total C N O 70 40 5 25	0
5	B	1	Total C N O 70 40 5 25	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0
5	C	1	Total C N O 112 64 8 40	0
5	D	1	Total C N O 70 40 5 25	0
5	D	1	Total C N O 70 40 5 25	0
5	D	1	Total C N O 70 40 5 25	0

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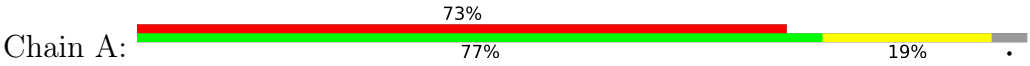
Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			70	40	5	25	
5	D	1	Total	C	N	O	0
			70	40	5	25	

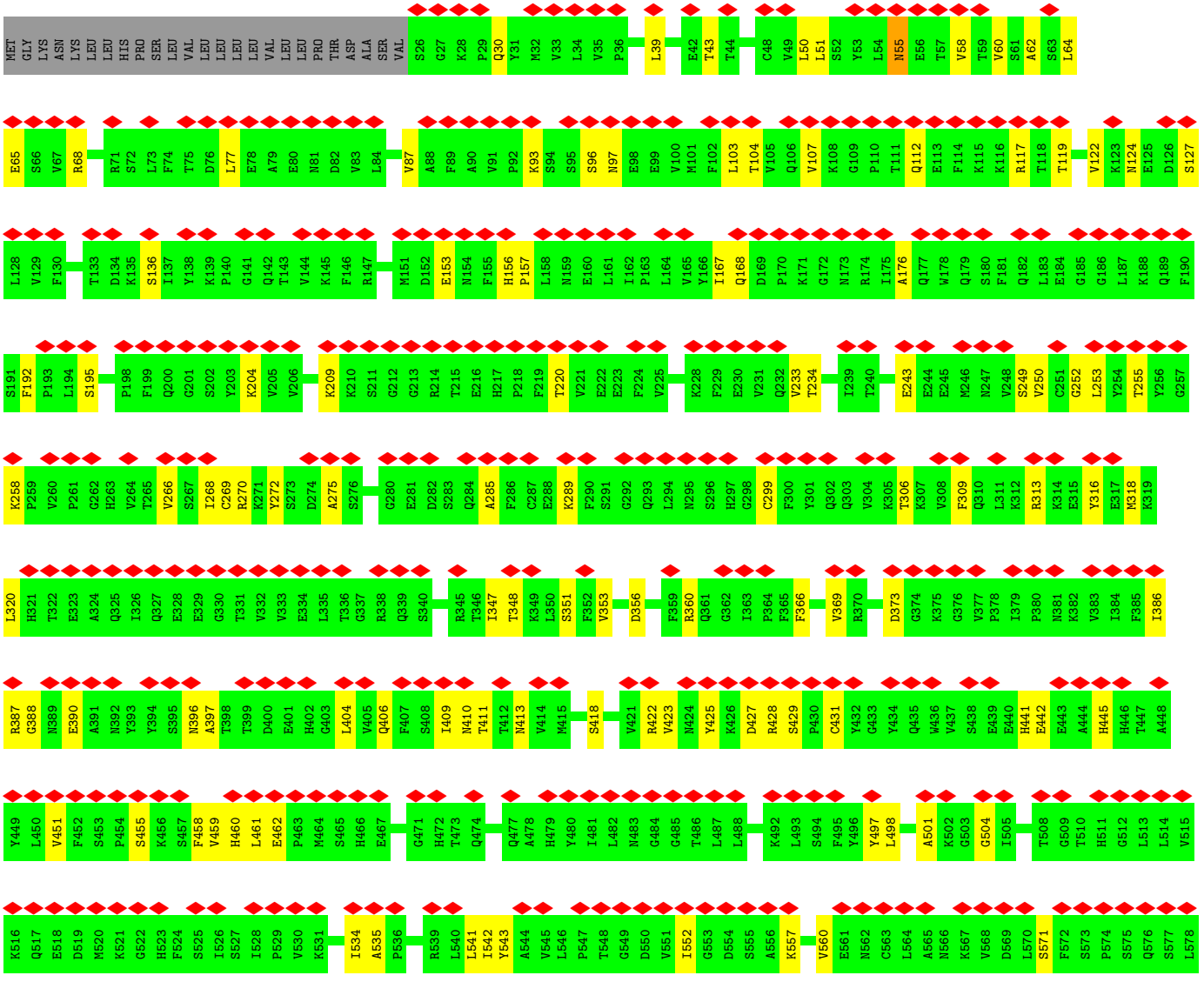
3 Residue-property plots (i)

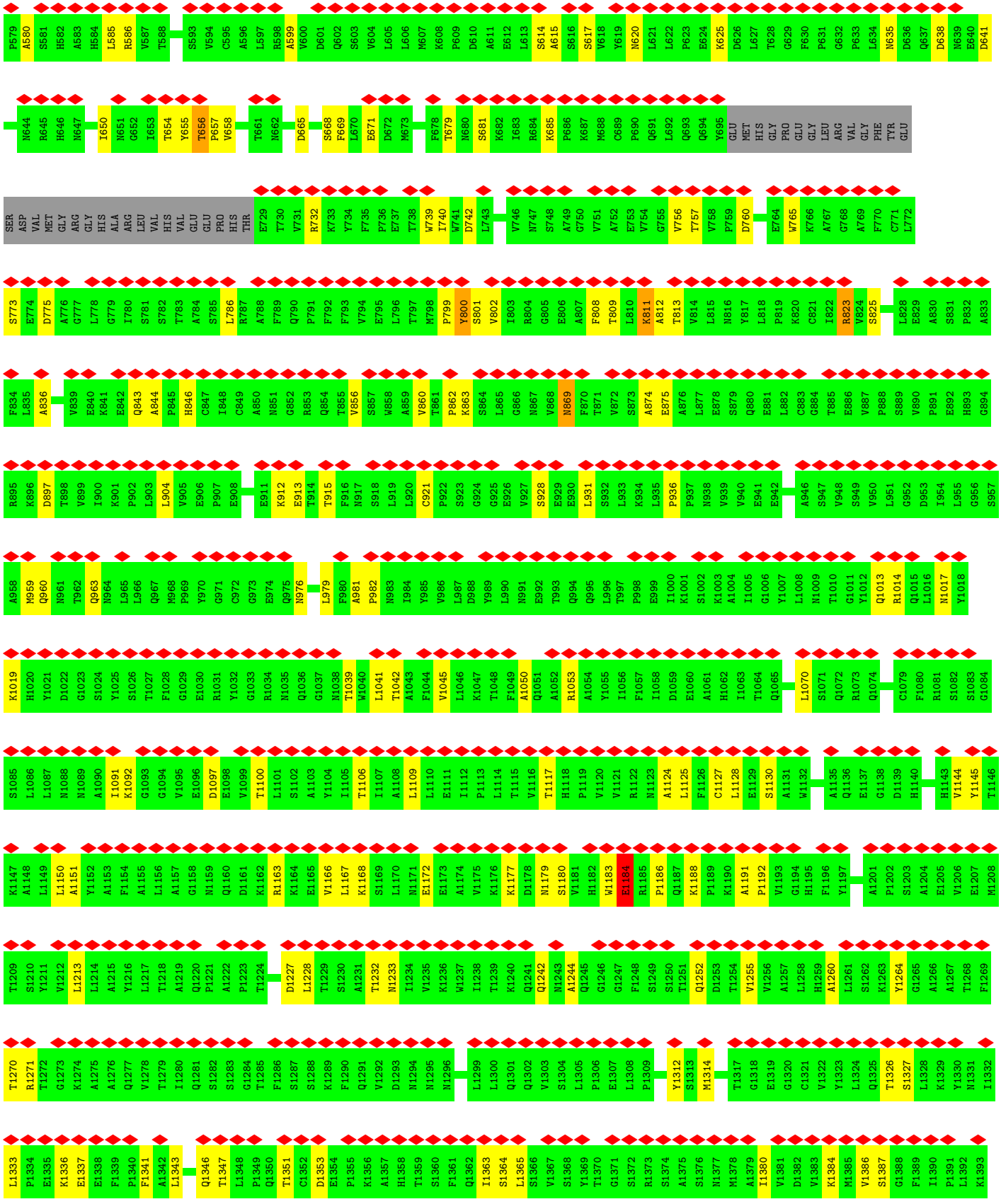
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Alpha-2-macroglobulin

Chain A:



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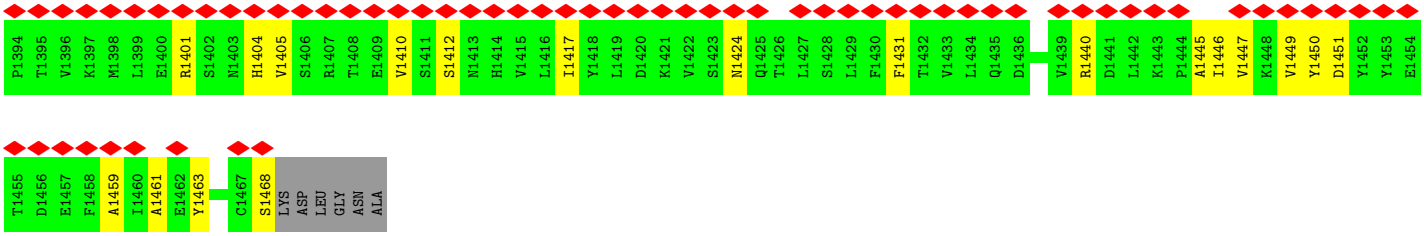
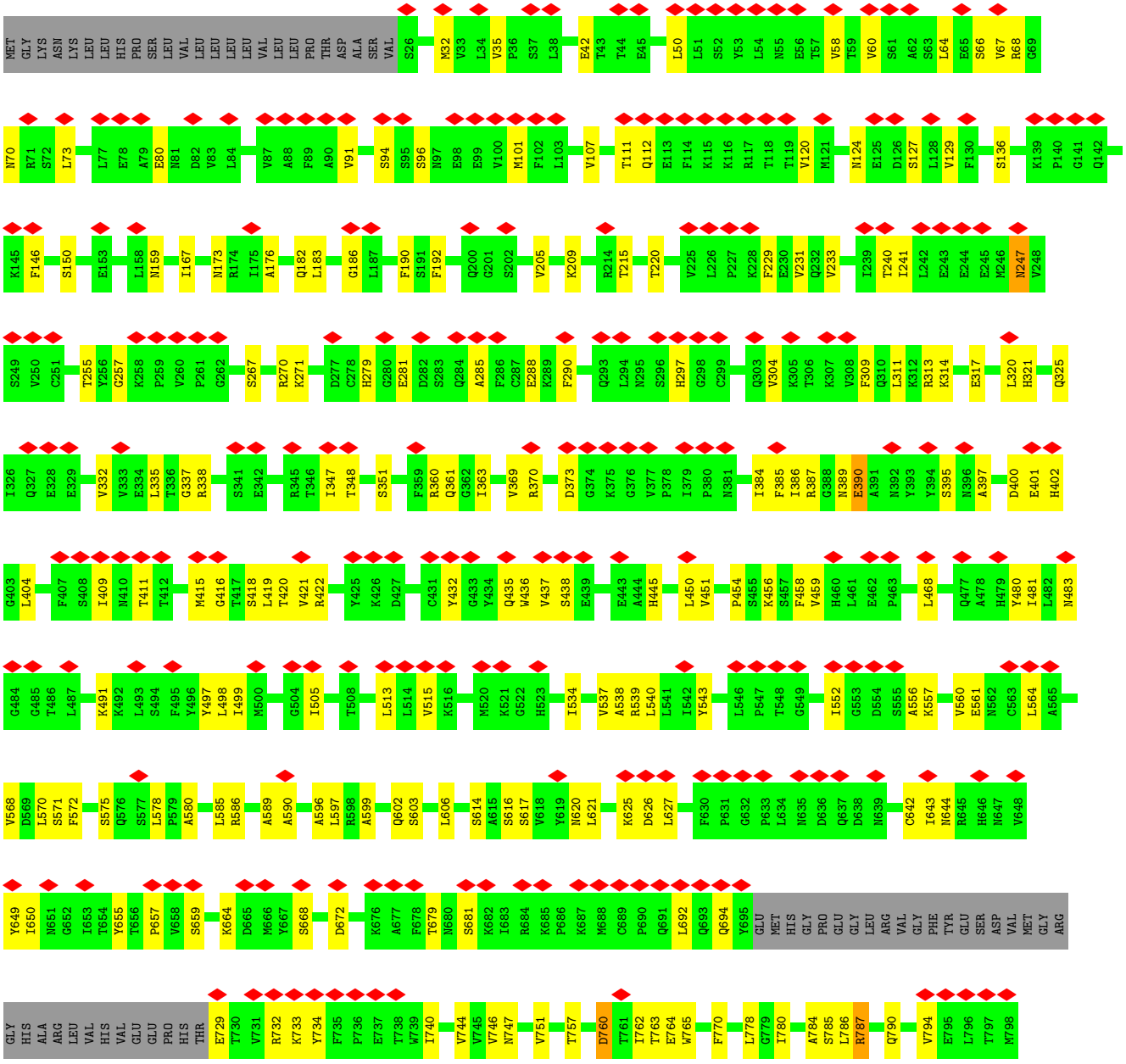
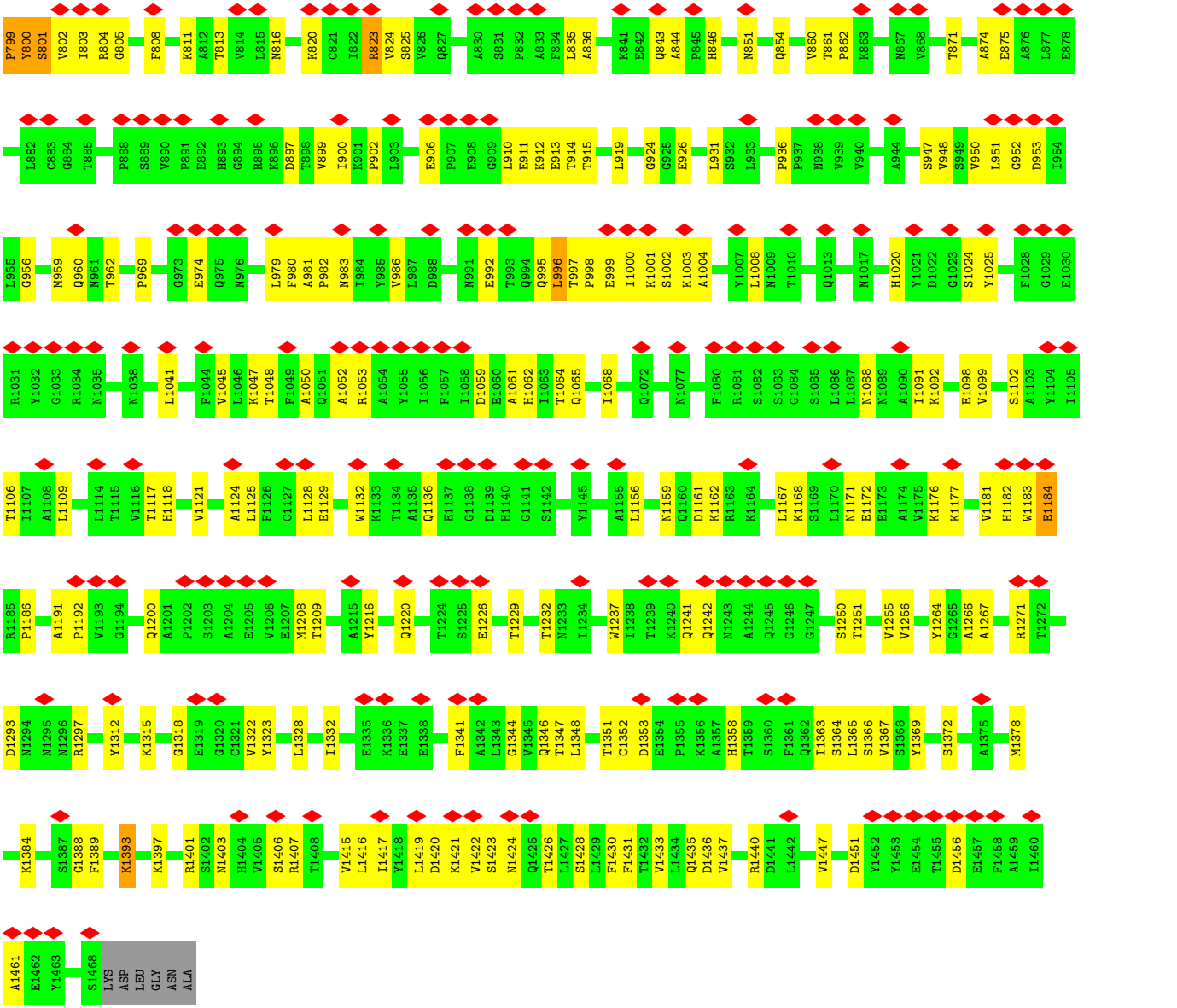
W644 R645 H646 N647 I650 N651 G652 I653 T654 Y655 T656 P657 V658 T661 N662 D665 S668 F669 L670 E671 D672 M673 F678 T679 N680 S681 K682 I683 R684 K685 P686 K687 M688 C689 P690 Q691 L692 Q693 Q694 Y695 GLU MET HIS GLY PRO GLU GLY LEU ARG VAL GLY PHE TYR GLU
SER ASP VAL MET GLY ARG GLY HIS ALA ARG LEU VAL HIS VAL GLU GLU PRO HIS THR E729 T730 V731 R732 K733 Y734 F735 P736 E737 T738 W739 I740 W741 D742 L743 V746 N747 S748 A749 G750 V751 A752 E753 V754 G755 V756 T757 V758 P759 D760 E764 W765 K766 A767 G768 A769 F770 C771 L772
S773 E774 D775 A776 G777 L778 G779 I780 S781 S782 T783 A784 S785 L786 R787 A788 F789 Q790 P791 F792 F793 V794 E795 L796 T797 M798 P799 Y800 S801 V802 I803 R804 G805 E806 A807 F808 T809 L810 K811 A812 T813 V814 L815 N816 Y817 L818 P819 K820 C821 I822 R823 V824 S825 L828 E829 A830 S831 P832 A833
F834 L835 A836 V839 E840 K841 E842 Q843 A844 P845 H846 C847 I848 C849 A850 N851 G852 R853 Q854 T855 V856 S857 W858 A859 V860 T861 P862 K863 S864 L865 G866 N867 V868 N869 F870 T871 V872 S873 A874 E875 A876 L877 E878 S879 Q880 E881 L882 C883 G884 T885 E886 V887 P888 S889 V890 P891 E892 H893 G894
R895 K896 D897 T898 V899 I900 K901 P902 L903 L904 V905 E906 P907 E908 E911 K912 E913 T914 T915 F916 N917 S918 L919 L920 C921 P922 S923 G924 G925 E926 V927 S928 E929 E930 L931 S932 L933 K934 L935 P936 P937 N938 V939 V940 E941 E942 A946 S947 V948 S949 V950 L951 G952 D953 I954 L955 G956 S957
A958 M959 Q960 N961 T962 Q963 N964 L965 L966 Q967 M968 P969 Y970 G971 C972 G973 E974 Q975 N976 L979 F980 A981 P982 N983 I984 Y985 V986 L987 D988 Y989 L990 N991 E992 T993 Q994 Q995 L996 T997 P998 E999 I1000 K1001 S1002 K1003 A1004 I1005 G1006 Y1007 L1008 N1009 T1010 G1011 Y1012 Q1013 R1014 Q1015 L1016 N1017 Y1018
K1019 H1020 Y1021 D1022 G1023 S1024 Y1025 S1026 T1027 F1028 G1029 E1030 R1031 Y1032 G1033 R1034 N1035 Q1036 G1037 N1038 T1039 W1040 L1041 T1042 A1043 F1044 V1045 L1046 K1047 T1048 F1049 A1050 Q1051 A1052 R1053 A1054 Y1055 I1056 F1057 I1058 D1059 E1060 A1061 H1062 I1063 T1064 Q1065 L1070 S1071 Q1072 R1073 Q1074 C1079 F1080 R1081 S1082 S1083 G1084
S1085 L1086 L1087 N1088 N1089 A1090 I1091 K1092 G1093 G1094 V1095 E1096 D1097 E1098 V1099 T1100 L1101 S1102 A1103 Y1104 I1105 T1106 I1107 A1108 L1109 L1110 E1111 I1112 P1113 L1114 T1115 V1116 T1117 H1118 P1119 V1120 V1121 R1122 N1123 A1124 L1125 F1126 C1127 L1128 E1129 S1130 A1131 W1132 A1135 Q1136 E1137 G1138 D1139 H1140 H1143 V1144 Y1145 T1146
K1147 A1148 L1149 L1150 A1151 Y1152 A1153 F1154 A1155 L1156 A1157 G1158 N1159 Q1160 D1161 K1162 R1163 K1164 E1165 V1166 L1167 K1168 S1169 L1170 N1171 E1172 E1173 A1174 V1175 K1176 K1177 D1178 N1179 S1180 V1181 H1182 W1183 E1184 R1185 P1186 Q1187 K1188 P1189 K1190 A1191 P1192 V1193 G1194 H1195 F1196 Y1197 A1201 P1202 S1203 A1204 E1205 V1206 E1207 M1208
T1209 S1210 Y1211 V1212 L1213 L1214 A1215 Y1216 L1217 T1218 A1219 Q1220 P1221 A1222 P1223 T1224 D1227 L1228 T1229 S1230 A1231 T1232 N1233 I1234 V1235 K1236 W1237 I1238 T1239 K1240 Q1241 Q1242 N1243 A1244 Q1245 G1246 G1247 F1248 S1249 S1250 T1251 Q1252 D1253 T1254 V1255 V1256 A1257 L1258 H1259 A1260 L1261 S1262 K1263 Y1264 G1265 A1266 A1267 T1268 F1269
T1270 R1271 T1272 G1273 K1274 A1275 A1276 Q1277 V1278 T1279 I1280 Q1281 S1282 S1283 G1284 T1285 F1286 S1287 S1288 K1289 F1290 Q1291 V1292 D1293 N1294 N1295 N1296 L1299 L1300 Q1301 Q1302 V1303 S1304 L1305 P1306 E1307 L1308 P1309 Y1312 S1313 M1314 T1317 G1318 E1319 G1320 C1321 V1322 Y1323 L1324 Q1325 T1326 S1327 L1328 K1329 Y1330 N1331 I1332
L1333 P1334 E1335 K1336 E1337 E1338 F1339 P1340 F1341 A1342 L1343 Q1346 T1347 L1348 P1349 Q1350 T1351 C1352 D1353 E1354 P1355 K1356 A1357 H1358 T1359 S1360 F1361 Q1362 I1363 S1364 L1365 S1366 V1367 S1368 Y1369 T1370 G1371 S1372 R1373 S1374 A1375 S1376 N1377 M1378 A1379 I1380 V1381 D1382 V1383 K1384 M1385 V1386 S1387 G1388 F1389 I1390 P1391 L1392 K1393



• Molecule 1: Alpha-2-macroglobulin

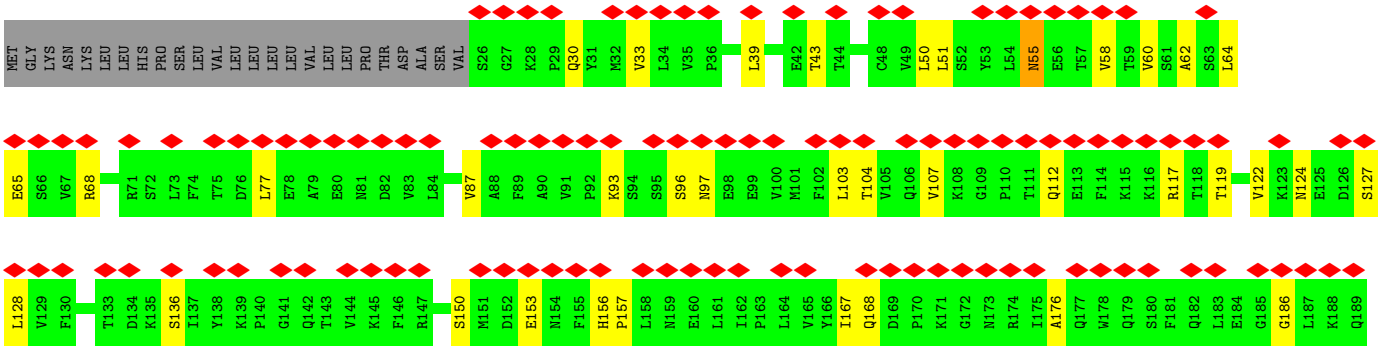
Chain B:

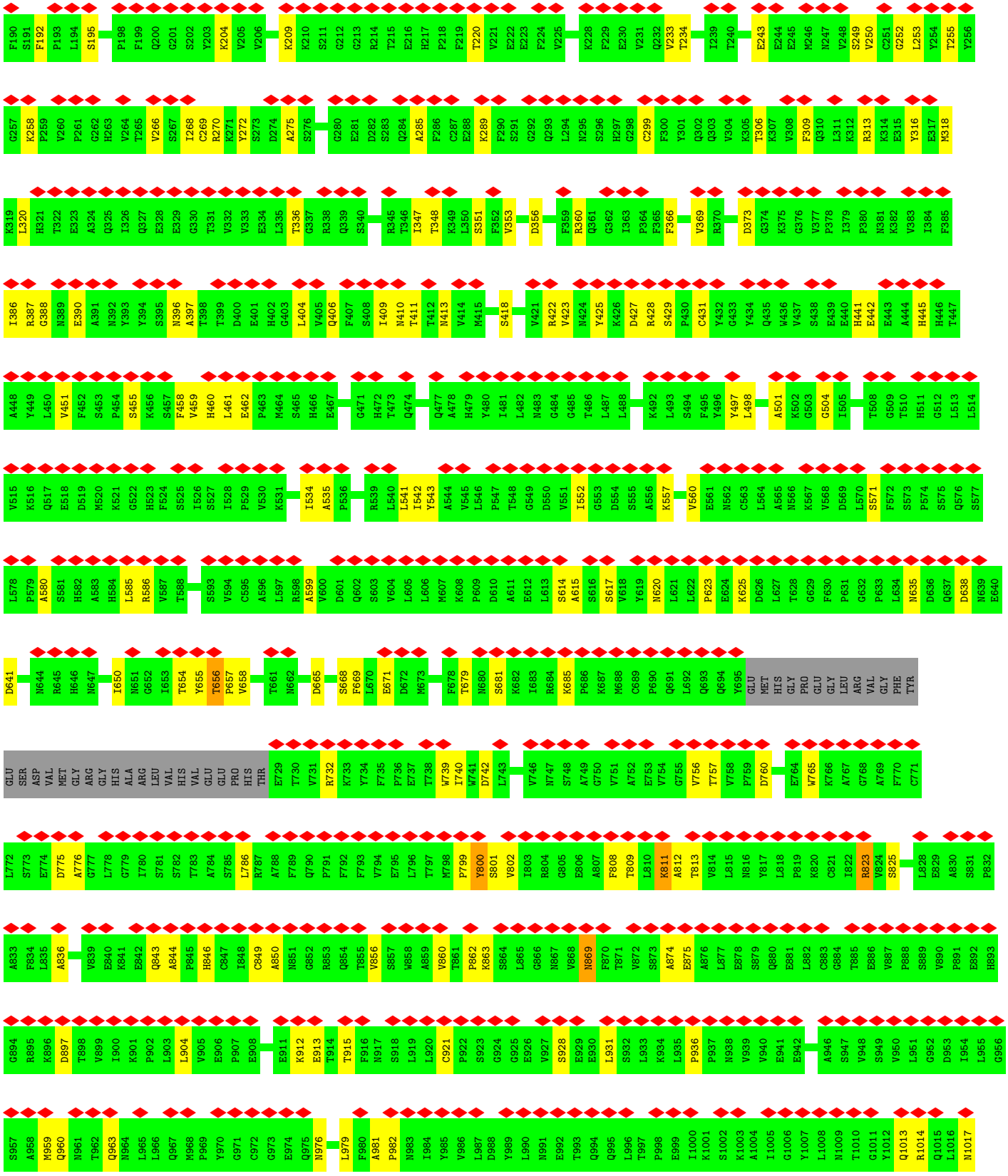




• Molecule 1: Alpha-2-macroglobulin

Chain C:




F190 S191 F192 P193 L194 S195 P198 F199 Q200 G201 S202 Y203 K204 V205 V206 K209 K210 S211 G212 G213 R214 T215 E216 H217 P218 F219 T220 V221 E222 E223 F224 V225 K228 F229 E230 V231 Q232 V233 T234 I239 T240 E243 E244 E245 M246 N247 V248 S249 V250 C251 G252 L253 Y254 T255 Y256
G257 K258 P259 V260 P261 C262 H263 V264 T265 V266 S267 I268 C269 R270 K271 Y272 S273 D274 A275 S276 G280 E281 D282 S283 Q284 A285 F286 C287 E288 K289 F290 S291 G292 Q293 L294 N295 S296 H297 G298 C299 F300 Y301 Q302 Q303 V304 K305 T306 K307 V308 F309 Q310 L311 K312 R313 K314 E315 Y316 E317 M318
K319 L320 H321 T322 E323 A324 Q325 I326 Q327 E328 E329 G330 T331 V332 V333 E334 L335 T336 G337 R338 Q339 S340 R345 T346 I347 T348 K349 L350 S351 F352 V353 D356 F359 R360 Q361 G362 I363 P364 F365 F366 V369 R370 D373 G374 K375 G376 V377 P378 I379 P380 N381 K382 V383 I384 F385
I386 R387 G388 N389 E390 A391 N392 Y393 Y394 S395 N396 A397 T398 T399 D400 E401 H402 G403 L404 V405 Q406 F407 S408 I409 N410 T411 T412 N413 V414 M415 S418 V421 R422 V423 N424 Y425 K426 D427 R428 S429 P430 C431 Y432 G433 Y434 Q435 W436 V437 S438 E439 E440 H441 E442 E443 A444 H445 H446 T447
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V515 K516 Q517 E518 D519 M520 K521 G522 H523 F524 S525 I526 S527 I528 P529 V530 K531 I534 A535 P536 R539 L540 L541 I542 Y543 A544 V545 L546 P547 T548 G549 D550 V551 I552 G553 D554 S555 A556 K557 V560 E561 N562 C563 L564 A565 N566 K567 V568 D569 L570 S571 F572 S573 P574 S575 Q576 S577
L578 P579 A580 S581 H582 A583 H584 L585 R586 V587 T588 S593 V594 C595 A596 L597 R598 A599 V600 D601 Q602 S603 V604 L605 L606 M607 K608 P609 D610 A611 E612 L613 S614 A615 S616 S617 V618 Y619 N620 L621 L622 P623 E624 K625 D626 L627 T628 G629 F630 P631 G632 P633 L634 N635 D636 Q637 D638 N639 E640
D641 N644 R645 H646 N647 I650 N651 G652 I653 T654 Y655 T656 P657 V658 T661 N662 D665 S668 F669 L670 E671 D672 M673 F678 T679 N680 S681 K682 I683 R684 K685 P686 K687 M688 G689 P690 Q691 L692 Q693 Q694 Y695 GLU MET HIS GLY PRO GLU GLY LEU ARG VAL GLY PHE TYR
GLU SER ASP VAL MET GLY ARG GLY HIS ALA ARG LEU VAL HIS VAL GLU GLU PRO HIS THR E729 T730 V731 R732 K733 Y734 F735 P736 E737 T738 W739 I740 W741 D742 L743 V746 N747 S748 A749 G750 V751 A752 E753 V754 G755 V756 T757 V758 P759 D760 E764 W765 K766 A767 G768 A769 F770 C771
L772 S773 E774 D775 A776 G777 L778 G779 I780 S781 S782 T783 A784 S785 L786 R787 A788 F789 Q790 P791 F792 F793 V794 E795 L796 T797 M798 P799 Y800 S801 V802 I803 R804 G805 E806 A807 F808 T809 L810 K811 A812 T813 V814 L815 N816 Y817 L818 P819 K820 C821 I822 R823 V824 S825 L828 E829 A830 S831 P832
A833 F834 L835 A836 V839 E840 K841 E842 Q843 A844 P845 H846 C847 I848 C849 A850 N851 Q852 R853 Q854 T855 V856 S857 W858 A859 V860 T861 P862 K863 S864 L865 G866 N867 V868 N869 F870 T871 V872 S873 A874 E875 A876 L877 E878 S879 Q880 E881 L882 C883 G884 T885 E886 V887 P888 S889 V890 P891 E892 H893
G894 R895 K896 D897 T898 V899 I900 K901 P902 L903 L904 V905 E906 P907 E908 E911 K912 E913 T914 T915 F916 N917 S918 L919 L920 C921 P922 S923 G924 G925 E926 V927 S928 E929 E930 L931 S932 L933 K934 L935 P936 P937 N938 V939 V940 E941 E942 A946 S947 V948 S949 V950 L951 G952 D953 I954 L955 G956
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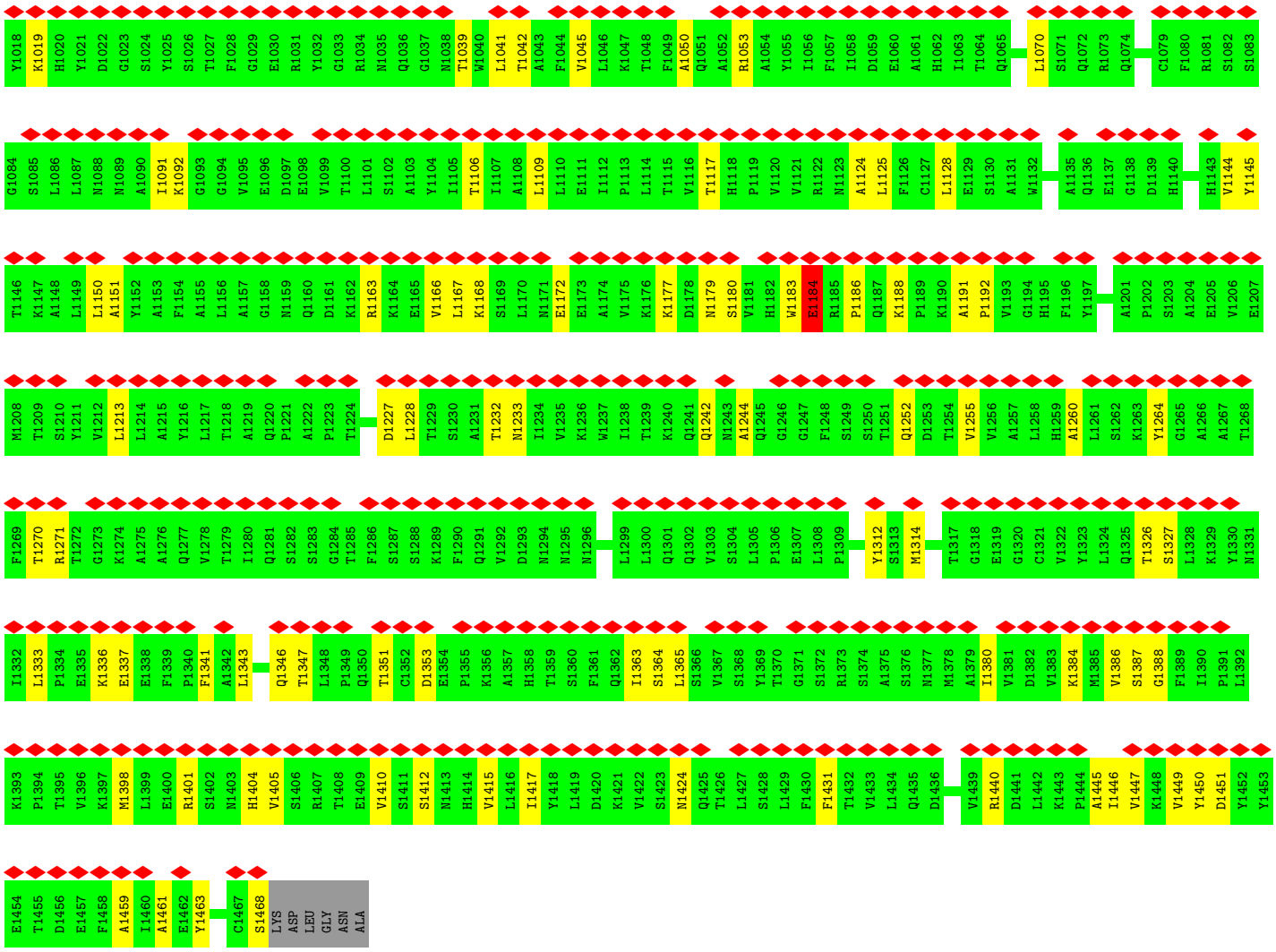
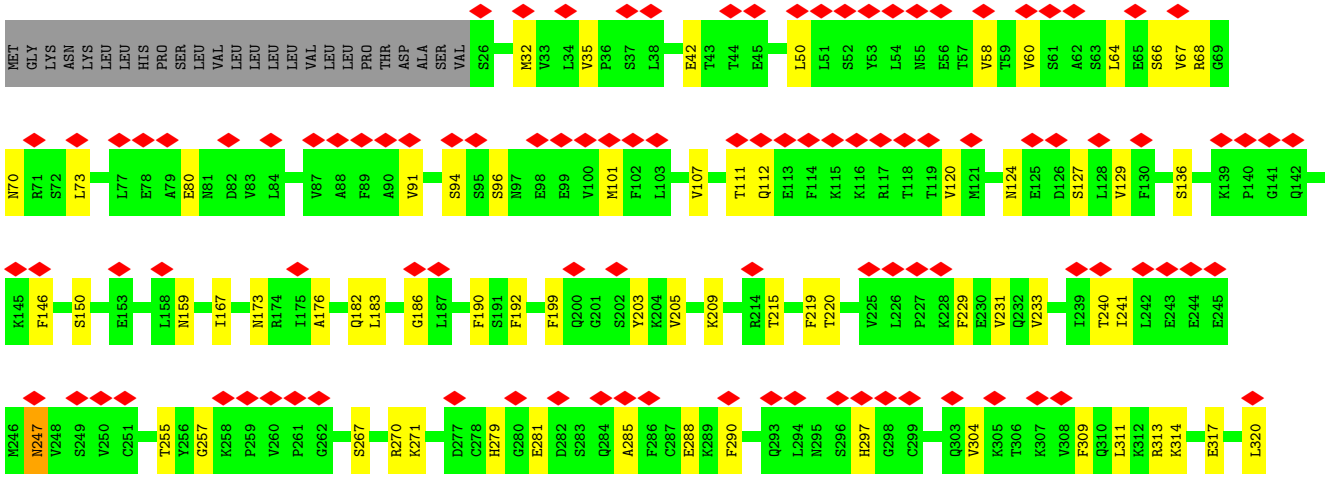
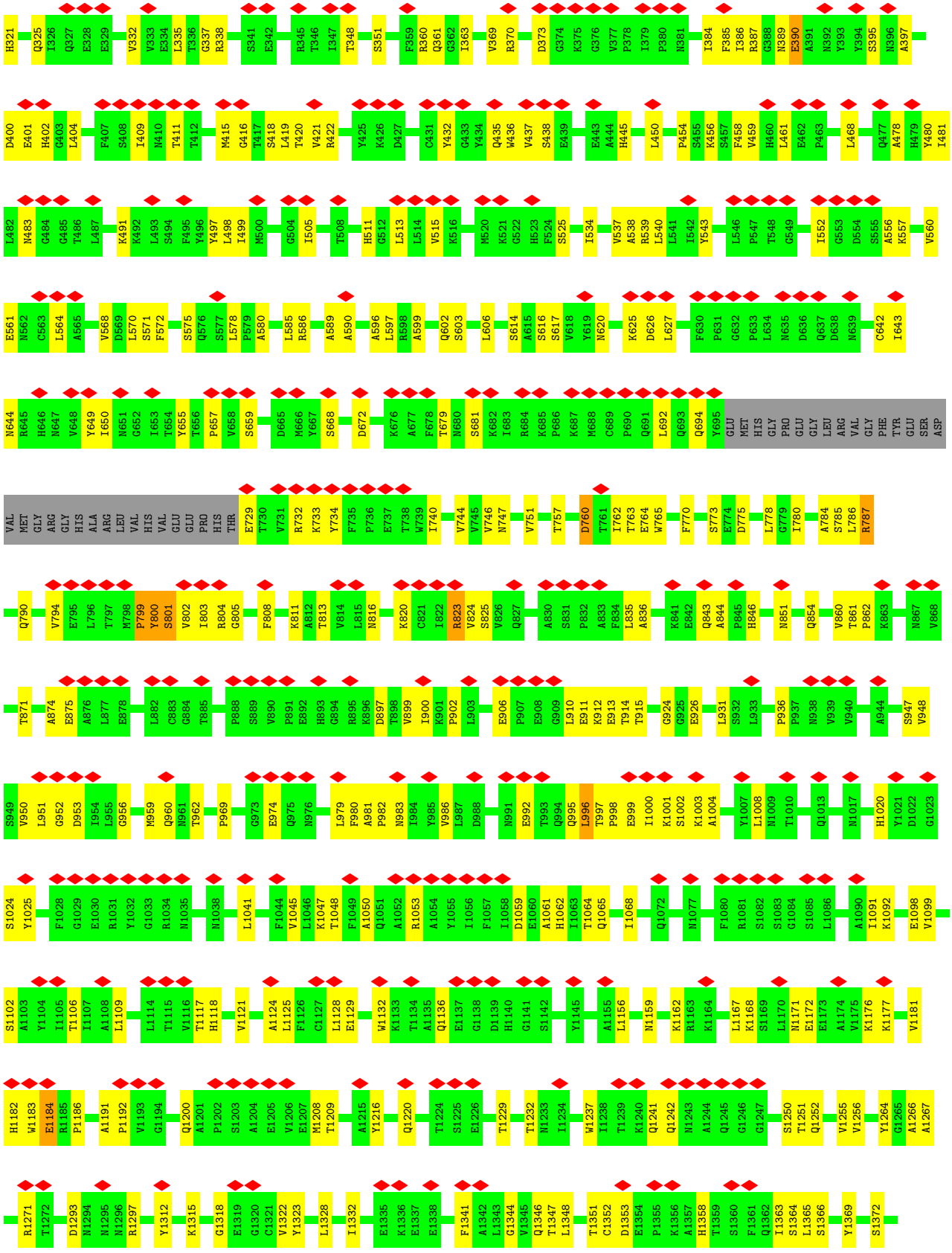
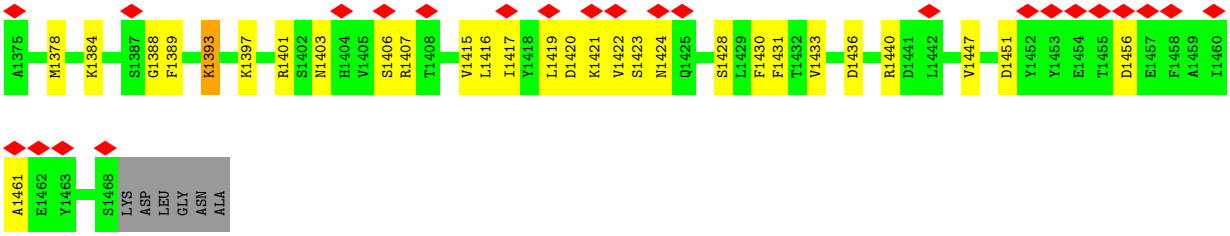


