wwPDB EM Validation Summary Report

Nov 19, 2022 – 09:40 PM EST

PDB ID	:	7S5Y
EMDB ID	:	EMD-24843
Title	:	Human KATP channel in open conformation, focused on Kir and one SUR, position 2
Authors	:	Zhao, C.; MacKinnon, R.
Deposited on	:	2021-09-12
Resolution	:	3.90 Å(reported)

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

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

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

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

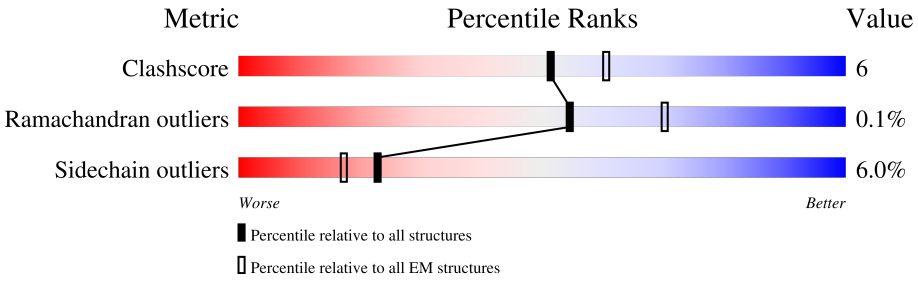
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.90 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	390	14% 62% 19% • 18%
1	B	390	20% 61% 20% • 18%
1	C	390	17% 62% 19% • 18%
1	D	390	18% 62% 19% • 18%
2	E	1582	26% 73% 15% • 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21106 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-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	0	0
			2519	1622	430	451	16		
1	B	321	Total	C	N	O	S	0	0
			2519	1622	430	451	16		
1	C	321	Total	C	N	O	S	0	0
			2519	1622	430	451	16		
1	D	321	Total	C	N	O	S	0	0
			2519	1622	430	451	16		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	SER	CYS	engineered mutation	UNP B2RC52
A	334	ASP	GLY	engineered mutation	UNP B2RC52
B	166	SER	CYS	engineered mutation	UNP B2RC52
B	334	ASP	GLY	engineered mutation	UNP B2RC52
C	166	SER	CYS	engineered mutation	UNP B2RC52
C	334	ASP	GLY	engineered mutation	UNP B2RC52
D	166	SER	CYS	engineered mutation	UNP B2RC52
D	334	ASP	GLY	engineered mutation	UNP B2RC52

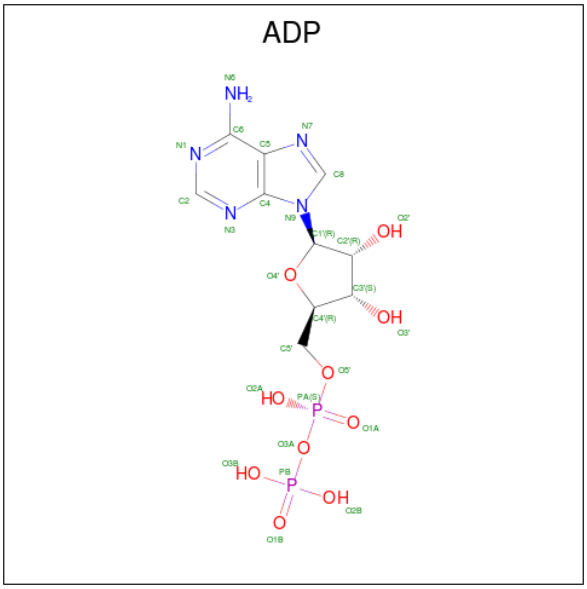
- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1402	Total	C	N	O	S	0	0
			10970	7131	1864	1920	55		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	expression tag	UNP Q09428
E	2	GLY	-	expression tag	UNP Q09428

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

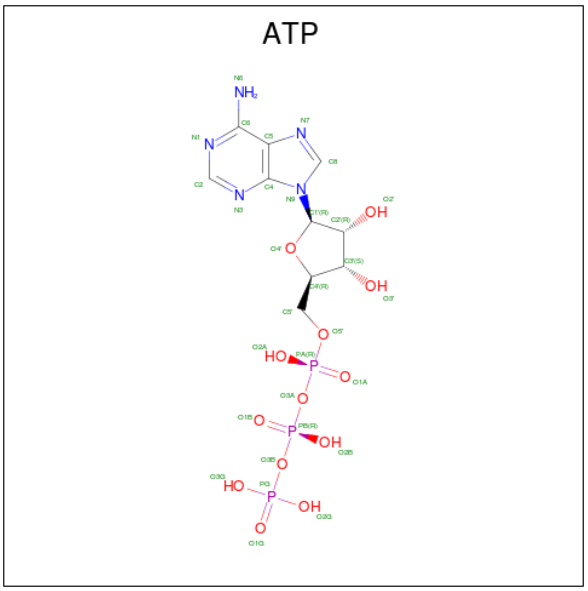


Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	E	2	Total	Mg	0
			2	2	

- Molecule 5 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).

