Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 04:49 PM EST

PDB ID	:	8DGF
EMDB ID	:	EMD-27422
Title	:	Avs4 bound to phage PhiV-1 portal
Authors	:	Wilkinson, M.E.; Gao, L.; Strecker, J.; Makarova, K.S.; Macrae, R.K.; Koonin, E.V.; Zhang, F.
Deposited on	:	2022-06-23
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

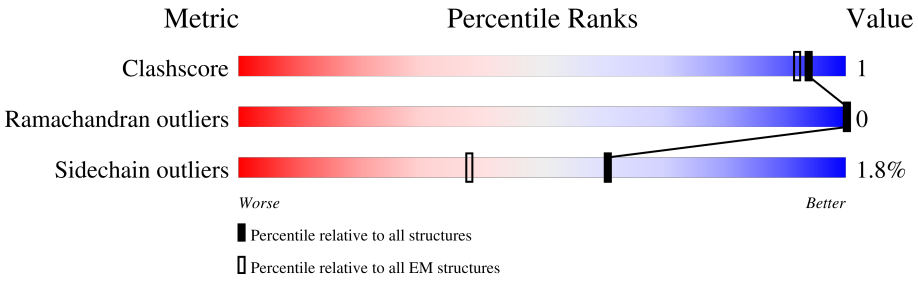
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1587	66% 93%
1	B	1587	69% 92%
1	C	1587	66% 94%
1	D	1587	69% 93%
2	E	535	82% 76% 5% 18%
2	F	535	82% 73% 8% 18%
2	G	535	82% 79% 18%
2	H	535	82% 74% 7% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 64958 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.

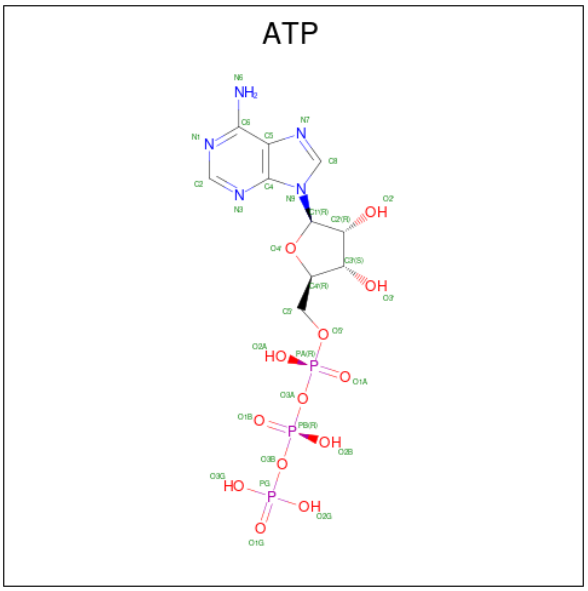
- Molecule 1 is a protein called ATP-binding protein Avs4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1541	Total	C	N	O	S	0	0
			12805	8291	2104	2370	40		
1	B	1534	Total	C	N	O	S	0	0
			12756	8265	2094	2358	39		
1	C	1541	Total	C	N	O	S	0	0
			12805	8291	2104	2370	40		
1	D	1534	Total	C	N	O	S	0	0
			12756	8265	2094	2358	39		

- Molecule 2 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	438	Total	C	N	O	S	0	0
			3427	2165	565	678	19		
2	F	438	Total	C	N	O	S	0	0
			3427	2165	565	678	19		
2	G	438	Total	C	N	O	S	0	0
			3427	2165	565	678	19		
2	H	438	Total	C	N	O	S	0	0
			3427	2165	565	678	19		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

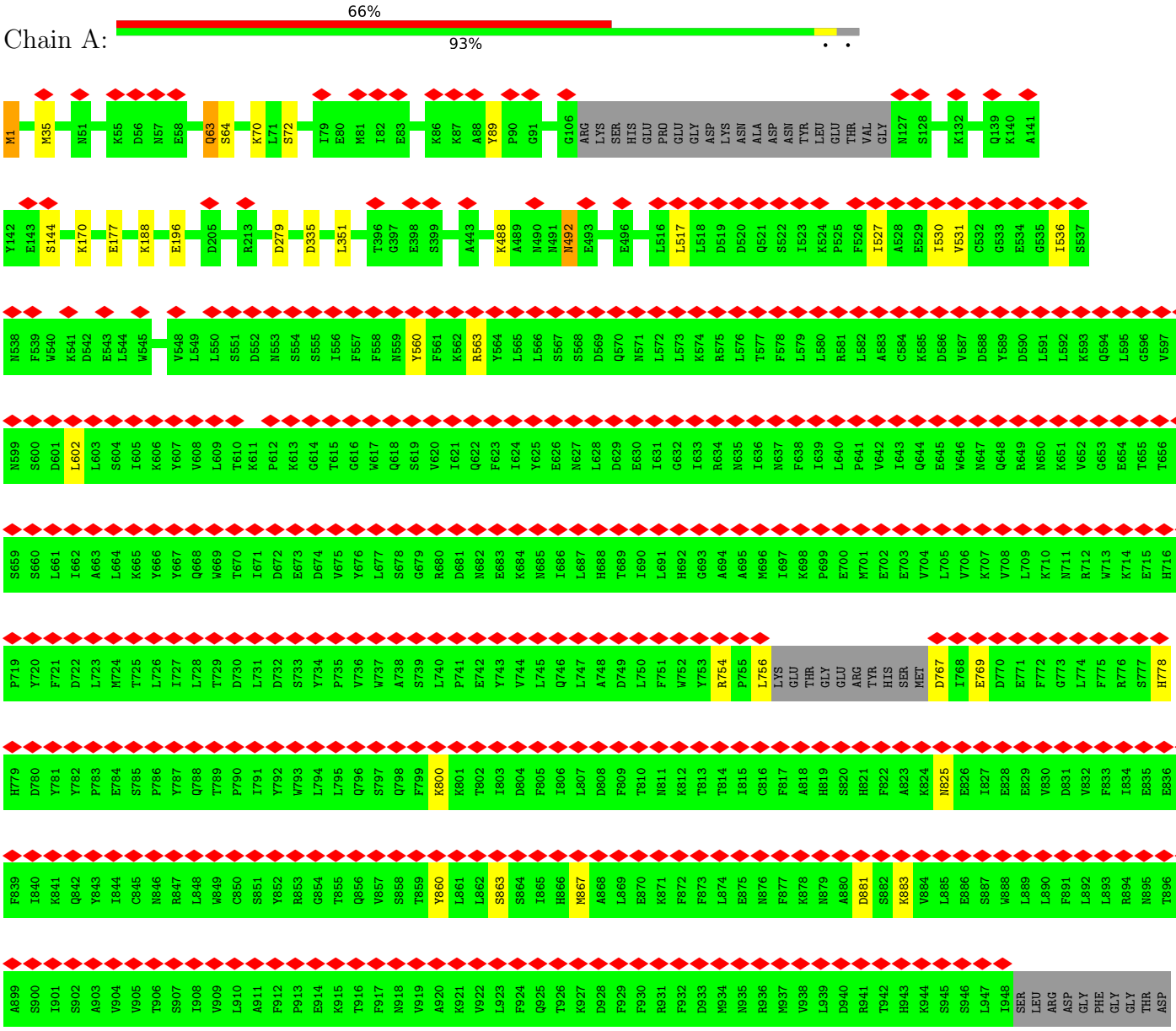
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	

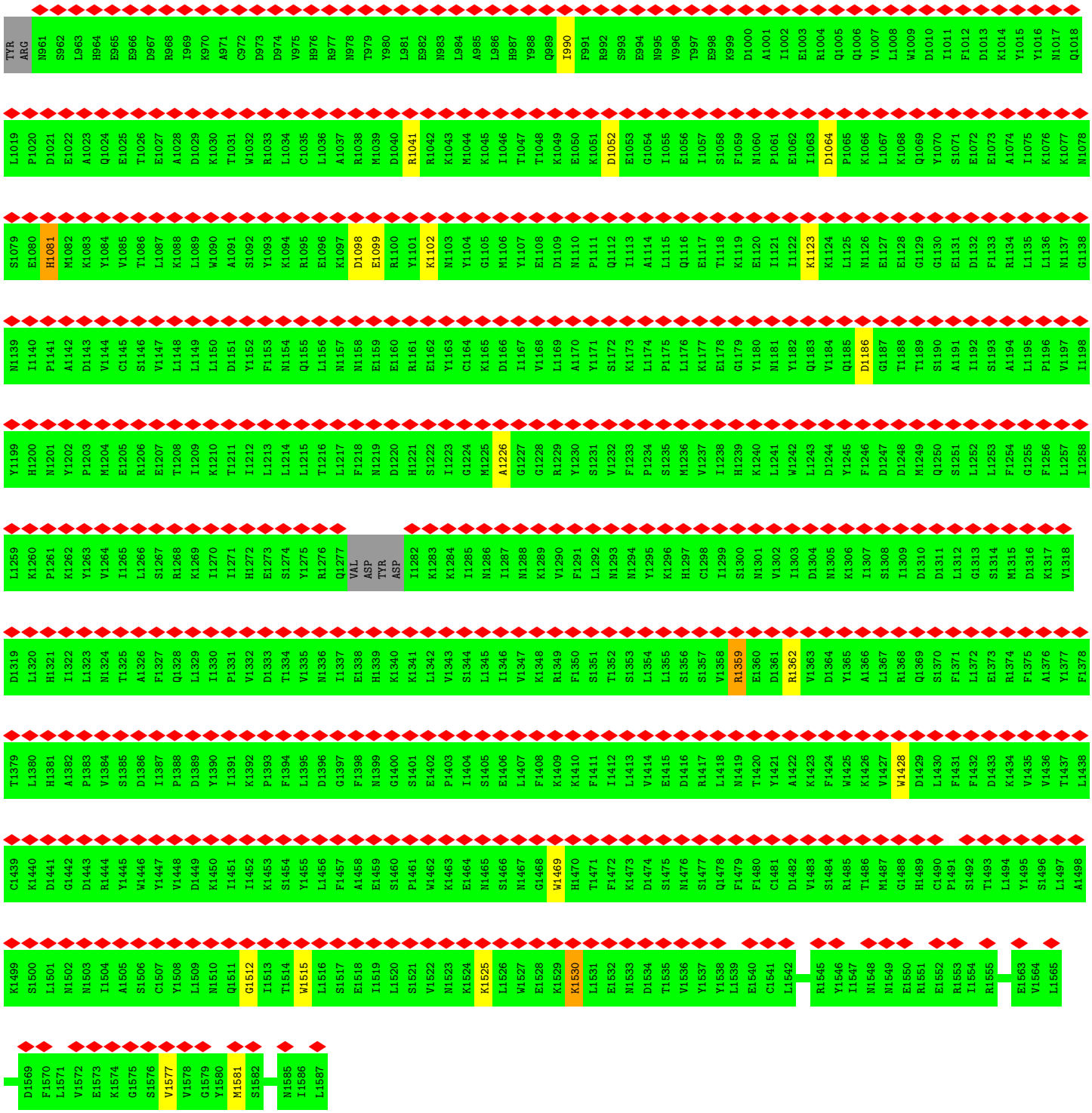
3 Residue-property plots (i)

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: ATP-binding protein Avs4

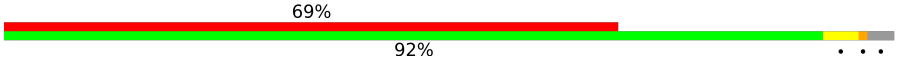
Chain A:

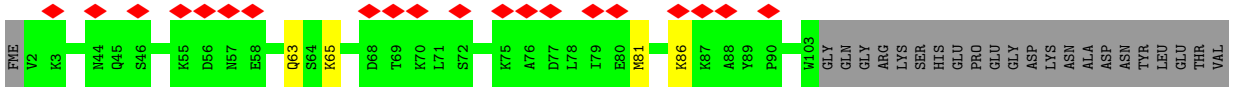


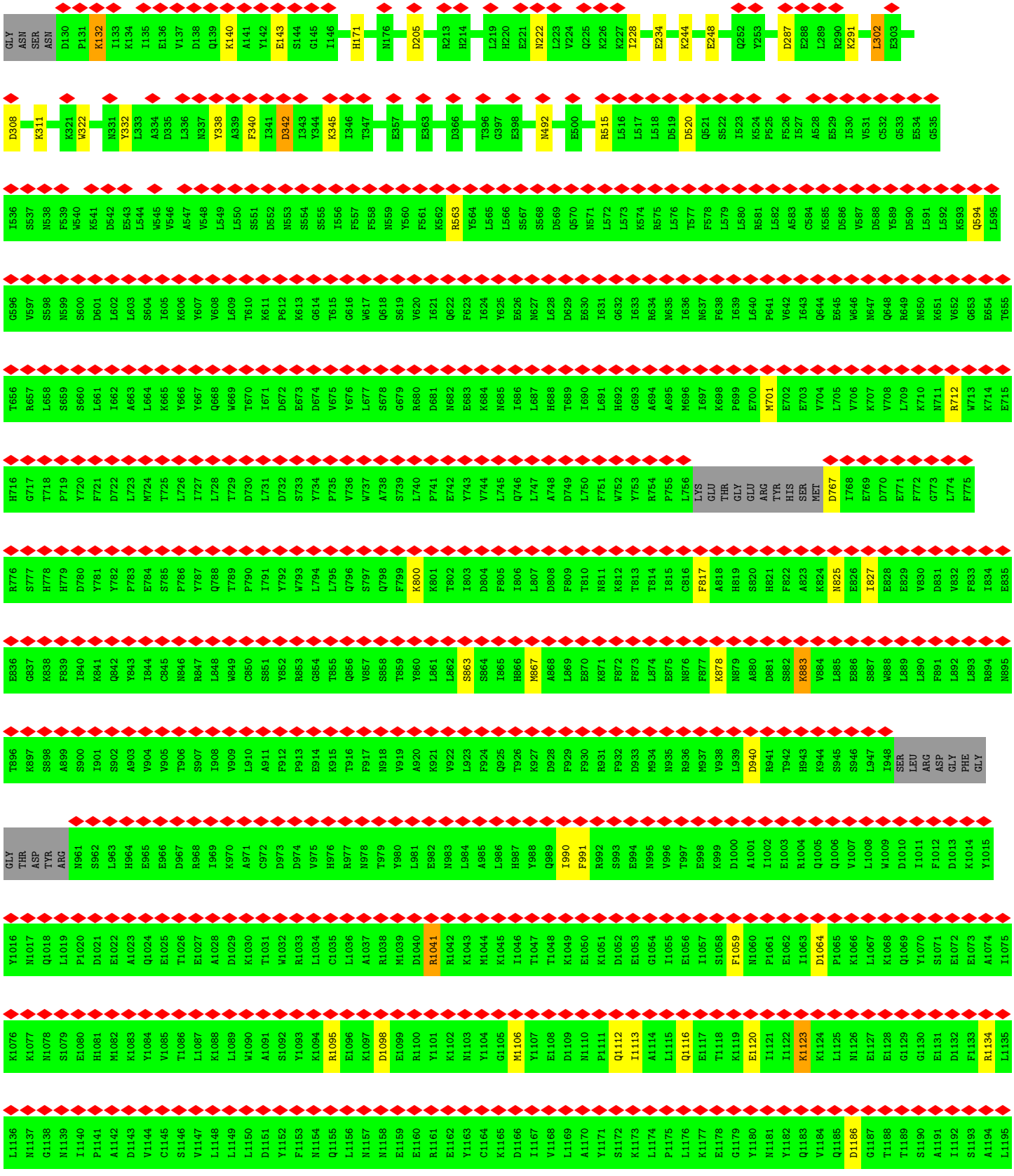


• Molecule 1: ATP-binding protein Avs4

Chain B:



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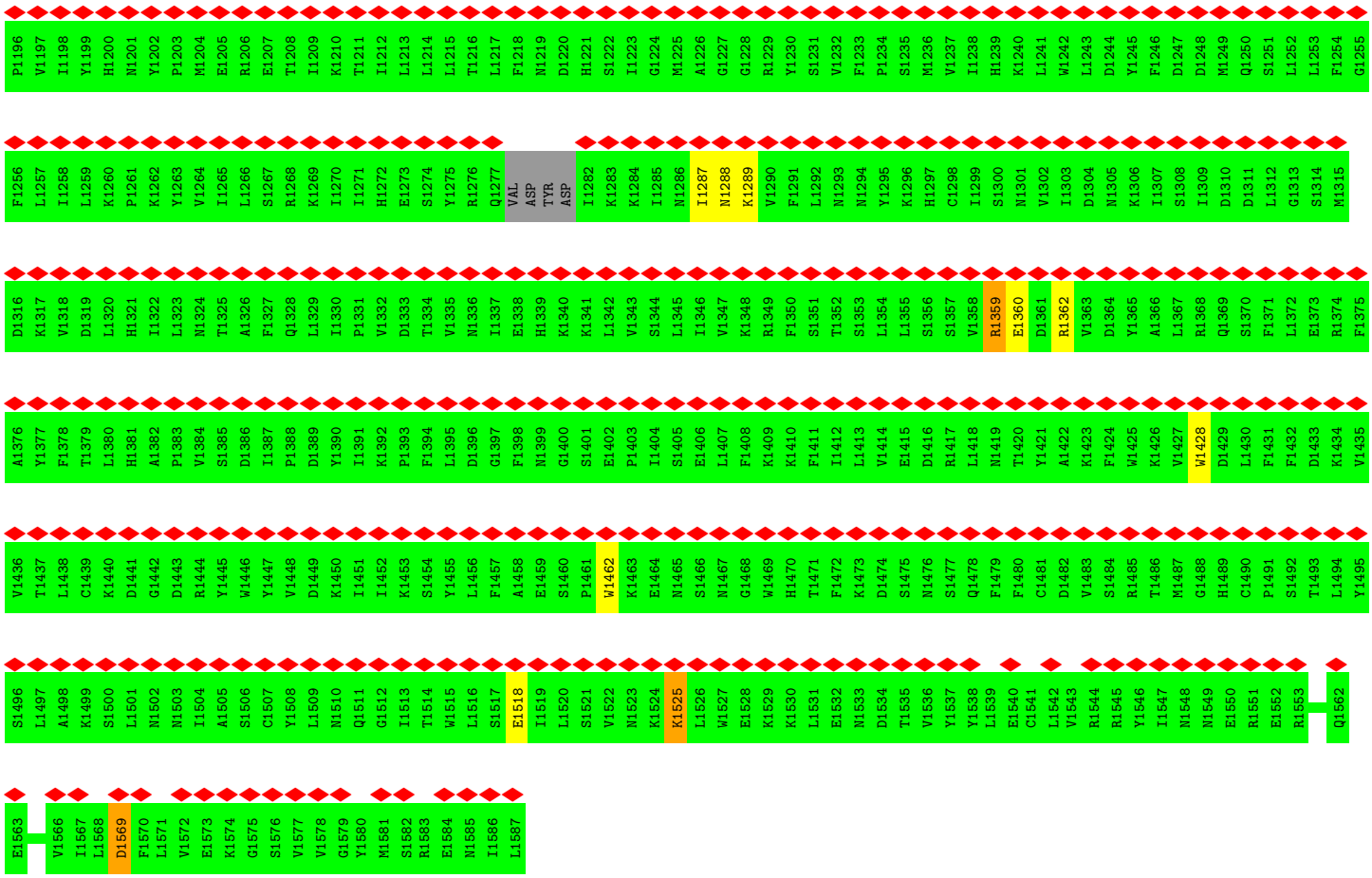
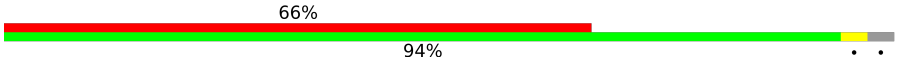
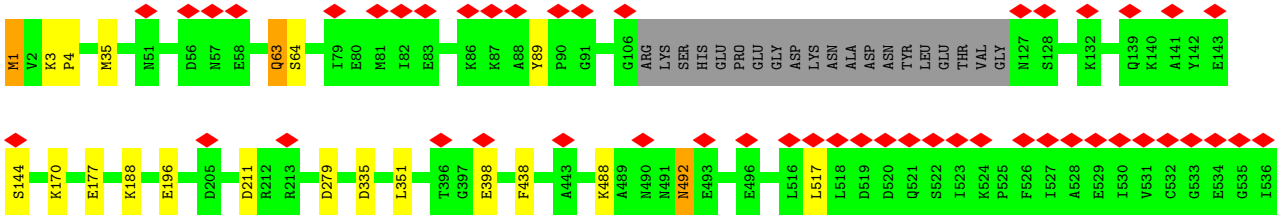
D308 K311 K321 W322 N331 Y332 L333 A334 D335 L336 N337 Y338 A339 F340 I341 D342 I343 Y344 K345 I346 T347 E357 E363 D366 T396 G397 E398 N492 E500 R515 L516 L517 L518 D519 D520 Q521 S522 I523 K524 P525 F526 I527 A528 E529 I530 V531 C532 G533 E534 G535
I536 S537 N538 F539 W540 K541 D542 E543 L544 W545 V546 A547 V548 L549 L550 S551 D552 N553 S554 S555 I556 F557 F558 N559 Y560 F561 K562 R563 Y564 L565 L566 S567 S568 D569 Q570 N571 L572 L573 K574 R575 L576 T577 F578 L579 L580 R581 L582 A583 C584 K585 D586 V587 D588 Y589 D590 L591 L592 K593 Q594 L595
G596 V597 S598 N599 S600 D601 L602 L603 S604 I605 K606 Y607 V608 L609 T610 K611 P612 K613 G614 T615 G616 W617 Q618 S619 V620 I621 Q622 F623 I624 Y625 E626 N627 L628 D629 E630 I631 G632 I633 R634 N635 I636 N637 F638 I639 L640 P641 V642 I643 Q644 E645 W646 N647 Q648 R649 N650 K651 V652 G653 E654 T655
T656 R657 L658 S659 S660 L661 I662 A663 L664 K665 Y666 Y667 Q668 W669 T670 I671 D672 E673 D674 V675 Y676 L677 S678 G679 R680 D681 N682 E683 K684 N685 I686 L687 H688 T689 I690 L691 H692 G693 A694 A695 M696 I697 K698 P699 E700 M701 E702 E703 V704 L705 V706 K707 V708 L709 K710 N711 R712 W713 K714 E715
H716 G717 T718 P719 Y720 F721 D722 L723 M724 T725 L726 I727 L728 T729 D730 L731 D732 S733 Y734 P735 V736 W737 A738 S739 L740 P741 E742 Y743 V744 L745 Q746 L747 A748 D749 L750 F751 W752 Y753 R754 P755 L756 LYS GLU THR GLY GLU ARG TYR HIS SER MET D767 I768 E769 D770 E771 F772 G773 L774 F775
R776 S777 H778 H779 D780 Y781 Y782 P783 E784 S785 P786 Y787 Q788 T789 P790 I791 Y792 W793 L794 L795 Q796 S797 Q798 F799 K800 K801 T802 I803 D804 F805 I806 L807 D808 F809 T810 N811 K812 T813 T814 I815 C816 F817 A818 H819 S820 H821 F822 A823 K824 N825 E826 I827 E828 E829 V830 D831 V832 F833 I834 E835
E836 G837 K838 F839 I840 K841 Q842 Y843 I844 C845 N846 R847 L848 W849 C850 S851 Y852 R853 G854 T855 Q856 V857 S858 T859 Y860 L861 L862 S863 S864 I865 H866 M867 A868 L869 E870 K871 F872 F873 L874 E875 N876 F877 K878 N879 A880 D881 S882 K883 V884 L885 E886 S887 W888 L889 L890 F891 L892 L893 R894 N895
T896 K897 S898 A899 S900 I901 S902 A903 V904 V905 T906 S907 I908 V909 L910 A911 F912 P913 E914 K915 T916 F917 N918 V919 A920 K921 V922 L923 F924 Q925 T926 K927 D928 F929 F930 R931 F932 D933 M934 N935 R936 M937 V938 L939 D940 R941 T942 H943 K944 S945 S946 L947 I948 SER LEU ARG ASP GLY PHE GLY
GLY THR ASP TYR ARG N961 S962 L963 H964 E965 E966 D967 R968 I969 K970 A971 C972 D973 D974 V975 H976 R977 N978 T979 Y980 L981 E982 N983 L984 A985 L986 H987 Y988 Q989 I990 F991 R992 S993 E994 N995 V996 T997 E998 K999 D1000 A1001 I1002 E1003 R1004 Q1005 Q1006 V1007 L1008 W1009 D1010 I1011 F1012 D1013 K1014 Y1015
Y1016 N1017 Q1018 L1019 P1020 D1021 E1022 A1023 Q1024 E1025 T1026 E1027 A1028 D1029 K1030 T1031 W1032 R1033 L1034 C1035 L1036 A1037 R1038 M1039 D1040 R1041 R1042 K1043 M1044 K1045 I1046 T1047 T1048 K1049 E1050 K1051 D1052 E1053 G1054 I1055 E1056 I1057 S1058 F1059 N1060 P1061 E1062 I1063 D1064 P1065 K1066 L1067 K1068 Q1069 Y1070 S1071 E1072 E1073 A1074 I1075
K1076 K1077 N1078 S1079 E1080 H1081 M1082 K1083 Y1084 V1085 T1086 L1087 K1088 L1089 W1090 A1091 S1092 Y1093 K1094 R1095 E1096 K1097 D1098 E1099 R1100 Y1101 K1102 N1103 Y1104 G1105 M1106 Y1107 E1108 D1109 N1110 P1111 Q1112 I1113 A1114 L1115 Q1116 E1117 T1118 K1119 E1120 I1121 I1122 K1123 K1124 L1125 N1126 E1127 E1128 G1129 G1130 E1131 D1132 F1133 R1134 L1135
L1136 N1137 G1138 N1139 I1140 P1141 A1142 D1143 V1144 C1145 S1146 V1147 L1148 L1149 L1150 D1151 Y1152 F1153 N1154 Q1155 L1156 N1157 N1158 E1159 E1160 R1161 E1162 Y1163 C1164 K1165 D1166 I1167 V1168 L1169 A1170 Y1171 S1172 K1173 L1174 P1175 L1176 K1177 E1178 G1179 Y1180 N1181 Y1182 Q1183 V1184 Q1185 D1186 G1187 T1188 T1189 S1190 A1191 I1192 S1193 A1194 L1195

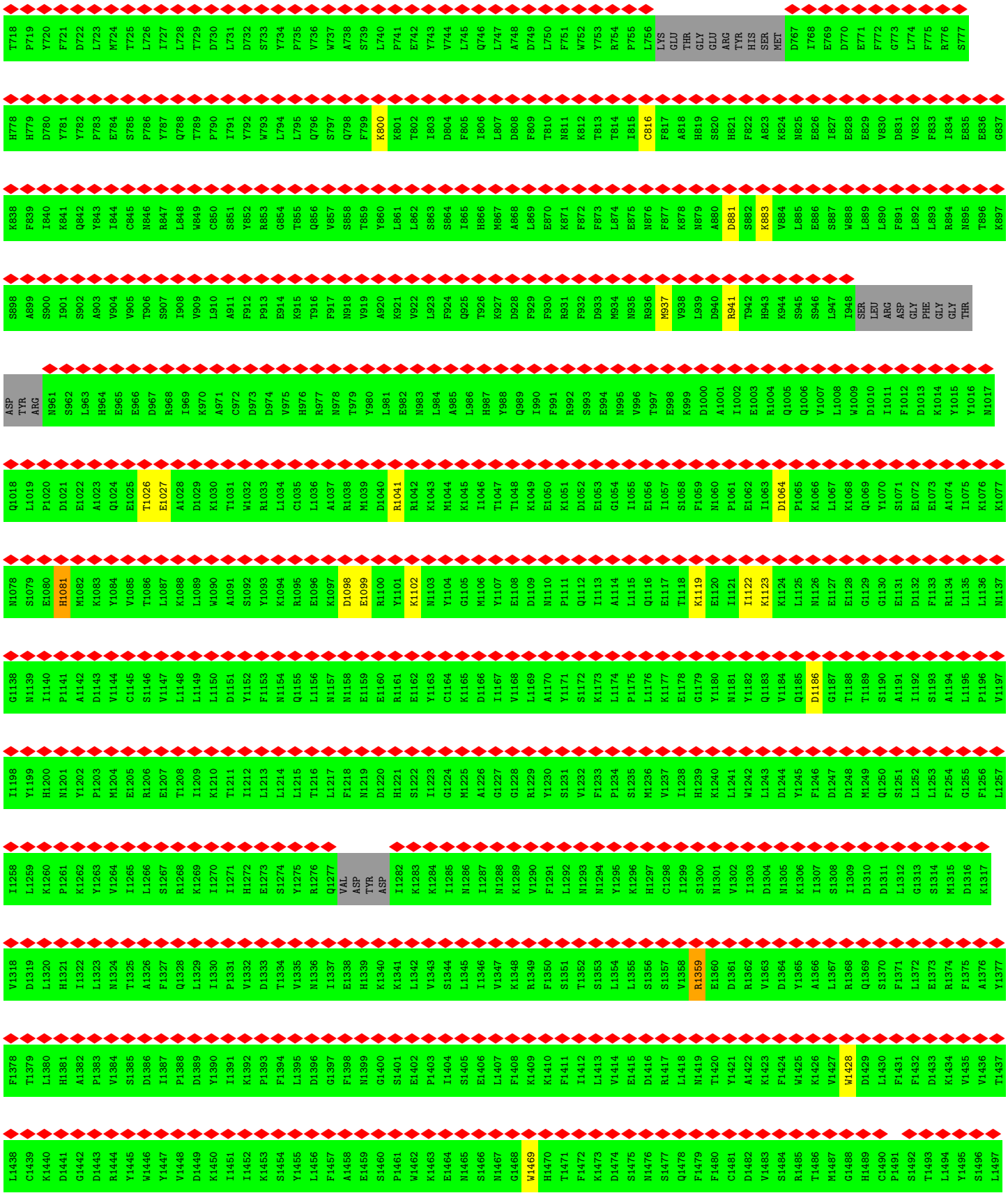


• Molecule 1: ATP-binding protein Avs4

Chain C:



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H778 H779 D780 Y781 Y782 P783 E784 S785 P786 Y787 Q788 T789 P790 I791 Y792 W793 L794 L795 Q796 S797 Q798 F799 K800 K801 T802 I803 D804 F805 I806 L807 D808 F809 T810 N811 K812 T813 T814 I815 C816 F817 A818 H819 S820 H821 F822 A823 K824 N825 E826 I827 E828 E829 V830 D831 V832 F833 I834 E835 E836 G837
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ASP TYR ARG N961 S962 L963 H964 E965 E966 D967 R968 I969 K970 A971 C972 D973 D974 V975 H976 R977 N978 T979 Y980 L981 E982 N983 L984 A985 L986 H987 Y988 Q989 I990 F991 R992 S993 E994 N995 V996 T997 E998 K999 D1000 A1001 I1002 E1003 R1004 Q1005 Q1006 V1007 L1008 W1009 D1010 I1011 F1012 D1013 K1014 Y1015 Y1016 N1017
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N1078 S1079 E1080 H1081 M1082 K1083 Y1084 V1085 T1086 L1087 K1088 L1089 W1090 A1091 S1092 Y1093 K1094 R1095 E1096 K1097 D1098 E1099 R1100 Y1101 K1102 N1103 Y1104 G1105 M1106 Y1107 E1108 D1109 N1110 P1111 Q1112 I1113 A1114 L1115 Q1116 E1117 T1118 K1119 E1120 I1121 I1122 K1123 K1124 L1125 N1126 E1127 E1128 G1129 G1130 E1131 D1132 F1133 R1134 L1135 L1136 N1137
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I1258 L1259 K1260 P1261 K1262 Y1263 V1264 I1265 L1266 S1267 R1268 K1269 I1270 I1271 H1272 E1273 S1274 Y1275 R1276 Q1277 VAL ASP TYR ASP I1282 K1283 K1284 I1285 N1286 I1287 N1288 K1289 V1290 F1291 L1292 N1293 N1294 Y1295 K1296 H1297 C1298 I1299 S1300 N1301 V1302 I1303 D1304 N1305 K1306 I1307 S1308 I1309 D1310 D1311 L1312 G1313 S1314 M1315 D1316 K1317
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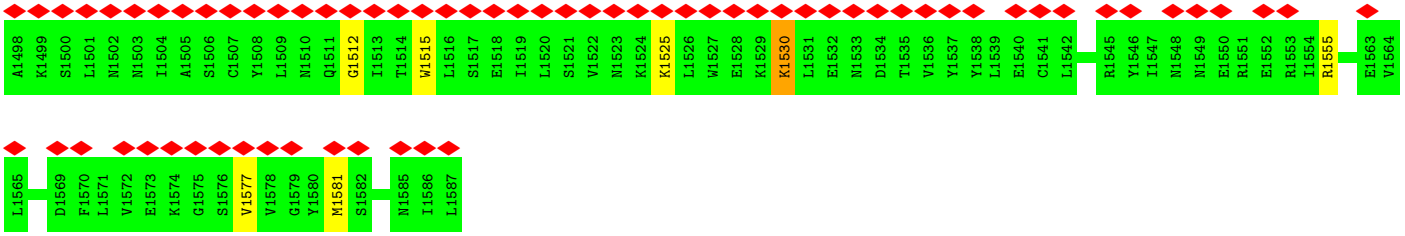
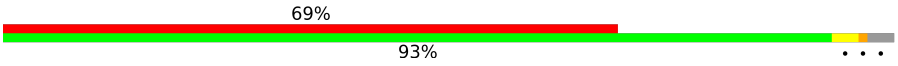
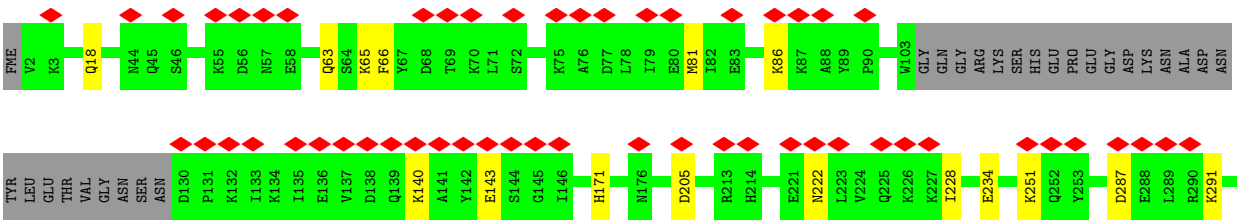
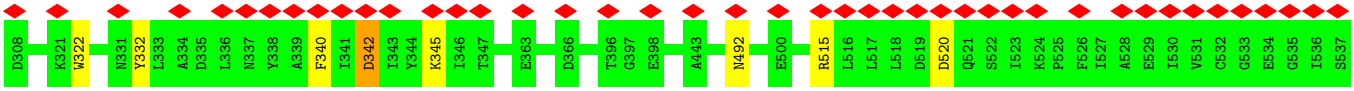


