wwPDB EM Validation Summary Report (i)

May 6, 2025 – 01:44 AM EDT

PDB ID	:	8E6S / pdb_00008e6s
EMDB ID	:	EMD-27924
Title	:	Human TRPM2 ion channel in 1 mM dADPR and Ca2+
Authors	:	Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on	:	2022-08-23
Resolution	:	4.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

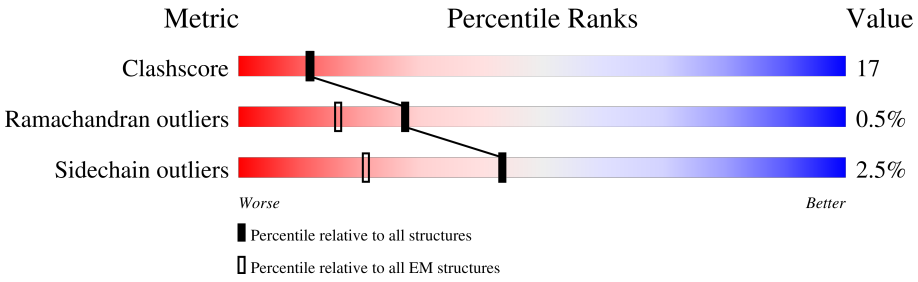
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 4.60 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	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	1503	39% 56% 31% • 12%
1	B	1503	39% 56% 31% • 12%
1	C	1503	40% 56% 30% • 12%
1	D	1503	39% 56% 31% • 12%

2 Entry composition (i)

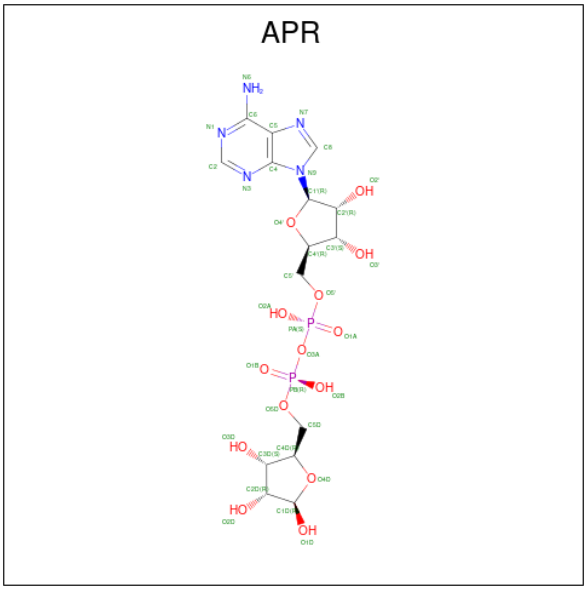
There are 5 unique types of molecules in this entry. The entry contains 42336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily M member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1330	Total	C	N	O	S	0	0
			10521	6791	1829	1851	50		
1	B	1330	Total	C	N	O	S	0	0
			10521	6791	1829	1851	50		
1	C	1330	Total	C	N	O	S	0	0
			10521	6791	1829	1851	50		
1	D	1330	Total	C	N	O	S	0	0
			10521	6791	1829	1851	50		

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			35	15	5	13	2	
2	B	1	Total	C	N	O	P	0
			35	15	5	13	2	

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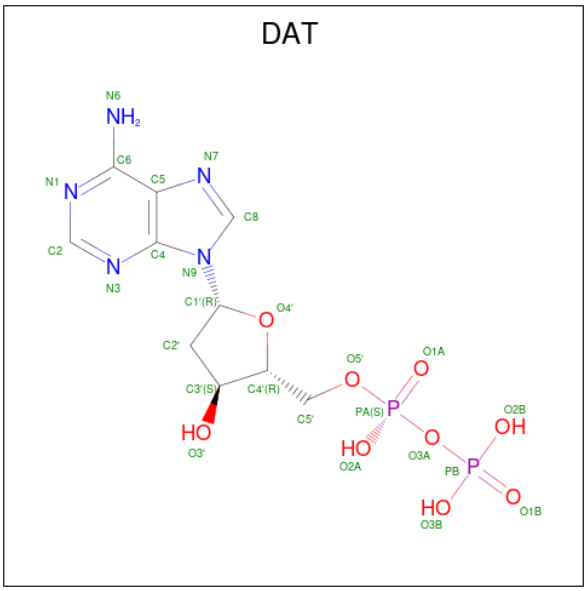
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			35	15	5	13	2	
2	D	1	Total	C	N	O	P	0
			35	15	5	13	2	

- Molecule 3 is 2'-DEOXYADENOSINE-5'-DIPHOSPHATE (CCD ID: DAT) (formula: $C_{10}H_{15}N_5O_9P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			26	10	5	9	2	
3	B	1	Total	C	N	O	P	0
			26	10	5	9	2	
3	C	1	Total	C	N	O	P	0
			26	10	5	9	2	
3	D	1	Total	C	N	O	P	0
			26	10	5	9	2	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total Zn 1 1	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

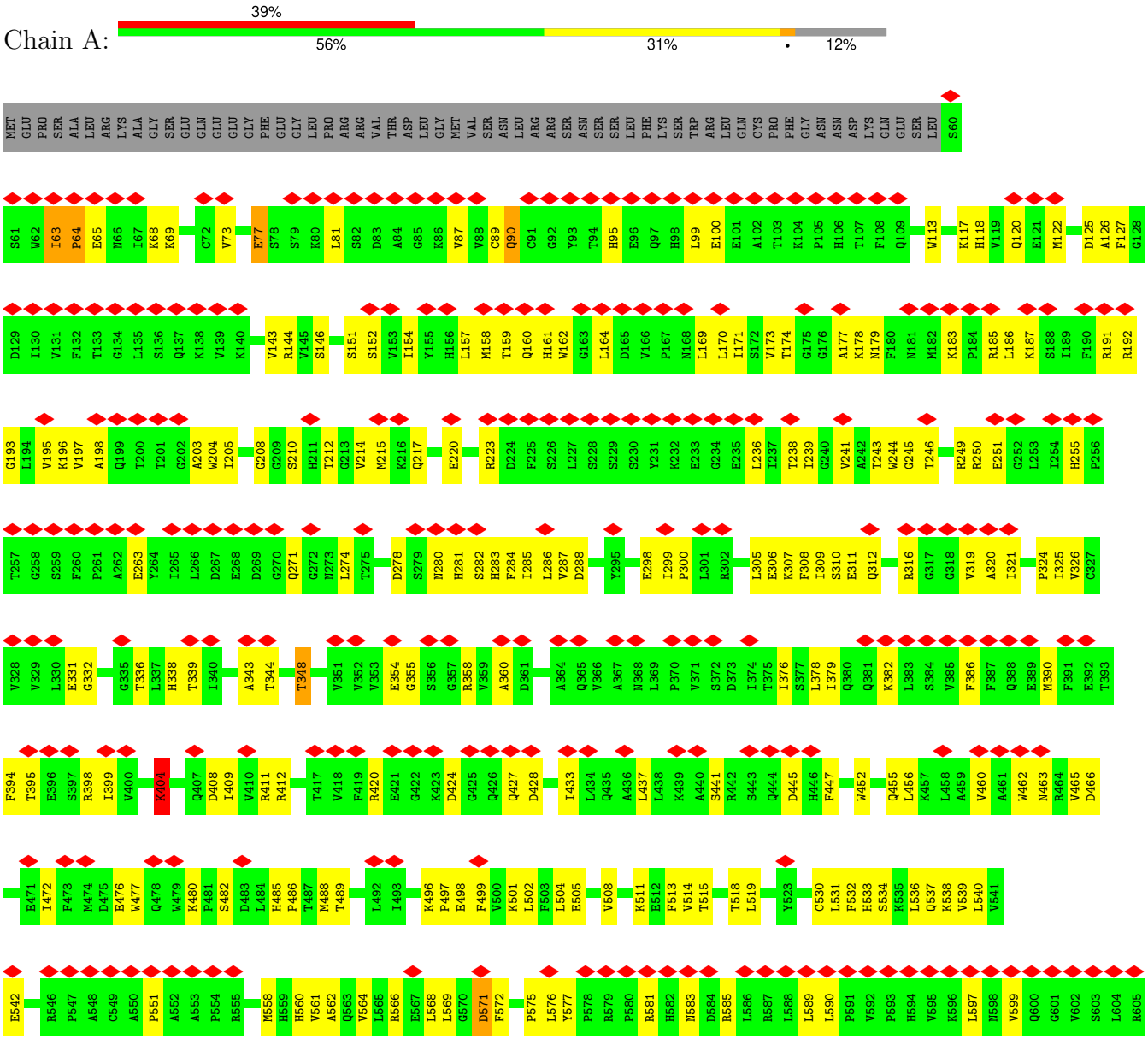
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Ca 1 1	0
5	B	1	Total Ca 1 1	0
5	C	1	Total Ca 1 1	0
5	D	1	Total Ca 1 1	0

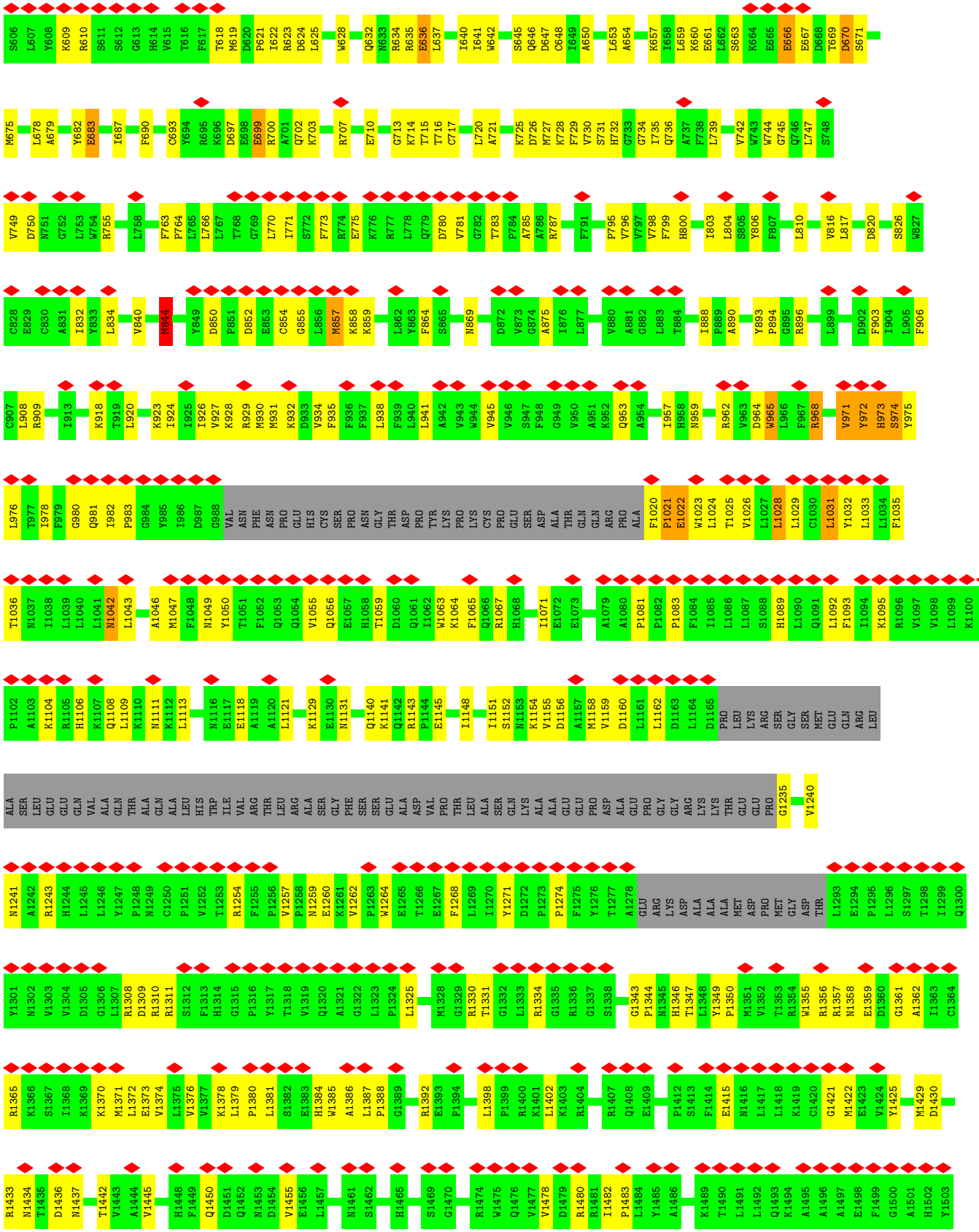
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain A:



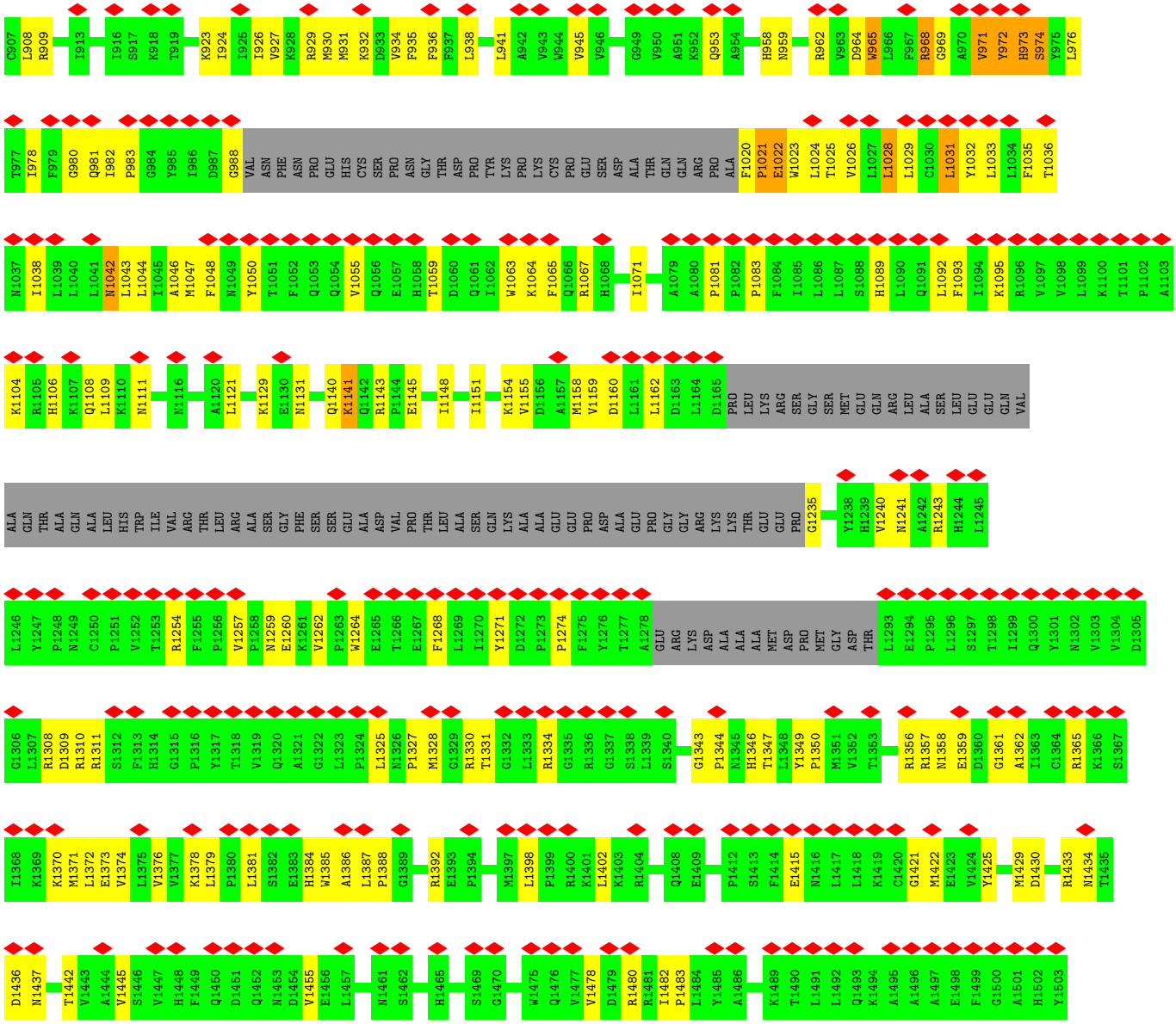


• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain B:

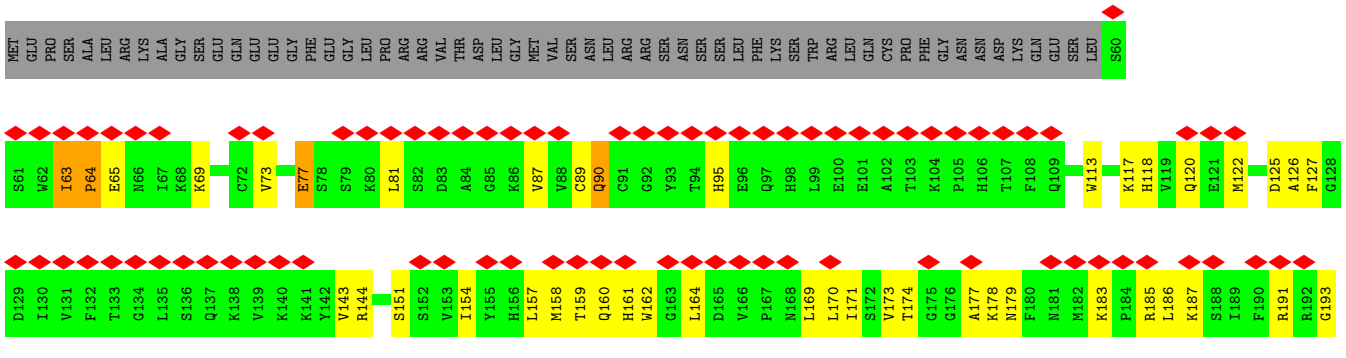

39%
56%
31%
12%

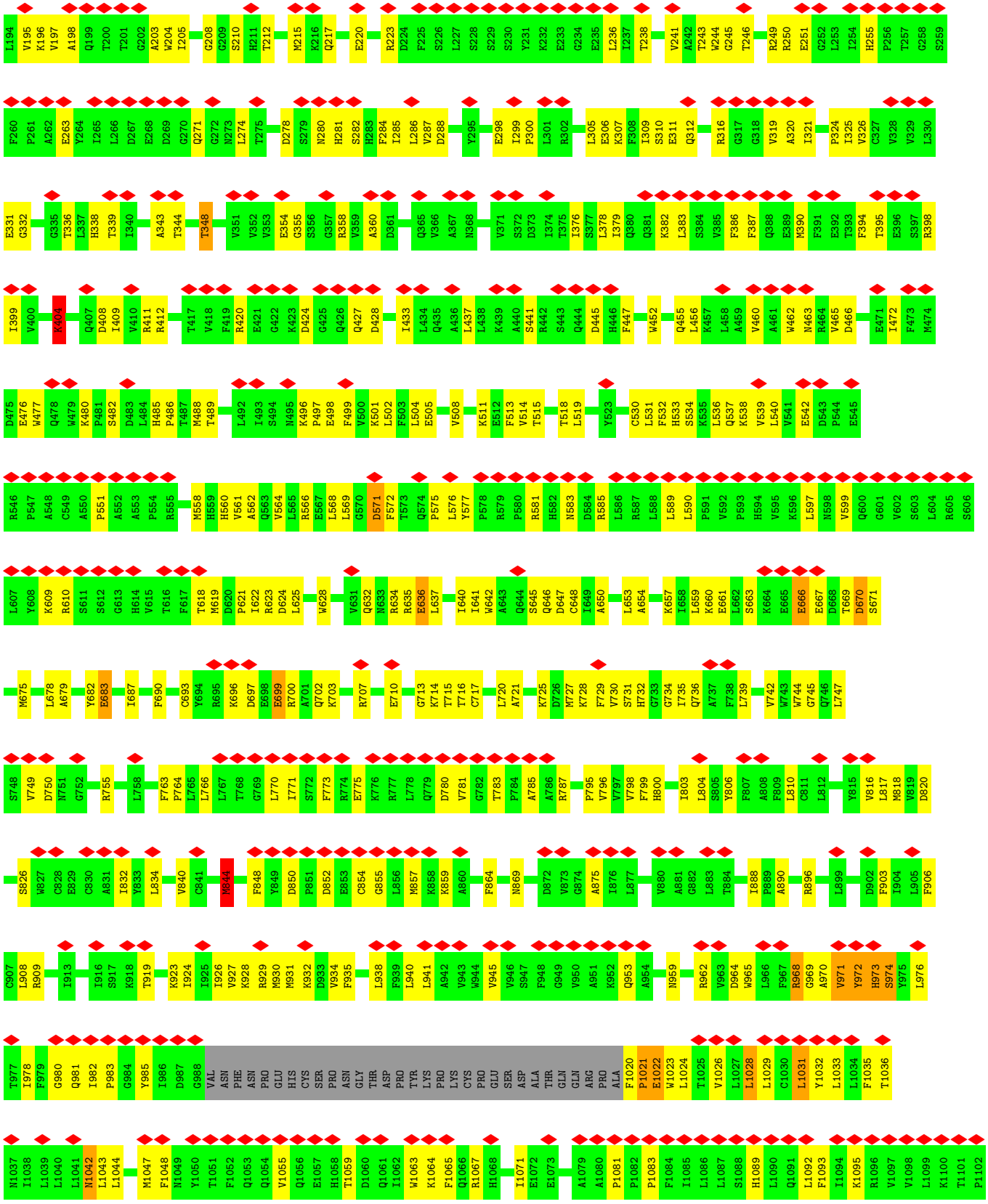

MET GLU PRO SER ALA LEU ARG LYS ALA GLY SER GLU GLN GLU GLU GLY PHE GLU GLY LEU PRO ARG ARG VAL THR ASP LEU GLY MET VAL SER ASN LEU ARG ARG SER ASN SER SER LEU PHE LYS SER TRP ARG LEU GLN CYS PRO PHE GLY ASN ASN ASP LYS GLN GLU SER LEU S60
S61 W62 I63 P64 E65 N66 I67 K68 K69 C72 V73 E77 S78 S79 K80 L81 S82 D83 A84 G85 K86 V87 V88 C89 Q90 C91 G92 Y93 T94 H95 E96 Q97 H98 L99 E100 E101 A102 T103 K104 P105 H106 T107 F108 Q109 W113 K117 H118 V119 Q120 E121 M122 D125 A126 F127 G128
D129 I130 V131 F132 T133 G134 L135 S136 Q137 K138 V139 K140 K141 Y142 V143 R144 V145 S146 S151 S152 V153 I154 Y155 H156 L157 M158 T159 Q160 H161 W162 G163 L164 D165 V166 P167 N168 L169 L170 I171 S172 V173 T174 G175 G176 A177 K178 N179 F180 N181 M182 K183 P184 R185 L186 K187 S188 R191 R192
G193 L194 V195 K196 V197 A198 Q199 T200 T201 G202 A203 W204 I205 G208 G209 S210 H211 T212 M215 K216 Q217 E220 R223 D224 F225 S226 L227 S228 S229 S230 Y231 K232 E233 G234 E235 L236 I237 T238 I239 G240 V241 A242 T243 W244 G245 T246 R249 R250 E251 G252 L253 I254 H255 P256 T257
G258 S259 F260 P261 A262 E263 Y264 I265 L266 D267 E268 D269 G270 Q271 G272 N273 L274 T275 D278 S279 N280 H281 S282 H283 F284 I285 L286 V287 D288 Y295 E298 I299 P300 L301 R302 L305 E306 K307 F308 I309 S310 E311 Q312 R316 G317 G318 V319 A320 I321 P324 I325 V326 C327 V328
V329 L330 E331 G332 G335 T336 L337 H338 T339 I340 A343 T344 T348 V351 V352 V353 E354 G355 S356 G357 R358 V359 A360 D361 A364 Q365 V366 A367 N368 L369 P370 V371 S372 D373 I374 T375 I376 S377 L378 I379 Q380 Q381 K382 L383 S384 V385 F386 F387 Q388 E389 M390 F391 E392 T393 F394
T395 E396 S397 R398 I399 V400 K404 Q407 D408 I409 V410 R411 R412 T417 V418 F419 R420 E421 G422 K423 D424 G425 Q426 Q427 D428 I433 L434 Q435 A436 L437 L438 K439 A440 S441 R442 S443 Q444 D445 H446 F447 W452 Q455 L458 A459 V460 A461 W462 N463 R464 V465 D466 E471
I472 F473 M474 W477 Q478 W479 K480 P481 S482 D483 L484 H485 P486 T487 M488 T489 L492 I493 K496 P497 E498 F499 V500 K501 L502 F503 L504 E505 V508 K511 E512 F513 V514 T515 T518 L519 Y523 C530 L531 F532 H533 S534 K535 L536 Q537 K538 V539 L540 V541 E542 R546
P547 A548 C549 A550 P551 A552 A553 P554 R555 K558 H559 H560 V561 A562 Q563 V564 L565 R566 E567 L568 L569 G570 D571 F572 P575 L576 Y577 P578 R579 P580 R581 H582 N583 D584 R585 L586 R587 L588 L589 L590 P591 V592 P593 H594 V595 K596 L597 N598 V599 Q600 G601 V602 S603 L604 R605 S606 L607 Y608
K609 R610 S611 S612 G613 H614 V615 T616 F617 T618 M619 D620 P621 I622 R623 D624 L625 W628 Q632 N633 R634 R635 E636 L637 I640 I641 W642 A643 Q644 S645 Q646 D647 C648 I649 A650 L653 A654 K657 I658 L659 K660 E661 L662 S663 K664 E665 E666 E667 D668 T669 D670 S671 M675
L678 A679 Y682 E683 I687 F690 C693 Y694 R695 K696 D697 E698 E699 R700 A701 Q702 K703 R707 E710 G713 K714 T715 T716 C717 L720 A721 A724 K725 D726 M727 K728 F729 V730 S731 H732 G733 G734 I735 Q736 A737 F738 L739 V742 W743 W744 G745 Q746 L747 S748 V749
D750 W751 G752 L753 W754 R755 L758 F763 P764 L765 L766 L767 T768 G769 L770 I771 S772 F773 R774 E775 K776 R777 L778 Q779 D780 V781 G782 T783 P784 A785 A786 R787 F791 P795 V796 V797 V798 F799 H800 I803 L804 S805 Y806 F807 A808 F809 L810 V816 L817 M818 V819 D820 S826
W827 C828 E829 C830 A831 I832 Y833 L834 L839 V840 M844 F848 Y849 D850 P851 D852 E853 C854 G855 L856 M857 K858 K859 L862 Y863 F864 N869 D872 V873 G874 A875 I876 F879 V880 A881 G882 L883 T884 I888 P889 A890 Y893 P894 G895 R896 L899 F903 F906



• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain C:

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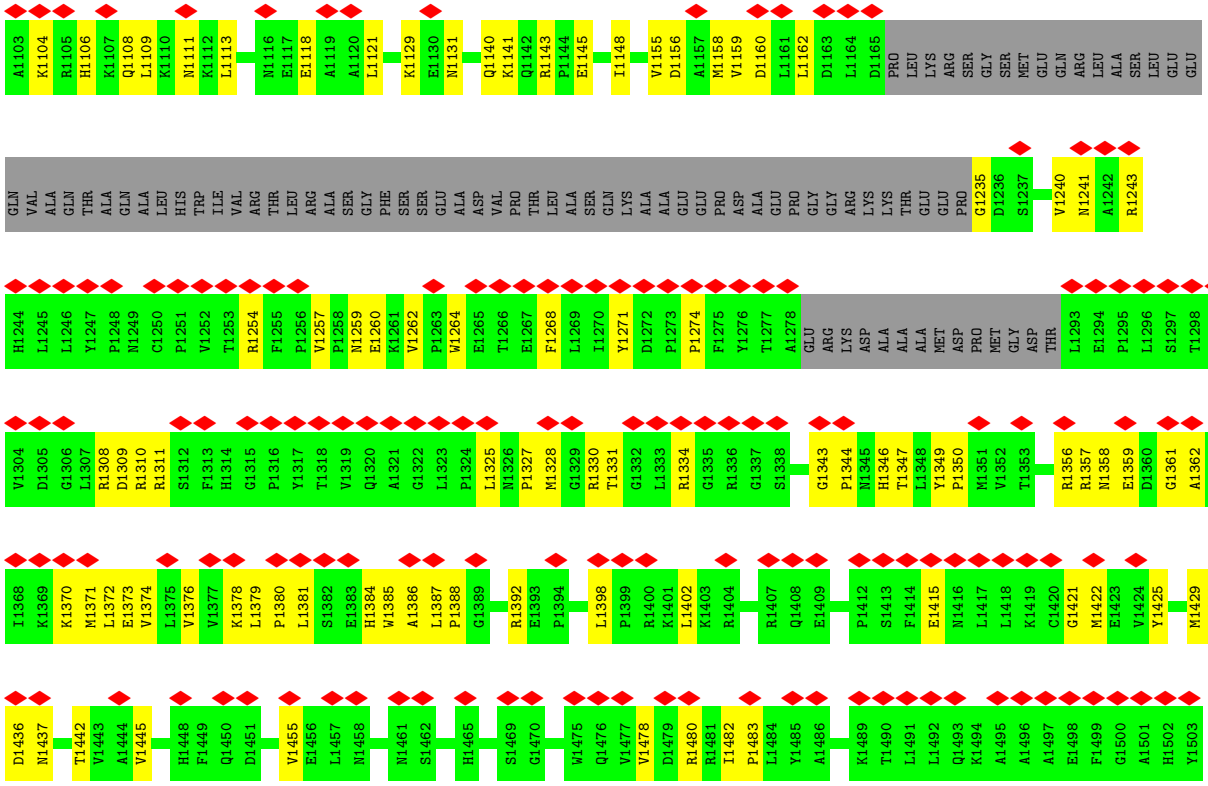
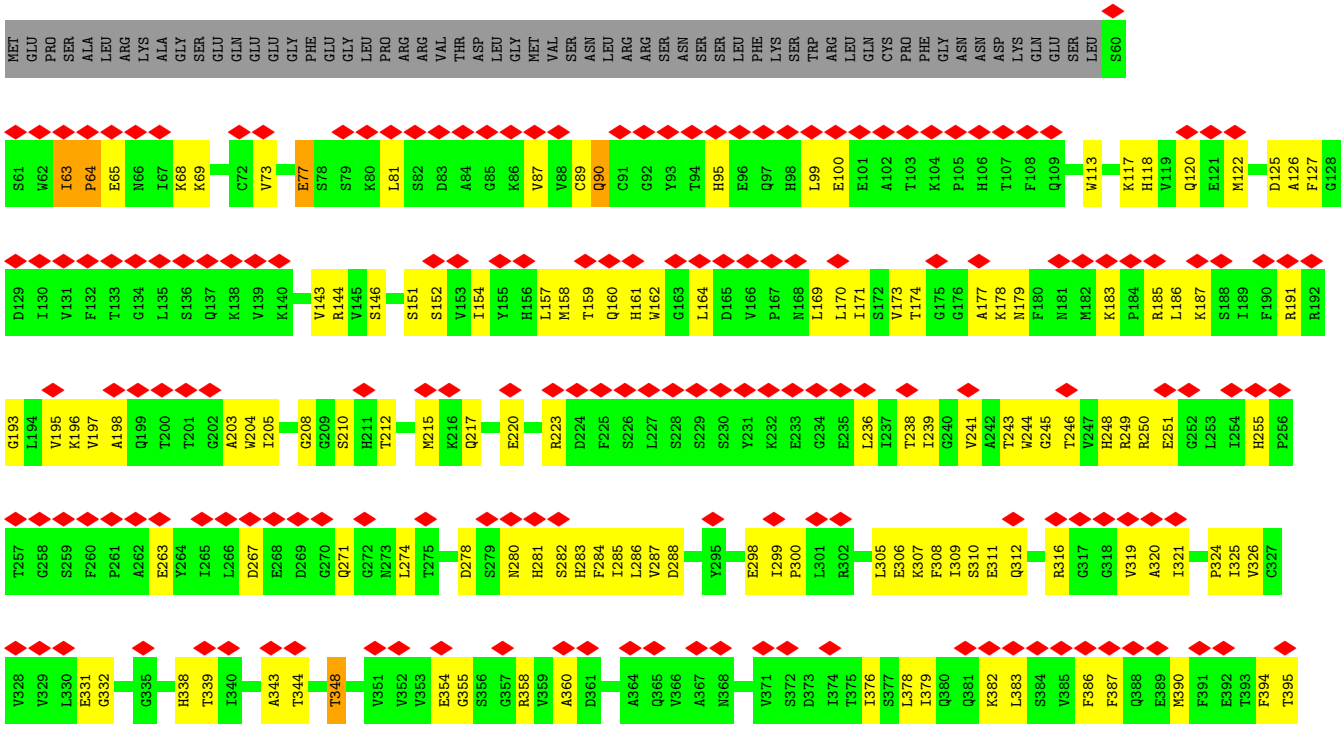
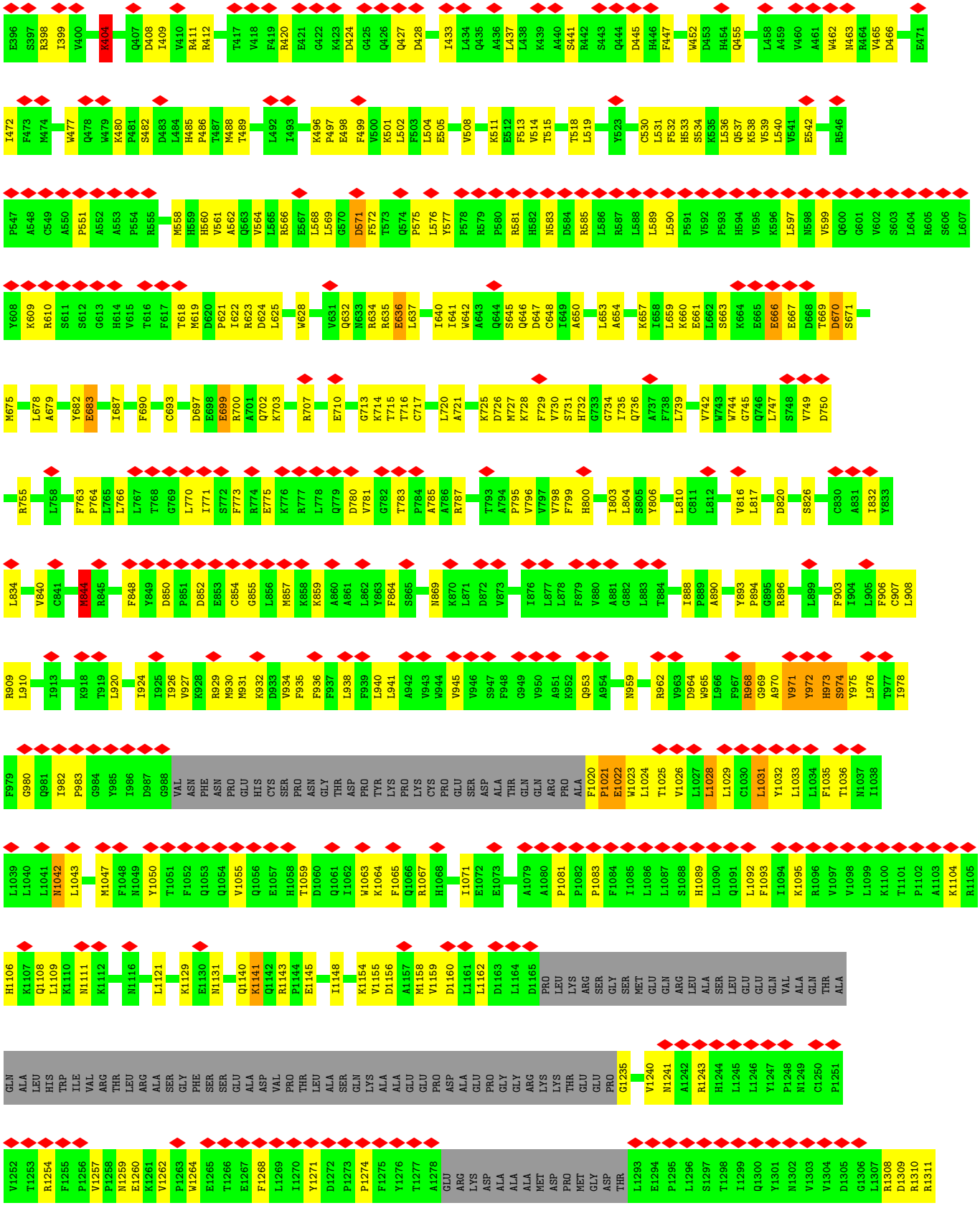
F260 P261 A262 E263 Y264 I265 L266 D267 E268 D269 G270 Q271 G272 N273 L274 T275 D278 S279 N280 H281 S282 H283 F284 I285 L286 V287 D288 Y295 E298 I299 P300 L301 R302 L305 E306 K307 F308 I309 S310 E311 Q312 R316 G317 G318 V319 A320 I321 P324 I325 V326 C327 V328 V329 L330
E331 G332 G335 T336 L337 H338 T339 I340 A343 T344 T348 V351 V352 V353 E354 G355 S366 G357 R358 V359 A360 D361 Q365 V366 A367 N368 V371 S372 D373 I374 T375 I376 S377 L378 I379 Q380 Q381 K382 L383 S384 V385 F386 F387 Q388 E389 M390 F391 E392 T393 F394 T395 E396 S397 R398
I399 V400 K404 Q407 D408 I409 V410 R411 R412 T417 V418 F419 R420 E421 G422 K423 D424 G425 Q426 Q427 D428 I433 L434 Q435 A436 L437 L438 K439 A440 S441 R442 S443 Q444 D445 H446 F447 W452 Q455 L456 K457 L458 A459 V460 A461 W462 N463 R464 V465 D466 E471 I472 F473 M474
D475 E476 W477 Q478 W479 K480 P481 S482 D483 L484 H485 P486 T487 M488 T489 L492 I493 S494 N495 K496 P497 E498 F499 V500 K501 L502 F503 L504 E505 V508 K511 E512 F513 V514 T515 T518 L519 Y523 C530 L531 F532 H533 S534 K535 L536 Q537 K538 V539 L540 V541 E542 D543 P544 E545
R546 P547 A548 C549 A550 P551 A552 A553 P554 R555 M558 H559 H560 V561 A562 Q563 V564 L565 R566 E567 L568 L569 G570 D571 F572 T573 Q574 P575 L576 Y577 P578 R579 P580 R581 H582 N583 D584 R585 L586 R587 L588 L589 L590 P591 V592 P593 H594 V595 K596 L597 N598 V599 Q600 G601 V602 S603 L604 R605 S606
L607 Y608 K609 R610 S611 S612 G613 H614 V615 T616 F617 T618 M619 D620 P621 I622 R623 D624 L625 W628 V631 Q632 N633 R634 R635 E636 L637 I640 I641 W642 A643 Q644 S645 Q646 D647 C648 I649 A650 L653 A654 K657 I658 L659 K660 E661 L662 S663 K664 E665 E666 E667 D668 T669 D670 S671
M675 L678 A679 Y682 E683 I687 F690 C693 Y694 R695 K696 D697 E698 E699 R700 A701 Q702 K703 R707 E710 G713 K714 T715 T716 C717 L720 A721 K725 D726 M727 K728 F729 V730 S731 H732 G733 G734 I735 Q736 A737 F738 L739 V742 W743 W744 G745 Q746 L747
S748 V749 D750 N751 G752 R755 L758 F763 P764 L765 L766 L767 T768 G769 L770 I771 S772 F773 R774 E775 K776 R777 L778 Q779 D780 V781 G782 T783 P784 A785 A786 R787 P795 V796 V797 V798 F799 H800 I803 L804 S805 Y806 F807 A808 F809 L810 C811 L812 Y815 V816 L817 M818 V819 D820
S826 W827 C828 E829 C830 A831 I832 Y833 L834 V840 C841 M844 F848 Y849 D850 P851 D852 E853 C854 G855 L856 M857 K858 K859 A860 F864 N869 D872 V873 G874 A875 I876 L877 V880 A881 G882 L883 T884 I888 P889 A890 R896 L899 D902 F903 I904 L905 F906
C907 L908 R909 T913 I916 S917 K918 T919 K923 I924 I925 I926 V927 K928 R929 M930 M931 K932 D933 V934 F935 L938 F939 L940 L941 A942 V943 W944 V945 V946 S947 F948 G949 V950 A951 K952 Q953 A954 N959 R962 V963 D964 W965 L966 F967 R968 G969 A970 V971 Y972 H973 S974 Y975 L976
T977 I978 F979 G980 Q981 I982 P983 G984 Y985 I986 D987 G988 VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN ARG PRO ALA F1020 P1021 E1022 W1023 L1024 T1025 V1026 L1027 L1028 L1029 C1030 L1031 Y1032 L1033 L1034 F1035 T1036
N1037 I1038 L1039 L1040 L1041 N1042 L1043 L1044 M1047 F1048 N1049 Y1050 T1051 F1052 Q1053 Q1054 V1055 Q1056 E1057 H1058 T1059 D1060 Q1061 I1062 W1063 K1064 F1065 Q1066 R1067 H1068 I1071 E1072 E1073 A1079 A1080 P1081 P1082 P1083 F1084 I1085 L1086 L1087 S1088 H1089 L1090 Q1091 L1092 F1093 I1094 K1095 R1096 V1097 V1098 L1099 K1100 T1101 P1102



• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain D:

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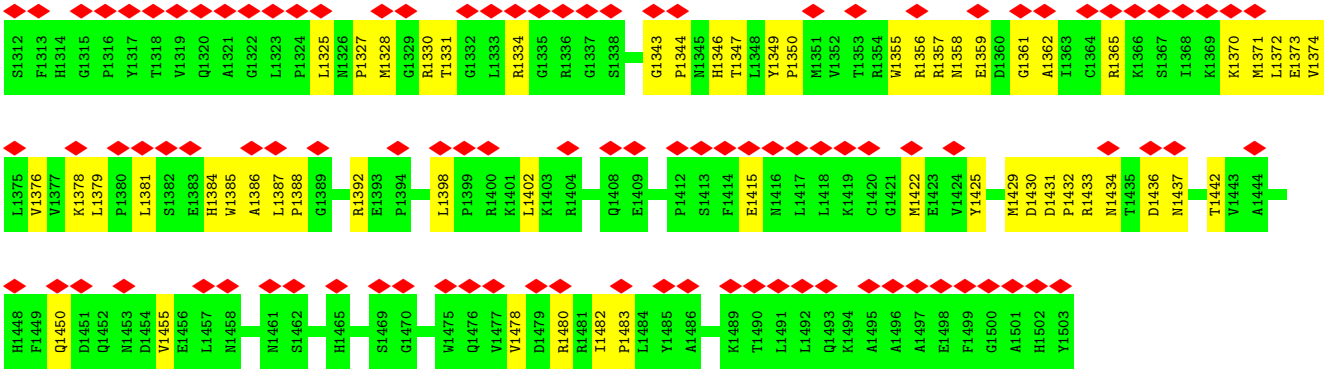
I472 F473 M474 W477 Q478 W479 K480 P481 S482 D483 I484 H485 P486 T487 M488 T489 L492 I493 K496 P497 E498 F499 V500 K501 L502 F503 L504 E505 V508 K511 E512 F513 V514 T515 T518 L519 Y523 C530 L531 F532 H533 S534 K535 L536 Q537 K538 V539 L540 V541 E542 R546
P547 A548 C549 A550 P551 A552 A553 P554 R555 M558 H559 H560 V561 A562 Q563 V564 L565 R566 E567 L568 L569 G570 D571 F572 T573 Q574 P575 L576 Y577 P578 R579 P580 R581 H582 N583 D584 R585 L586 R587 L588 L589 L590 P591 V592 P593 H594 V595 K596 L597 N598 V599 Q600 G601 V602 S603 L604 R605 S606 L607
Y608 K609 R610 S611 S612 G613 H614 V615 T616 F617 T618 M619 D620 P621 I622 R623 D624 L625 W628 V631 Q632 N633 R634 R635 E636 L637 I640 I641 W642 A643 Q644 S645 Q646 D647 C648 I649 A650 L653 A654 K657 I658 L659 K660 E661 L662 S663 K664 E665 E666 E667 D668 T669 D670 S671
M675 L678 A679 Y682 E683 I687 F690 C693 D697 E698 E699 R700 A701 Q702 K703 R707 E710 G713 K714 T715 T716 C717 L720 A721 K725 D726 M727 K728 F729 V730 S731 H732 G733 G734 I735 Q736 A737 F738 L739 V742 W743 W744 G745 Q746 L747 S748 V749 D750
R755 L758 F763 P764 L765 L766 L767 T768 G769 L770 I771 S772 F773 R774 E775 K776 R777 L778 Q779 D780 V781 G782 T783 P784 A785 A786 R787 T793 A794 P795 V796 V797 V798 F799 H800 I803 L804 S805 Y806 L810 C811 L812 V816 L817 D820 S826 C830 A831 I832 Y833
L834 V840 C841 M844 R845 F848 Y849 D850 P851 D852 E853 C854 G855 L856 M857 K858 K859 A860 A861 L862 Y863 F864 S865 N869 K870 L871 D872 V873 I876 L877 L878 F879 V880 A881 G882 L883 T884 I888 P889 A890 Y893 P894 G895 R896 L899 F903 I904 L905 F906 C907 L908
R909 L910 I913 K918 T919 L920 I924 I925 I926 V927 K928 R929 M930 M931 K932 D933 V934 F935 F936 F937 L938 F939 L940 L941 A942 V943 W944 V945 V946 S947 F948 G949 V950 A951 K952 Q953 A954 N959 R962 V963 D964 W965 L966 F967 R968 G969 A970 V971 Y972 H973 S974 Y975 L976 T977 I978
F979 G980 Q981 I982 P983 G984 Y985 I986 D987 G988 VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN ARG PRO ALA F1020 P1021 E1022 W1023 L1024 T1025 V1026 L1027 L1028 L1029 C1030 L1031 Y1032 L1033 L1034 F1035 T1036 N1037 I1038
L1039 L1040 L1041 N1042 L1043 M1047 F1048 N1049 Y1050 T1051 F1052 Q1053 Q1054 V1055 Q1056 E1057 H1058 T1059 D1060 Q1061 I1062 W1063 K1064 F1065 Q1066 R1067 H1068 I1071 E1072 E1073 A1079 A1080 P1081 P1082 P1083 F1084 I1085 L1086 L1087 S1088 H1089 L1090 Q1091 L1092 F1093 I1094 K1095 R1096 V1097 V1098 L1099 K1100 T1101 P1102 A1103 K1104 R1105
H1106 K1107 Q1108 L1109 K1110 N1111 K1112 N1116 L1121 K1129 E1130 N1131 Q1140 K1141 Q1142 R1143 P1144 E1145 I1148 K1154 V1155 D1156 A1157 M1158 V1159 D1160 L1161 L1162 D1163 L1164 D1165 PRO LEU LYS ARG SER GLY SER MET GLU GLN ARG LEU ALA SER LEU GLU GLU GLN VAL ALA GLN THR ALA
GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ARG ALA SER GLY PHE SER SER SER GLU ALA ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA ALA GLU GLU PRO ASP ALA ALA GLU PRO GLY GLY GLY ARG LYS LYS THR GLU GLU PRO G1235 V1240 N1241 A1242 R1243 H1244 L1245 L1246 Y1247 P1248 N1249 C1250 P1251
V1252 T1253 R1254 F1255 P1256 V1257 P1258 N1259 E1260 K1261 V1262 P1263 W1264 E1265 T1266 E1267 F1268 L1269 I1270 Y1271 D1272 P1273 P1274 F1275 Y1276 T1277 A1278 GLU ARG LYS ASP ALA ALA ALA MET ASP PRO MET GLY ASP THR L1293 E1294 P1295 L1296 S1297 T1298 I1299 Q1300 Y1301 N1302 V1303 V1304 D1305 G1306 L1307 R1308 D1309 R1310 R1311


S1312 F1313 H1314 G1315 P1316 Y1317 T1318 V1319 Q1320 A1321 G1322 L1323 P1324 L1325 N1326 P1327 M1328 G1329 R1330 T1331 G1332 L1333 R1334 G1335 R1336 G1337 S1338 G1343 P1344 N1345 H1346 T1347 L1348 Y1349 P1350 M1351 V1352 T1353 R1354 W1355 R1356 R1357 N1358 E1359 D1360 G1361 A1362 I1363 C1364 R1365 K1366 S1367 I1368 K1369 K1370 M1371 L1372 E1373 V1374
L1375 V1376 V1377 K1378 L1379 P1380 L1381 S1382 E1383 H1384 W1385 A1386 L1387 P1388 G1389 R1392 E1393 P1394 L1398 P1399 R1400 K1401 L1402 K1403 R1404 Q1408 E1409 P1412 S1413 F1414 E1415 N1416 L1417 L1418 K1419 C1420 G1421 M1422 E1423 V1424 Y1425 M1429 D1430 D1431 P1432 R1433 N1434 T1435 D1436 N1437 T1442 V1443 A1444
H1448 F1449 Q1450 D1451 Q1452 N1453 D1454 V1455 E1456 L1457 N1458 N1461 S1462 H1465 S1469 G1470 W1475 Q1476 V1477 V1478 D1479 R1480 R1481 I1482 P1483 L1484 Y1485 A1486 K1489 T1490 L1491 L1492 Q1493 K1494 A1495 A1496 A1497 E1498 F1499 G1500 A1501 H1502 Y1503

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95674	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 ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	22000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.852	Depositor
Minimum map value	-0.361	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.169	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	0/10787	0.52	6/14658 (0.0%)
1	B	0.18	0/10787	0.52	6/14658 (0.0%)
1	C	0.18	0/10787	0.52	6/14658 (0.0%)
1	D	0.18	0/10787	0.52	6/14658 (0.0%)
All	All	0.18	0/43148	0.52	24/58632 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	6
1	D	0	6
All	All	0	24

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	974	SER	N-CA-C	5.98	121.14	113.18
1	B	974	SER	N-CA-C	5.96	121.11	113.18
1	D	974	SER	N-CA-C	5.96	121.10	113.18
1	A	974	SER	N-CA-C	5.93	121.07	113.18
1	A	404	LYS	CB-CG-CD	5.82	124.69	111.30

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	ILE	Peptide
1	A	666	GLU	Peptide
1	A	965	TRP	Peptide
1	A	968	ARG	Peptide
1	A	971	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10521	0	10407	395	0
1	B	10521	0	10407	409	0
1	C	10521	0	10407	392	0
1	D	10521	0	10407	373	0
2	A	35	0	19	1	0
2	B	35	0	19	1	0
2	C	35	0	19	1	0
2	D	35	0	19	0	0
3	A	26	0	12	1	0
3	B	26	0	12	1	0
3	C	26	0	12	1	0
3	D	26	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	42336	0	41752	1451	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 17.

The worst 5 of 1451 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:1022:GLU:HB3	1:D:975:TYR:N	1.66	1.09
1:A:1024:LEU:H	1:B:972:TYR:C	1.70	0.99
1:C:1022:GLU:HB3	1:D:975:TYR:H	0.84	0.99
1:C:1022:GLU:CB	1:D:975:TYR:H	1.78	0.95
1:B:981:GLN:NE2	1:C:981:GLN:OE1	1.99	0.95

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	1322/1503 (88%)	1169 (88%)	147 (11%)	6 (0%)	25	64
1	B	1322/1503 (88%)	1170 (88%)	145 (11%)	7 (0%)	25	64
1	C	1322/1503 (88%)	1171 (89%)	144 (11%)	7 (0%)	25	64
1	D	1322/1503 (88%)	1171 (89%)	145 (11%)	6 (0%)	25	64
All	All	5288/6012 (88%)	4681 (88%)	581 (11%)	26 (0%)	27	64

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	PRO
1	A	87	VAL
1	B	64	PRO
1	B	87	VAL
1	C	64	PRO

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	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
1	B	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
1	C	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
1	D	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
All	All	4436/5272 (84%)	4324 (98%)	112 (2%)	43	62

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	195	VAL
1	D	1371	MET
1	C	834	LEU
1	D	1160	ASP
1	D	834	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	732	HIS
1	D	732	HIS
1	C	118	HIS
1	D	684	HIS
1	D	1437	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	APR	A	1601	-	35,38,39	0.63	0	43,58,60	0.83	2 (4%)
2	APR	B	1601	-	35,38,39	0.63	0	43,58,60	0.83	2 (4%)
2	APR	C	1601	-	35,38,39	0.62	0	43,58,60	0.83	2 (4%)
3	DAT	C	1602	-	24,28,28	0.78	0	30,43,43	0.86	1 (3%)
3	DAT	B	1602	-	24,28,28	0.77	0	30,43,43	0.86	1 (3%)
3	DAT	A	1602	-	24,28,28	0.77	0	30,43,43	0.87	1 (3%)
3	DAT	D	1602	-	24,28,28	0.78	0	30,43,43	0.86	1 (3%)
2	APR	D	1601	-	35,38,39	0.63	0	43,58,60	0.83	2 (4%)

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	APR	A	1601	-	-	0/18/50/54	0/4/4/4
2	APR	B	1601	-	-	0/18/50/54	0/4/4/4
2	APR	C	1601	-	-	0/18/50/54	0/4/4/4
3	DAT	C	1602	-	-	1/12/28/28	0/3/3/3
3	DAT	B	1602	-	-	1/12/28/28	0/3/3/3
3	DAT	A	1602	-	-	1/12/28/28	0/3/3/3
3	DAT	D	1602	-	-	1/12/28/28	0/3/3/3
2	APR	D	1601	-	-	0/18/50/54	0/4/4/4

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1601	APR	C1D-C2D-C3D	-3.04	98.54	102.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1601	APR	C1D-C2D-C3D	-3.04	98.55	102.29
2	B	1601	APR	C1D-C2D-C3D	-3.02	98.57	102.29
2	C	1601	APR	C1D-C2D-C3D	-3.01	98.59	102.29
2	D	1601	APR	C5-C6-N6	2.34	123.87	120.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1602	DAT	PB-O3A-PA-O5'
3	B	1602	DAT	PB-O3A-PA-O5'
3	C	1602	DAT	PB-O3A-PA-O5'
3	D	1602	DAT	PB-O3A-PA-O5'

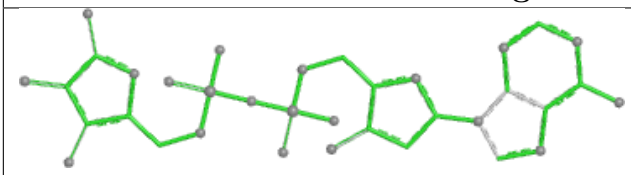
There are no ring outliers.