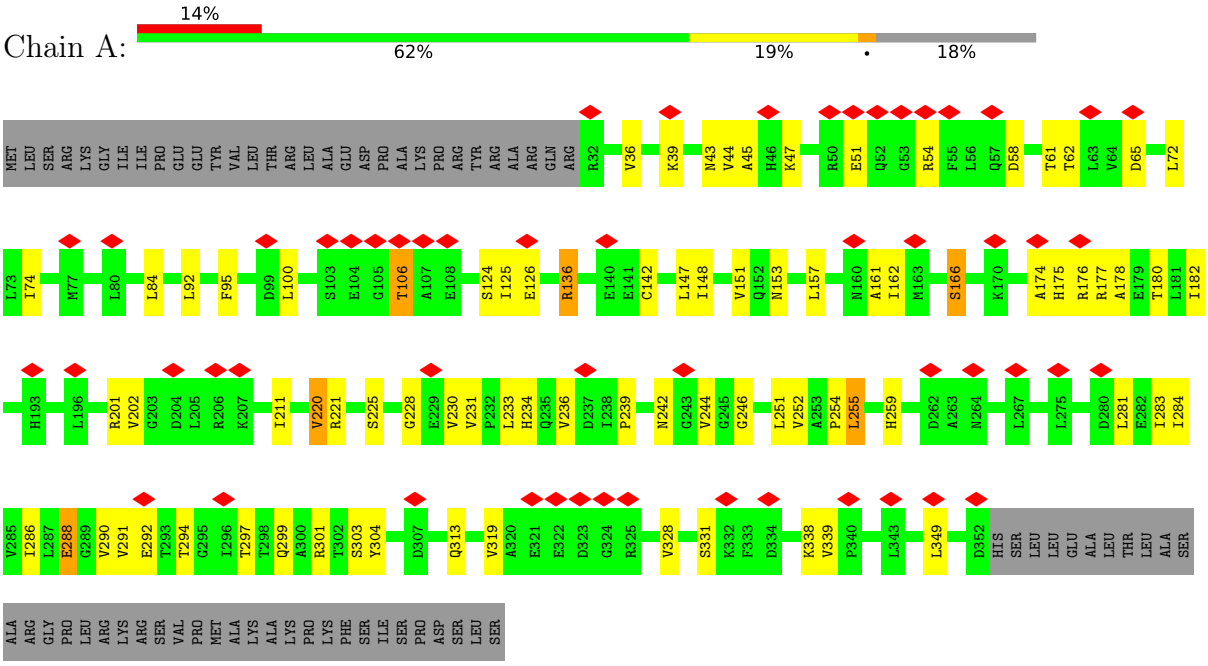


Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

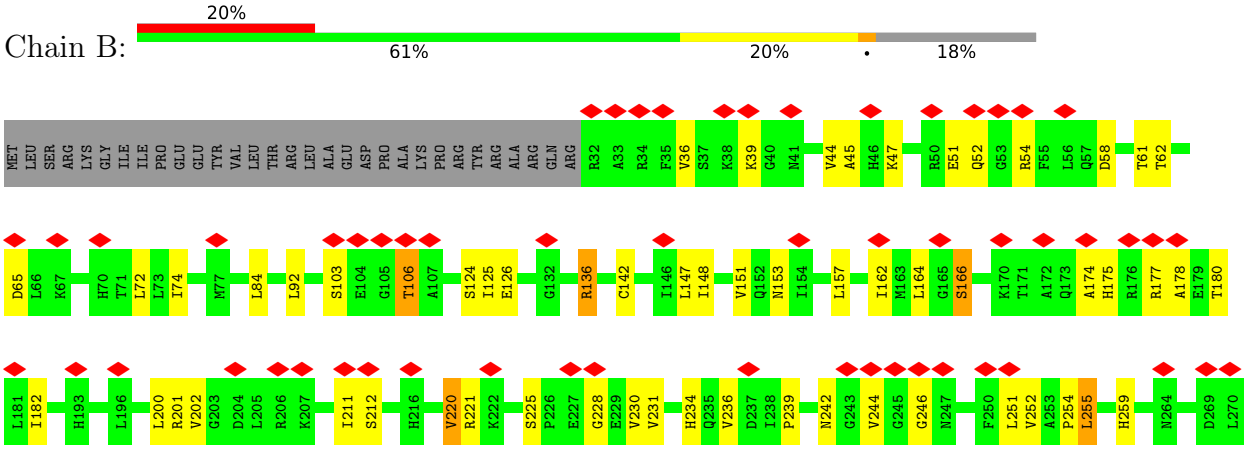
3 Residue-property plots (i)

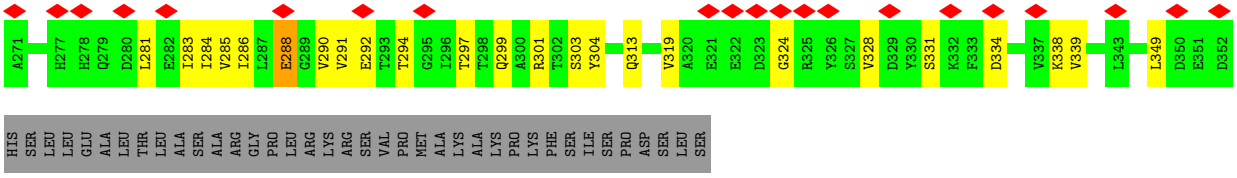
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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-sensitive inward rectifier potassium channel 11



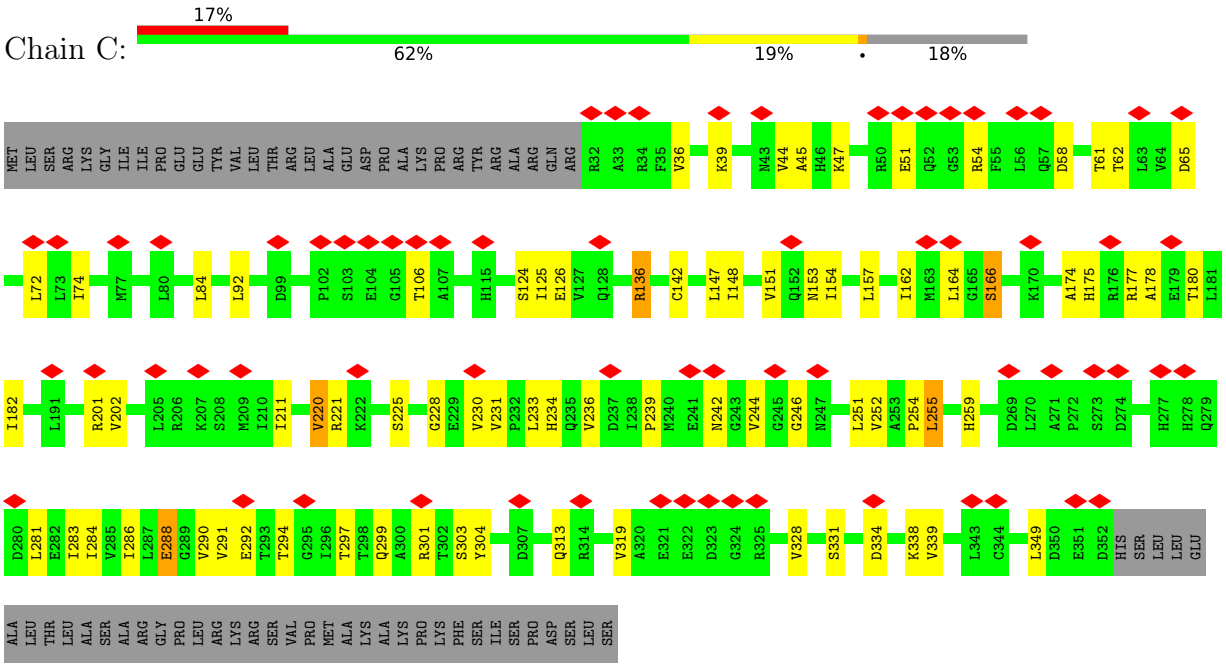
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11





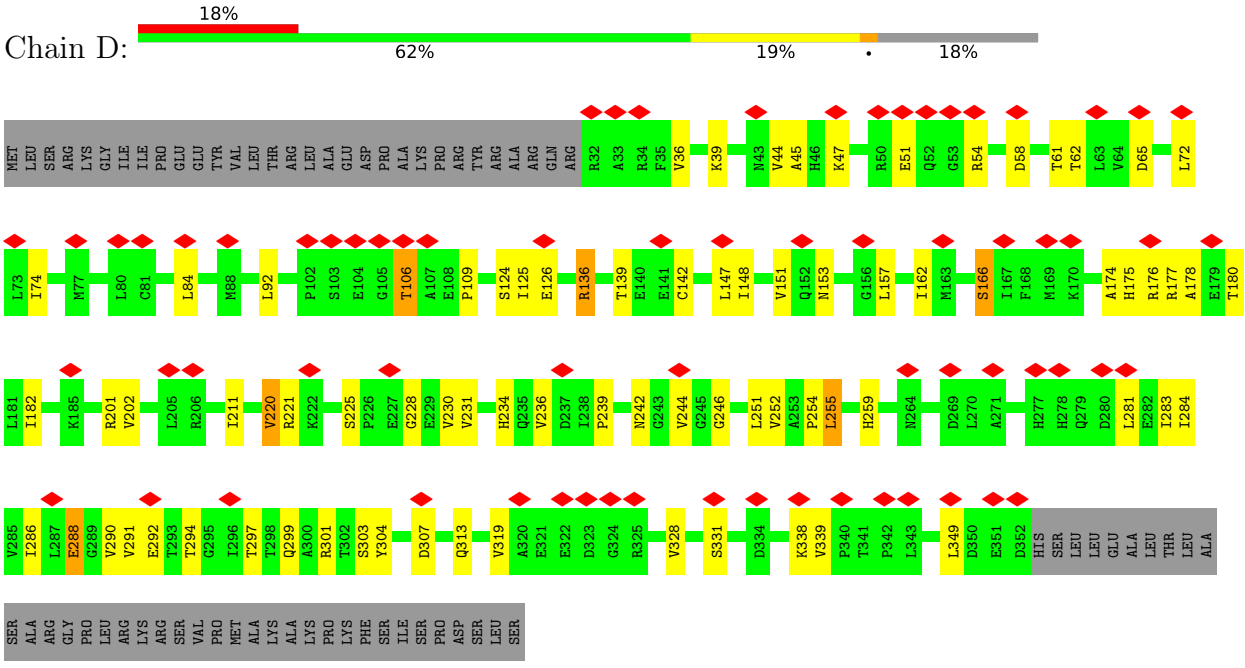
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain C:



• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

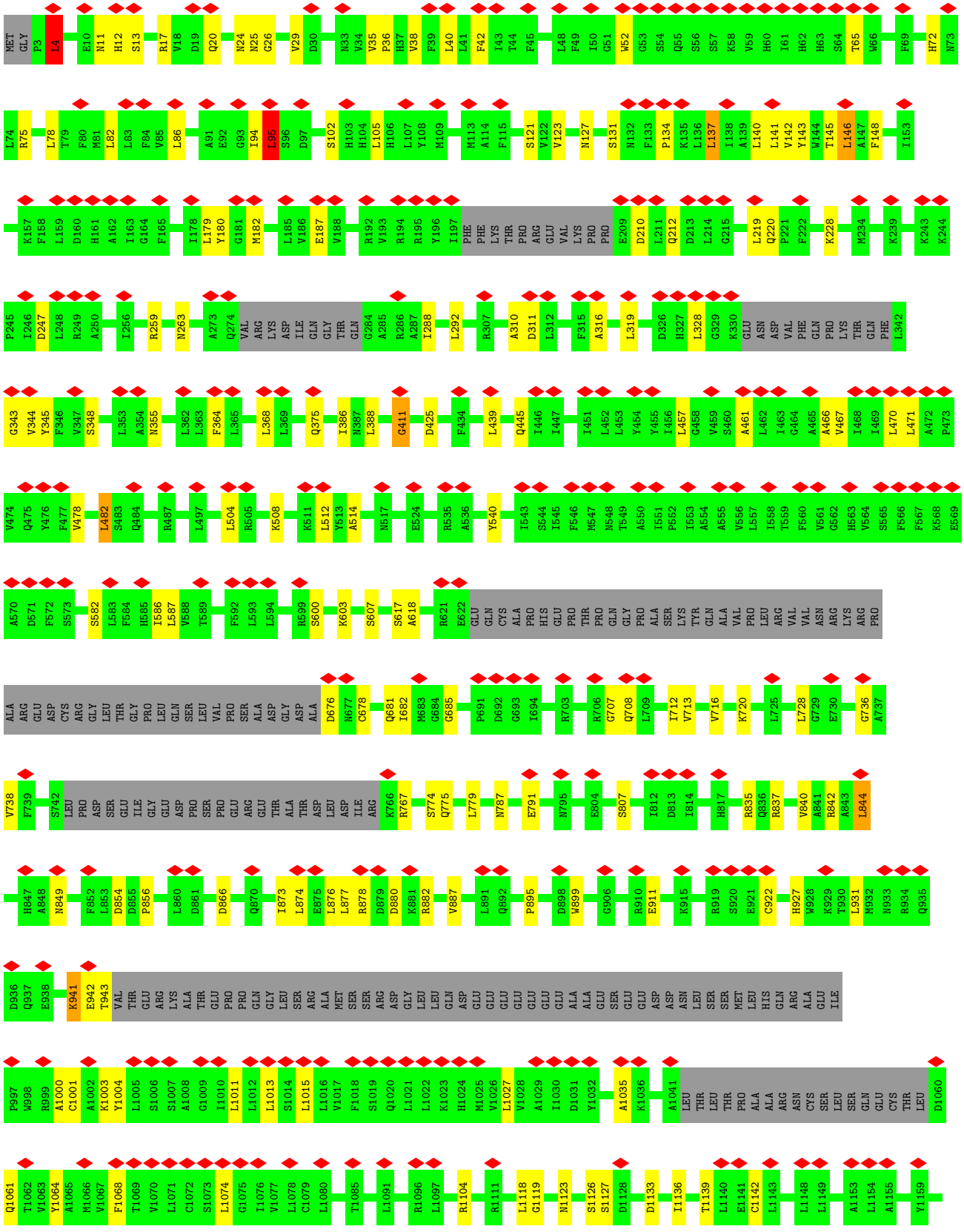
Chain D:

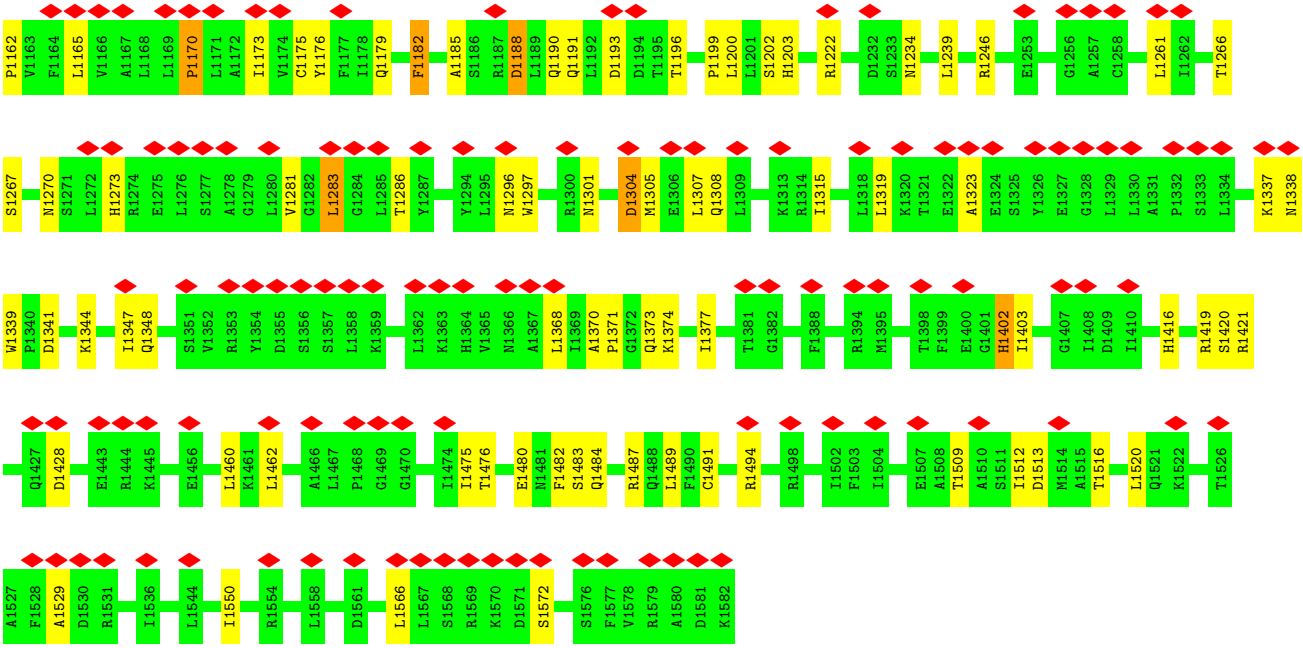


• Molecule 2: ATP-binding cassette sub-family C member 8

Chain E:


26%
73%
15%
11%


MET GLY P3 L4 E10 N11 H12 S13 R17 V18 D19 Q20 N24 N25 G26 V29 D30 N33 V34 V35 P36 H37 V38 F39 L40 L41 F42 I43 T44 F45 L48 F49 I50 G51 W52 G53 S54 Q55 S56 S57 K58 V59 H60 I61 H62 H63 S64 T65 W66 F69 H72 W73
L74 R75 L78 T79 F80 M81 L82 L83 F84 V85 L86 A91 E92 G93 I94 L95 S96 D97 S102 H103 H104 L105 H106 L107 Y108 M109 M113 A114 F115 S121 V122 V123 N127 S131 N132 F133 P134 K135 L136 L137 I138 A139 L140 L141 V142 Y143 W144 T145 L146 A147 F148 I153
K157 F158 L159 D160 H161 A162 I163 G164 F165 I178 L179 Y180 G181 M182 L185 V186 E187 V188 R192 V193 R194 R195 Y196 I197 PHE PHE LYS THR PRO ARG GLU VAL LYS PRO PRO E209 D210 L211 Q212 D213 L214 G215 L219 Q220 P221 F222 K228 M234 K239 K243 K244
P245 I246 D247 L248 R249 A250 I256 R259 N263 A273 Q274 VAL ARG LYS ASP ILE GLN GLY THR GLN G284 A285 R286 A287 I288 L292 R307 A310 D311 L312 F315 A316 L319 D326 H327 L328 G329 K330 GLU ASN ASP VAL PHE GLN PRO LYS THR GLN PHE L342
G343 V344 Y345 F346 V347 S348 L353 A354 N355 L362 L363 F364 L365 L368 L369 Q375 I386 N387 L388 G411 D425 F434 L439 Q445 I446 I447 T451 L452 L453 Y454 Y455 I456 L457 G458 V459 S460 A461 L462 I463 G464 A465 A466 V467 I468 I469 L470 L471 A472 P473
V474 Q475 Y476 F477 V478 L482 S483 Q484 R487 L497 L504 R505 K508 K511 L512 Y513 A514 N517 E524 R535 A536 Y540 I543 S544 I545 F546 M547 N548 T549 A550 I551 P552 I553 A554 A555 V556 L557 I558 T559 F560 V561 G562 H563 V564 S565 F566 F567 K568 E569
A570 D571 F572 S573 S582 L583 F584 H585 I586 L587 V588 T589 F592 L593 L594 R599 S600 K603 S607 S617 A618 R621 E622 GLU GLN CYS ALA PRO HIS GLU PRO THR PRO GLN GLY PRO ALA SER LYS TYR GLN ALA VAL PRO LEU ARG VAL VAL ASN ARG LYS ARG PRO
ALA ARG GLU ASP CYS ARG GLY LEU THR GLY PRO LEU GLN SER LEU VAL PRO SER ALA ASP GLY ASP ALA D676 N677 C678 Q681 I682 M683 G684 G685 P691 D692 G693 I694 R703 R706 G707 Q708 L709 I712 V713 V716 K720 L725 L728 G729 E730 G736 A737
V738 F739 S742 LEU PRO ASP SER GLU ILE GLY GLU ASP PRO SER PRO GLU ARG GLU THR ALA THR ASP LEU ASP ILE ARG K766 R767 S774 Q775 L779 N787 E791 N795 E804 S807 I812 D813 I814 H817 R835 Q836 R837 V840 A841 R842 A843 L844
H847 A848 N849 F852 L853 D854 D855 P856 L860 D861 D866 Q870 I873 L874 E875 L876 L877 R878 D879 D880 K881 R882 V887 L891 Q892 P895 D898 W899 G906 R910 E911 K915 R919 S920 E921 C922 H927 W928 K929 T930 L931 M932 N933 R934 Q935
D936 Q937 E938 K941 E942 T943 VAL THR GLU ARG LYS ALA THR GLU PRO PRO GLN GLY LEU SER ARG ALA MET SER SER ARG ASP GLY LEU LEU GLN ASP GLU GLU GLU GLU GLU GLU GLU ALA ALA GLU SER GLU GLU ASP ASP ASN LEU SER SER MET LEU HIS GLN ARG ALA GLU ILE
P997 W998 R999 A1000 C1001 A1002 K1003 Y1004 L1005 S1006 S1007 A1008 G1009 I1010 L1011 L1012 L1013 S1014 L1015 L1016 V1017 F1018 S1019 Q1020 L1021 L1022 K1023 H1024 M1025 V1026 L1027 V1028 A1029 I1030 D1031 Y1032 A1035 K1036 A1041 LEU THR LEU THR PRO ALA ALA ARG ASN CYS SER LEU SER GLN GLU CYS THR LEU D1060
Q1061 T1062 V1063 Y1064 A1065 M1066 V1067 F1068 T1069 V1070 L1071 C1072 S1073 L1074 G1075 I1076 V1077 L1078 C1079 L1080 T1085 L1091 R1096 L1097 R1104 R1111 L1118 G1119 N1123 S1126 S1127 D1128 D1133 I1136 T1139 L1140 E1141 C1142 L1143 L1148 L1149 A1153 L1154 A1155 Y1159


P1162 V1163 F1164 L1165 V1166 A1167 L1168 L1169 P1170 L1171 A1172 I1173 V1174 C1175 Y1176 F1177 I1178 Q1179 F1182 A1185 S1186 R1187 D1188 L1189 Q1190 Q1191 L1192 D1193 D1194 T1195 T1196 P1199 L1200 L1201 S1202 H1203 R1222 D1232 S1233 N1234 L1239 R1246 E1253 G1256 A1257 C1258 L1261 I1262 T1266
S1267 N1270 S1271 L1272 H1273 R1274 E1275 L1276 S1277 A1278 G1279 L1280 V1281 G1282 L1283 G1284 L1285 T1286 Y1287 Y1294 L1295 N1296 W1297 R1300 N1301 D1304 M1305 E1306 L1307 Q1308 L1309 K1313 R1314 I1315 L1318 L1319 K1320 T1321 E1322 A1323 E1324 S1325 Y1326 E1327 G1328 L1329 L1330 A1331 P1332 S1333 L1334 K1337 N1338
W1339 P1340 D1341 K1344 I1347 Q1348 S1351 V1352 R1353 Y1354 D1355 S1356 S1357 L1358 K1359 L1362 K1363 H1364 V1365 N1366 A1367 L1368 I1369 A1370 P1371 G1372 Q1373 K1374 I1377 T1381 G1382 F1388 R1394 M1395 T1398 F1399 E1400 G1401 H1402 I1403 G1407 I1408 D1409 I1410 H1416 R1419 S1420 R1421
Q1427 D1428 E1443 R1444 K1445 E1456 L1460 K1461 L1462 A1466 L1467 P1468 G1469 G1470 I1474 I1475 T1476 E1480 N1481 F1482 S1483 Q1484 R1487 Q1488 L1489 F1490 C1491 R1494 R1498 I1502 F1503 I1504 E1507 A1508 T1509 A1510 S1511 I1512 D1513 M1514 A1515 T1516 L1520 Q1521 K1522 T1526
A1527 F1528 A1529 D1530 R1531 I1536 L1544 I1550 R1554 L1558 D1561 L1566 L1567 S1568 R1569 K1570 D1571 S1572 S1576 F1577 V1578 R1579 A1580 D1581 K1582

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24689	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 ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.090	Depositor
Minimum map value	-0.791	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	473.19998, 473.19998, 473.19998	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.50	0/2576	0.76	0/3502
1	B	0.50	0/2576	0.76	0/3502
1	C	0.50	0/2576	0.76	0/3502
1	D	0.50	0/2576	0.76	0/3502
2	E	0.50	1/11201 (0.0%)	0.83	28/15205 (0.2%)
All	All	0.50	1/21505 (0.0%)	0.80	28/29213 (0.1%)

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
2	E	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1136	ILE	C-N	6.05	1.45	1.34

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	311	ASP	CB-CG-OD1	11.02	128.22	118.30
2	E	874	LEU	CA-CB-CG	8.97	135.94	115.30
2	E	844	LEU	CA-CB-CG	8.74	135.40	115.30
2	E	95	LEU	CA-CB-CG	8.50	134.84	115.30
2	E	179	LEU	CA-CB-CG	7.99	133.67	115.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	102	SER	Peptide
2	E	131	SER	Peptide
2	E	137	LEU	Peptide
2	E	4	LEU	Peptide
2	E	95	LEU	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	2519	0	2549	32	0
1	B	2519	0	2549	35	0
1	C	2519	0	2549	31	0
1	D	2519	0	2549	31	0
2	E	10970	0	11215	124	0
3	E	27	0	12	0	0
4	E	2	0	0	0	0
5	E	31	0	12	1	0
All	All	21106	0	21435	246	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 6.