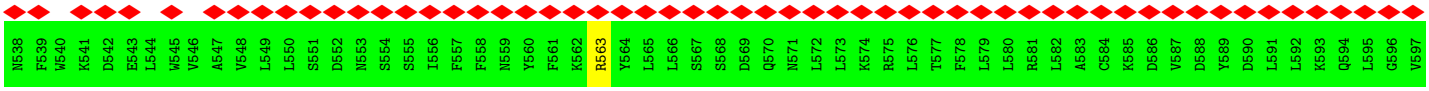
• Molecule 1: ATP-binding protein Avs4

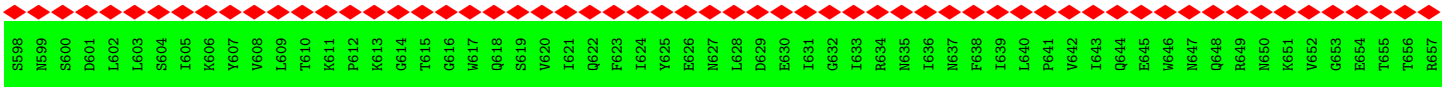
Chain D:

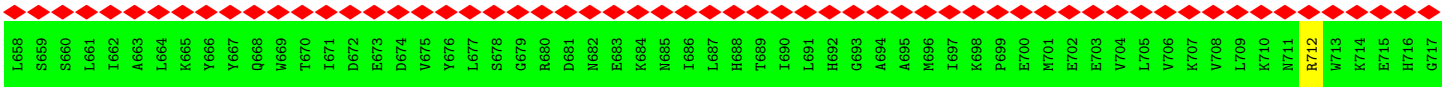


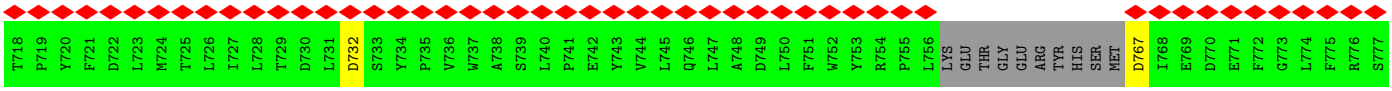


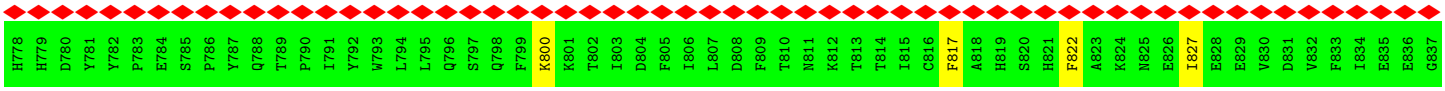


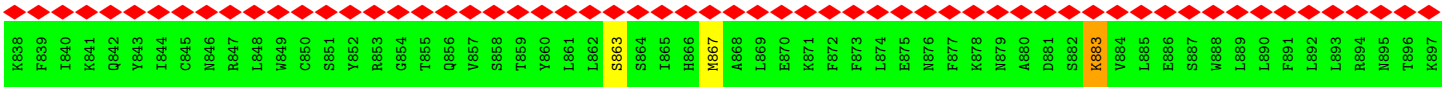


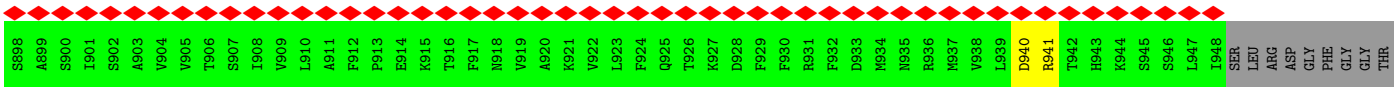


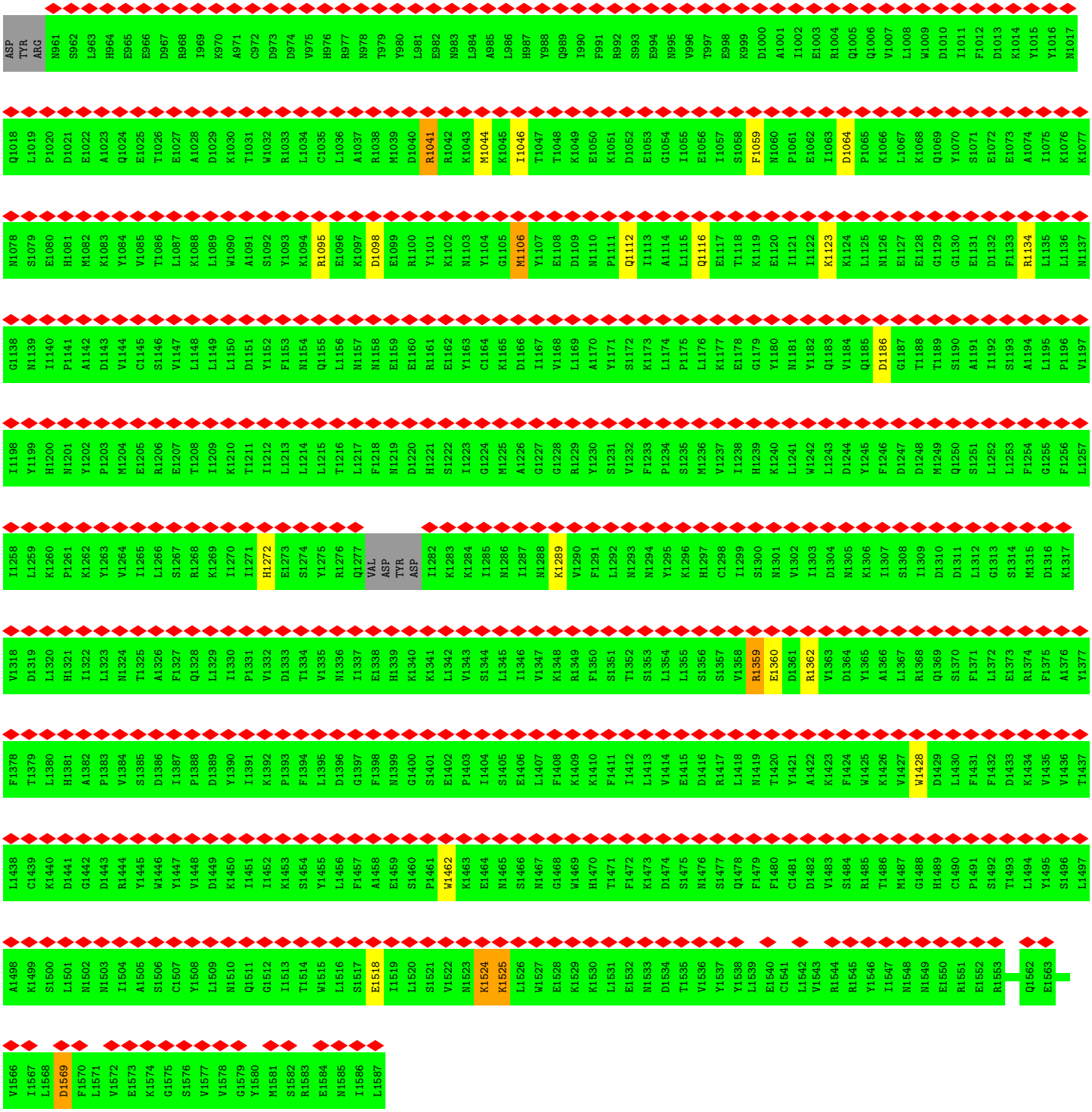






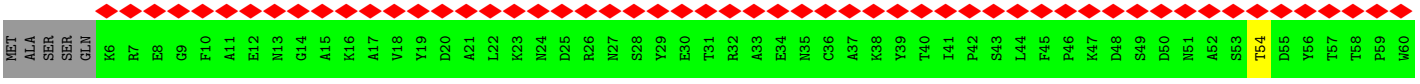


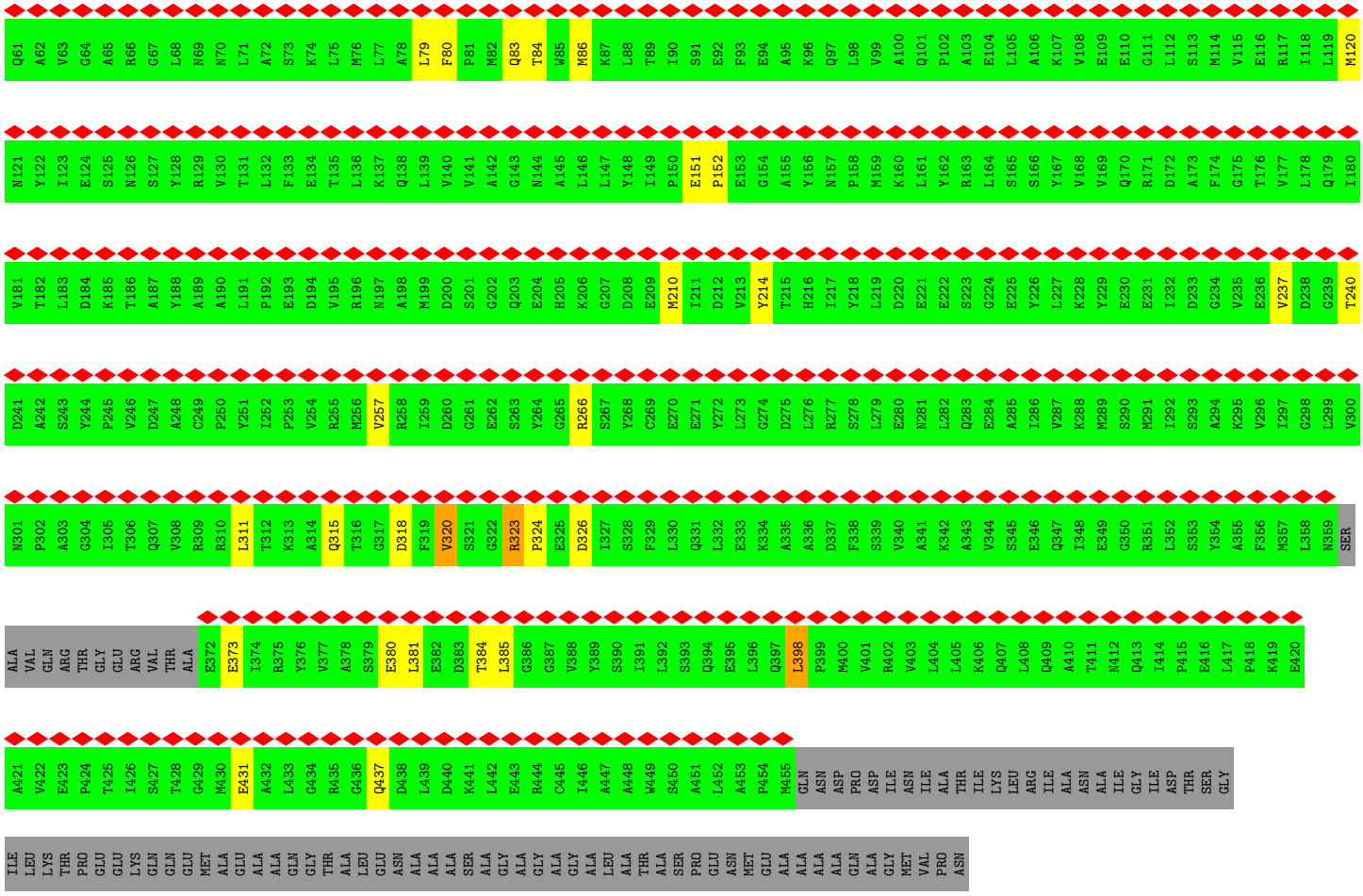




• Molecule 2: Portal protein

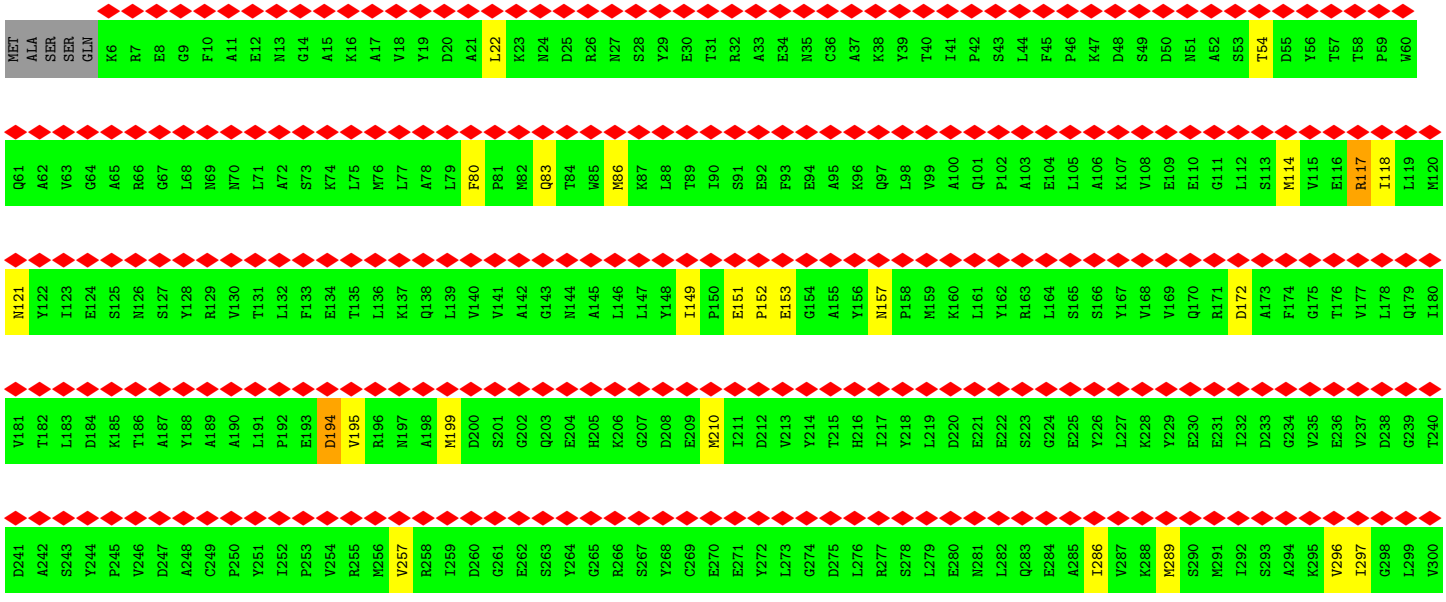
Chain E:

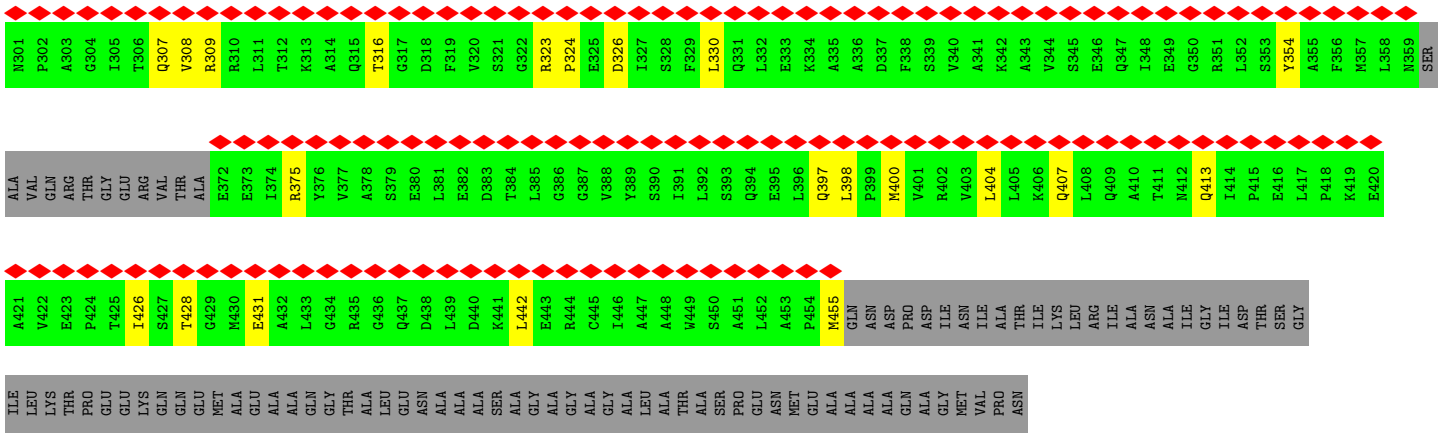




- Molecule 2: Portal protein

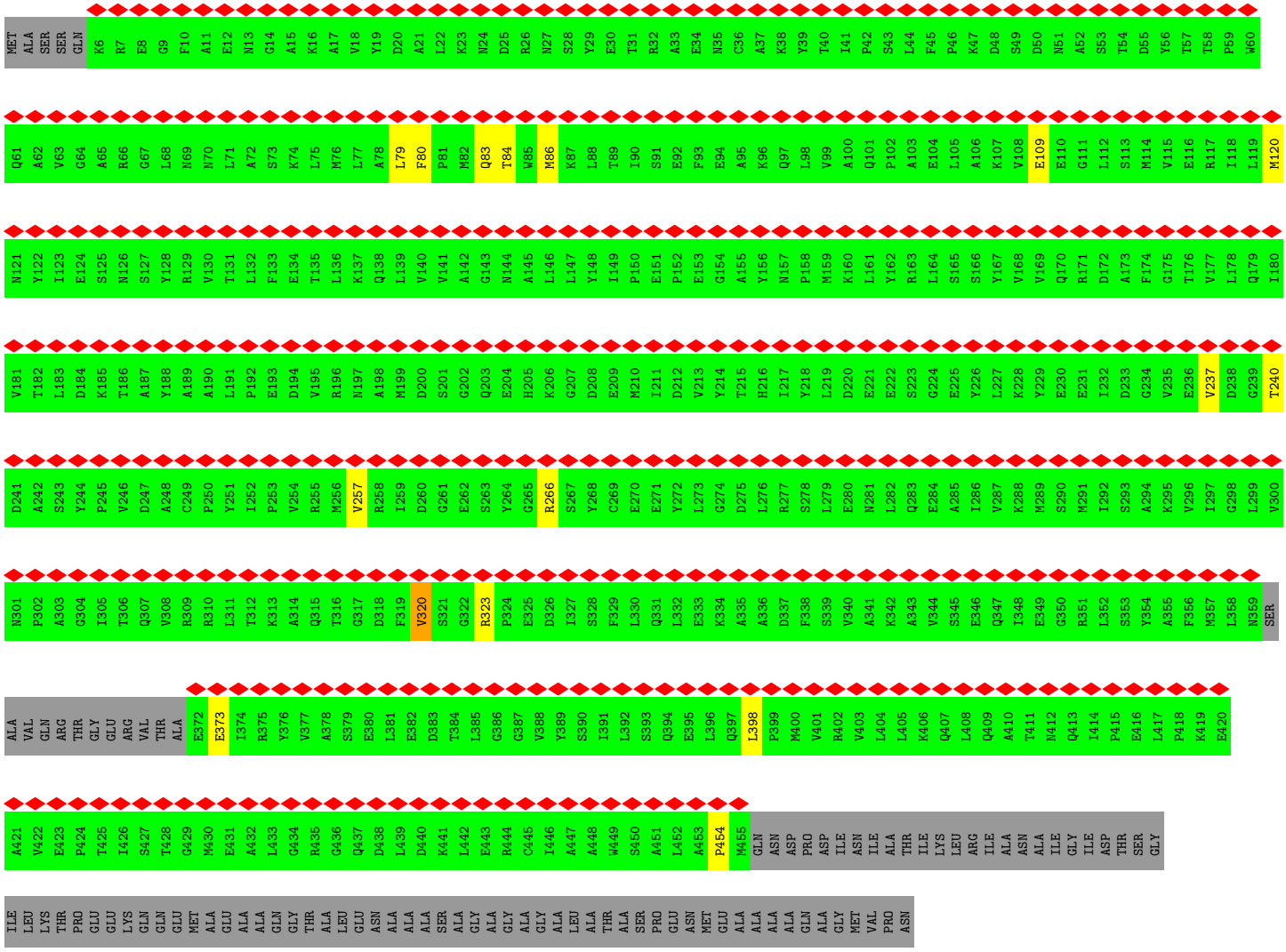
Chain F:





• Molecule 2: Portal protein

Chain G:



• Molecule 2: Portal protein

Chain H:

MET ALA SER SER GLN K6 R7 E8 G9 F10 A11 E12 N13 G14 A15 K16 A17 V18 Y19 D20 A21 L22 K23 N24 D25 R26 N27 S28 Y29 E30 T31 R32 A33 E34 N35 C36 A37 K38 Y39 T40 I41 P42 S43 L44 F45 P46 K47 D48 S49 D50 N51 A52 S53 T54 D55 Y56 T57 T58 P59 W60

Q61 A62 V63 G64 A65 R66 G67 L68 N69 N70 L71 A72 S73 K74 L75 M76 L77 A78 L79 F80 P81 M82 Q83 T84 W85 M86 K87 L88 T89 I90 S91 E92 F93 E94 A95 K96 Q97 L98 V99 A100 Q101 P102 A103 E104 L105 A106 K107 V108 E109 E110 G111 L112 S113 M114 V115 E116 R117 I118 L119 M120

N121 Y122 I123 E124 S125 N126 S127 Y128 R129 V130 T131 L132 F133 E134 T135 L136 K137 Q138 L139 V140 V141 A142 G143 N144 A145 L146 L147 Y148 I149 P150 E151 P152 E153 G154 A155 Y156 N157 P158 M159 K160 L161 Y162 R163 L164 S165 S166 Y167 V168 V169 Q170 R171 D172 A173 F174 G175 T176 V177 L178 Q179 I180

V181 T182 L183 D184 K185 T186 A187 Y188 A189 A190 L191 P192 E193 D194 V195 R196 N197 A198 M199 D200 S201 G202 Q203 E204 H205 K206 G207 D208 E209 M210 I211 D212 V213 Y214 T215 H216 I217 Y218 L219 D220 E221 E222 S223 G224 E225 Y226 L227 K228 Y229 E230 E231 I232 D233 G234 V235 E236 V237 D238 G239 T240

D241 A242 S243 Y244 P245 V246 D247 A248 C249 P250 Y251 I252 P253 V254 R255 M256 V257 R258 I259 D260 G261 E262 S263 Y264 G265 R266 S267 Y268 C269 E270 E271 Y272 L273 G274 D275 L276 R277 S278 L279 E280 N281 L282 Q283 E284 A285 I286 V287 K288 M289 S290 M291 I292 S293 A294 K295 V296 I297 G298 L299 V300

N301 P302 A303 G304 I305 T306 Q307 V308 R309 R310 L311 T312 K313 A314 Q315 T316 G317 D318 F319 V320 S321 G322 R323 P324 E325 D326 I327 S328 F329 L330 Q331 L332 E333 K334 A335 A336 D337 F338 S339 V340 A341 K342 A343 V344 S345 E346 Q347 I348 E349 G350 R351 L352 S353 Y354 A355 F356 M357 L358 N359 SER

ALA VAL GLN ARG THR GLY GLU ARG VAL THR ALA E372 E373 I374 R375 Y376 V377 A378 S379 E380 L381 E382 D383 T384 L385 G386 G387 V388 Y389 S390 I391 L392 S393 Q394 E395 L396 Q397 L398 P399 M400 V401 R402 V403 L404 L405 K406 Q407 L408 Q409 A410 T411 N412 Q413 I414 P415 E416 L417 P418 K419 E420

A421 V422 E423 P424 T425 I426 S427 T428 G429 M430 E431 A432 L433 G434 R435 G436 Q437 D438 L439 D440 K441 L442 E443 R444 C445 I446 A447 A448 W449 S450 A451 L452 A453 P454 M455 GLN ASN ASP PRO ASP ILE ASN ILE ALA THR ILE LYS LEU ARG ILE ALA ASN ALA ILE GLY ILE ASP THR SER GLY

ILE LEU LYS THR PRO GLU GLU LYS GLN GLN GLU MET ALA GLU ALA ALA ALA GLN GLY THR ALA ALA LEU GLU ASN ALA ALA ALA SER ALA ALA GLY ALA GLY ALA ALA GLY ALA ALA LEU ALA THR ALA SER PRO GLU ASN MET GLU ALA ALA ALA ALA ALA GLN ALA GLY MET VAL PRO ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	169977	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 ($e^-/Å^2$)	31	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	372.3703, 372.3703, 372.3703	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.034362, 1.034362, 1.034362	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, ATP, MG

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	0.39	0/13095	0.66	6/17695 (0.0%)
1	B	0.40	0/13056	0.67	8/17643 (0.0%)
1	C	0.39	0/13095	0.66	6/17695 (0.0%)
1	D	0.40	0/13056	0.66	8/17643 (0.0%)
2	E	0.73	3/3485 (0.1%)	0.89	8/4720 (0.2%)
2	F	0.48	2/3485 (0.1%)	0.80	10/4720 (0.2%)
2	G	0.54	1/3485 (0.0%)	0.81	6/4720 (0.1%)
2	H	0.47	1/3485 (0.0%)	0.82	13/4720 (0.3%)
All	All	0.44	7/66242 (0.0%)	0.70	65/89556 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	324	PRO	CG-CD	-32.03	0.45	1.50
2	G	454	PRO	CG-CD	-19.71	0.85	1.50
2	F	324	PRO	CG-CD	-11.44	1.12	1.50
2	E	324	PRO	CB-CG	11.21	2.06	1.50
2	H	324	PRO	CG-CD	-10.89	1.14	1.50
2	F	257	VAL	CB-CG1	-5.43	1.41	1.52
2	E	324	PRO	CA-C	5.39	1.63	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	324	PRO	CB-CG-CD	-27.29	0.07	106.50
2	G	454	PRO	N-CD-CG	-20.29	72.77	103.20
2	E	324	PRO	CA-N-CD	-15.21	90.20	111.50
2	F	398	LEU	CB-CG-CD2	-12.07	90.47	111.00
2	F	324	PRO	N-CD-CG	-11.55	85.88	103.20
2	G	454	PRO	CA-CB-CG	-11.32	82.49	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	324	PRO	N-CD-CG	-10.84	86.94	103.20
2	E	324	PRO	CA-CB-CG	-10.32	84.40	104.00
2	G	398	LEU	CB-CG-CD2	-10.07	93.89	111.00
2	E	398	LEU	CB-CG-CD2	-9.63	94.63	111.00
1	B	342	ASP	CB-CG-OD1	8.81	126.23	118.30
1	D	342	ASP	CB-CG-OD1	8.80	126.22	118.30
2	H	383	ASP	CB-CG-OD2	8.77	126.19	118.30
2	H	398	LEU	CB-CG-CD2	-8.40	96.71	111.00
2	F	324	PRO	CA-N-CD	-8.37	99.78	111.50
2	H	324	PRO	CA-N-CD	-8.12	100.13	111.50
2	H	330	LEU	CB-CG-CD1	-8.02	97.37	111.00
2	H	330	LEU	CA-CB-CG	7.93	133.54	115.30
2	F	324	PRO	CA-CB-CG	-7.62	89.52	104.00
2	H	324	PRO	CA-CB-CG	-7.08	90.55	104.00
1	D	287	ASP	CB-CG-OD1	7.02	124.62	118.30
1	B	287	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	351	LEU	CA-CB-CG	6.86	131.08	115.30
2	H	199	MET	CG-SD-CE	6.84	111.14	100.20
1	D	302	LEU	CB-CG-CD1	-6.79	99.46	111.00
2	E	323	ARG	C-N-CD	6.68	142.43	128.40
1	A	351	LEU	CA-CB-CG	6.67	130.65	115.30
2	E	324	PRO	N-CD-CG	-6.66	93.22	103.20
2	F	398	LEU	CB-CG-CD1	6.63	122.28	111.00
1	C	1186	ASP	CB-CG-OD1	6.14	123.83	118.30
2	H	172	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	1064	ASP	CB-CG-OD1	6.10	123.79	118.30
2	F	172	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	1186	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	1186	ASP	CB-CG-OD1	6.05	123.75	118.30
1	C	1064	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	1186	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	1064	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	517	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	517	LEU	CA-CB-CG	5.97	129.04	115.30
1	B	302	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	1064	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	1098	ASP	CB-CG-OD1	5.92	123.62	118.30
1	C	1098	ASP	CB-CG-OD1	5.81	123.53	118.30
2	H	326	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	1569	ASP	CB-CG-OD2	5.72	123.45	118.30
2	E	320	VAL	CG1-CB-CG2	-5.63	101.89	110.90
1	D	1098	ASP	CB-CG-OD1	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1569	ASP	CB-CG-OD2	5.60	123.34	118.30
2	G	454	PRO	N-CA-CB	-5.59	96.45	102.60
1	B	1098	ASP	CB-CG-OD1	5.53	123.28	118.30
1	D	251	LYS	CD-CE-NZ	5.51	124.36	111.70
2	F	194	ASP	CB-CG-OD2	5.51	123.26	118.30
2	G	320	VAL	CG1-CB-CG2	-5.38	102.29	110.90
2	E	324	PRO	N-CA-CB	-5.36	96.70	102.60
2	H	330	LEU	CB-CG-CD2	5.34	120.07	111.00
1	A	881	ASP	CB-CG-OD1	5.29	123.06	118.30
2	G	454	PRO	CA-N-CD	-5.27	104.13	111.50
2	F	442	LEU	CA-CB-CG	5.24	127.36	115.30
2	F	404	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	B	878	LYS	CD-CE-NZ	5.20	123.66	111.70
1	C	881	ASP	CB-CG-OD1	5.19	122.97	118.30
2	H	114	MET	CG-SD-CE	5.16	108.45	100.20
2	H	132	LEU	CA-CB-CG	-5.09	103.60	115.30
2	F	199	MET	CG-SD-CE	5.01	108.21	100.20

There are no chirality outliers.

There are no planarity outliers.