• Molecule 1: Alpha-2-macroglobulin

Chain D:

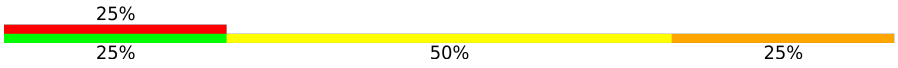



H321 Q325 I326 Q327 E328 E329 V332 V333 E334 L335 T336 G337 R338 S341 E342 R345 T346 I347 T348 S351 F359 R360 Q361 G362 I363 V369 R370 D373 G374 K375 G376 V377 P378 I379 P380 N381 I384 F385 I386 R387 G388 N389 E390 A391 N392 Y393 Y394 S395 N396 A397
D400 E401 H402 G403 L404 F407 S408 I409 N410 T411 T412 M415 G416 T417 S418 L419 T420 V421 R422 Y425 K426 D427 C431 Y432 G433 Y434 Q435 W436 V437 S438 E439 E443 A444 H445 L450 P454 S455 K456 S457 F458 V459 H460 L461 E462 P463 L468 Q477 A478 H479 Y480 I481
L482 N483 G484 G485 T486 L487 K491 K492 L493 S494 P495 Y496 Y497 L498 I499 M500 G504 I505 T508 H511 G512 L513 L514 V515 K516 M520 K521 G522 H523 F524 S525 I534 V537 A538 R539 L540 L541 I542 Y543 L546 P547 T548 G549 I552 G553 D554 S555 A556 K557 V560
E561 N562 C563 L564 A565 V568 D569 L570 S571 F572 S575 Q576 S577 L578 P579 A580 L585 R586 A589 A590 A596 L597 R598 A599 Q602 S603 L606 S614 A615 S616 S617 V618 Y619 N620 K625 D626 L627 F630 P631 G632 P633 L634 N635 D636 Q637 D638 N639 C642 I643
N644 R645 H646 N647 V648 Y649 I650 N651 G652 I653 T654 Y655 T656 P657 V658 S659 D665 M666 Y667 S668 D672 K676 A677 F678 T679 N680 S681 K682 I683 K684 K685 P686 K687 M688 C689 P690 Q691 L692 Q693 Q694 Y695 GLU MET HIS GLY PRO GLU GLY LEU ARG VAL GLY PHE TYR GLU SER ASP
VAL MET GLY ARG GLY HIS ALA ARG LEU VAL HIS VAL GLU GLU PRO HIS THR E729 T730 V731 R732 K733 Y734 F735 P736 E737 T738 W739 I740 V744 V745 V746 N747 V751 T757 D760 T761 I762 T763 E764 W765 F770 S773 E774 D775 L778 G779 I780 A784 S785 L786 R787
Q790 V794 E795 L796 T797 M798 P799 Y800 S801 V802 I803 R804 C805 F808 K811 A812 T813 V814 L815 N816 K820 C821 I822 R823 V824 S825 V826 Q827 A830 S831 P832 A833 F834 L835 A836 K841 E842 Q843 A844 P845 H846 N851 Q854 V860 T861 P862 K863 N867 V868
T871 A874 E875 A876 L877 E878 L882 C883 G884 T885 P888 S889 V890 P891 E892 H893 G894 R895 K896 D897 T898 V899 I900 K901 P902 L903 E906 P907 E908 G909 L910 E911 K912 E913 T914 T915 G924 G925 E926 L931 S932 L933 P936 P937 N938 V939 V940 A944 S947 V948
S949 V950 L951 G952 D953 I954 L955 G956 M959 Q960 N961 T962 P969 G973 E974 Q975 N976 L979 F980 A981 P982 N983 I984 Y985 V986 L987 D988 N991 E992 T993 Q994 Q995 L996 T997 P998 E999 I1000 K1001 S1002 K1003 A1004 Y1007 L1008 N1009 T1010 Q1013 N1017 H1020 Y1021 D1022 G1023
S1024 Y1025 F1028 G1029 E1030 R1031 Y1032 G1033 R1034 N1035 N1038 L1041 F1044 V1045 L1046 K1047 T1048 F1049 A1050 Q1051 A1052 R1053 A1054 Y1055 I1056 F1057 I1058 D1059 E1060 A1061 H1062 I1063 T1064 Q1065 I1068 Q1072 N1077 F1080 R1081 S1082 S1083 G1084 S1085 L1086 A1090 I1091 K1092 E1098 V1099
S1102 A1103 Y1104 I1105 T1106 I1107 A1108 L1109 L1114 T1115 V1116 T1117 H1118 V1121 A1124 L1125 F1126 C1127 L1128 E1129 W1132 K1133 T1134 A1135 Q1136 E1137 G1138 D1139 H1140 G1141 S1142 Y1145 A1155 L1156 N1159 K1162 R1163 K1164 L1167 K1168 S1169 L1170 N1171 E1172 E1173 A1174 V1175 K1176 K1177 V1181
H1182 W1183 E1184 R1185 P1186 A1191 P1192 V1193 G1194 Q1200 A1201 P1202 S1203 A1204 E1205 V1206 E1207 M1208 T1209 A1215 Y1216 Q1220 T1224 S1225 E1226 T1229 T1232 N1233 I1234 W1237 I1238 T1239 K1240 Q1241 Q1242 N1243 A1244 Q1245 G1246 G1247 S1250 T1251 Q1252 V1255 V1256 Y1264 G1265 A1266 A1267
R1271 T1272 D1293 N1294 N1295 N1296 R1297 Y1312 K1315 G1318 E1319 G1320 C1321 V1322 Y1323 L1328 I1332 E1335 K1336 E1337 E1338 F1341 A1342 L1343 G1344 V1345 Q1346 T1347 L1348 T1351 C1352 D1353 E1354 P1355 K1356 A1357 H1358 T1359 S1360 F1361 Q1362 I1363 S1364 L1365 S1366 Y1369 S1372



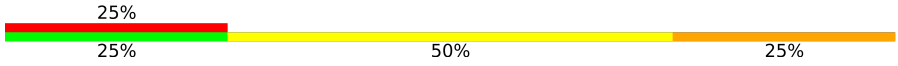
• Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

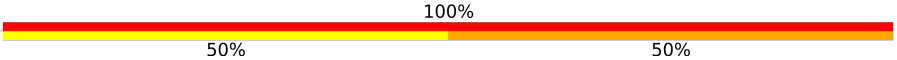
Chain F:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

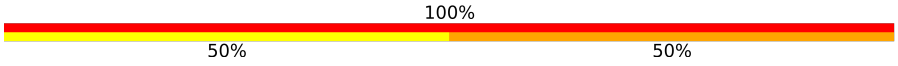
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	30618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	47775	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	335.04, 335.04, 335.04	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	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, MAN, BMA

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	0/11249	0.61	4/15286 (0.0%)
1	B	0.33	0/11248	0.62	3/15283 (0.0%)
1	C	0.32	0/11249	0.61	4/15286 (0.0%)
1	D	0.33	0/11248	0.62	3/15283 (0.0%)
All	All	0.33	0/44994	0.62	14/61138 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	801	SER	N-CA-C	-6.57	93.27	111.00
1	D	801	SER	N-CA-C	-6.57	93.27	111.00
1	A	55	ASN	CB-CA-C	6.51	123.43	110.40
1	C	55	ASN	CB-CA-C	6.51	123.43	110.40
1	B	760	ASP	CB-CG-OD1	5.91	123.62	118.30

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	11004	0	10891	186	0
1	B	11004	0	10888	271	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	11004	0	10891	193	0
1	D	11004	0	10888	267	0
2	E	50	0	43	3	0
2	H	50	0	43	3	0
3	F	39	0	34	1	0
3	I	39	0	34	1	0
4	G	28	0	25	3	0
4	J	28	0	25	3	0
5	A	112	0	104	5	0
5	B	70	0	65	6	0
5	C	112	0	104	5	0
5	D	70	0	65	6	0
All	All	44614	0	44100	915	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 10.