The worst 5 of 246 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:E:942:GLU:OE1	2:E:942:GLU:HA	1.73	0.88
2:E:466:ALA:O	2:E:470:LEU:HB2	1.79	0.83
1:C:61:THR:O	1:C:65:ASP:HB2	1.81	0.81
1:B:61:THR:O	1:B:65:ASP:HB2	1.81	0.81
1:A:61:THR:O	1:A:65:ASP:HB2	1.81	0.80

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	319/390 (82%)	306 (96%)	13 (4%)	0	100 100
1	B	319/390 (82%)	306 (96%)	13 (4%)	0	100 100
1	C	319/390 (82%)	306 (96%)	13 (4%)	0	100 100
1	D	319/390 (82%)	306 (96%)	13 (4%)	0	100 100
2	E	1386/1582 (88%)	1296 (94%)	88 (6%)	2 (0%)	51 84
All	All	2662/3142 (85%)	2520 (95%)	140 (5%)	2 (0%)	54 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	344	VAL
2	E	345	TYR

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	278/337 (82%)	245 (88%)	33 (12%)	5 25
1	B	278/337 (82%)	245 (88%)	33 (12%)	5 25
1	C	278/337 (82%)	245 (88%)	33 (12%)	5 25
1	D	278/337 (82%)	245 (88%)	33 (12%)	5 25
2	E	1181/1368 (86%)	1175 (100%)	6 (0%)	88 93
All	All	2293/2716 (84%)	2155 (94%)	138 (6%)	23 49

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	182	ILE
1	D	236	VAL
1	D	339	VAL
1	B	180	THR
1	B	166	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	375	GLN
2	E	1301	ASN
2	E	486	GLN
2	E	1486	GLN
2	E	787	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\|>2$
5	ATP	E	1604	4	26,33,33	0.93	1 (3%)	31,52,52	1.55	5 (16%)
3	ADP	E	1601	4	24,29,29	0.95	1 (4%)	29,45,45	1.44	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	E	1604	4	-	7/18/38/38	0/3/3/3
3	ADP	E	1601	4	-	4/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1601	ADP	C5-C4	2.30	1.47	1.40
5	E	1604	ATP	C5-C4	2.08	1.46	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1604	ATP	N3-C2-N1	-4.02	122.40	128.68
3	E	1601	ADP	N3-C2-N1	-3.88	122.62	128.68
5	E	1604	ATP	PB-O3B-PG	-3.14	122.05	132.83
3	E	1601	ADP	C3'-C2'-C1'	3.13	105.70	100.98
5	E	1604	ATP	C3'-C2'-C1'	2.84	105.25	100.98

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1604	ATP	C5'-O5'-PA-O1A
5	E	1604	ATP	C5'-O5'-PA-O2A
3	E	1601	ADP	PB-O3A-PA-O1A
5	E	1604	ATP	O4'-C4'-C5'-O5'
5	E	1604	ATP	C3'-C4'-C5'-O5'

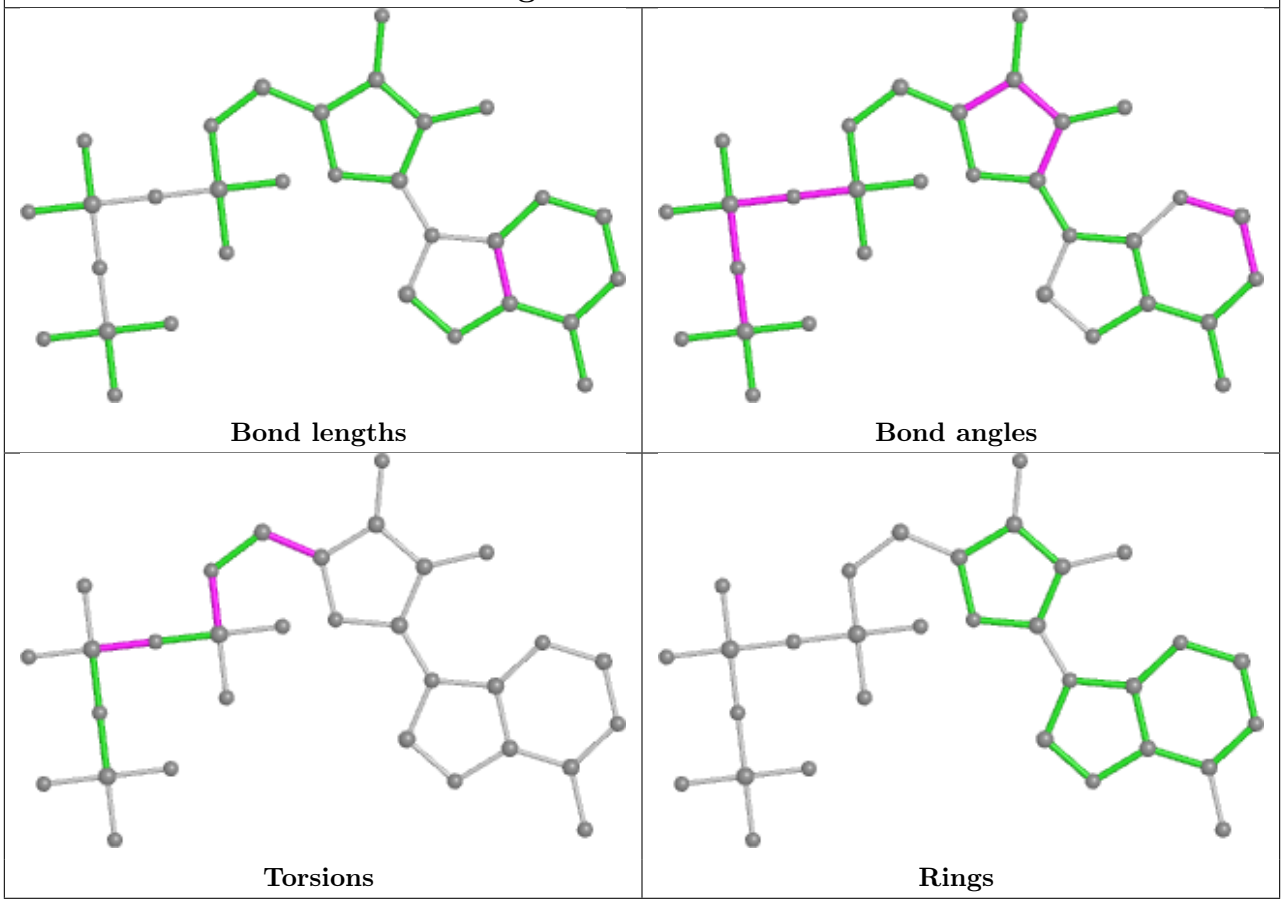
There are no ring outliers.

1 monomer is involved in 1 short contact:

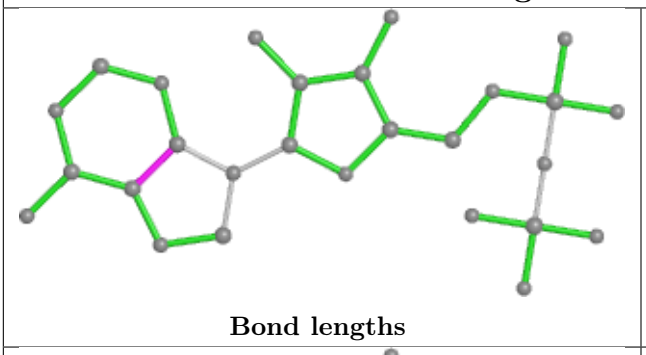
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1604	ATP	1	0

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.

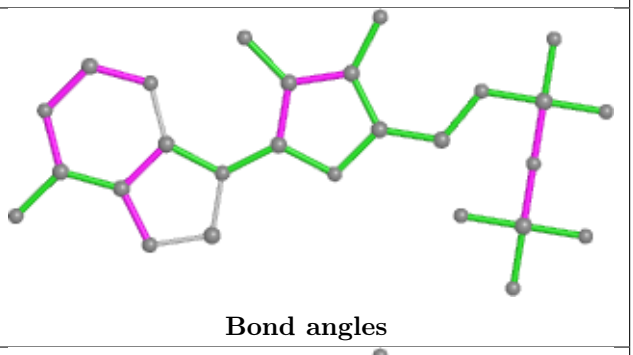
Ligand ATP E 1604



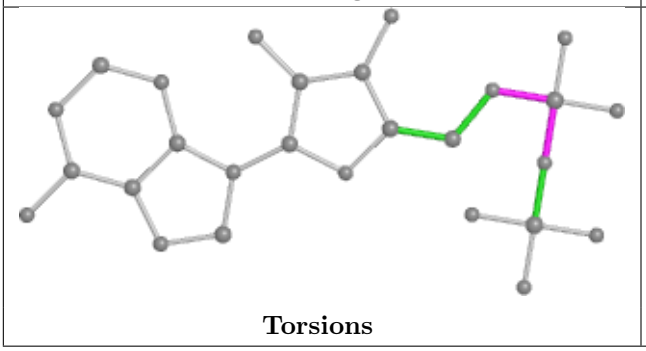
Ligand ADP E 1601



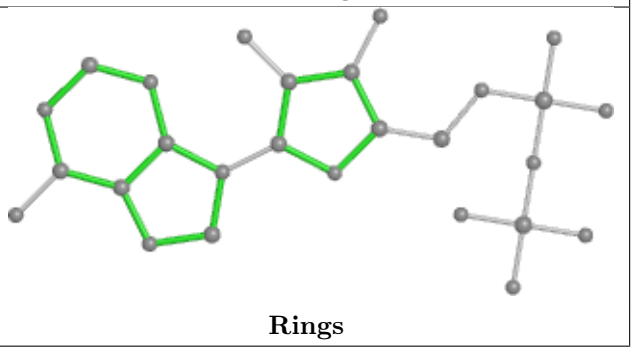
Bond lengths



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.