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	12805	0	12724	25	0
1	B	12756	0	12683	32	0
1	C	12805	0	12724	22	0
1	D	12756	0	12683	26	0
2	E	3427	0	3400	16	0
2	F	3427	0	3400	22	0
2	G	3427	0	3400	9	0
2	H	3427	0	3400	21	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	64958	0	64462	156	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 1.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:117:ARG:HH12	2:F:121:ASN:HB2	1.39	0.87
2:H:117:ARG:HH12	2:H:121:ASN:HB2	1.46	0.79
1:C:937:MET:HG2	1:C:941:ARG:HH12	1.51	0.76
1:A:1359:ARG:O	1:A:1359:ARG:NH1	2.25	0.69
1:C:1359:ARG:O	1:C:1359:ARG:NH1	2.26	0.69
2:E:257:VAL:HG12	2:E:266:ARG:H	1.58	0.68
2:G:257:VAL:HG12	2:G:266:ARG:H	1.59	0.68
2:E:83:GLN:HG3	2:E:431:GLU:HG2	1.77	0.67
1:C:1026:THR:OG1	1:C:1027:GLU:OE2	2.13	0.66
2:H:83:GLN:HG3	2:H:431:GLU:HG2	1.78	0.66
1:D:515:ARG:NH2	1:D:520:ASP:OD2	2.30	0.64
1:A:1226:ALA:HB2	2:E:384:THR:HG23	1.81	0.63
2:F:83:GLN:HG3	2:F:431:GLU:HG2	1.82	0.62
1:B:1106:MET:SD	1:B:1106:MET:N	2.73	0.61
1:B:1462:TRP:O	2:F:375:ARG:NH2	2.34	0.61
1:D:1462:TRP:O	2:H:375:ARG:NH2	2.34	0.61
1:C:1027:GLU:OE2	1:C:1027:GLU:N	2.33	0.61
2:F:149:ILE:HD11	2:F:400:MET:HG3	1.83	0.60
1:D:302:LEU:HD11	1:D:332:TYR:CD1	2.37	0.60
1:B:302:LEU:HD11	1:B:332:TYR:CD1	2.37	0.59
1:D:1106:MET:N	1:D:1106:MET:SD	2.74	0.59
1:B:308:ASP:HA	1:B:311:LYS:HG3	1.83	0.59
2:H:315:GLN:HG2	2:H:318:ASP:HB2	1.85	0.58
1:A:1525:LYS:H	1:A:1525:LYS:HD2	1.69	0.58
2:F:308:VAL:HG22	2:F:309:ARG:HH21	1.69	0.58
1:C:1525:LYS:HD2	1:C:1525:LYS:H	1.69	0.58
2:E:237:VAL:O	2:E:240:THR:OG1	2.21	0.57
2:H:257:VAL:HG12	2:H:266:ARG:H	1.69	0.57
2:G:237:VAL:O	2:G:240:THR:OG1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1359:ARG:HH11	1:B:1362:ARG:HD3	1.69	0.56
2:H:330:LEU:HG	2:H:334:LYS:HB2	1.87	0.56
2:F:118:ILE:HG21	2:F:413:GLN:HE21	1.72	0.55
2:H:330:LEU:HD12	2:H:333:GLU:HB3	1.88	0.55
2:H:152:PRO:HA	2:H:157:ASN:OD1	2.06	0.55
2:H:149:ILE:HD11	2:H:400:MET:HG3	1.88	0.55
1:A:196:GLU:OE1	1:A:196:GLU:N	2.40	0.54
1:C:196:GLU:N	1:C:196:GLU:OE2	2.40	0.54
1:D:302:LEU:HD21	1:D:332:TYR:CE1	2.43	0.54
2:F:118:ILE:HD13	2:F:413:GLN:NE2	2.23	0.53
2:H:309:ARG:HH12	2:H:313:LYS:HD3	1.74	0.53
1:A:1:FME:O1	1:D:171:HIS:ND1	2.43	0.52
1:B:1112:GLN:O	1:B:1116:GLN:HG3	2.09	0.52
1:D:1041:ARG:HE	2:H:316:THR:HG23	1.73	0.52
1:B:1525:LYS:H	1:B:1525:LYS:HE2	1.74	0.52
1:C:941:ARG:HB2	1:C:941:ARG:NH1	2.24	0.52
1:B:171:HIS:ND1	1:C:1:FME:O1	2.43	0.52
1:D:1112:GLN:O	1:D:1116:GLN:HG3	2.09	0.52
1:D:1525:LYS:HE2	1:D:1525:LYS:H	1.75	0.52
1:C:1469:TRP:CD1	2:G:373:GLU:HG3	2.45	0.51
1:A:1469:TRP:CD1	2:E:373:GLU:HG3	2.45	0.51
2:F:153:GLU:H	2:F:157:ASN:HD21	1.58	0.50
1:D:63:GLN:HG2	1:D:81:MET:SD	2.52	0.50
1:B:515:ARG:NH2	1:B:520:ASP:OD2	2.44	0.50
1:D:228:ILE:HG21	1:D:340:PHE:CZ	2.47	0.50
1:B:244:LYS:O	1:B:248:GLU:HG2	2.12	0.50
1:B:63:GLN:HG2	1:B:81:MET:SD	2.52	0.49
1:B:228:ILE:HG21	1:B:340:PHE:CZ	2.48	0.49
1:B:302:LEU:HD21	1:B:332:TYR:CE1	2.48	0.49
1:B:1059:PHE:HB2	2:F:296:VAL:HG13	1.95	0.48
2:F:297:ILE:HG22	2:F:330:LEU:HD23	1.94	0.48
1:A:1530:LYS:HA	1:A:1530:LYS:HE2	1.95	0.48
1:B:1134:ARG:HH11	1:B:1134:ARG:HB3	1.78	0.48
2:F:152:PRO:HA	2:F:157:ASN:ND2	2.29	0.48
1:A:825:ASN:HD22	2:E:54:THR:C	2.17	0.47
1:C:1530:LYS:HA	1:C:1530:LYS:HE2	1.95	0.47
2:F:80:PHE:CE2	2:F:397:GLN:HG2	2.49	0.47
2:F:118:ILE:HD13	2:F:413:GLN:HE22	1.80	0.47
2:F:80:PHE:HE2	2:F:397:GLN:HG2	1.78	0.47
1:A:530:ILE:HD12	1:A:536:ILE:HD13	1.96	0.47
2:H:302:PRO:HD3	2:H:326:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:HB3	1:B:322:TRP:CE3	2.50	0.46
1:D:1134:ARG:HB3	1:D:1134:ARG:HH11	1.79	0.46
2:F:151:GLU:HA	2:F:407:GLN:HE21	1.80	0.46
1:A:170:LYS:NZ	1:A:177:GLU:O	2.48	0.46
1:B:990:ILE:HG23	1:B:991:PHE:HD2	1.80	0.46
1:B:132:LYS:H	1:B:132:LYS:HE2	1.81	0.46
1:D:291:LYS:HB3	1:D:322:TRP:CE3	2.50	0.46
2:F:286:ILE:HA	2:F:289:MET:HE3	1.96	0.46
2:F:426:ILE:HG22	2:F:428:THR:HG23	1.98	0.46
2:H:117:ARG:NH1	2:H:121:ASN:HB2	2.24	0.46
1:B:65:LYS:HA	1:B:65:LYS:HD3	1.81	0.45
1:B:1041:ARG:HE	2:F:316:THR:HG23	1.81	0.45
2:H:80:PHE:CE2	2:H:397:GLN:HG2	2.51	0.45
2:G:84:THR:HA	2:G:120:MET:CE	2.46	0.45
1:A:754:ARG:HH12	1:A:756:LEU:HD23	1.81	0.45
1:C:1469:TRP:HD1	2:G:373:GLU:HG3	1.81	0.45
1:A:863:SER:O	1:A:867:MET:HG3	2.17	0.45
1:D:65:LYS:HD3	1:D:65:LYS:HA	1.82	0.45
1:D:205:ASP:OD2	1:D:205:ASP:N	2.50	0.45
1:C:170:LYS:NZ	1:C:177:GLU:O	2.50	0.45
1:B:1134:ARG:HB3	1:B:1134:ARG:NH1	2.32	0.44
1:D:1134:ARG:HB3	1:D:1134:ARG:NH1	2.32	0.44
1:D:1059:PHE:HB2	2:H:296:VAL:HG13	1.98	0.44
1:A:1081:HIS:HD1	1:A:1081:HIS:C	2.21	0.44
1:B:1287:ILE:HD12	1:B:1288:ASN:N	2.33	0.44
1:C:492:ASN:OD1	1:C:492:ASN:N	2.50	0.44
1:B:205:ASP:OD2	1:B:205:ASP:N	2.49	0.44
2:E:84:THR:HA	2:E:120:MET:CE	2.47	0.44
2:H:157:ASN:HD22	2:H:157:ASN:HA	1.53	0.44
2:G:79:LEU:HB3	2:G:80:PHE:CD2	2.52	0.44
1:B:1120:GLU:O	1:B:1123:LYS:HE2	2.18	0.43
1:A:778:HIS:CE1	1:A:860:TYR:HD1	2.36	0.43
1:A:1469:TRP:HD1	2:E:373:GLU:HG3	1.82	0.43
2:G:83:GLN:O	2:G:120:MET:HE1	2.18	0.43
1:D:1046:ILE:HD12	2:H:311:LEU:HB3	2.01	0.43
1:A:527:ILE:O	1:A:531:VAL:HG23	2.19	0.43
1:D:1359:ARG:NH1	1:D:1362:ARG:HD3	2.34	0.43
1:D:1524:LYS:HD2	1:D:1524:LYS:HA	1.78	0.43
2:F:307:GLN:OE1	2:F:309:ARG:HG2	2.18	0.43
2:E:79:LEU:HB3	2:E:80:PHE:CD2	2.53	0.43
2:H:295:LYS:HE3	2:H:334:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:883:LYS:HD3	1:C:883:LYS:N	2.34	0.42
2:H:77:LEU:HD12	2:H:77:LEU:HA	1.89	0.42
1:A:492:ASN:OD1	1:A:492:ASN:N	2.50	0.42
1:C:1099:GLU:O	1:C:1102:LYS:HG3	2.20	0.42
2:E:151:GLU:HA	2:E:152:PRO:HD3	1.90	0.42
2:H:151:GLU:HA	2:H:407:GLN:HE21	1.83	0.42
2:G:257:VAL:HG11	2:G:266:ARG:HB2	2.01	0.42
1:B:883:LYS:HD2	1:B:883:LYS:H	1.85	0.42
1:C:1577:VAL:O	1:C:1581:MET:HG3	2.20	0.42
1:D:863:SER:O	1:D:867:MET:HG3	2.20	0.42
1:D:883:LYS:H	1:D:883:LYS:HD2	1.85	0.42
1:D:1569:ASP:N	1:D:1569:ASP:OD1	2.53	0.42
2:G:83:GLN:OE1	2:G:84:THR:N	2.53	0.42
1:B:817:PHE:CE2	1:B:827:ILE:HD11	2.54	0.41
2:F:194:ASP:OD2	2:F:195:VAL:N	2.52	0.41
1:B:825:ASN:HD22	2:F:54:THR:C	2.23	0.41
1:B:1113:ILE:H	1:B:1113:ILE:HG12	1.70	0.41
1:C:3:LYS:HG2	1:C:4:PRO:HD2	2.02	0.41
1:A:1577:VAL:O	1:A:1581:MET:HG3	2.20	0.41
1:B:140:LYS:O	1:B:143:GLU:HG3	2.21	0.41
1:C:1081:HIS:HD1	1:C:1081:HIS:C	2.24	0.41
2:E:257:VAL:HG11	2:E:266:ARG:HB2	2.02	0.41
2:F:117:ARG:HH22	2:F:121:ASN:HD22	1.69	0.41
1:A:1512:GLY:HA2	1:A:1515:TRP:CE3	2.56	0.41
1:D:18:GLN:NE2	1:D:66:PHE:O	2.54	0.41
1:A:883:LYS:N	1:A:883:LYS:HD3	2.35	0.41
1:C:438:PHE:HE1	1:C:1555:ARG:HH12	1.68	0.41
1:A:990:ILE:HD11	2:E:311:LEU:HD13	2.03	0.41
1:C:1512:GLY:HA2	1:C:1515:TRP:CE3	2.56	0.41
1:B:863:SER:O	1:B:867:MET:HG3	2.21	0.41
1:C:1119:LYS:HA	1:C:1122:ILE:HG22	2.03	0.41
2:E:380:GLU:HA	2:E:384:THR:OG1	2.21	0.41
2:E:315:GLN:HG2	2:E:318:ASP:HB2	2.02	0.40
1:A:1099:GLU:O	1:A:1102:LYS:HG3	2.20	0.40
1:B:228:ILE:HD13	1:B:340:PHE:CZ	2.57	0.40
1:C:63:GLN:OE1	1:C:64:SER:N	2.54	0.40
1:A:70:LYS:NZ	1:A:72:SER:OG	2.54	0.40
1:A:769:GLU:HG2	1:A:778:HIS:CE1	2.57	0.40
1:D:140:LYS:O	1:D:143:GLU:HG3	2.20	0.40
1:D:817:PHE:CE2	1:D:827:ILE:HD11	2.56	0.40
2:E:381:LEU:O	2:E:385:LEU:HD23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:398:LEU:HA	2:E:398:LEU:HD23	1.93	0.40
2:H:84:THR:HA	2:H:120:MET:HE3	2.04	0.40
1:A:63:GLN:OE1	1:A:64:SER:N	2.54	0.40
1:B:1569:ASP:N	1:B:1569:ASP:OD1	2.51	0.40

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	1531/1587 (96%)	1499 (98%)	32 (2%)	0	100	100
1	B	1524/1587 (96%)	1490 (98%)	34 (2%)	0	100	100
1	C	1531/1587 (96%)	1501 (98%)	30 (2%)	0	100	100
1	D	1524/1587 (96%)	1490 (98%)	34 (2%)	0	100	100
2	E	434/535 (81%)	422 (97%)	12 (3%)	0	100	100
2	F	434/535 (81%)	422 (97%)	12 (3%)	0	100	100
2	G	434/535 (81%)	419 (96%)	15 (4%)	0	100	100
2	H	434/535 (81%)	425 (98%)	9 (2%)	0	100	100
All	All	7846/8488 (92%)	7668 (98%)	178 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1422/1461 (97%)	1400 (98%)	22 (2%)	65 87
1	B	1418/1461 (97%)	1393 (98%)	25 (2%)	59 85
1	C	1422/1461 (97%)	1400 (98%)	22 (2%)	65 87
1	D	1418/1461 (97%)	1390 (98%)	28 (2%)	55 82
2	E	370/435 (85%)	363 (98%)	7 (2%)	57 84
2	F	370/435 (85%)	361 (98%)	9 (2%)	49 79
2	G	370/435 (85%)	366 (99%)	4 (1%)	73 92
2	H	370/435 (85%)	361 (98%)	9 (2%)	49 79
All	All	7160/7584 (94%)	7034 (98%)	126 (2%)	61 85

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET
1	A	63	GLN
1	A	89	TYR
1	A	144	SER
1	A	188	LYS
1	A	279	ASP
1	A	335	ASP
1	A	488	LYS
1	A	492	ASN
1	A	560	TYR
1	A	563	ARG
1	A	602	LEU
1	A	767	ASP
1	A	800	LYS
1	A	1041	ARG
1	A	1052	ASP
1	A	1081	HIS
1	A	1123	LYS
1	A	1359	ARG
1	A	1362	ARG
1	A	1428	TRP
1	A	1530	LYS
1	B	86	LYS
1	B	132	LYS
1	B	222	ASN

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Mol	Chain	Res	Type
1	B	234	GLU
1	B	338	TYR
1	B	342	ASP
1	B	345	LYS
1	B	492	ASN
1	B	563	ARG
1	B	594	GLN
1	B	701	MET
1	B	712	ARG
1	B	767	ASP
1	B	800	LYS
1	B	883	LYS
1	B	940	ASP
1	B	1041	ARG
1	B	1095	ARG
1	B	1123	LYS
1	B	1289	LYS
1	B	1359	ARG
1	B	1360	GLU
1	B	1428	TRP
1	B	1518	GLU
1	B	1525	LYS
1	C	35	MET
1	C	63	GLN
1	C	89	TYR
1	C	144	SER
1	C	188	LYS
1	C	211	ASP
1	C	279	ASP
1	C	335	ASP
1	C	398	GLU
1	C	488	LYS
1	C	492	ASN
1	C	560	TYR
1	C	563	ARG
1	C	602	LEU
1	C	800	LYS
1	C	816	CYS
1	C	1041	ARG
1	C	1081	HIS
1	C	1123	LYS
1	C	1359	ARG

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Mol	Chain	Res	Type
1	C	1428	TRP
1	C	1530	LYS
1	D	86	LYS
1	D	222	ASN
1	D	234	GLU
1	D	342	ASP
1	D	345	LYS
1	D	492	ASN
1	D	563	ARG
1	D	712	ARG
1	D	732	ASP
1	D	767	ASP
1	D	800	LYS
1	D	822	PHE
1	D	883	LYS
1	D	940	ASP
1	D	941	ARG
1	D	1041	ARG
1	D	1044	MET
1	D	1095	ARG
1	D	1106	MET
1	D	1123	LYS
1	D	1272	HIS
1	D	1289	LYS
1	D	1359	ARG
1	D	1360	GLU
1	D	1428	TRP
1	D	1518	GLU
1	D	1524	LYS
1	D	1525	LYS
2	E	86	MET
2	E	210	MET
2	E	214	TYR
2	E	320	VAL
2	E	323	ARG
2	E	326	ASP
2	E	437	GLN
2	F	22	LEU
2	F	86	MET
2	F	114	MET
2	F	117	ARG
2	F	210	MET

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Mol	Chain	Res	Type
2	F	323	ARG
2	F	326	ASP
2	F	354	TYR
2	F	455	MET
2	G	86	MET
2	G	109	GLU
2	G	320	VAL
2	G	323	ARG
2	H	22	LEU
2	H	86	MET
2	H	114	MET
2	H	117	ARG
2	H	194	ASP
2	H	199	MET
2	H	210	MET
2	H	323	ARG
2	H	354	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	825	ASN
1	B	825	ASN
2	F	157	ASN
2	F	413	GLN
2	H	205	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	1.04	0	7,9,11	2.72	2 (28%)
1	FME	C	1	1	8,9,10	1.05	0	7,9,11	2.81	2 (28%)

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
1	FME	A	1	1	-	6/7/9/11	-
1	FME	C	1	1	-	6/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	FME	CA-N-CN	-5.49	114.38	122.82
1	A	1	FME	CA-N-CN	-5.30	114.67	122.82
1	C	1	FME	O1-CN-N	4.50	137.12	125.27
1	A	1	FME	O1-CN-N	4.36	136.74	125.27

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	O-C-CA-CB
1	C	1	FME	O1-CN-N-CA
1	C	1	FME	O-C-CA-CB
1	A	1	FME	CB-CG-SD-CE
1	C	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
1	C	1	FME	N-CA-CB-CG
1	A	1	FME	CA-CB-CG-SD
1	C	1	FME	CA-CB-CG-SD
1	A	1	FME	C-CA-CB-CG
1	C	1	FME	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
1	C	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	C	1601	4	26,33,33	0.70	0	31,52,52	0.81	2 (6%)
3	ATP	B	1601	4	26,33,33	0.67	0	31,52,52	0.78	2 (6%)
3	ATP	A	1601	4	26,33,33	0.70	0	31,52,52	0.81	2 (6%)
3	ATP	D	1601	4	26,33,33	0.67	0	31,52,52	0.78	2 (6%)

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
3	ATP	C	1601	4	-	1/18/38/38	0/3/3/3
3	ATP	B	1601	4	-	0/18/38/38	0/3/3/3
3	ATP	A	1601	4	-	1/18/38/38	0/3/3/3
3	ATP	D	1601	4	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1601	ATP	PB-O3B-PG	2.24	140.50	132.83
3	A	1601	ATP	PB-O3B-PG	2.23	140.47	132.83
3	A	1601	ATP	C5-C6-N6	2.11	123.56	120.35
3	C	1601	ATP	C5-C6-N6	2.07	123.49	120.35
3	B	1601	ATP	PB-O3B-PG	2.06	139.91	132.83
3	D	1601	ATP	PB-O3B-PG	2.06	139.89	132.83
3	D	1601	ATP	C5-C6-N6	2.06	123.48	120.35
3	B	1601	ATP	C5-C6-N6	2.03	123.44	120.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

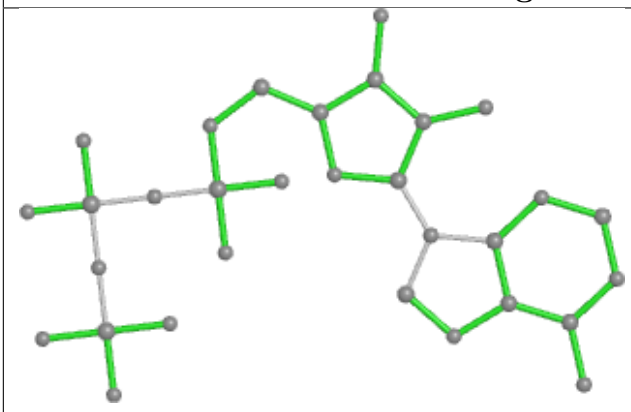
Mol	Chain	Res	Type	Atoms
3	A	1601	ATP	PA-O3A-PB-O2B
3	C	1601	ATP	PA-O3A-PB-O2B

There are no ring outliers.

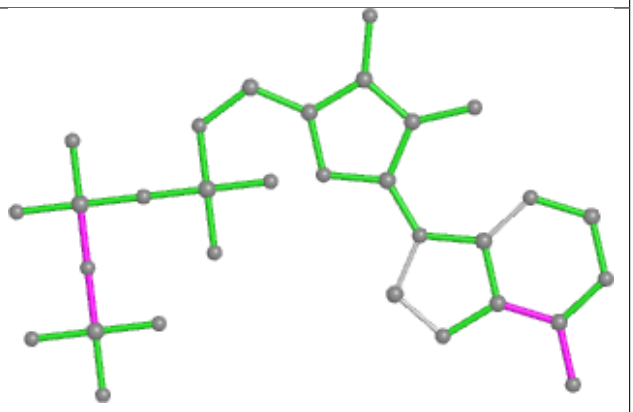
No monomer is involved in short contacts.