The worst 5 of 915 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:55:ASN:HD22	5:C:2001:NAG:C1	1.06	1.57
1:A:55:ASN:HD22	5:A:2001:NAG:C1	1.06	1.55
1:B:1424:ASN:ND2	4:G:1:NAG:C1	1.70	1.52
1:D:1424:ASN:ND2	4:J:1:NAG:C1	1.70	1.51
1:B:247:ASN:HD21	5:B:2003:NAG:C1	1.27	1.45

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	1406/1474 (95%)	1190 (85%)	209 (15%)	7 (0%)	29	69
1	B	1404/1474 (95%)	1163 (83%)	233 (17%)	8 (1%)	25	66
1	C	1406/1474 (95%)	1190 (85%)	209 (15%)	7 (0%)	29	69
1	D	1404/1474 (95%)	1163 (83%)	233 (17%)	8 (1%)	25	66
All	All	5620/5896 (95%)	4706 (84%)	884 (16%)	30 (0%)	32	69

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	800	TYR
1	A	1184	GLU
1	B	1184	GLU
1	C	800	TYR
1	C	1184	GLU

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	1236/1290 (96%)	1220 (99%)	16 (1%)	69	82
1	B	1236/1290 (96%)	1227 (99%)	9 (1%)	84	90
1	C	1236/1290 (96%)	1220 (99%)	16 (1%)	69	82
1	D	1236/1290 (96%)	1227 (99%)	9 (1%)	84	90
All	All	4944/5160 (96%)	4894 (99%)	50 (1%)	77	86

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	313	ARG
1	C	863	LYS
1	D	1397	LYS
1	C	396	ASN
1	C	732	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1425	GLN
1	C	182	GLN
1	D	435	GLN
1	C	112	GLN
1	C	474	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)

18 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	$\#\|Z\| > 2$
2	NAG	E	1	2	14,14,15	0.38	0	17,19,21	0.57	0
2	NAG	E	2	2	14,14,15	0.39	0	17,19,21	1.07	1 (5%)
2	BMA	E	3	2	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
2	MAN	E	4	2	11,11,12	0.23	0	15,15,17	0.58	0
3	NAG	F	1	1,3	14,14,15	0.33	0	17,19,21	0.84	0
3	NAG	F	2	3	14,14,15	0.29	0	17,19,21	0.73	0
3	BMA	F	3	3	11,11,12	0.23	0	15,15,17	0.63	0
4	NAG	G	1	4	14,14,15	0.63	0	17,19,21	1.66	4 (23%)
4	NAG	G	2	4	14,14,15	0.38	0	17,19,21	0.83	1 (5%)
2	NAG	H	1	2	14,14,15	0.38	0	17,19,21	0.57	0
2	NAG	H	2	2	14,14,15	0.39	0	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	H	3	2	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
2	MAN	H	4	2	11,11,12	0.23	0	15,15,17	0.58	0
3	NAG	I	1	1,3	14,14,15	0.33	0	17,19,21	0.84	0
3	NAG	I	2	3	14,14,15	0.29	0	17,19,21	0.73	0
3	BMA	I	3	3	11,11,12	0.23	0	15,15,17	0.63	0
4	NAG	J	1	4	14,14,15	0.63	0	17,19,21	1.66	4 (23%)
4	NAG	J	2	4	14,14,15	0.38	0	17,19,21	0.83	1 (5%)

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
2	NAG	E	1	2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	MAN	E	4	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	5/6/23/26	0/1/1/1
2	NAG	H	1	2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	MAN	H	4	2	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
4	NAG	J	1	4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	NAG	O5-C1-C2	-4.00	104.98	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1	NAG	O5-C1-C2	-4.00	104.98	111.29
2	E	2	NAG	C1-O5-C5	3.42	116.83	112.19
2	H	2	NAG	C1-O5-C5	3.42	116.83	112.19
4	G	1	NAG	O4-C4-C3	3.32	118.03	110.35

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

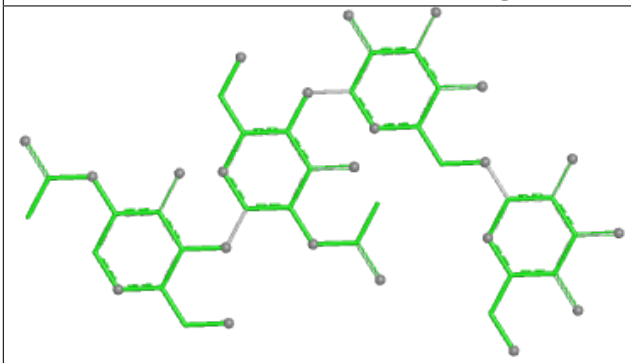
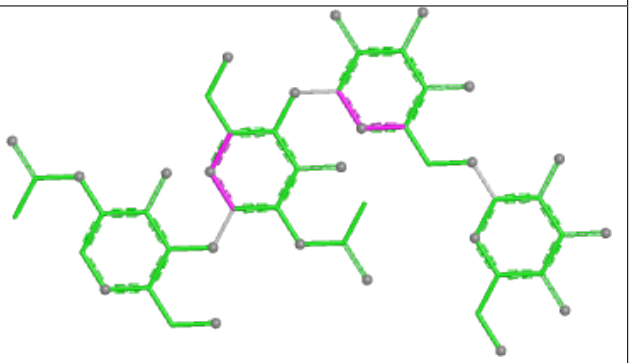
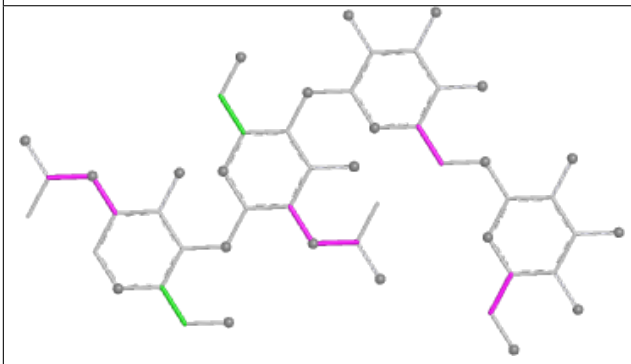
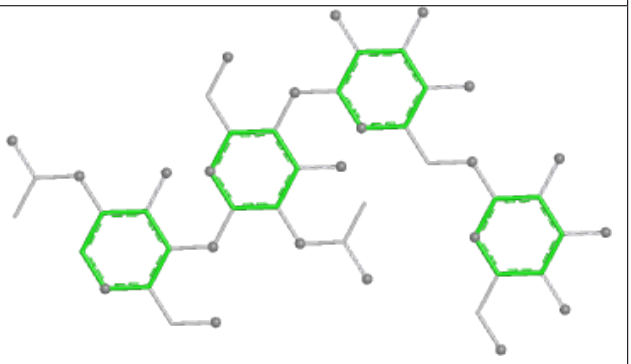
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

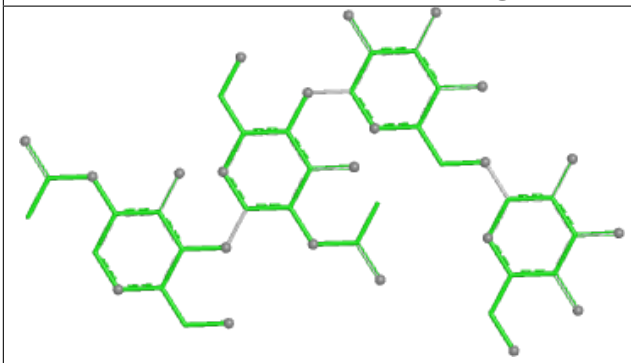
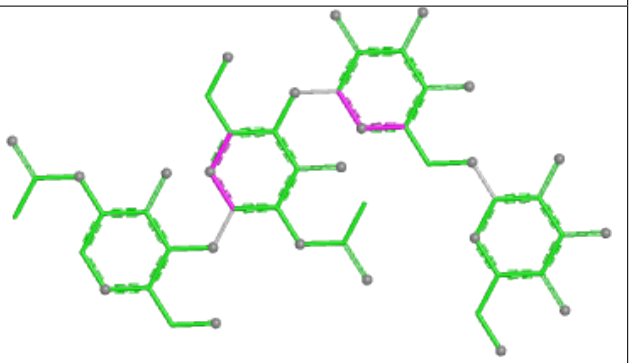
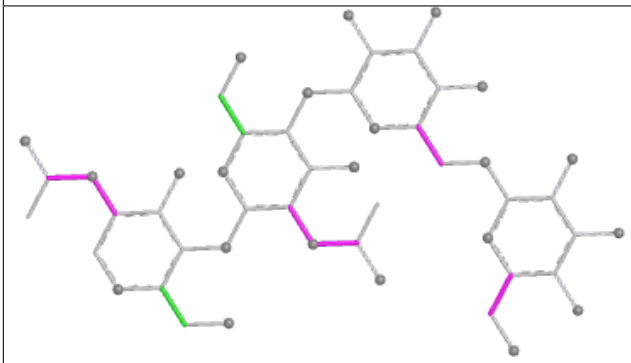
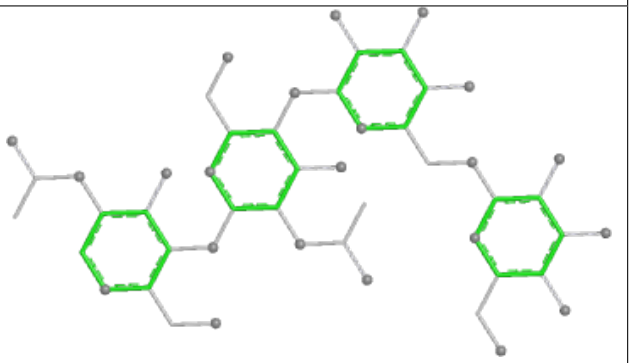
There are no ring outliers.