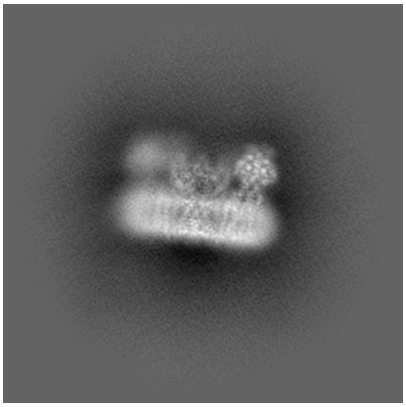
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24843. These allow visual inspection of the internal detail of the map and identification of artifacts.

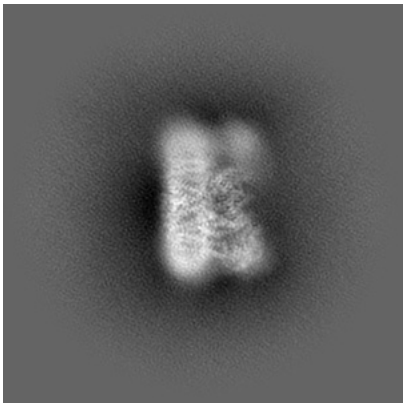
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

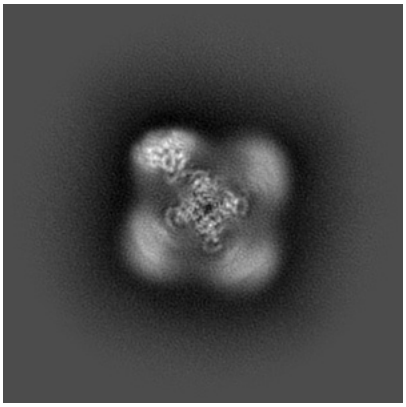
6.1.1 Primary map



X



Y

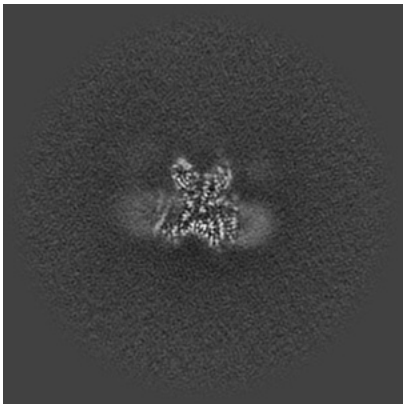


Z

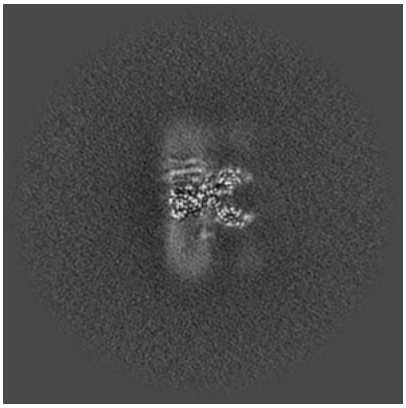
The images above show the map projected in three orthogonal directions.

6.2 Central slices

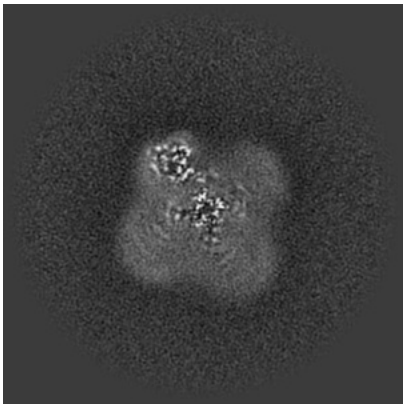
6.2.1 Primary map



X Index: 182



Y Index: 182



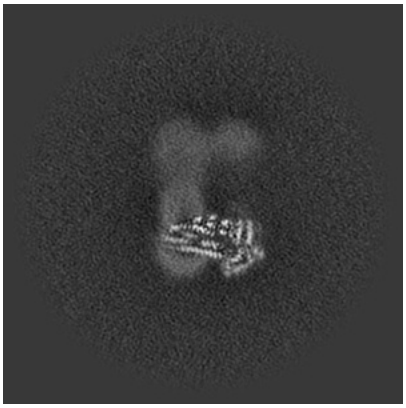
Z Index: 182

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

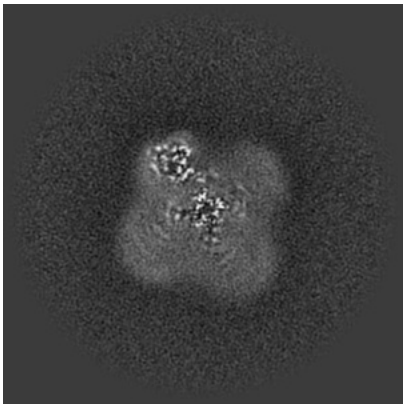
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 163



Y Index: 224

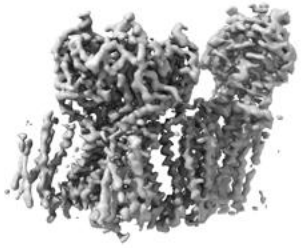


Z Index: 182

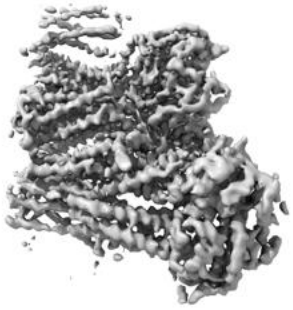
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

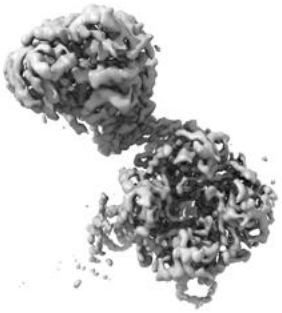
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