7 monomers are involved in 7 short contacts:

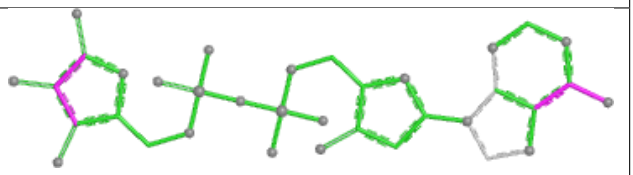
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	APR	1	0
2	B	1601	APR	1	0
2	C	1601	APR	1	0
3	C	1602	DAT	1	0
3	B	1602	DAT	1	0
3	A	1602	DAT	1	0
3	D	1602	DAT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand APR A 1601



Bond lengths



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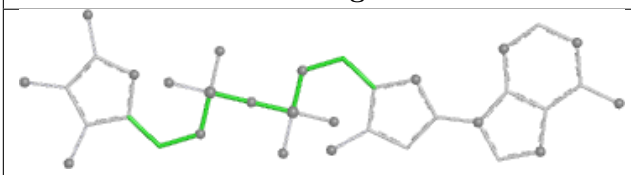
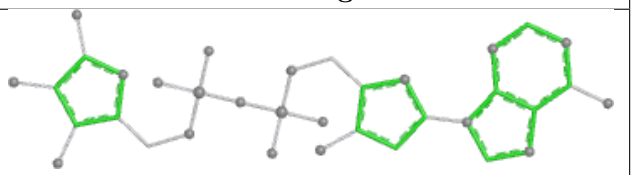
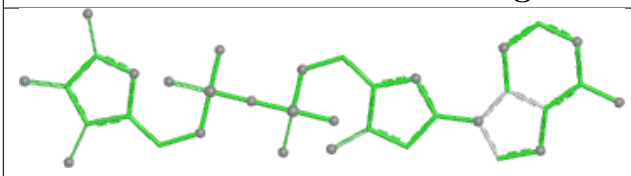


Torsions



Rings

Ligand APR B 1601



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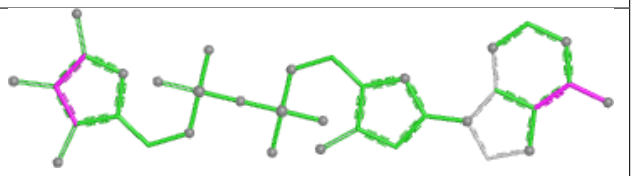

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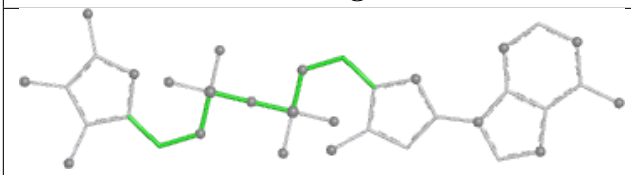

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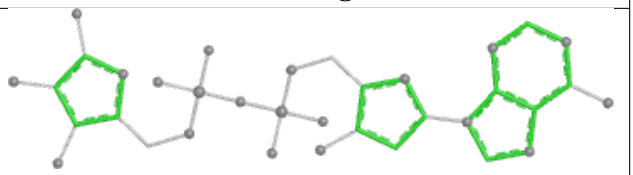
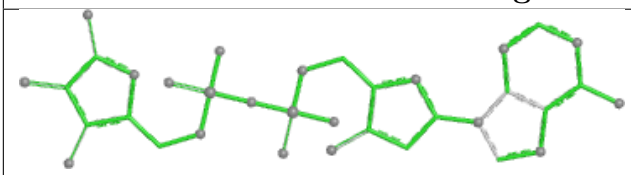


Rings

Ligand APR C 1601



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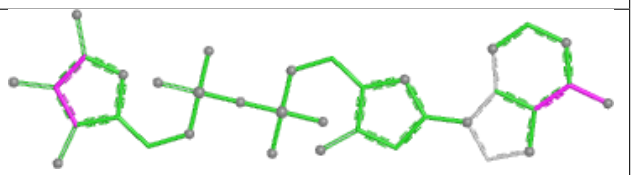

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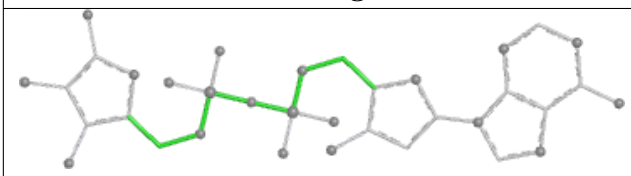

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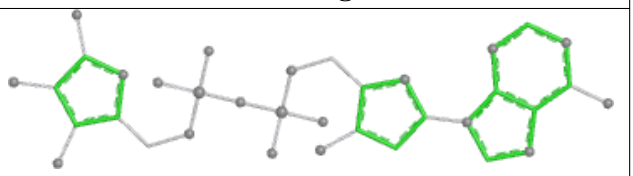

Rings

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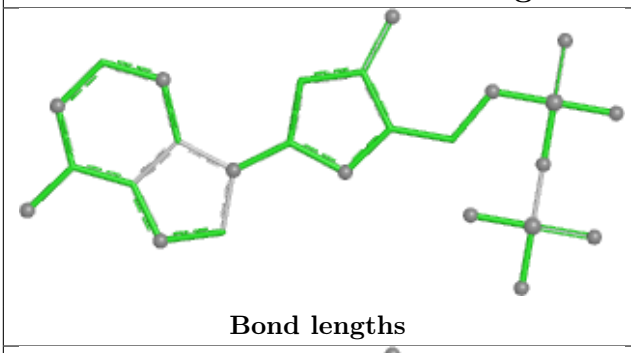

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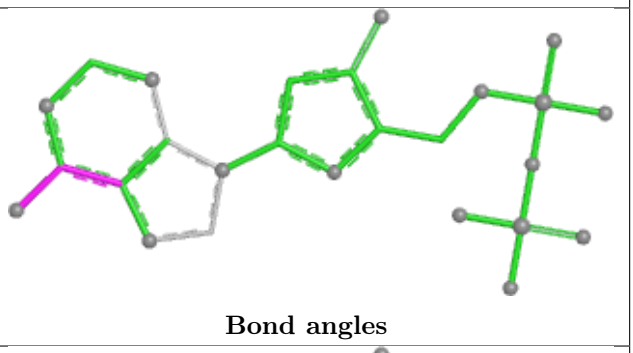
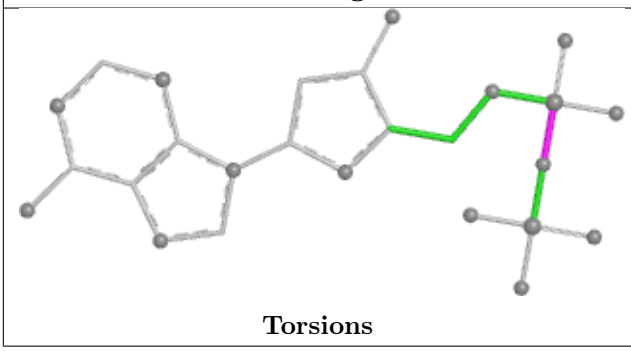


Bond angles



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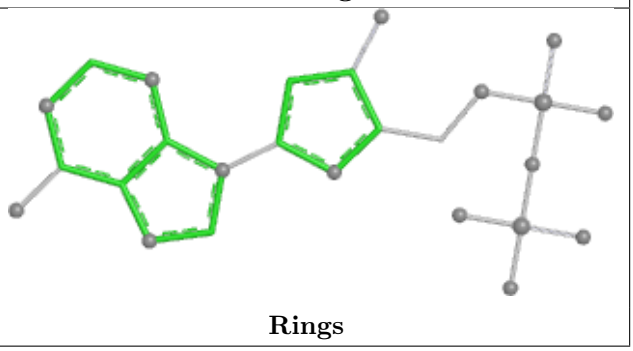
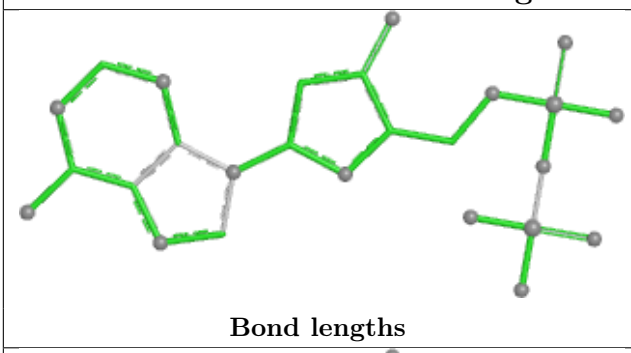
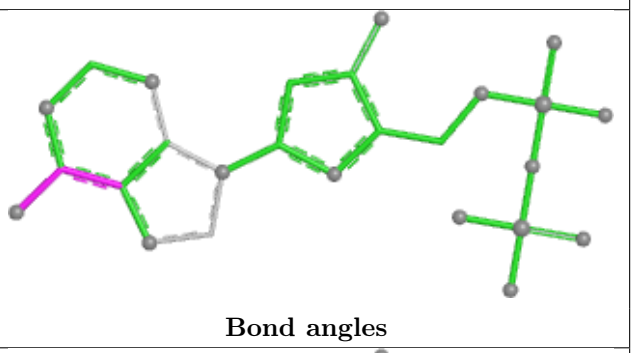


Rings

Ligand DAT B 1602



Bond lengths



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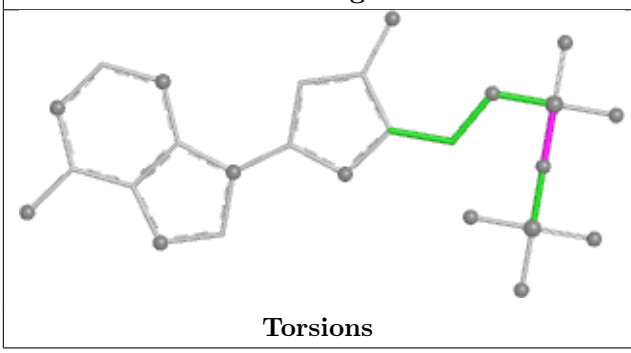

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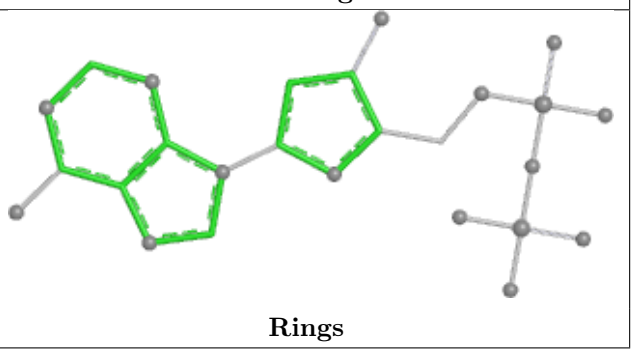
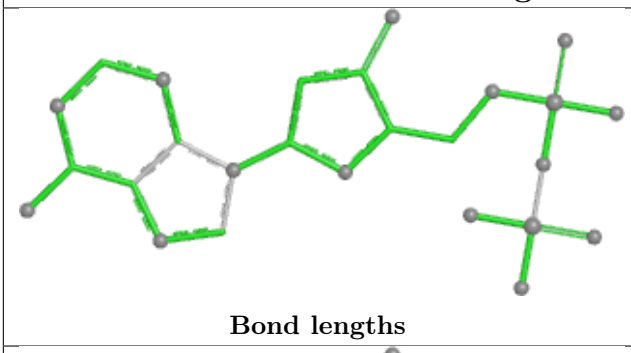
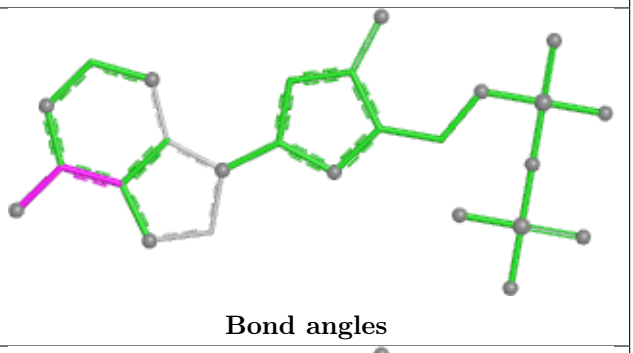