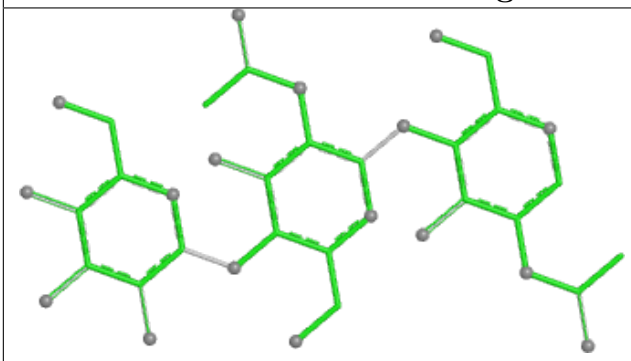
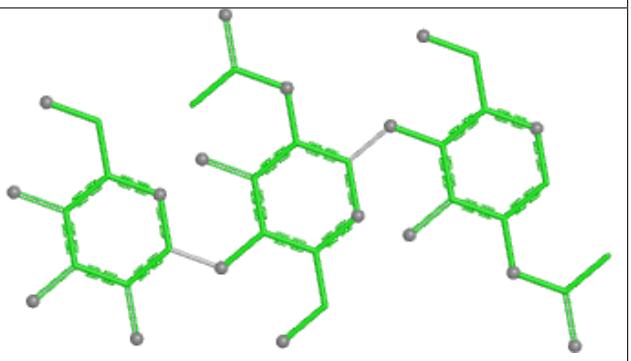
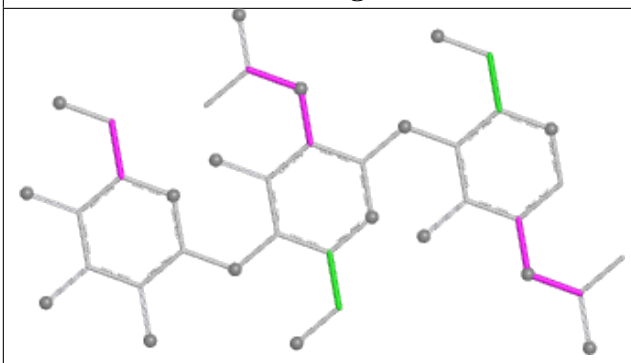
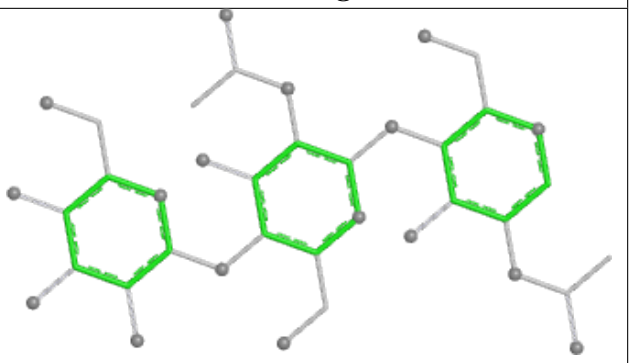
10 monomers are involved in 14 short contacts:

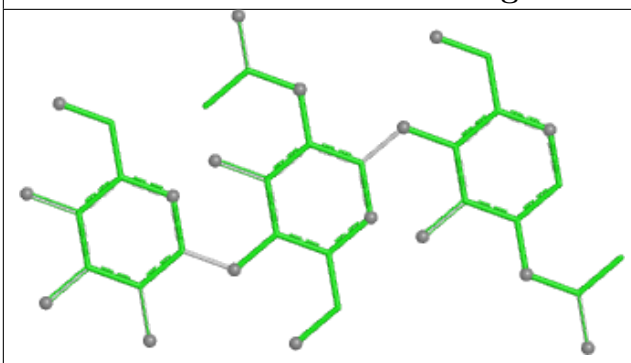
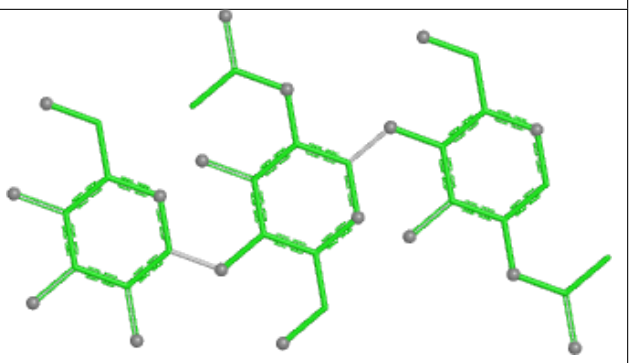
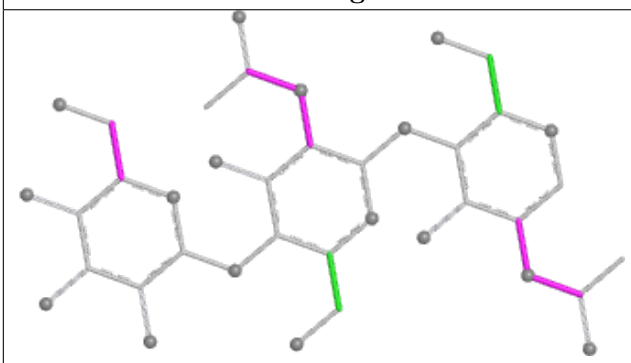
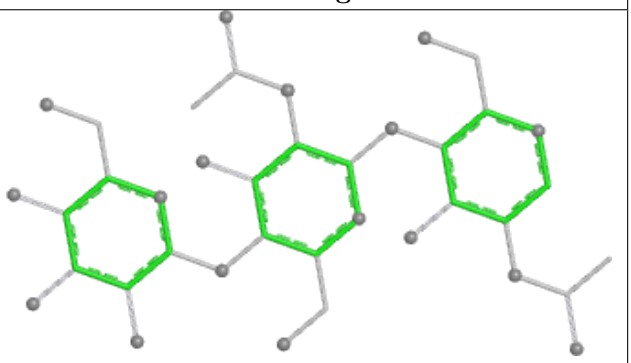
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	3	0
2	H	2	NAG	2	0
2	H	1	NAG	1	0
2	E	2	NAG	2	0
3	F	1	NAG	1	0
3	F	2	NAG	1	0
4	J	1	NAG	3	0
2	E	1	NAG	1	0
3	I	2	NAG	1	0
3	I	1	NAG	1	0

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

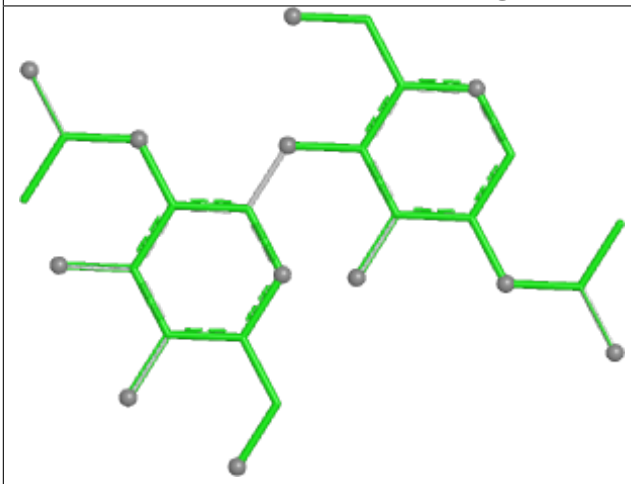
Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

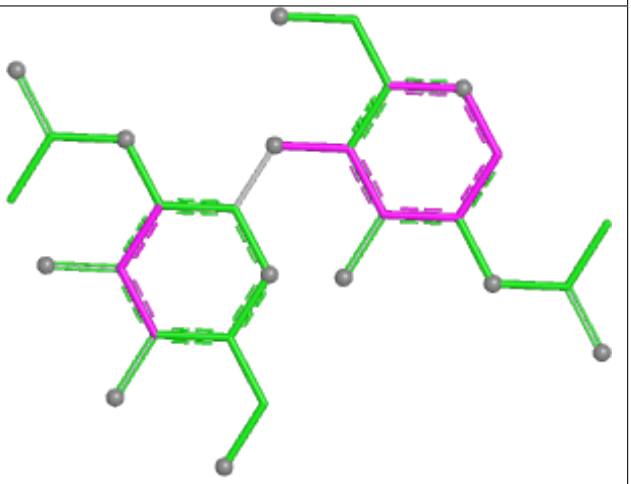
Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain I	
 Bond lengths	 Bond angles
 Torsions	 Rings