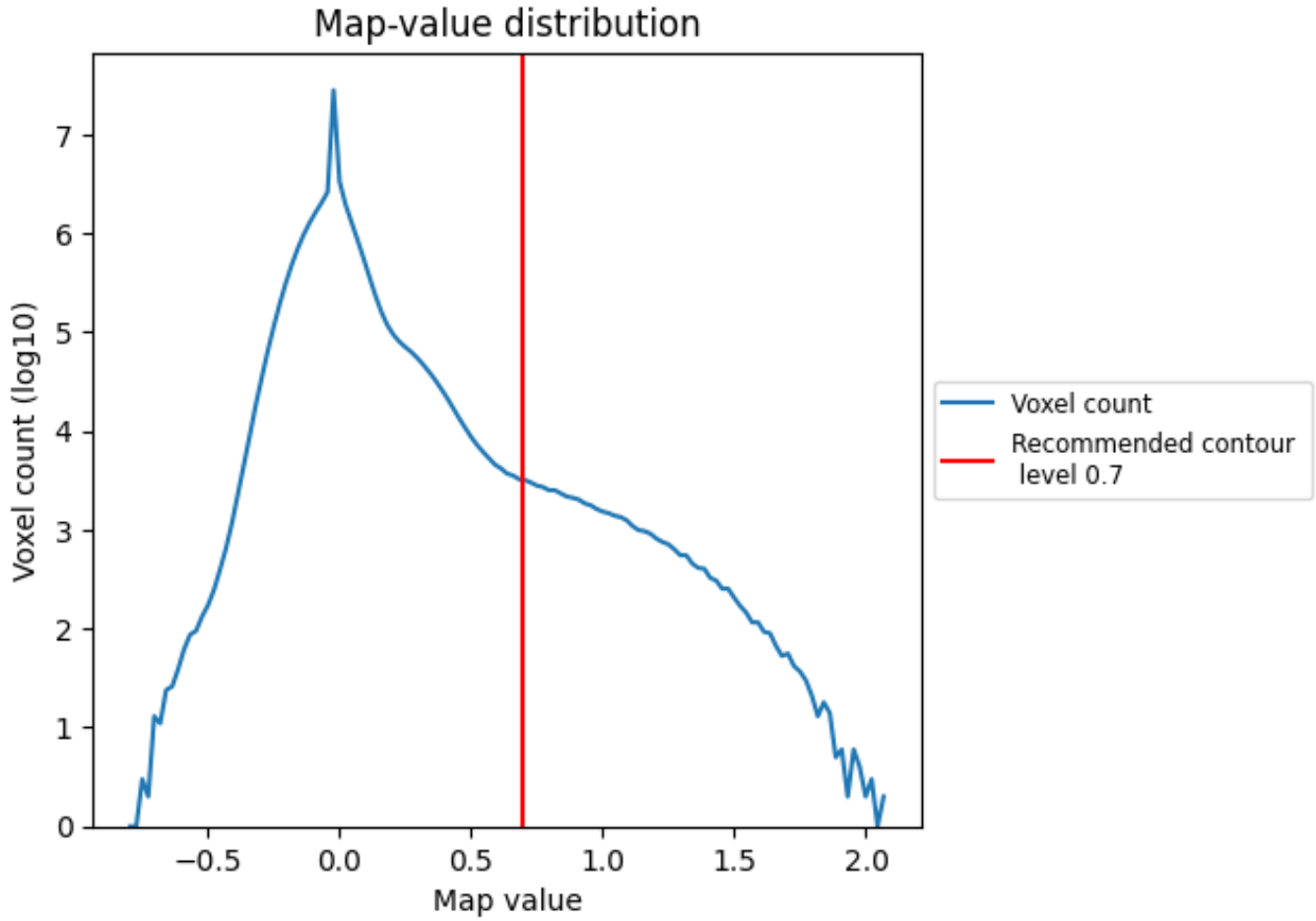
6.5 Mask visualisation (i)

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

7 Map analysis

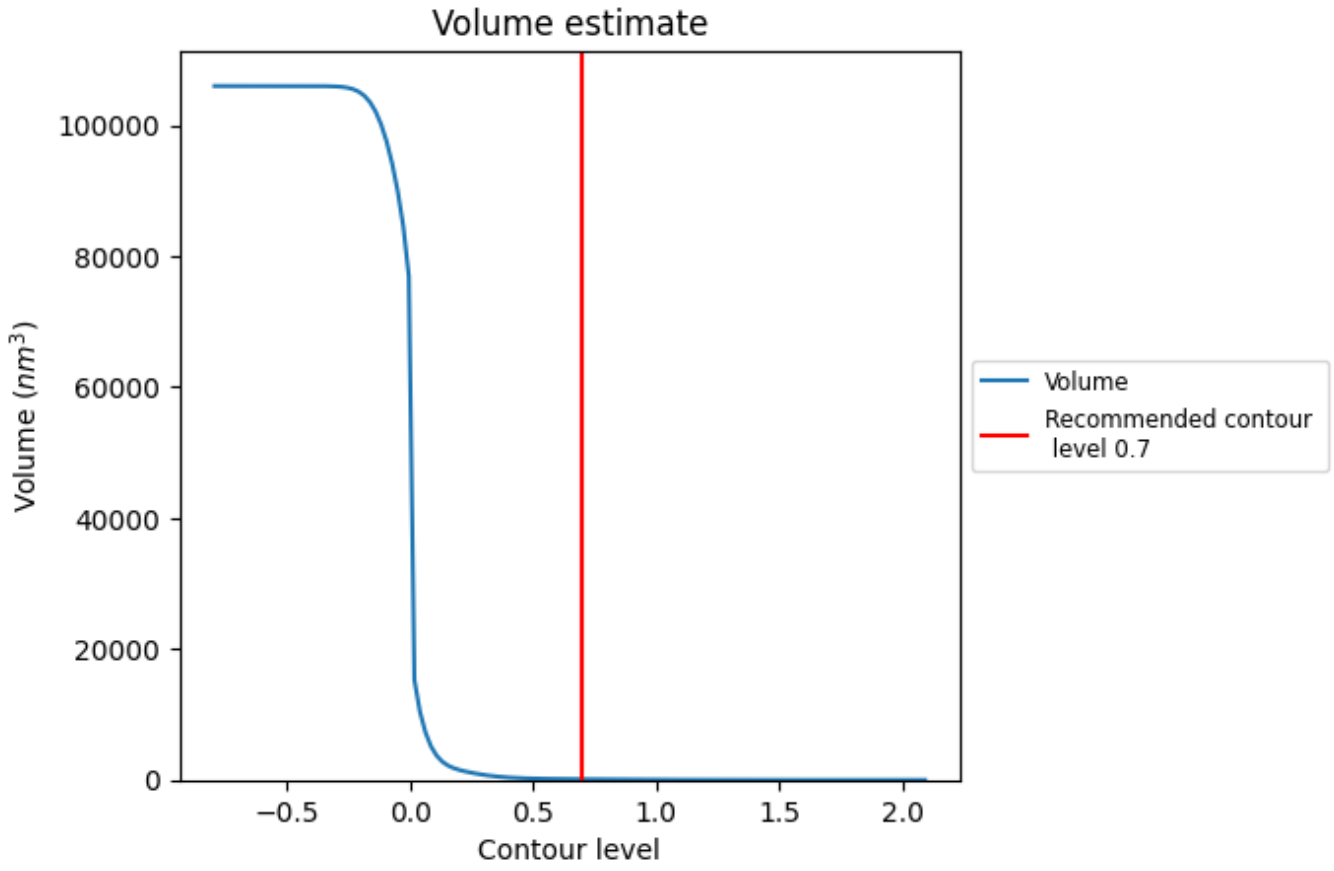
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