Rings

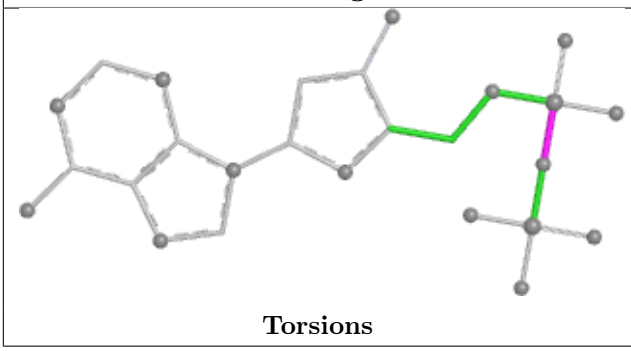
Ligand DAT A 1602



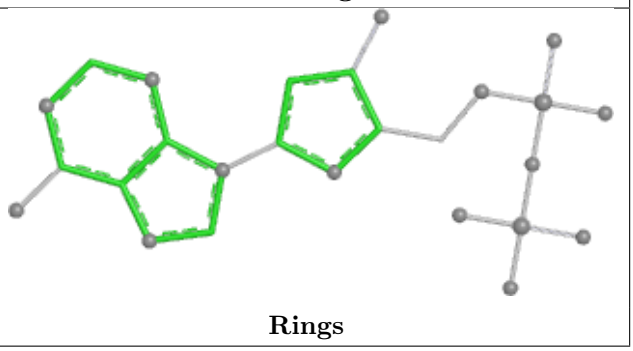
Bond lengths



Bond angles

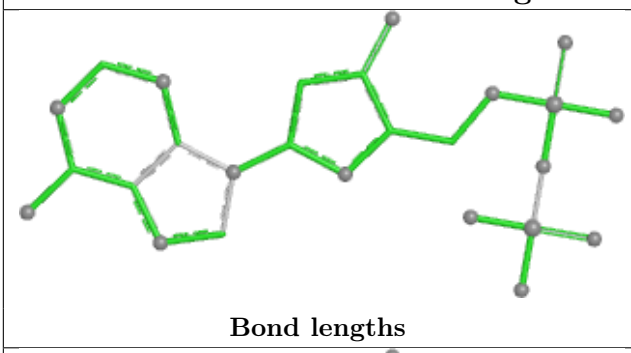


Torsions

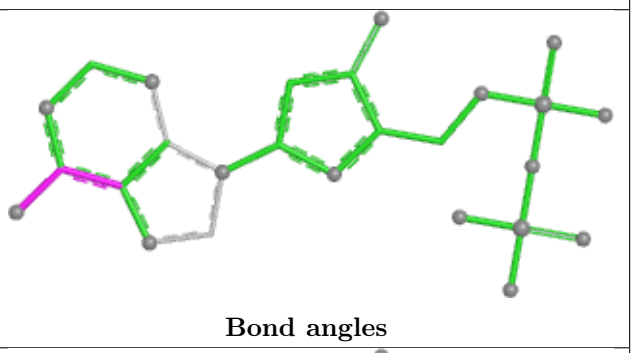


Rings

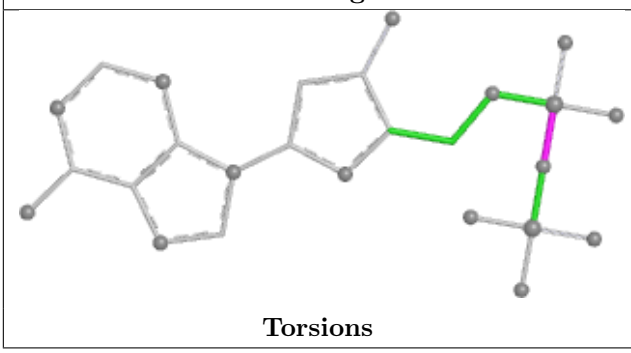
Ligand DAT D 1602



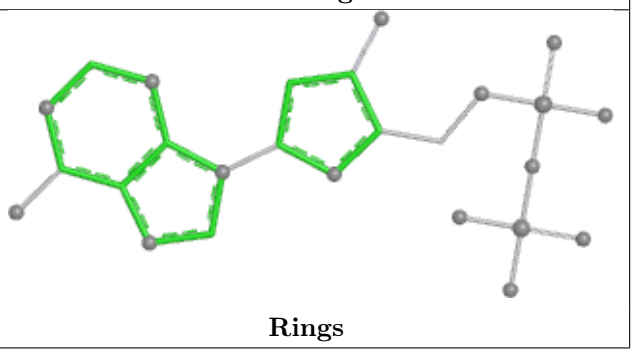
Bond lengths



Bond angles

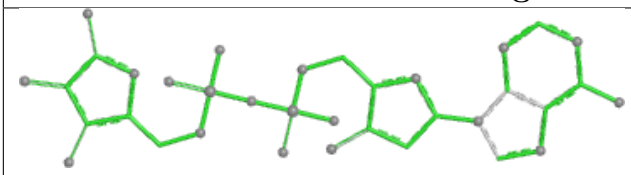


Torsions

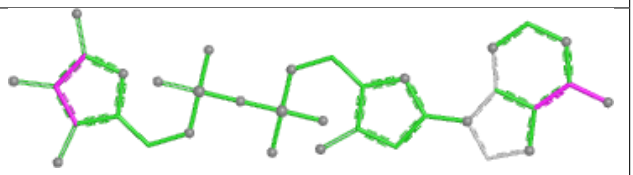


Rings

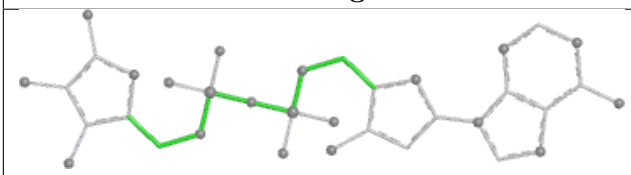
Ligand APR D 1601



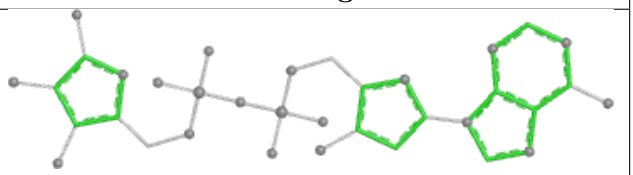
Bond lengths



Bond angles



Torsions



Rings

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.

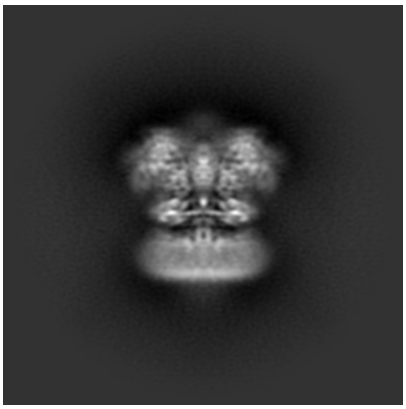
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27924. These allow visual inspection of the internal detail of the map and identification of artifacts.

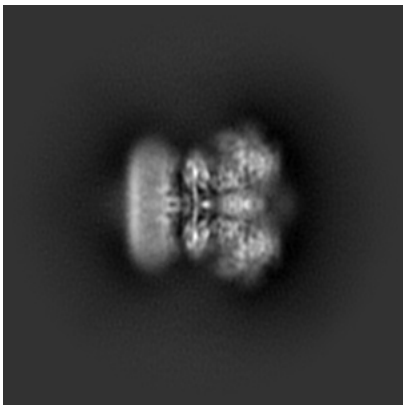
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

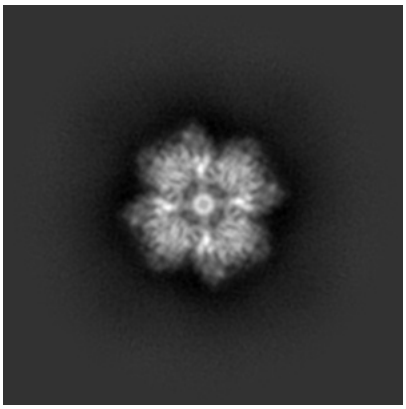
6.1.1 Primary map



X

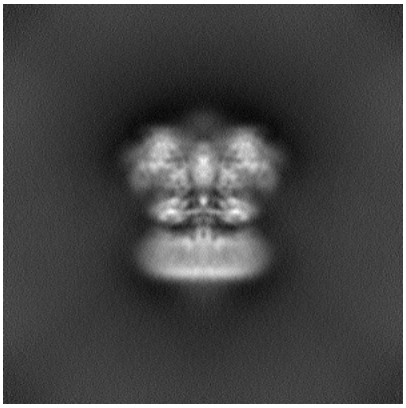


Y

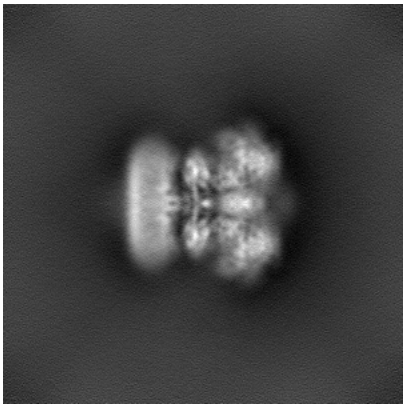


Z

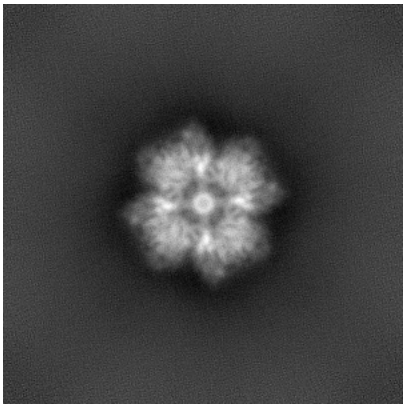
6.1.2 Raw map



X



Y

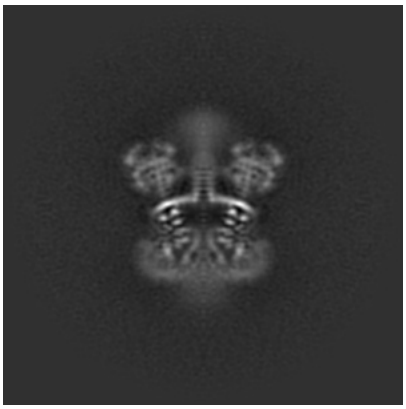


Z

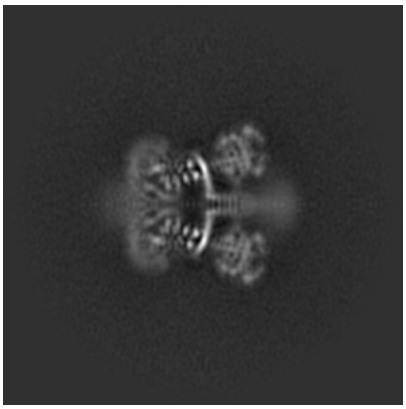
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

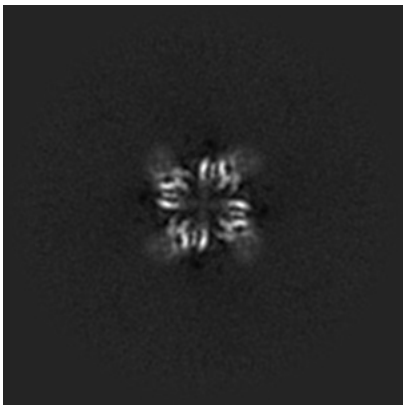
6.2.1 Primary map



X Index: 180

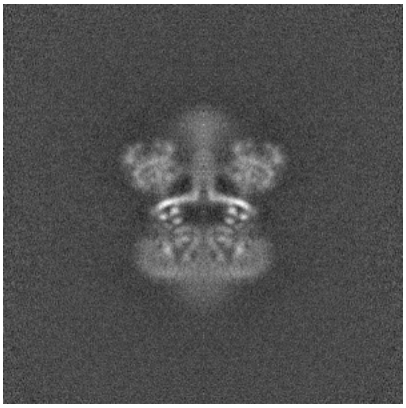


Y Index: 180

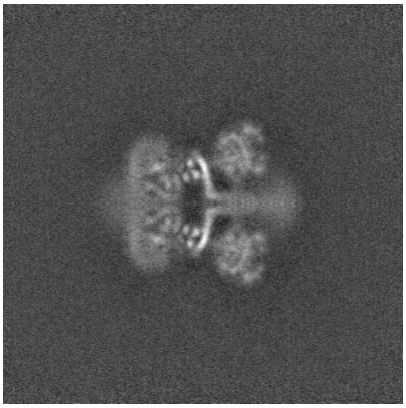


Z Index: 180

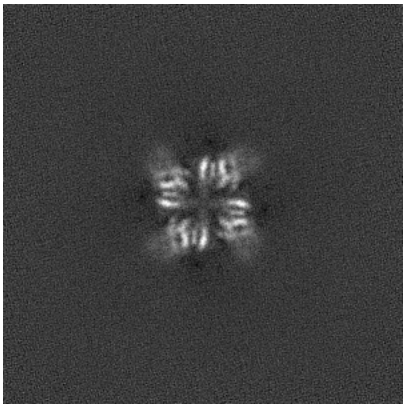
6.2.2 Raw map



X Index: 180



Y Index: 180

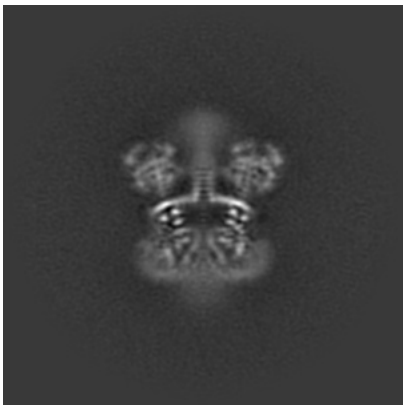


Z Index: 180

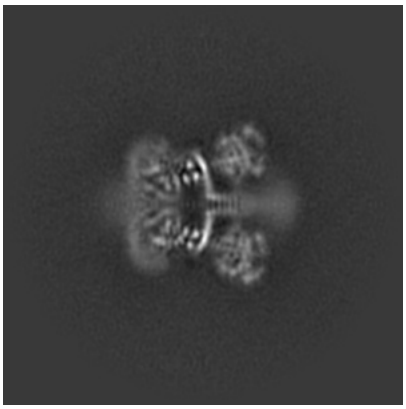
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

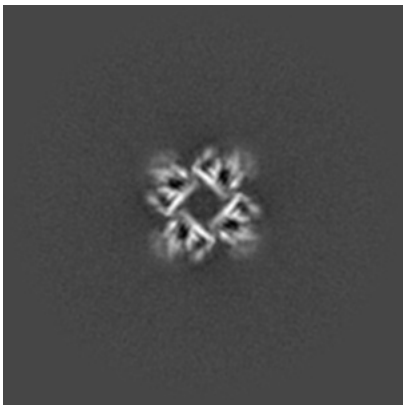
6.3.1 Primary map



X Index: 179

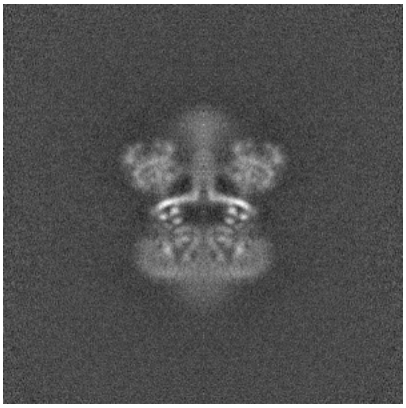


Y Index: 179

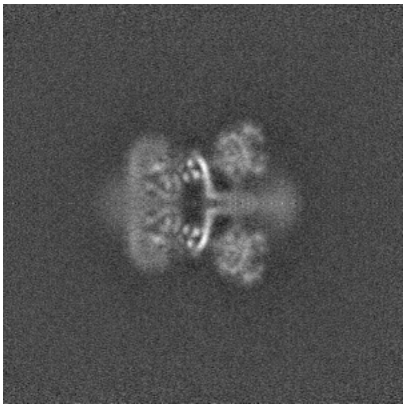


Z Index: 173

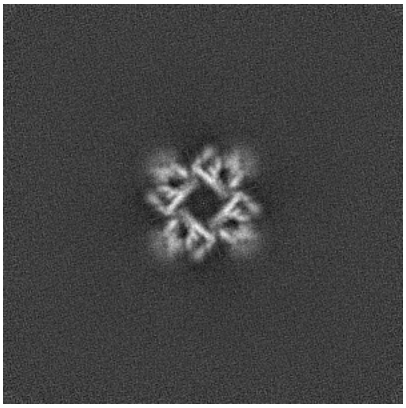
6.3.2 Raw map



X Index: 180



Y Index: 180

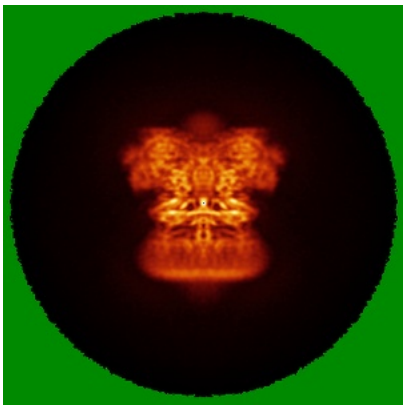


Z Index: 173

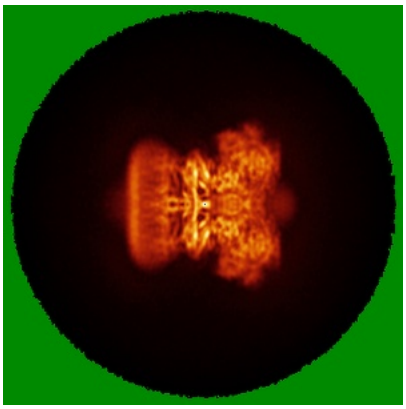
The images above show the largest variance slices of the map in three orthogonal directions.