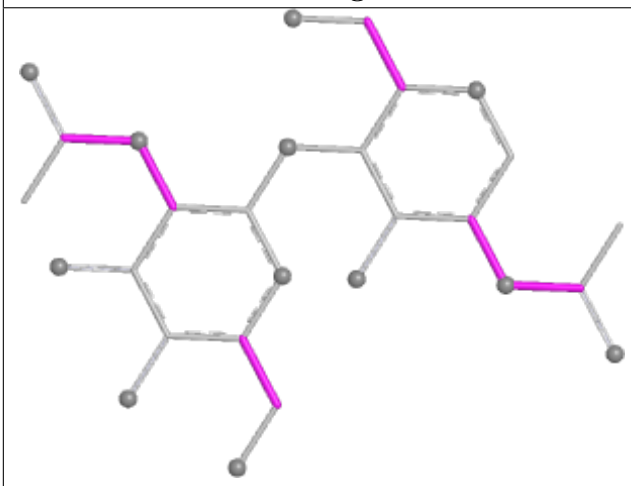
Oligosaccharide Chain G



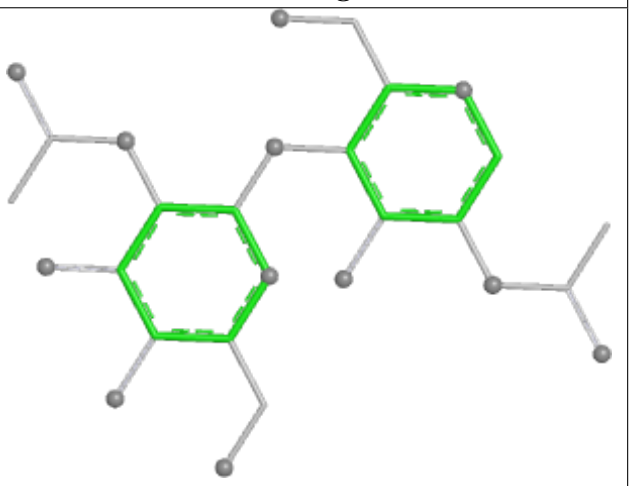
Bond lengths



Bond angles

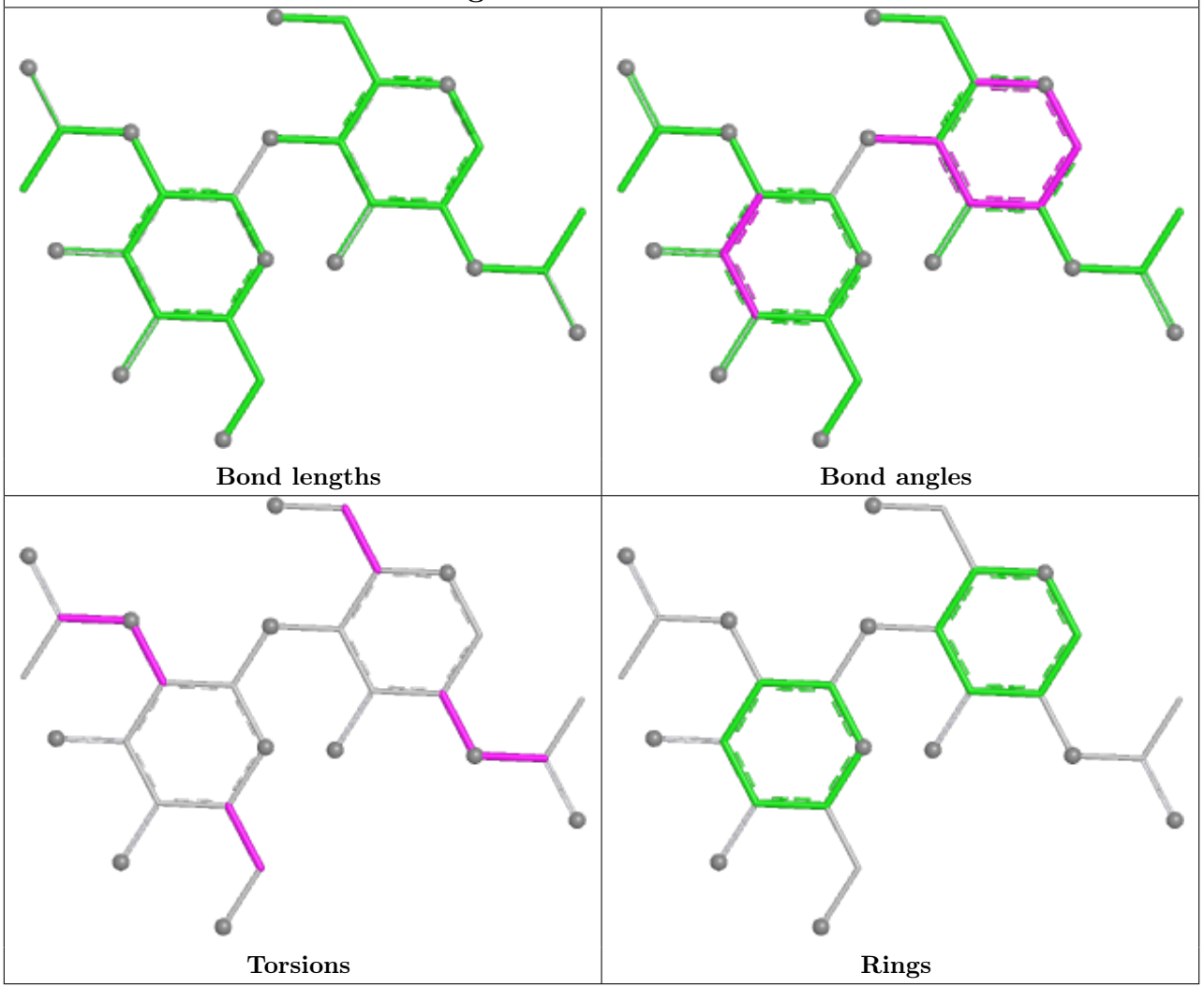


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

26 ligands 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	$\#\|Z\| > 2$
5	NAG	A	2006	1	14,14,15	0.33	0	17,19,21	0.84	0
5	NAG	B	2002	-	14,14,15	0.27	0	17,19,21	0.79	0
5	NAG	A	2002	-	14,14,15	0.32	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	C	2005	1	14,14,15	0.36	0	17,19,21	0.75	1 (5%)
5	NAG	D	2005	1	14,14,15	0.29	0	17,19,21	0.91	1 (5%)
5	NAG	A	2001	-	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	A	2003	1	14,14,15	0.29	0	17,19,21	0.92	1 (5%)
5	NAG	C	2008	1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	D	2001	1	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	D	2004	-	14,14,15	0.37	0	17,19,21	0.96	1 (5%)
5	NAG	B	2003	-	14,14,15	0.32	0	17,19,21	0.51	0
5	NAG	A	2008	1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	B	2001	1	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	A	2004	1	14,14,15	0.33	0	17,19,21	0.64	0
5	NAG	A	2005	1	14,14,15	0.36	0	17,19,21	0.75	1 (5%)
5	NAG	B	2005	1	14,14,15	0.29	0	17,19,21	0.91	1 (5%)
5	NAG	B	2004	-	14,14,15	0.37	0	17,19,21	0.96	1 (5%)
5	NAG	C	2001	-	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	C	2004	1	14,14,15	0.33	0	17,19,21	0.64	0
5	NAG	C	2007	1	14,14,15	0.30	0	17,19,21	0.67	0
5	NAG	C	2003	1	14,14,15	0.29	0	17,19,21	0.92	1 (5%)
5	NAG	C	2002	-	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	D	2002	-	14,14,15	0.27	0	17,19,21	0.79	0
5	NAG	D	2003	-	14,14,15	0.32	0	17,19,21	0.51	0
5	NAG	C	2006	1	14,14,15	0.33	0	17,19,21	0.84	0
5	NAG	A	2007	1	14,14,15	0.30	0	17,19,21	0.67	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
5	NAG	A	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2002	-	-	4/6/23/26	0/1/1/1
5	NAG	A	2002	-	-	3/6/23/26	0/1/1/1
5	NAG	C	2005	1	-	3/6/23/26	0/1/1/1
5	NAG	D	2005	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2001	-	-	1/6/23/26	0/1/1/1
5	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2008	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	2001	1	-	1/6/23/26	0/1/1/1
5	NAG	D	2004	-	-	4/6/23/26	0/1/1/1
5	NAG	B	2003	-	-	4/6/23/26	0/1/1/1
5	NAG	A	2008	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2001	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2004	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2005	1	-	3/6/23/26	0/1/1/1
5	NAG	B	2005	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2004	-	-	4/6/23/26	0/1/1/1
5	NAG	C	2001	-	-	1/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	4/6/23/26	0/1/1/1
5	NAG	C	2007	1	-	3/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2002	-	-	3/6/23/26	0/1/1/1
5	NAG	D	2002	-	-	4/6/23/26	0/1/1/1
5	NAG	D	2003	-	-	4/6/23/26	0/1/1/1
5	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2007	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2001	NAG	C1-O5-C5	3.89	117.47	112.19
5	C	2001	NAG	C1-O5-C5	3.89	117.47	112.19
5	B	2001	NAG	C1-O5-C5	3.84	117.40	112.19
5	D	2001	NAG	C1-O5-C5	3.84	117.40	112.19
5	B	2004	NAG	O5-C5-C6	2.48	111.10	107.20

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2002	NAG	C3-C2-N2-C7
5	A	2002	NAG	C8-C7-N2-C2
5	A	2002	NAG	O7-C7-N2-C2
5	A	2004	NAG	C8-C7-N2-C2
5	A	2004	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2005	NAG	1	0
5	A	2001	NAG	5	0
5	D	2004	NAG	1	0
5	B	2003	NAG	4	0
5	B	2005	NAG	1	0
5	B	2004	NAG	1	0
5	C	2001	NAG	5	0
5	D	2003	NAG	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	629:GLY	C	630:PHE	N	5.14
1	D	629:GLY	C	630:PHE	N	5.14

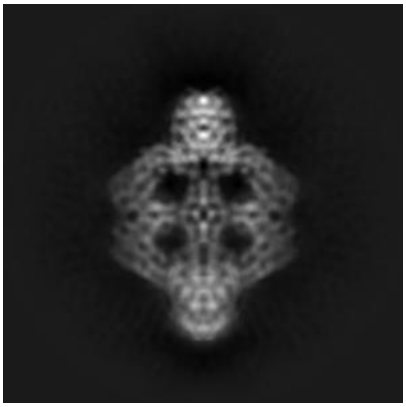
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12748. These allow visual inspection of the internal detail of the map and identification of artifacts.

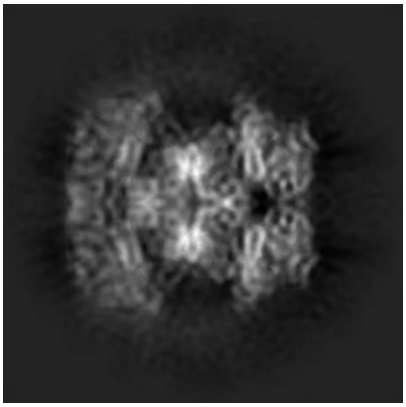
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

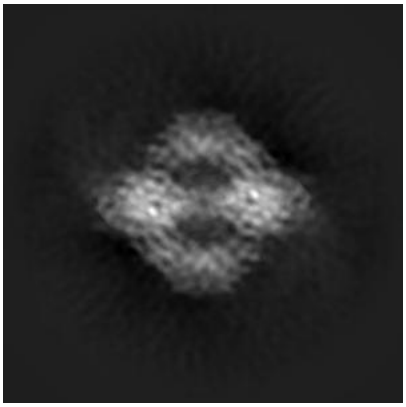
6.1.1 Primary map



X



Y



Z

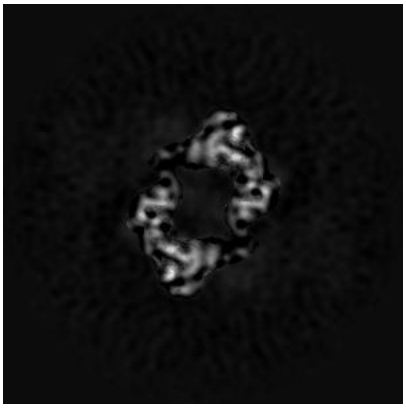
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 160

Y Index: 160



Z Index: 160

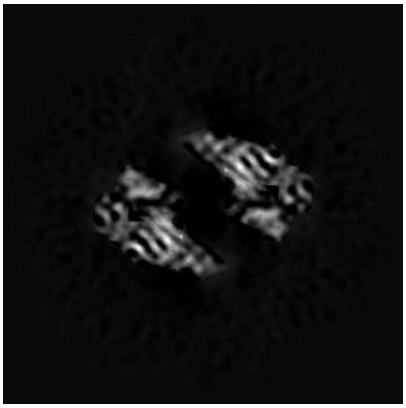
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 130

Y Index: 160

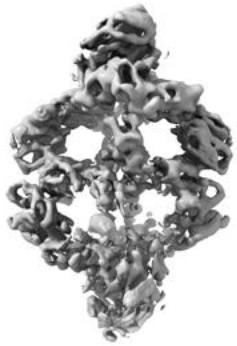


Z Index: 195

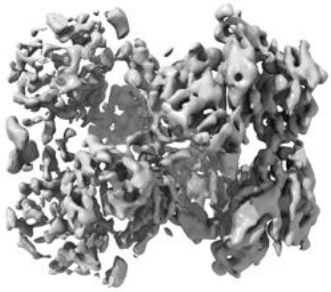
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

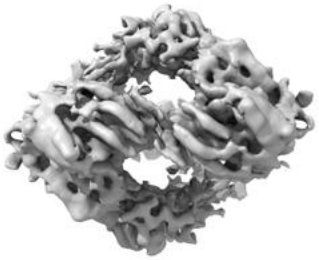
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

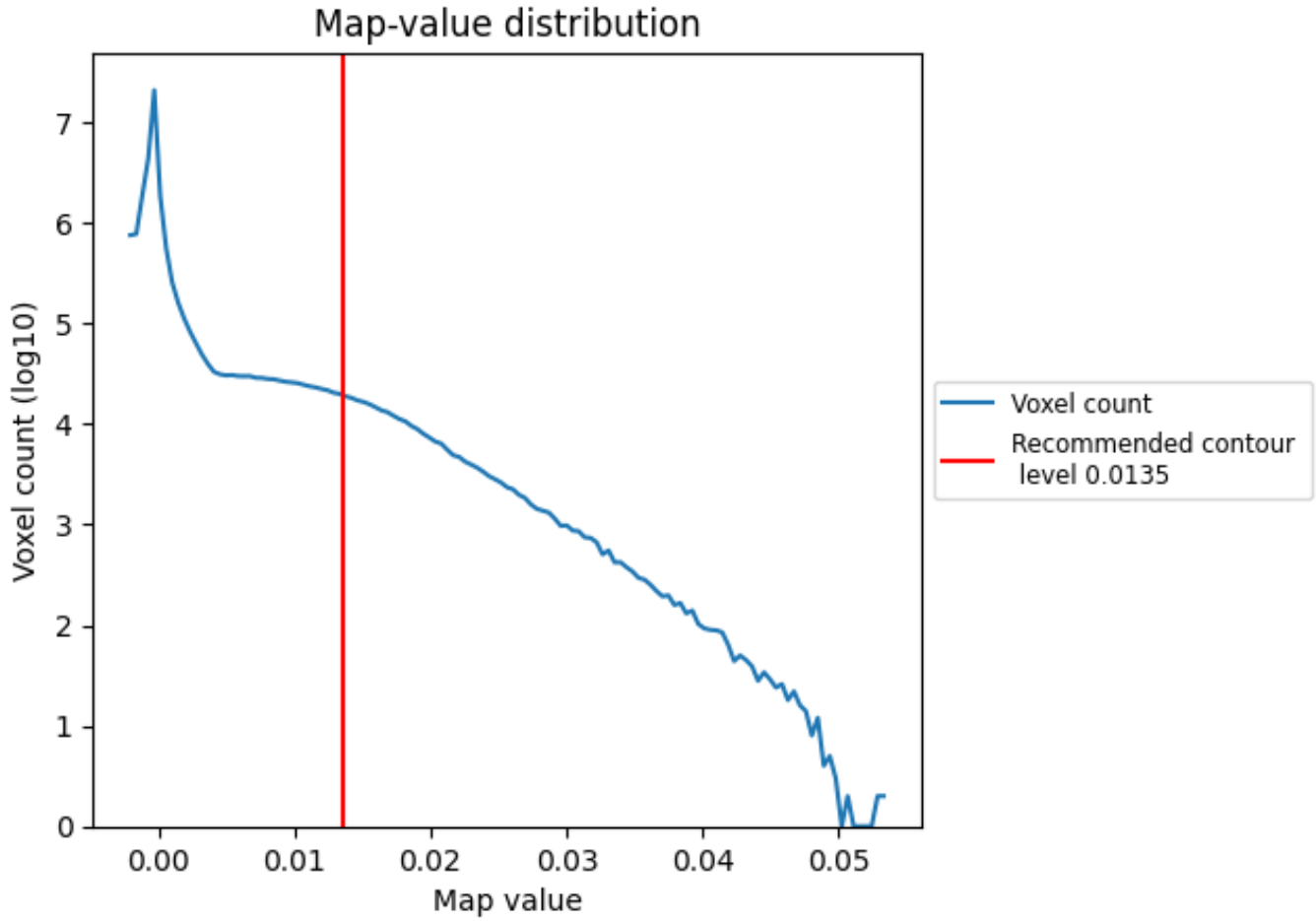
6.5 Mask visualisation (i)