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.

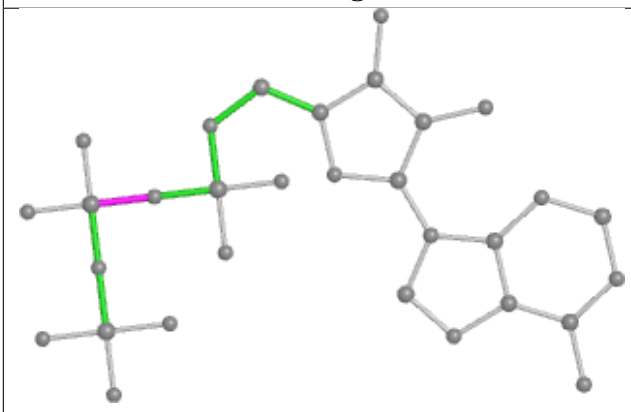
Ligand ATP C 1601



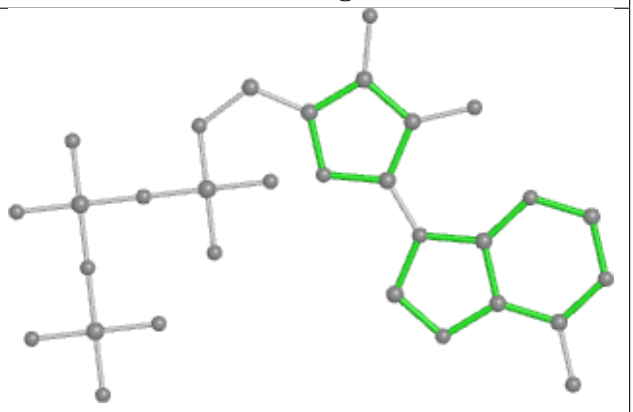
Bond lengths



Bond angles

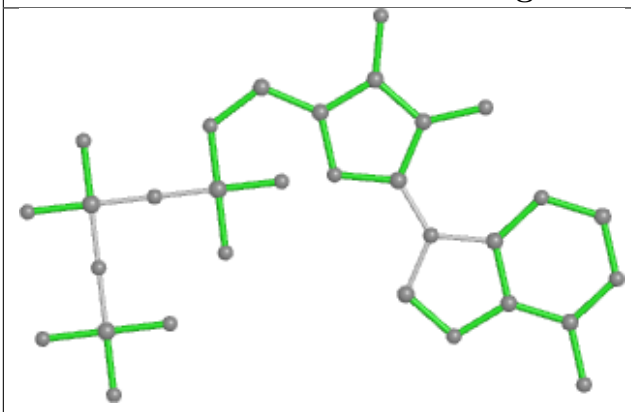


Torsions

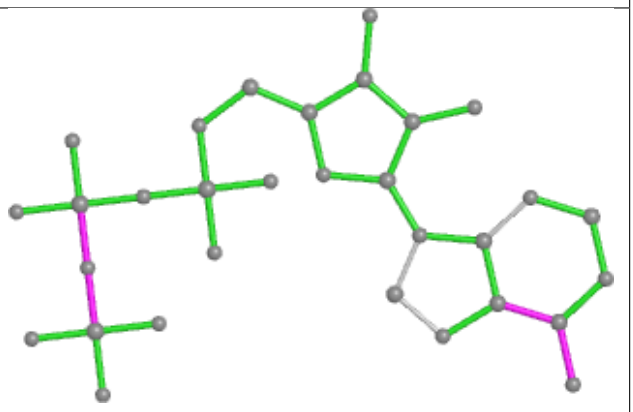


Rings

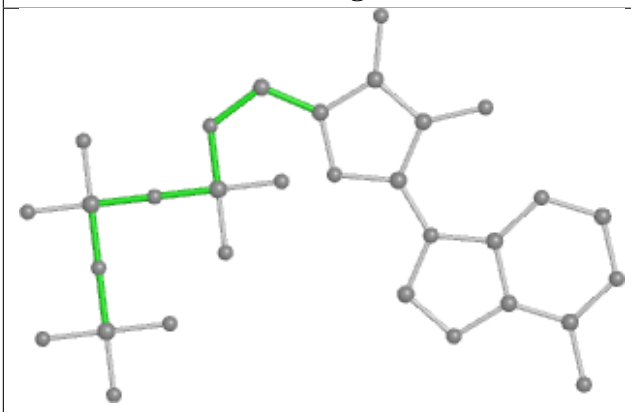
Ligand ATP B 1601



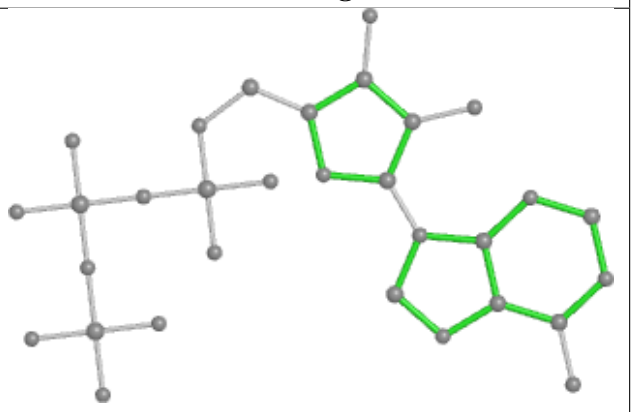
Bond lengths



Bond angles

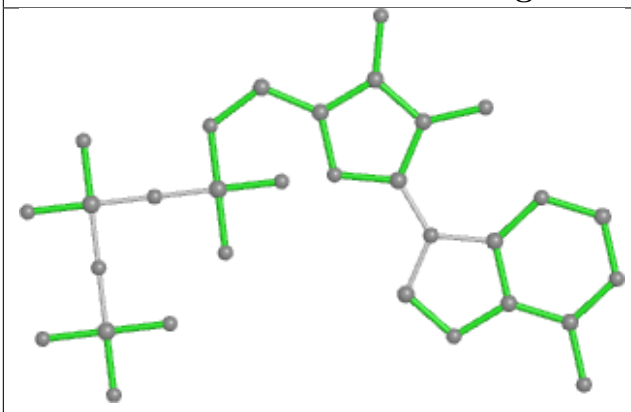


Torsions

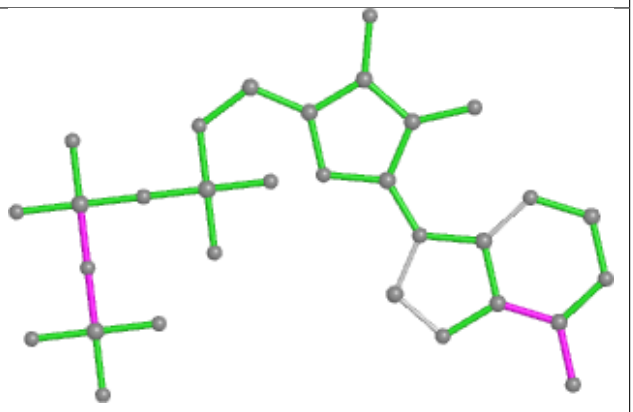


Rings

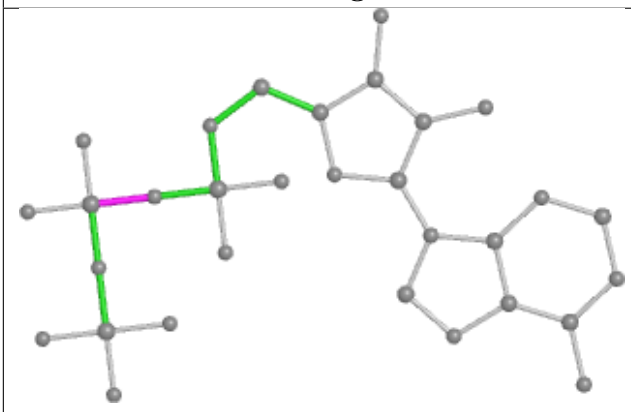
Ligand ATP A 1601



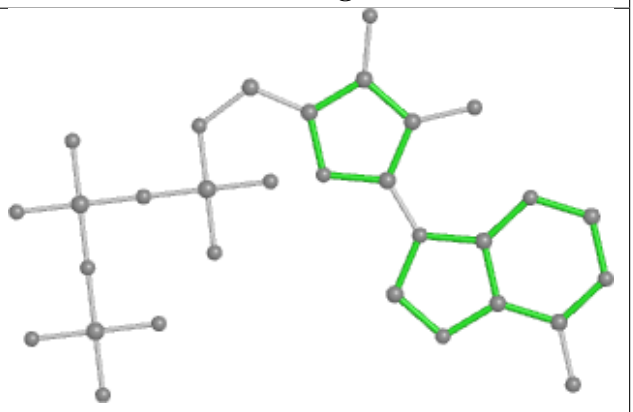
Bond lengths



Bond angles

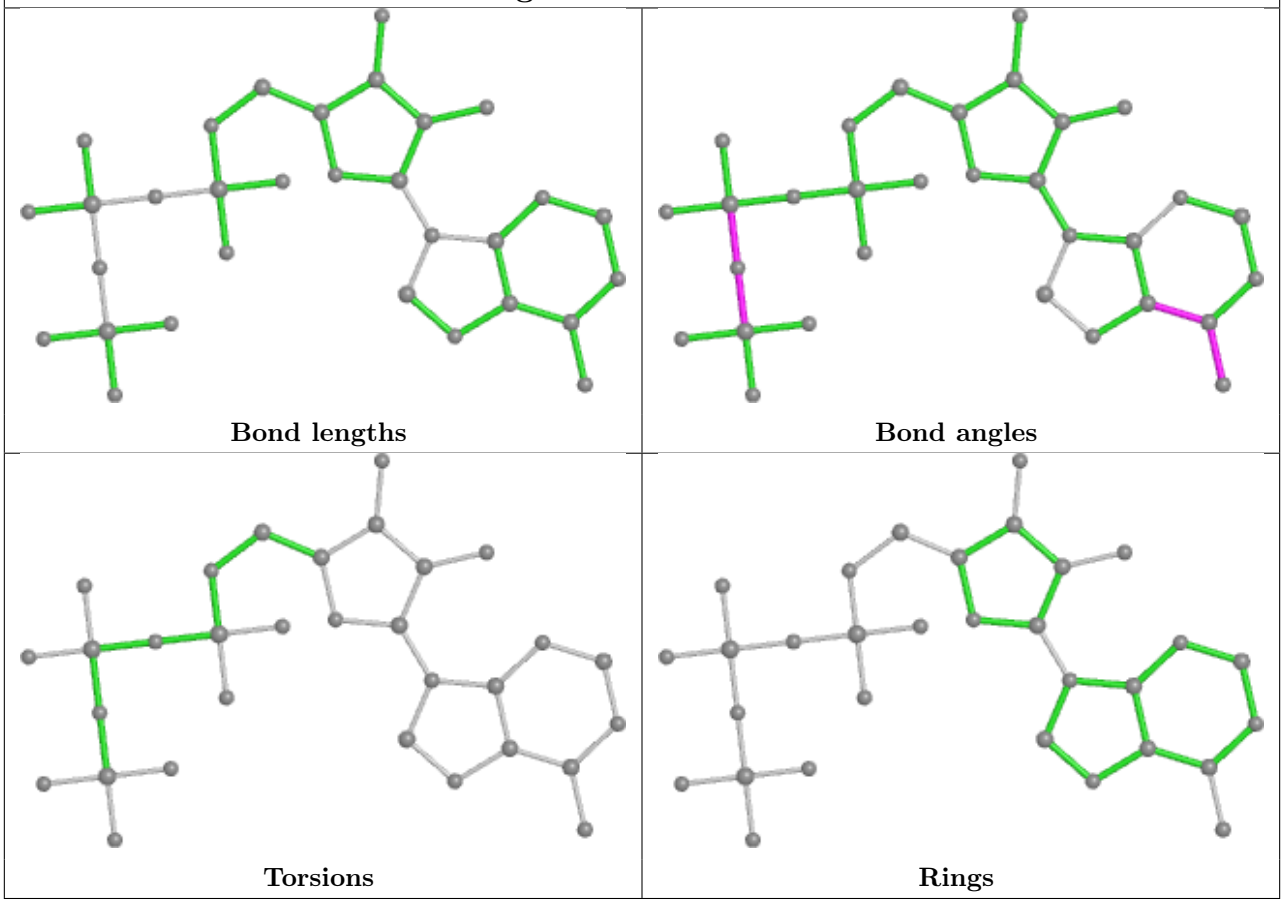


Torsions



Rings

Ligand ATP D 1601



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.

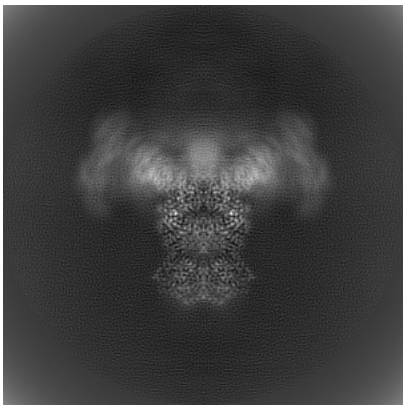
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27422. These allow visual inspection of the internal detail of the map and identification of artifacts.

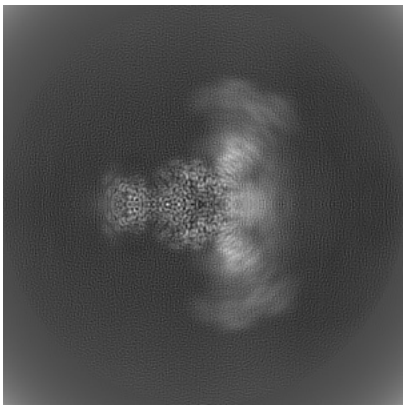
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

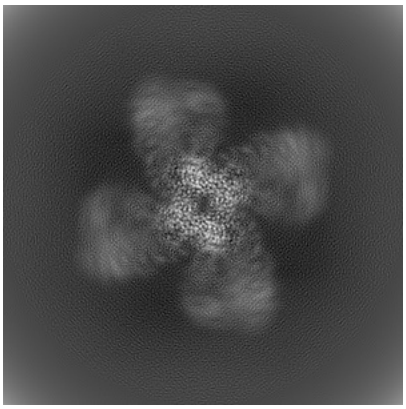
6.1.1 Primary map



X

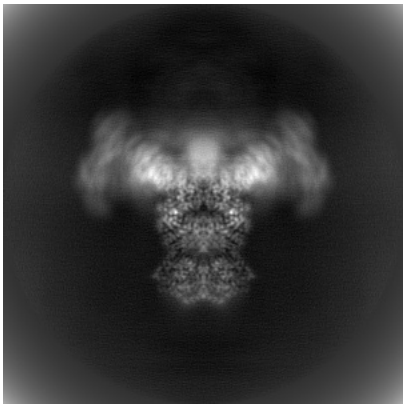


Y

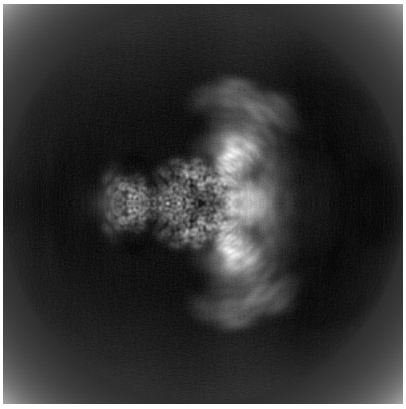


Z

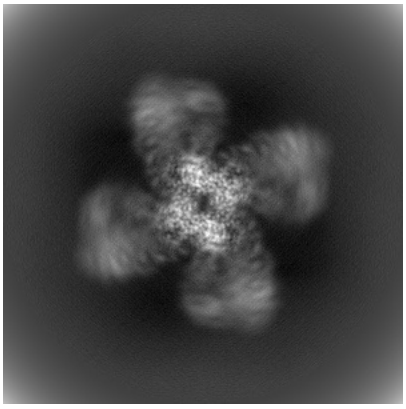
6.1.2 Raw map



X



Y

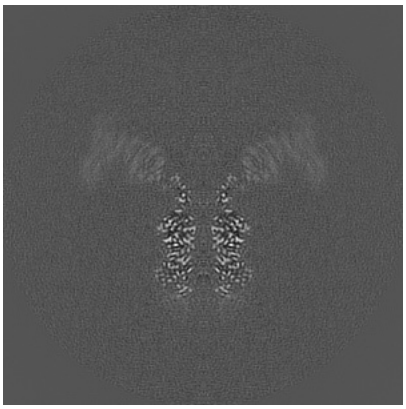


Z

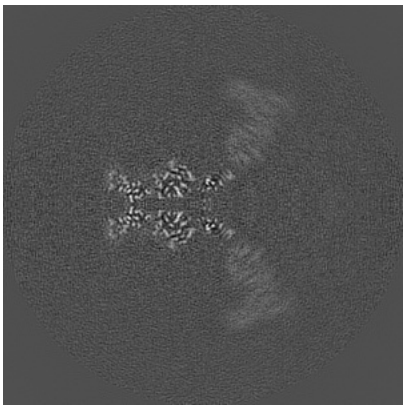
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