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

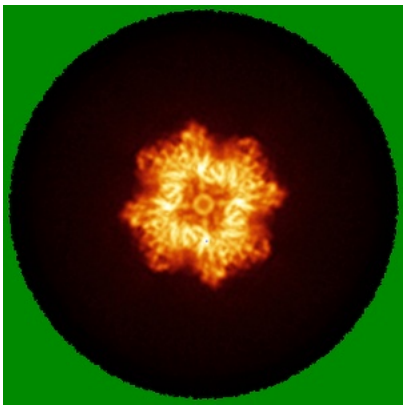
6.4.1 Primary map



X

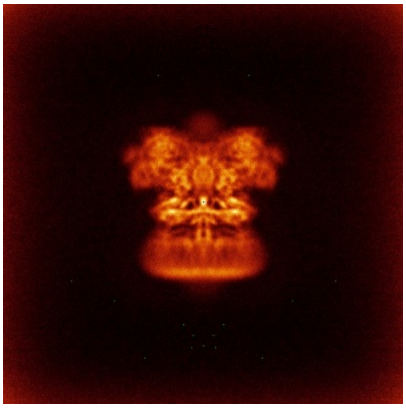


Y

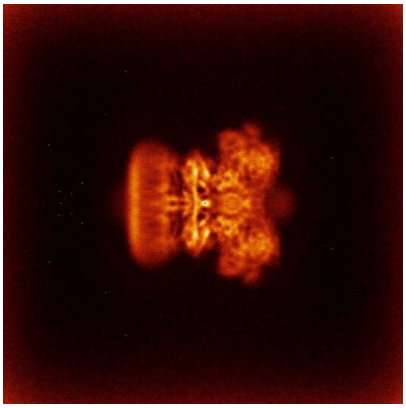


Z

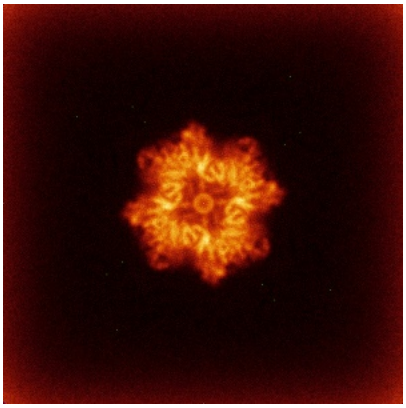
6.4.2 Raw map



X



Y

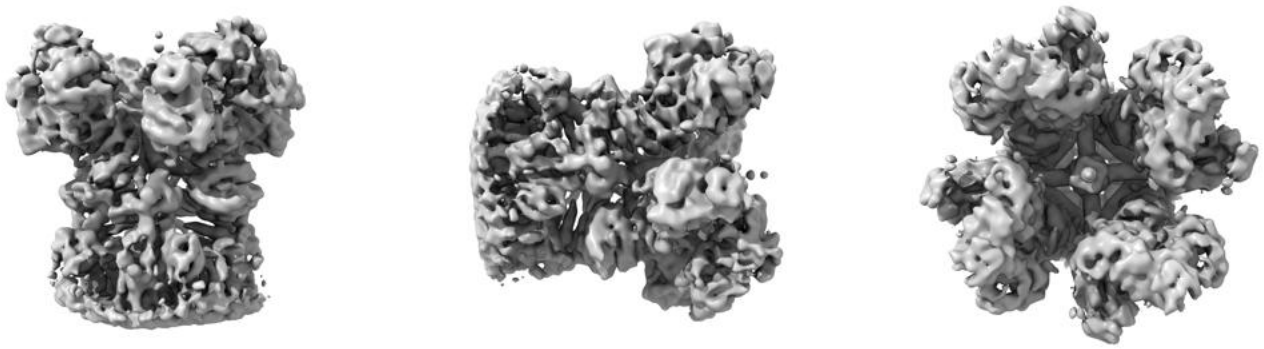


Z

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 0.169. 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.

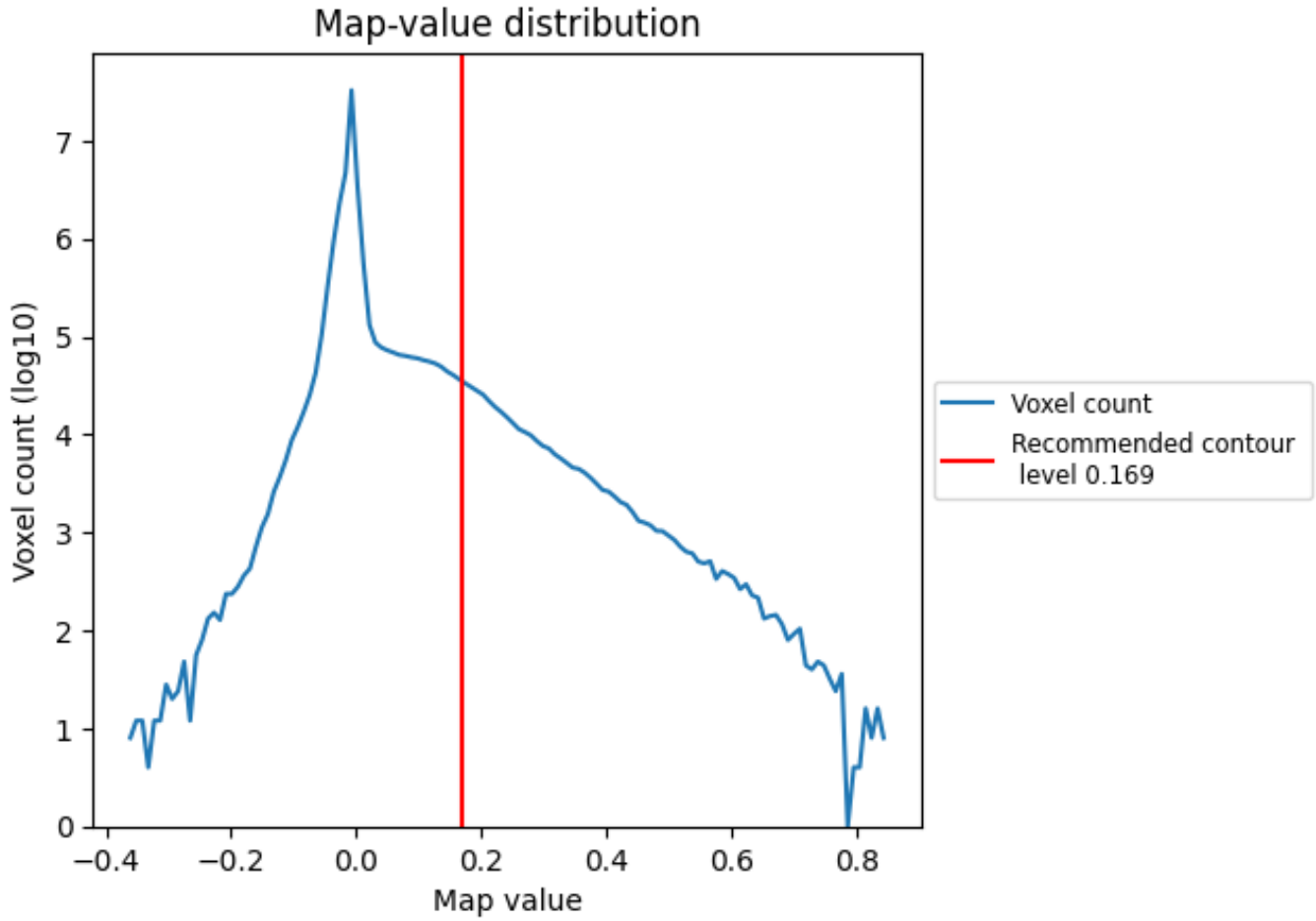
6.6 Mask visualisation (i)

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

7 Map analysis

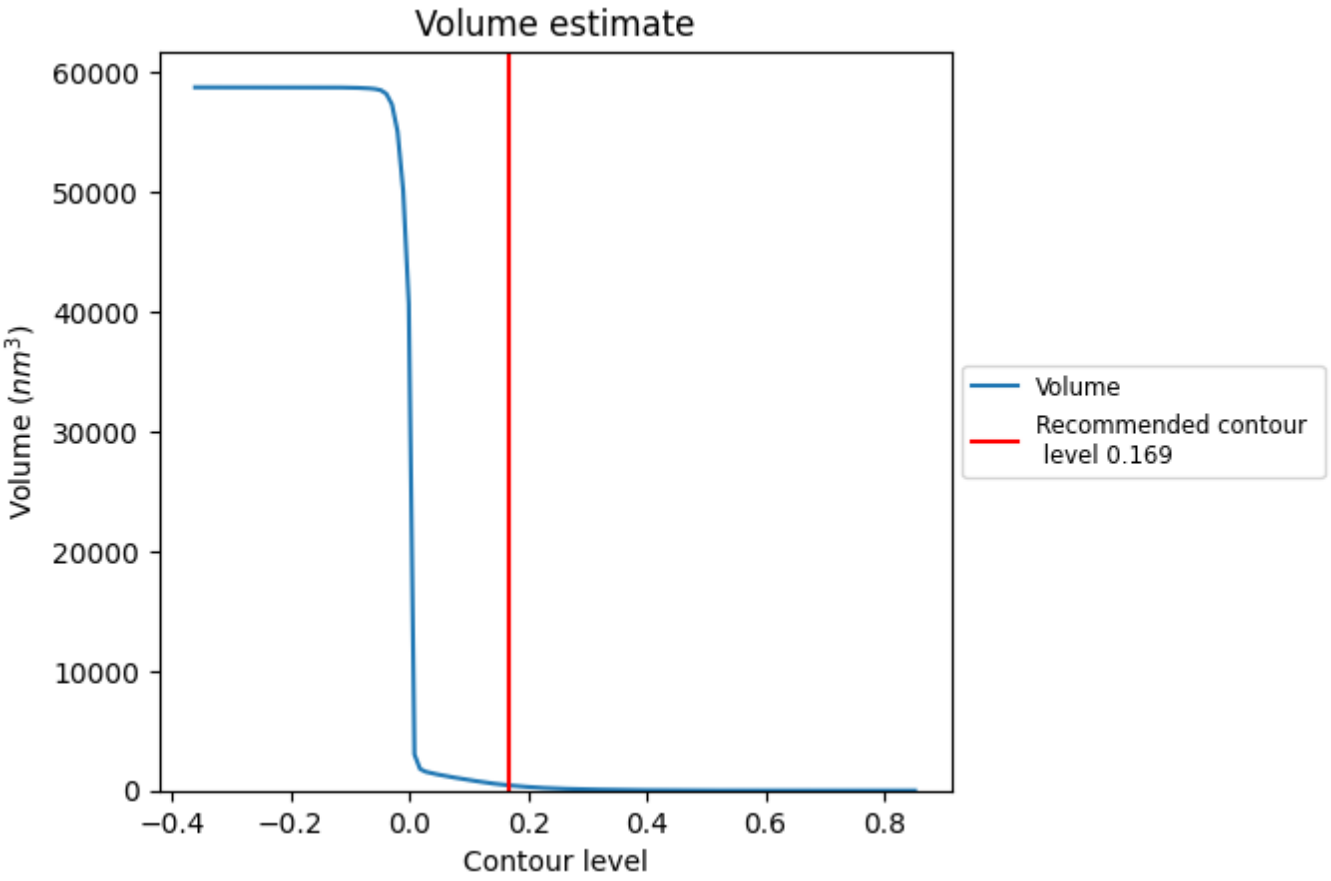
This section contains the results of statistical analysis of the map.

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.

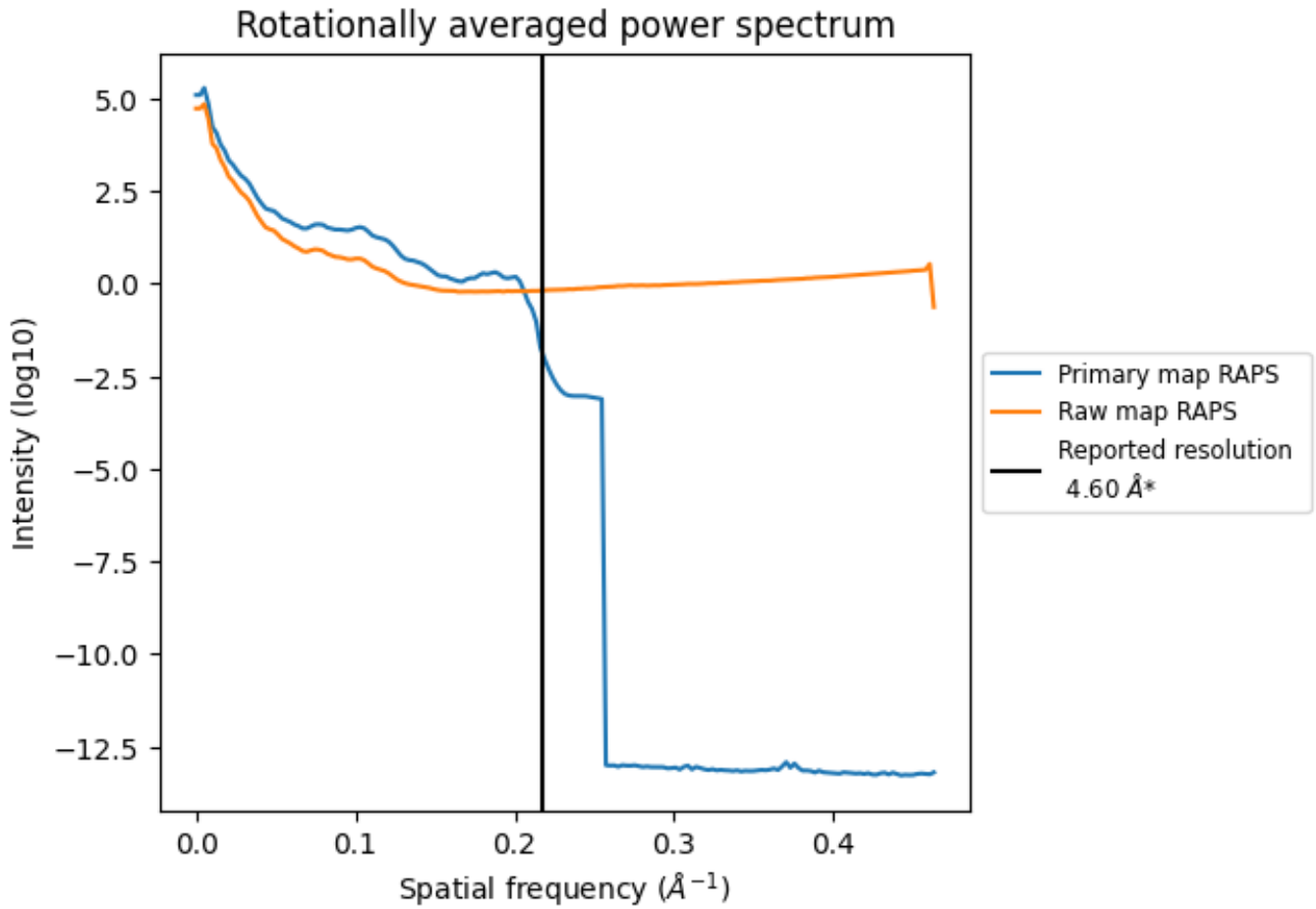
7.2 Volume estimate (i)