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

7 Map analysis

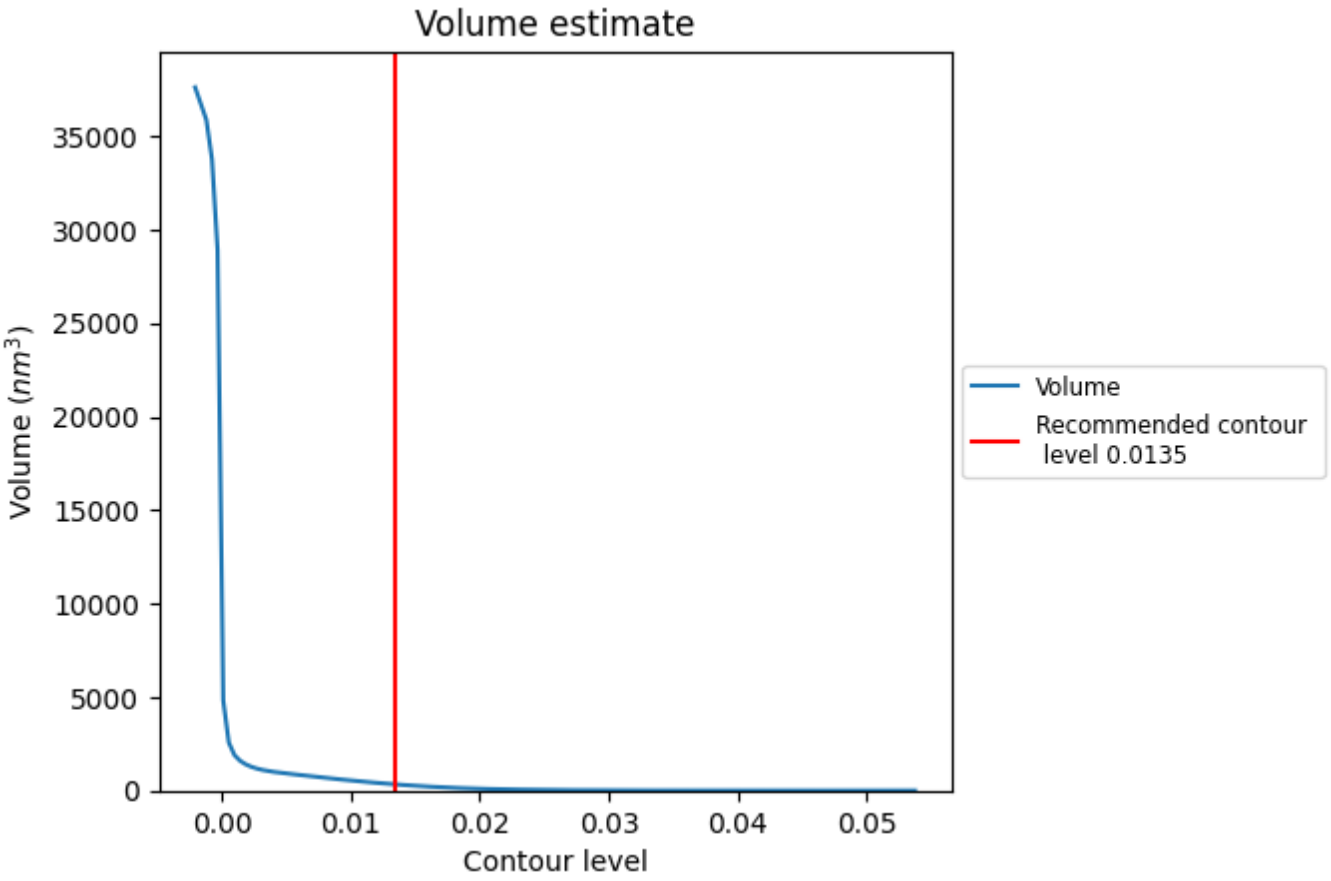
This section contains the results of statistical analysis of the map.

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.

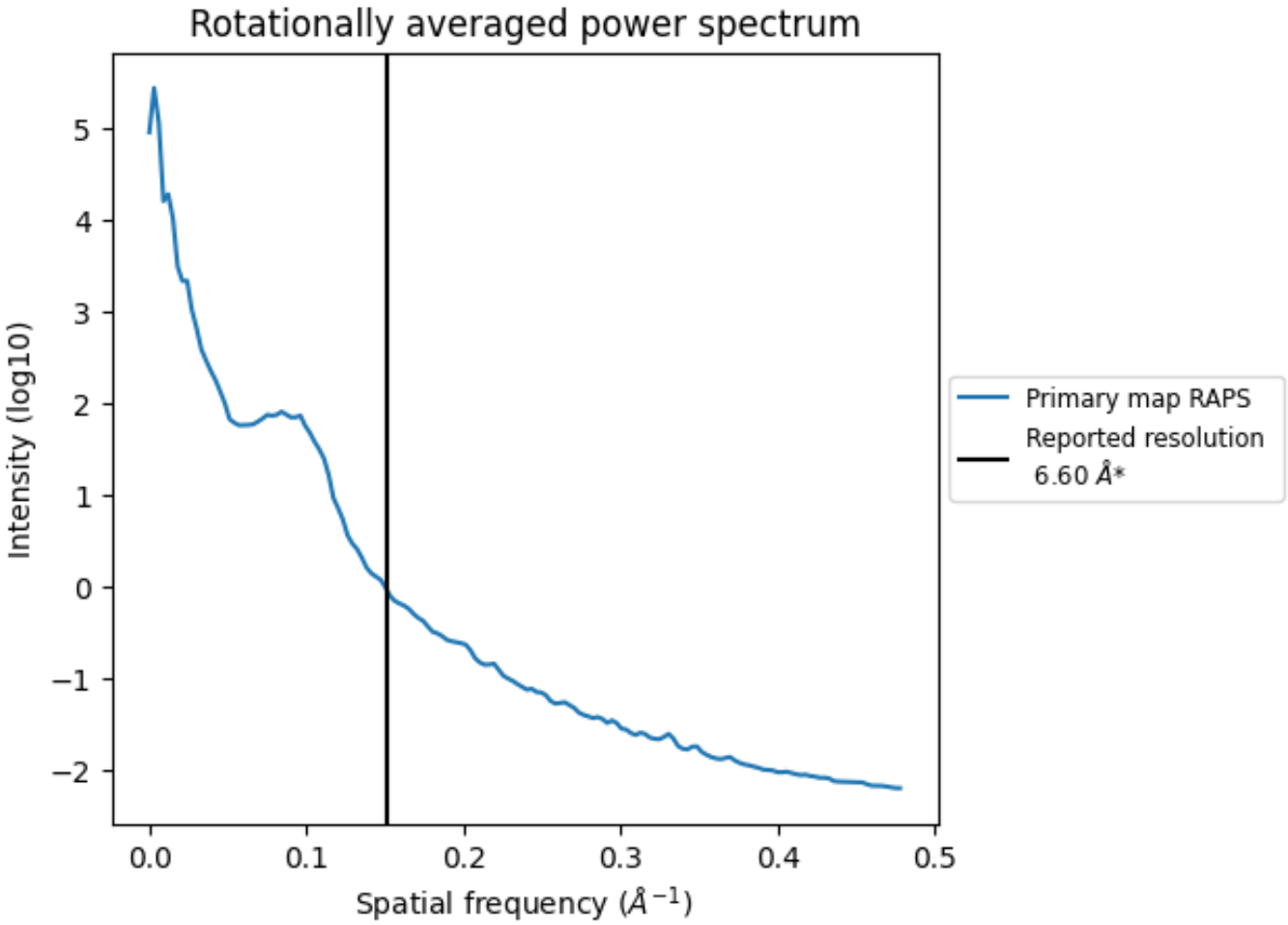
7.2 Volume estimate (i)



The volume at the recommended contour level is 329 nm^3; this corresponds to an approximate mass of 297 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 0.152 Å^{-1}

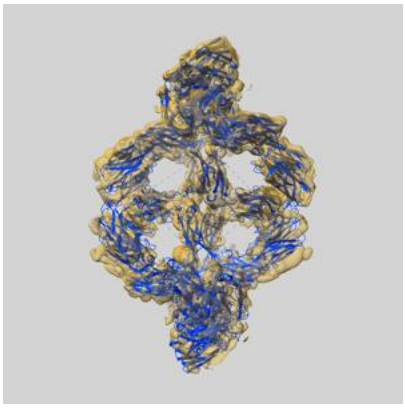
8 Fourier-Shell correlation (i)

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

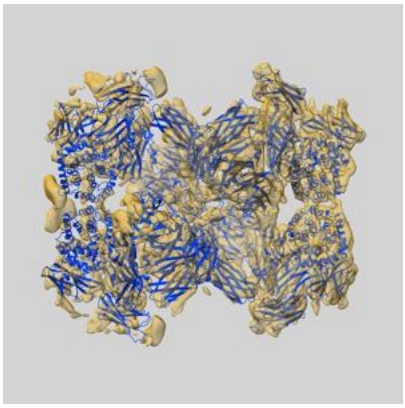
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12748 and PDB model 7O7M. Per-residue inclusion information can be found in section 3 on page 8.

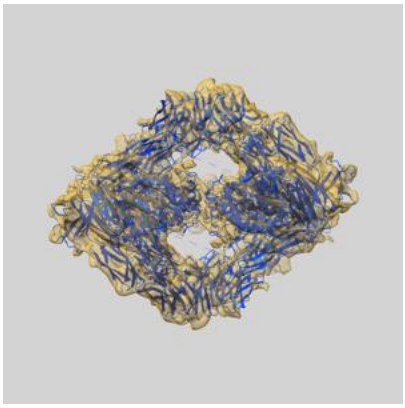
9.1 Map-model overlay



X



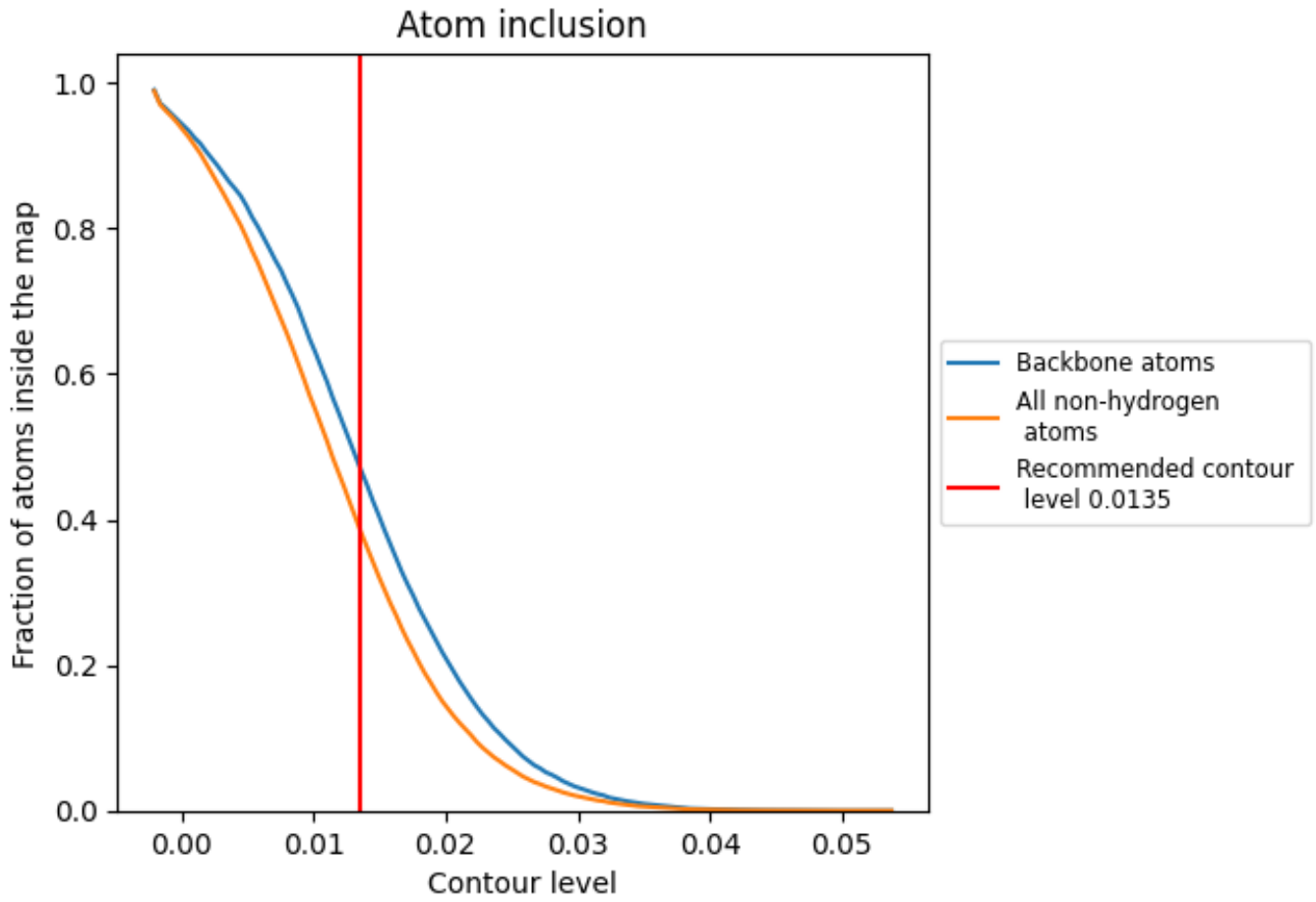
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135 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 Atom inclusion (i)



At the recommended contour level, 47% of all backbone atoms, 39% of all non-hydrogen atoms, are inside the map.