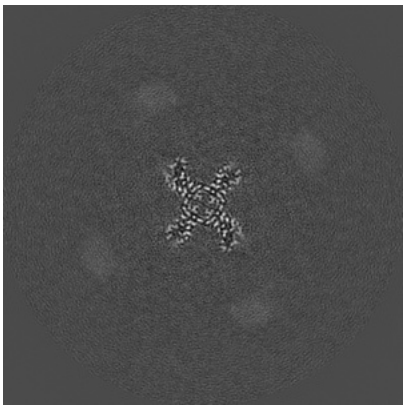
6.2.1 Primary map



X Index: 180

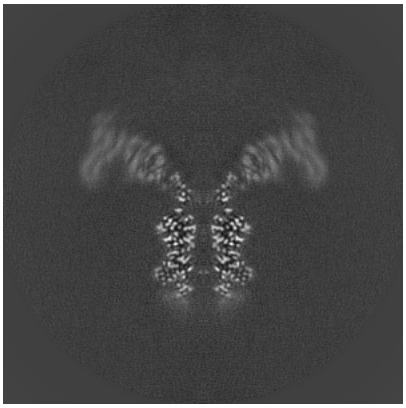


Y Index: 180

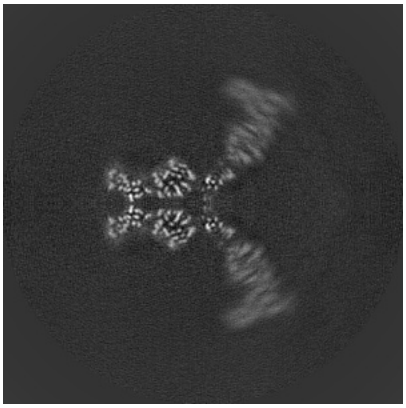


Z Index: 180

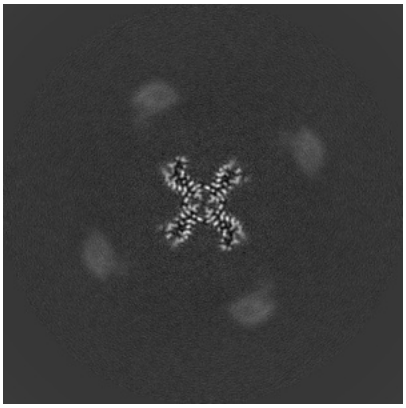
6.2.2 Raw map



X Index: 180



Y Index: 180

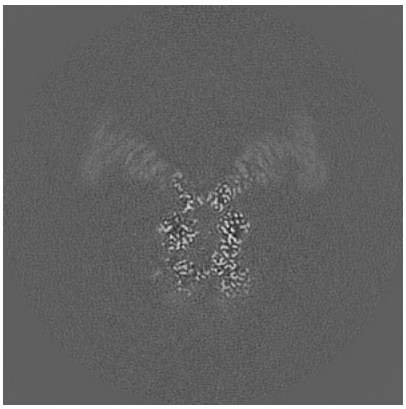


Z Index: 180

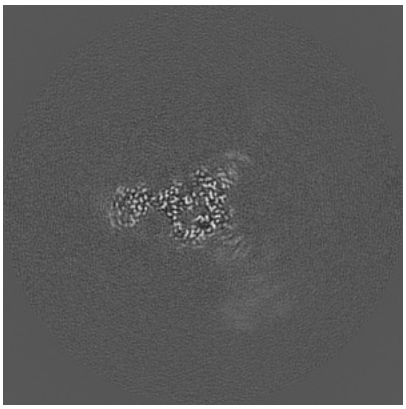
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

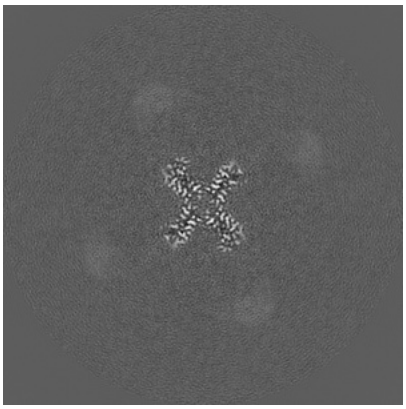
6.3.1 Primary map



X Index: 175

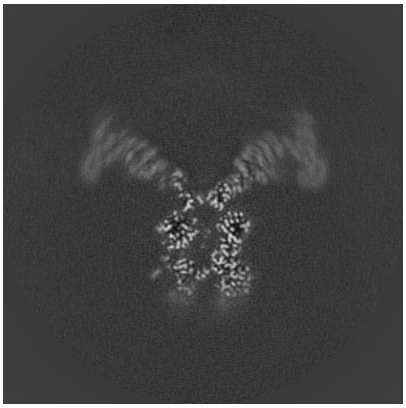


Y Index: 160

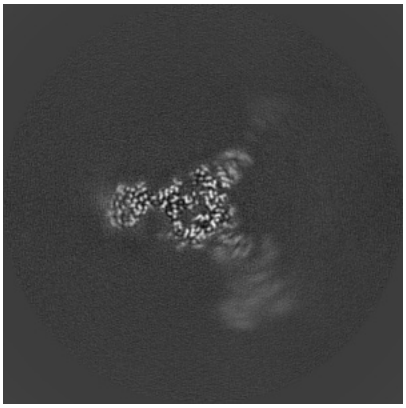


Z Index: 179

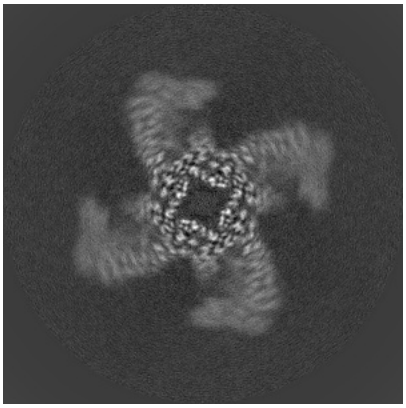
6.3.2 Raw map



X Index: 175



Y Index: 160

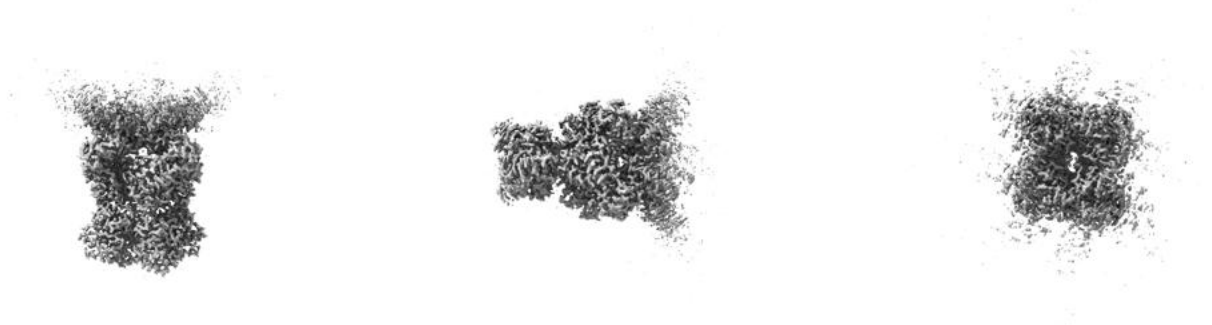


Z Index: 204

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

6.4 Orthogonal surface views (i)

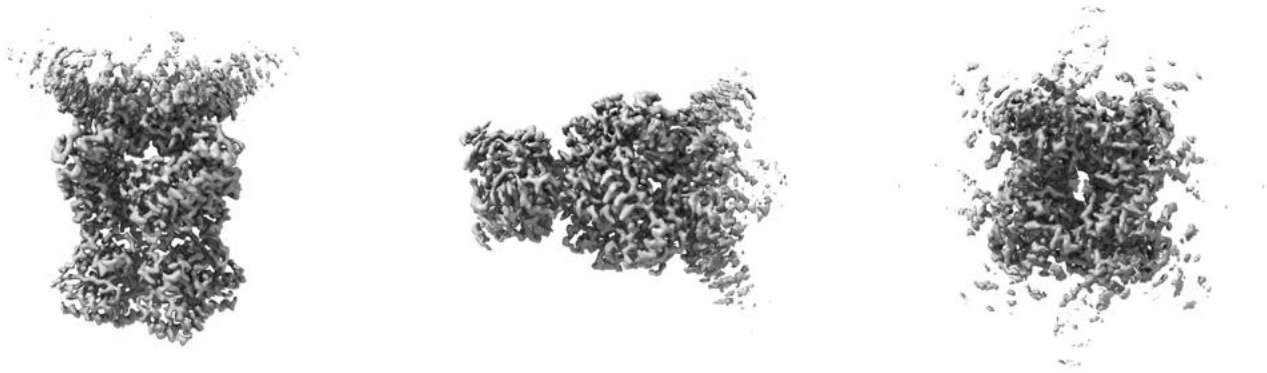
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

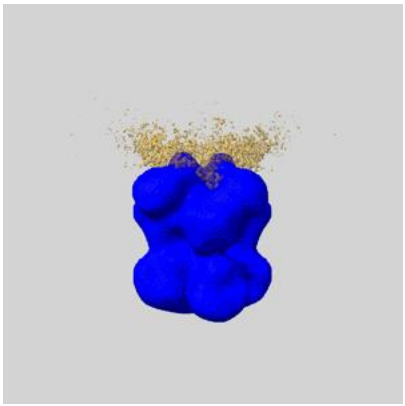
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

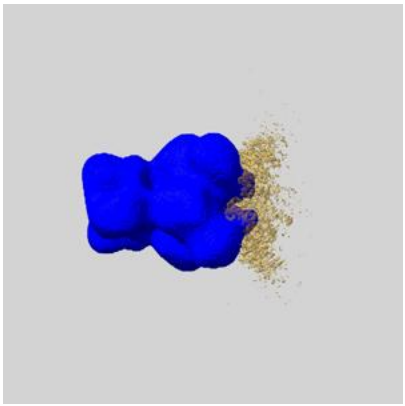
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

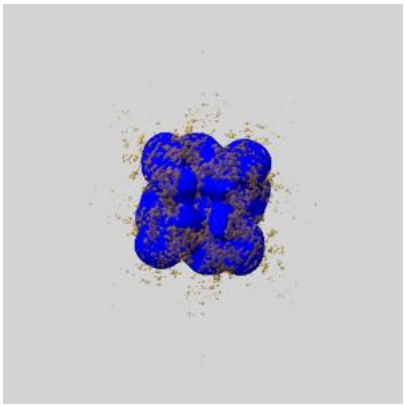
6.5.1 emd_27422_msk_1.map (i)



X



Y

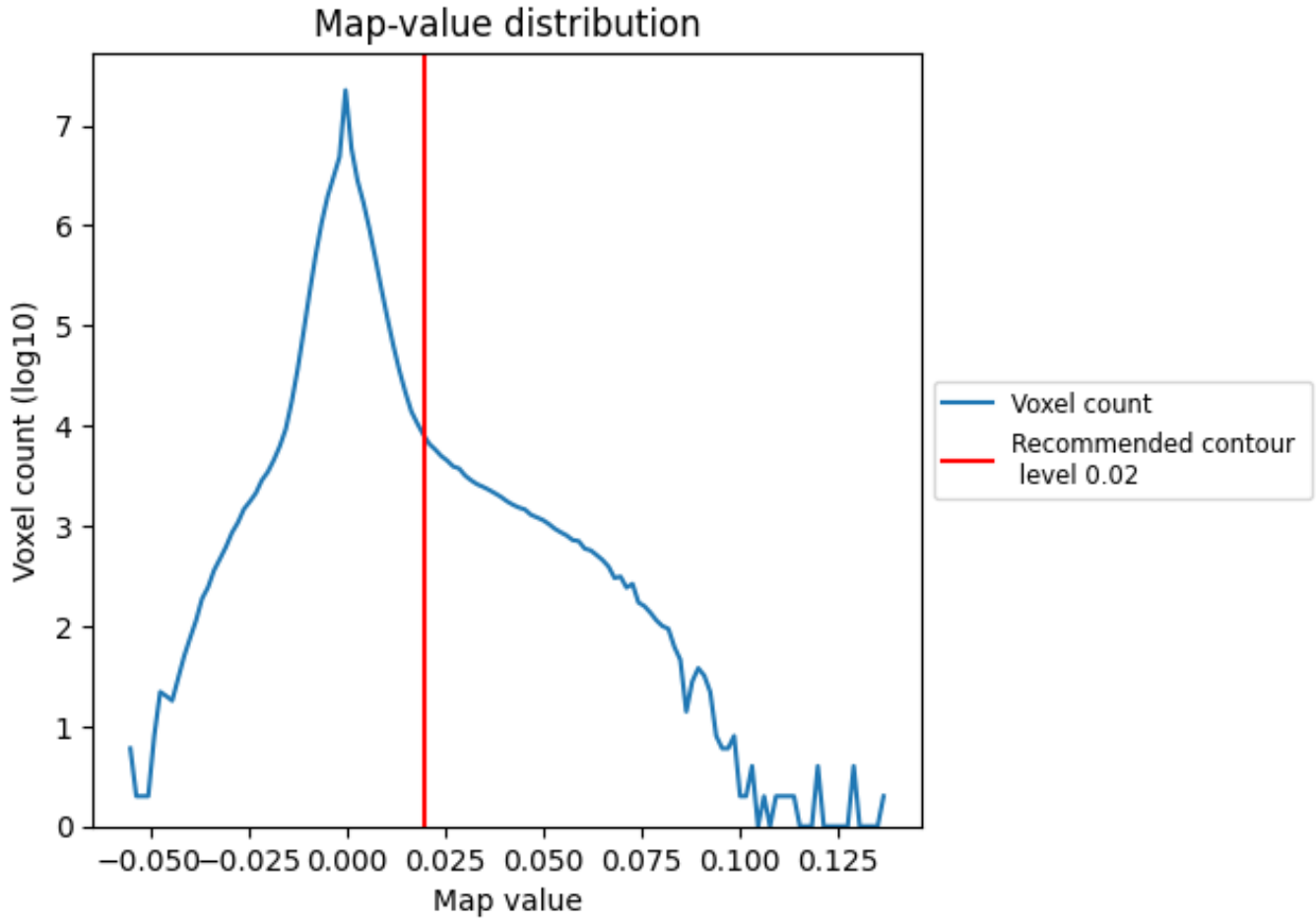


Z

7 Map analysis

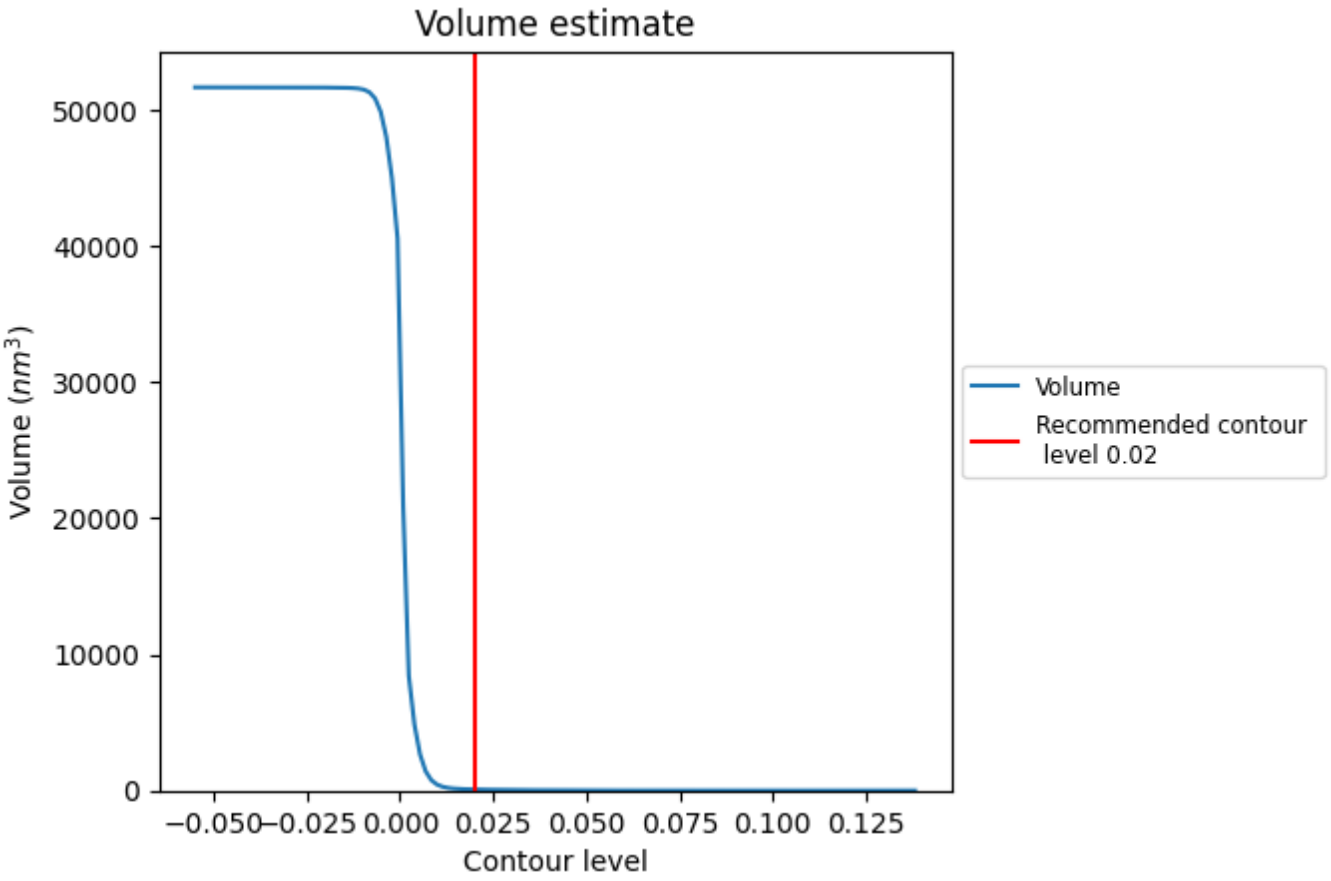
This section contains the results of statistical analysis of the map.