The volume at the recommended contour level is 431 nm^3; this corresponds to an approximate mass of 390 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)

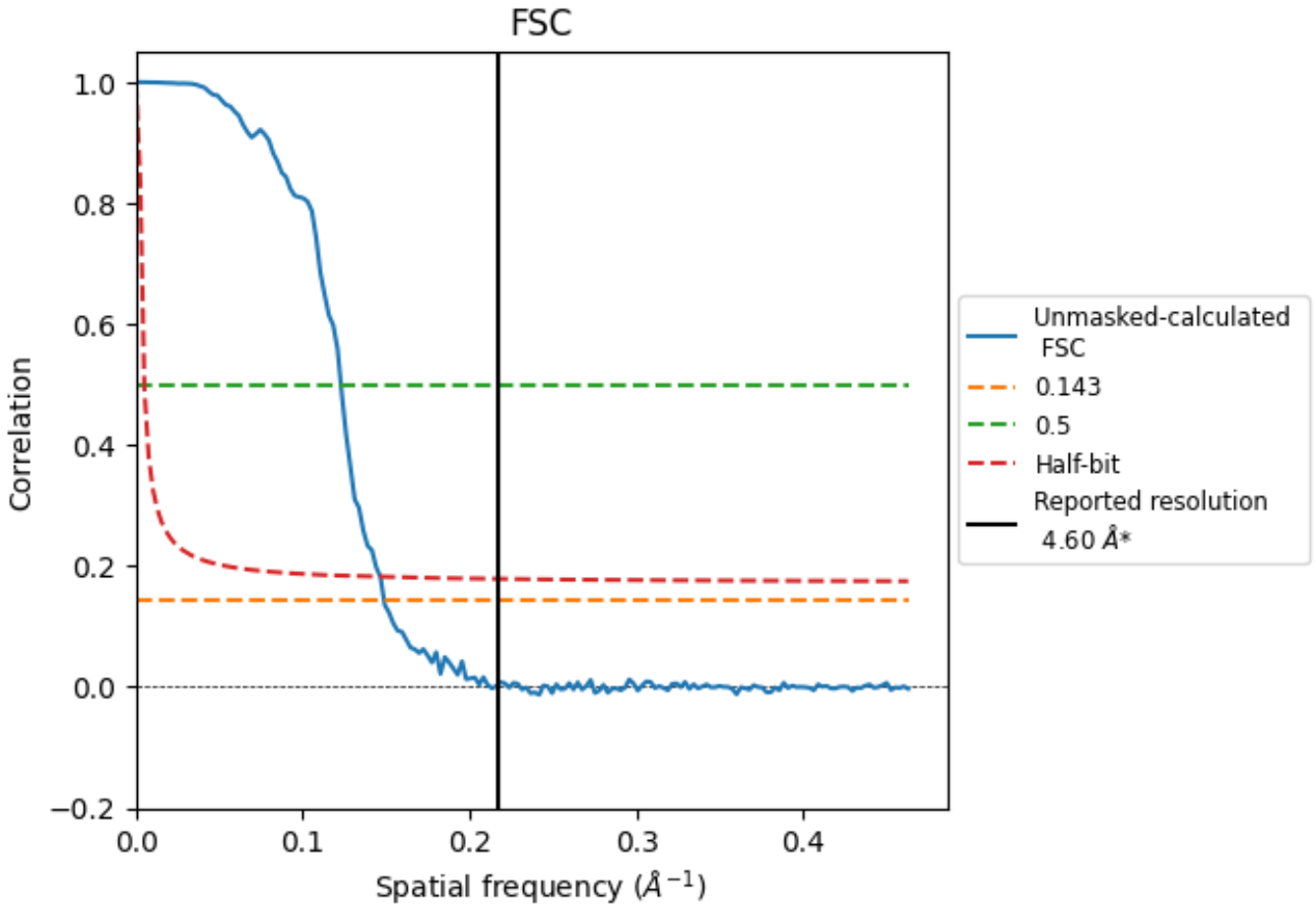


*Reported resolution corresponds to spatial frequency of 0.217 $Å^{-1}$

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

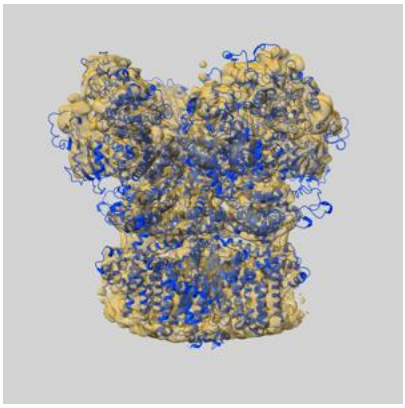
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.72	8.14	6.82

*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 6.72 differs from the reported value 4.6 by more than 10 %

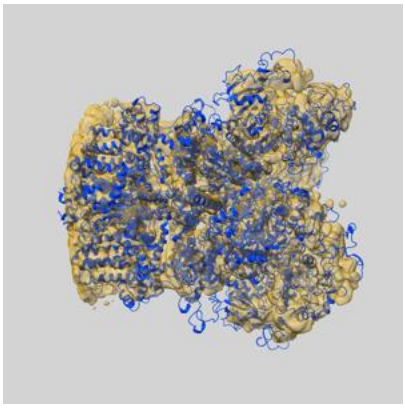
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27924 and PDB model 8E6S. Per-residue inclusion information can be found in section 3 on page 6.

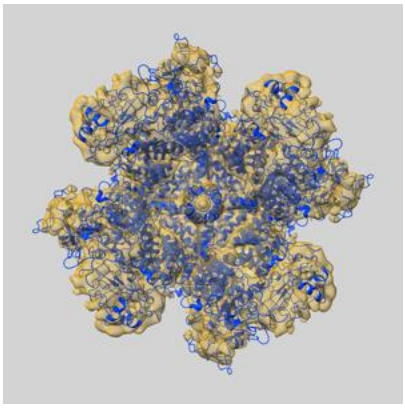
9.1 Map-model overlay



X



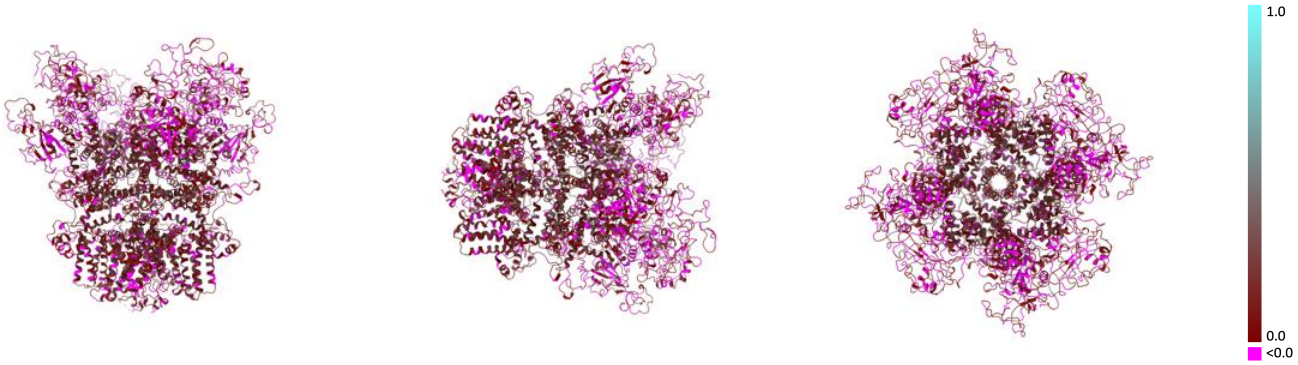
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.169 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.

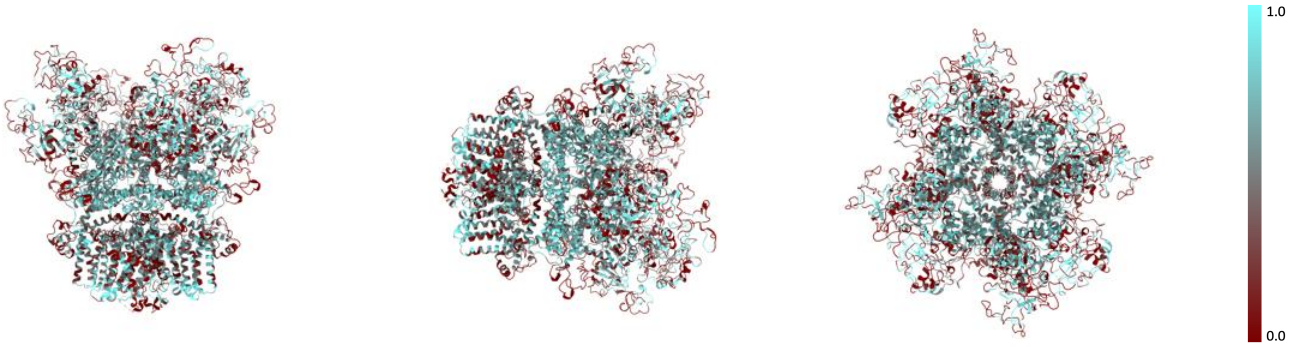
9.2 Q-score mapped to coordinate model (i)



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.

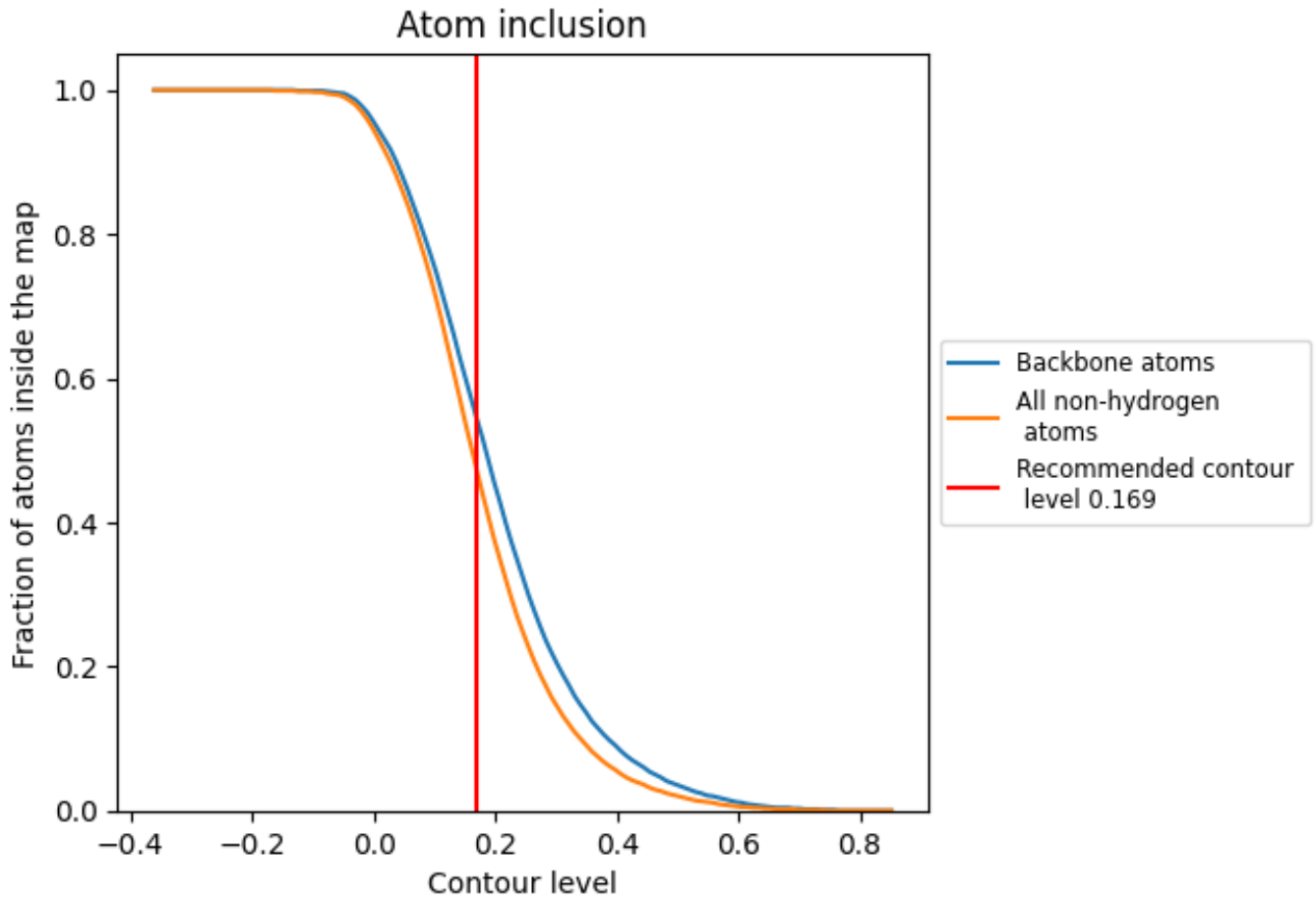
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.169).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 48% 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 (0.169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4750	0.0970
A	0.4750	0.0990
B	0.4760	0.0970
C	0.4710	0.0940
D	0.4760	0.0970