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.

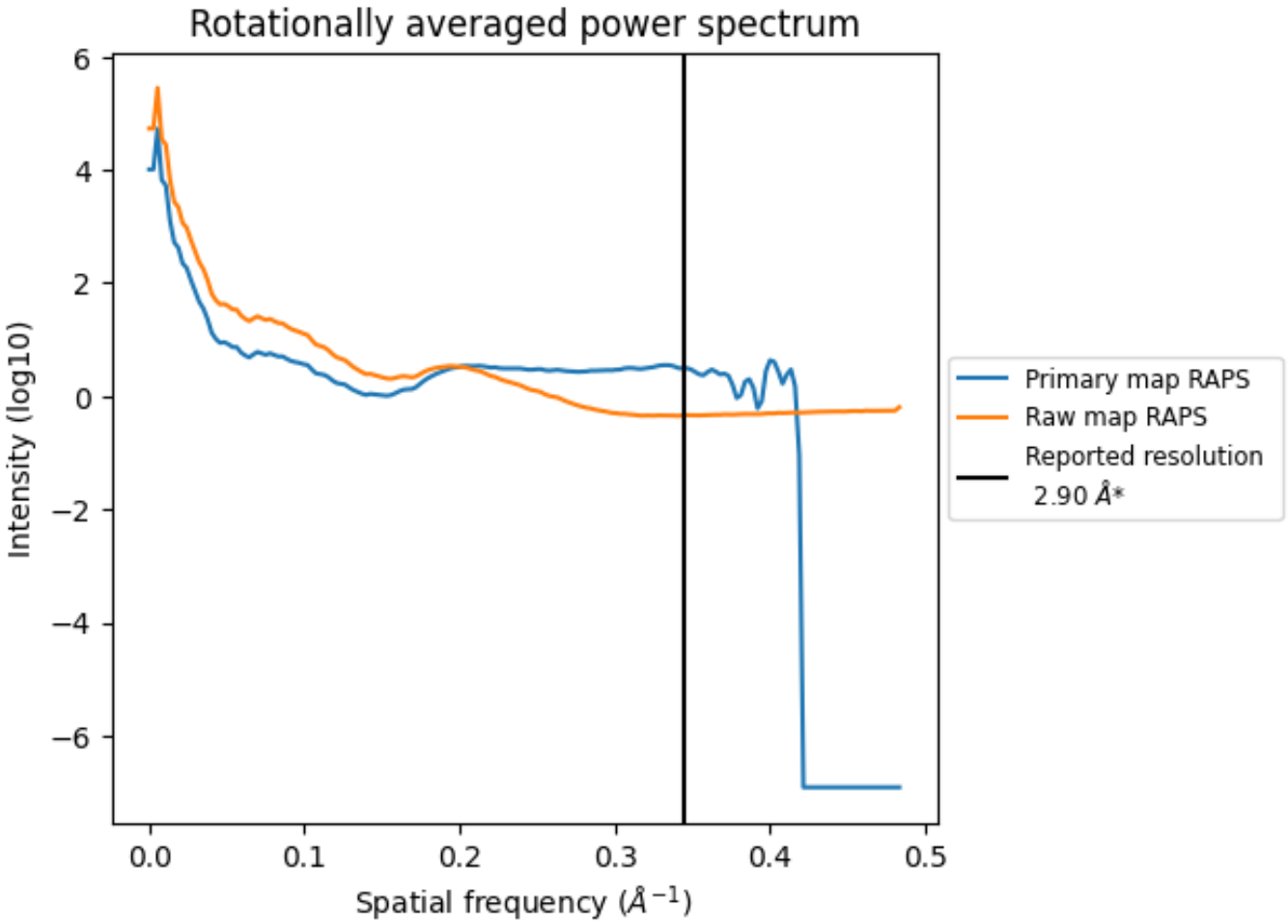
7.2 Volume estimate (i)



The volume at the recommended contour level is 80 nm^3; this corresponds to an approximate mass of 73 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)

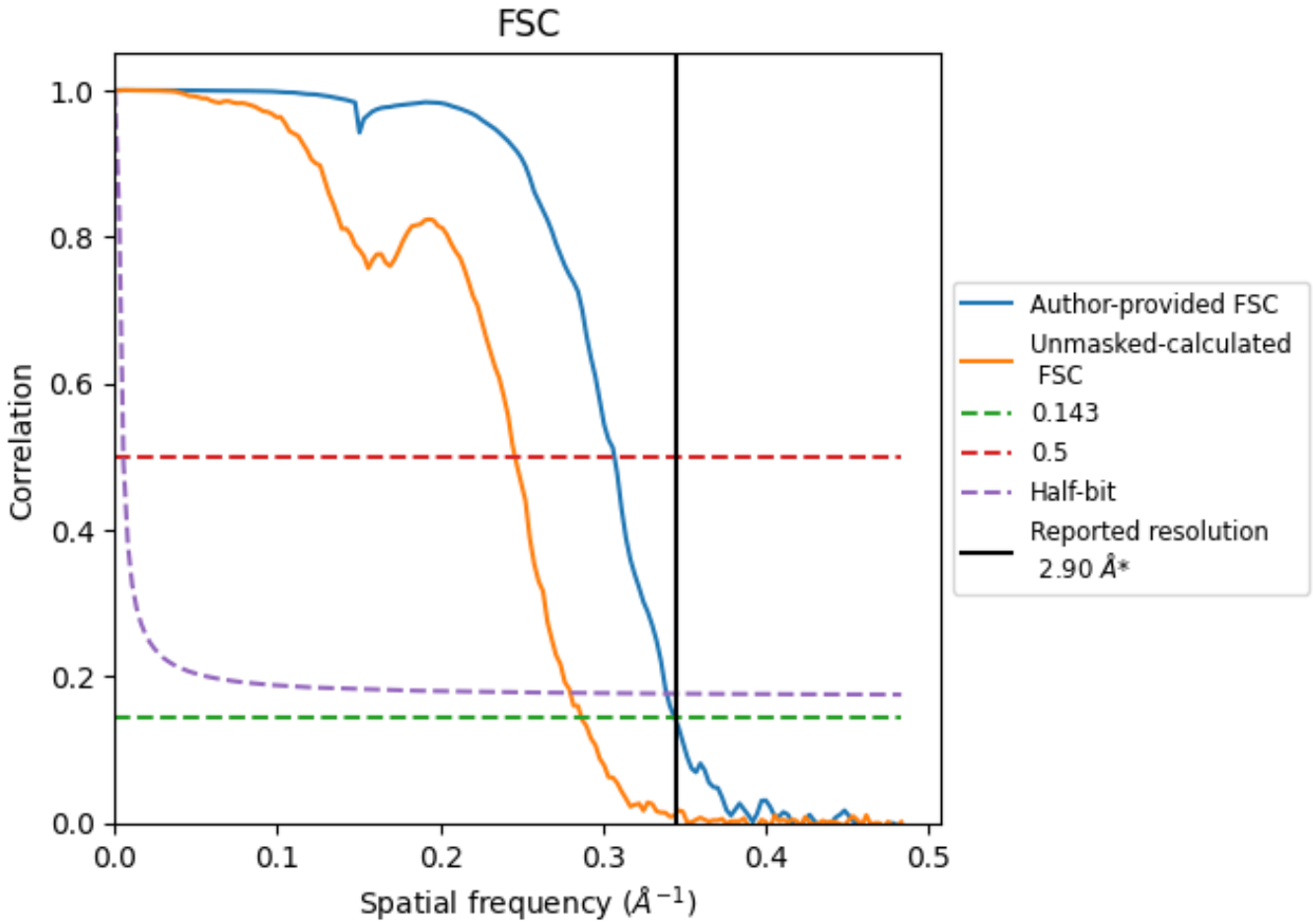


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 $Å^{-1}$

8.2 Resolution estimates (i)

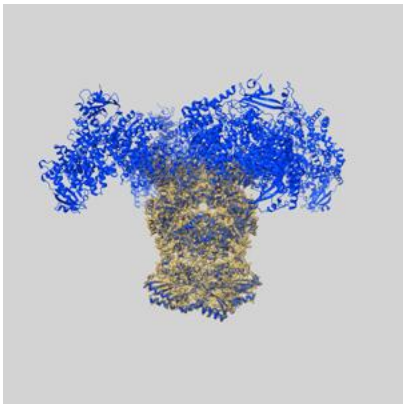
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.26	2.95
Unmasked-calculated*	3.48	4.07	3.57

*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 3.48 differs from the reported value 2.9 by more than 10 %

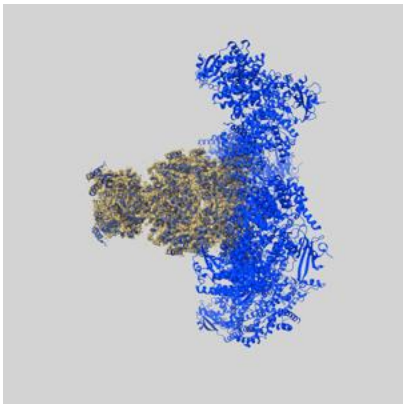
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27422 and PDB model 8DGF. Per-residue inclusion information can be found in section 3 on page 5.

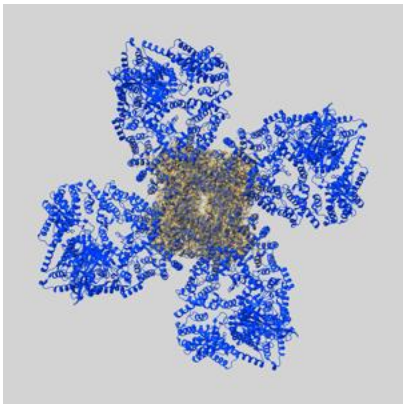
9.1 Map-model overlay



X



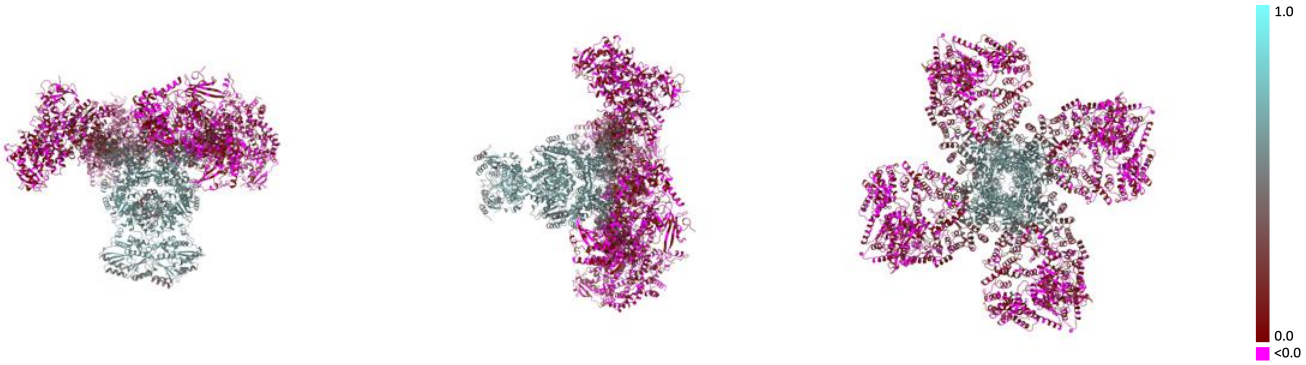
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

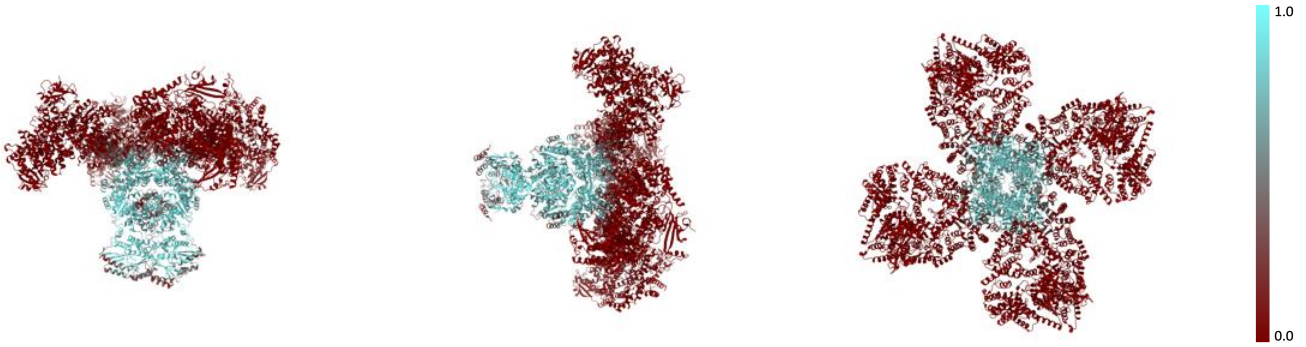
9.2 Q-score mapped to coordinate model (i)



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.

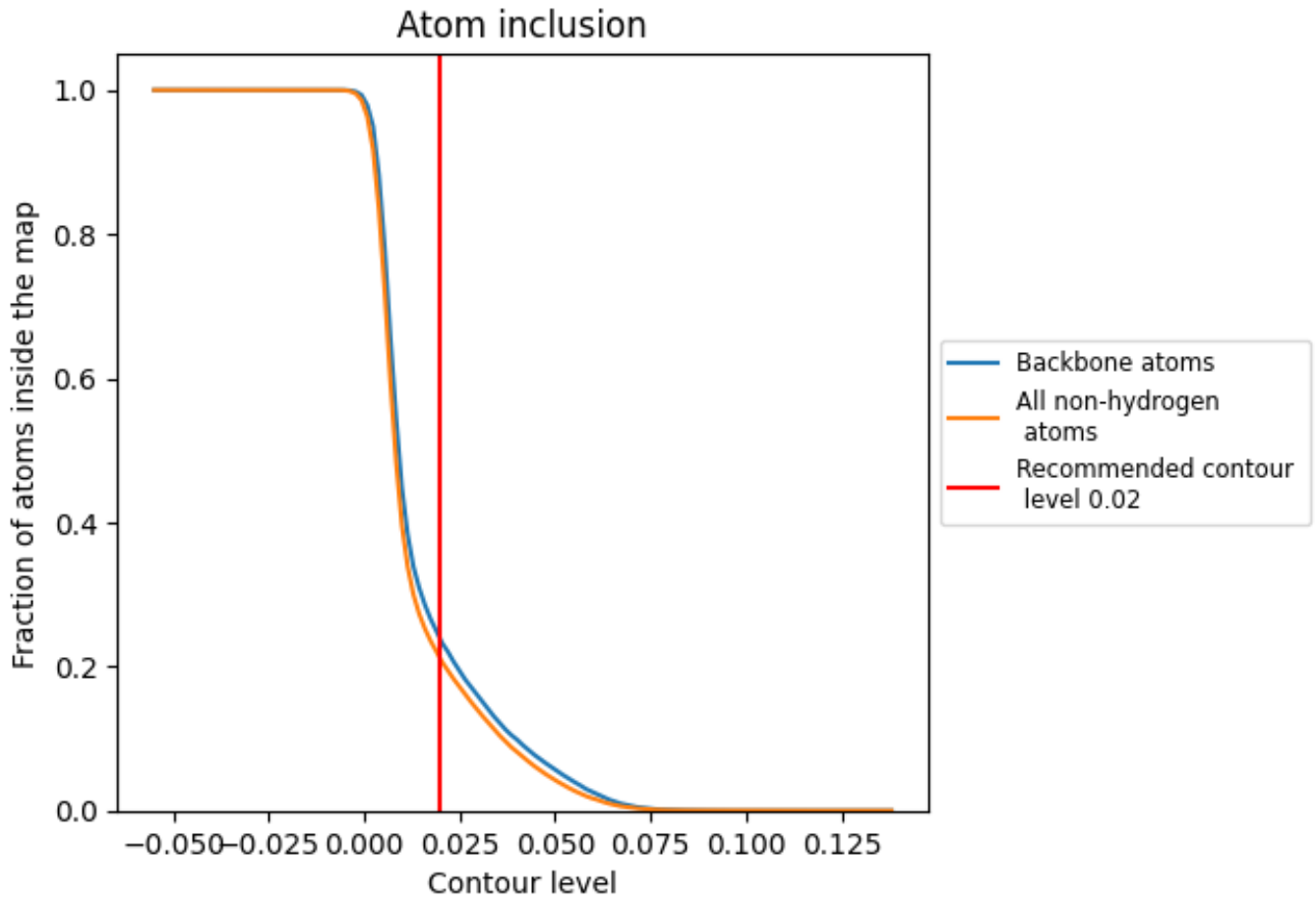
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 24% of all backbone atoms, 21% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2108	0.2340
A	0.2863	0.2990
B	0.2481	0.2640
C	0.2865	0.3000
D	0.2473	0.2650
E	0.0000	0.0570
F	0.0000	0.0470
G	0.0000	0.0570
H	0.0000	0.0470