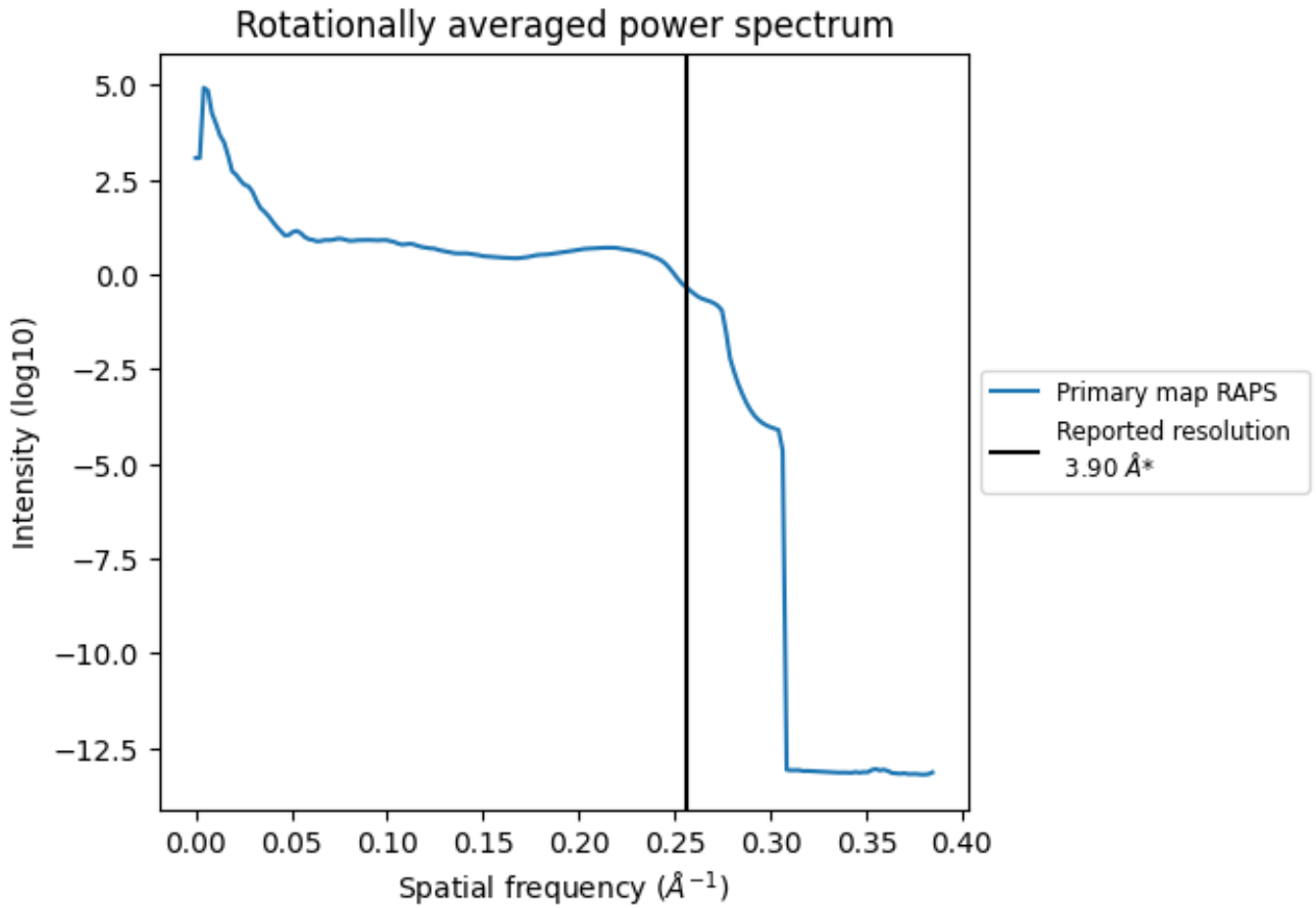
7.2 Volume estimate (i)



The volume at the recommended contour level is 110 nm^3; this corresponds to an approximate mass of 100 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)

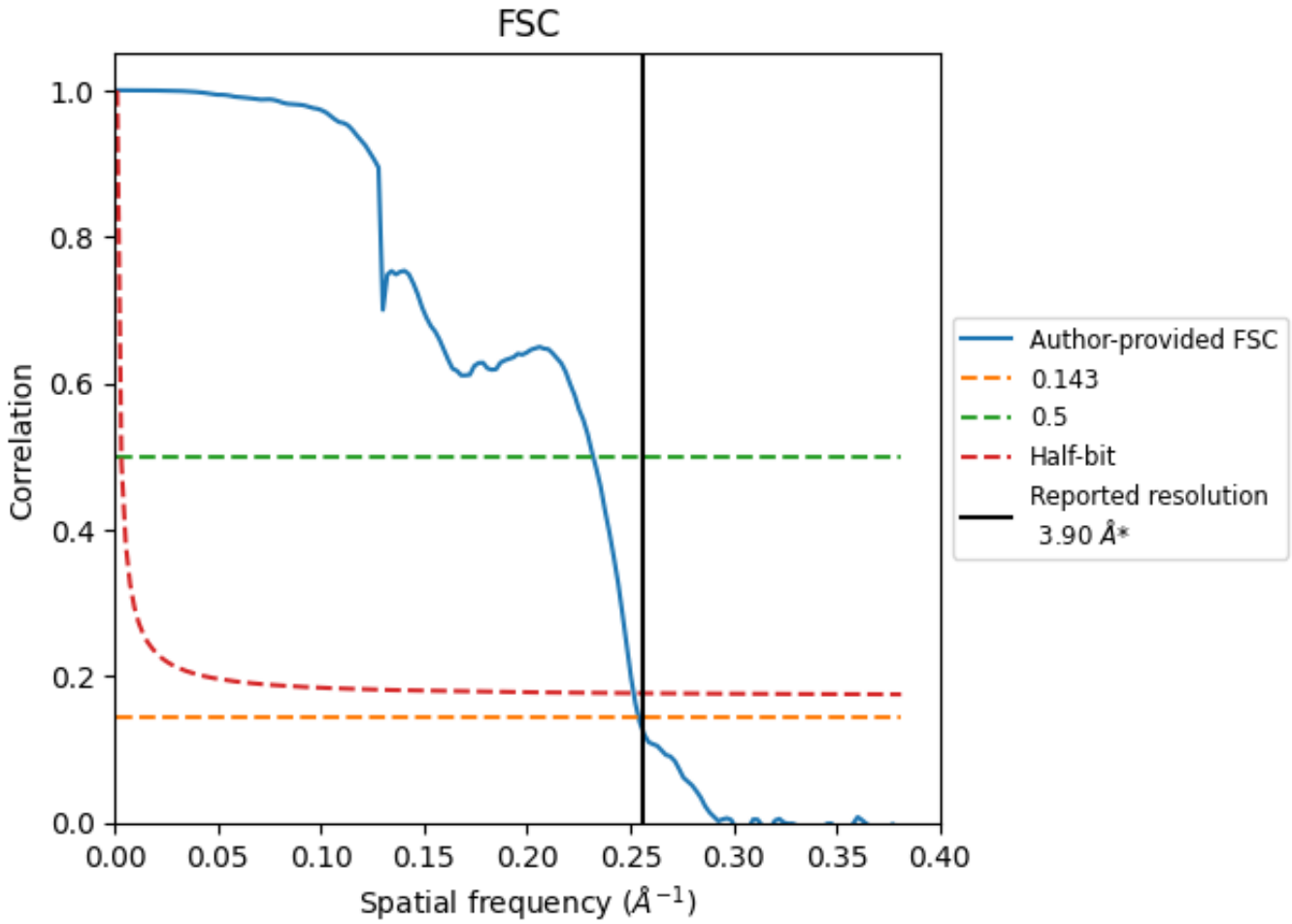


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

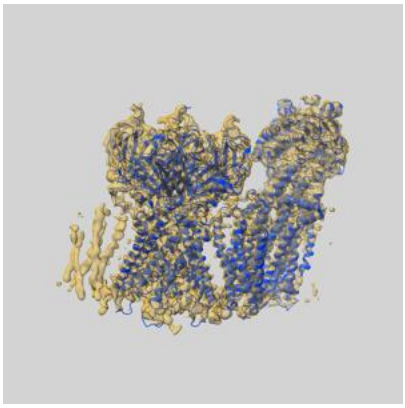
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.94	4.31	3.97
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

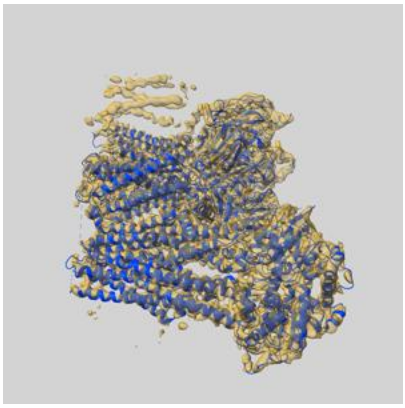
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24843 and PDB model 7S5Y. Per-residue inclusion information can be found in section 3 on page 6.

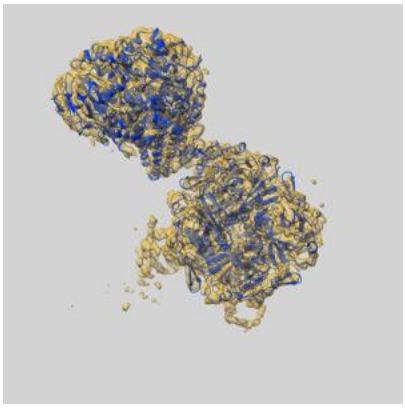
9.1 Map-model overlay



X



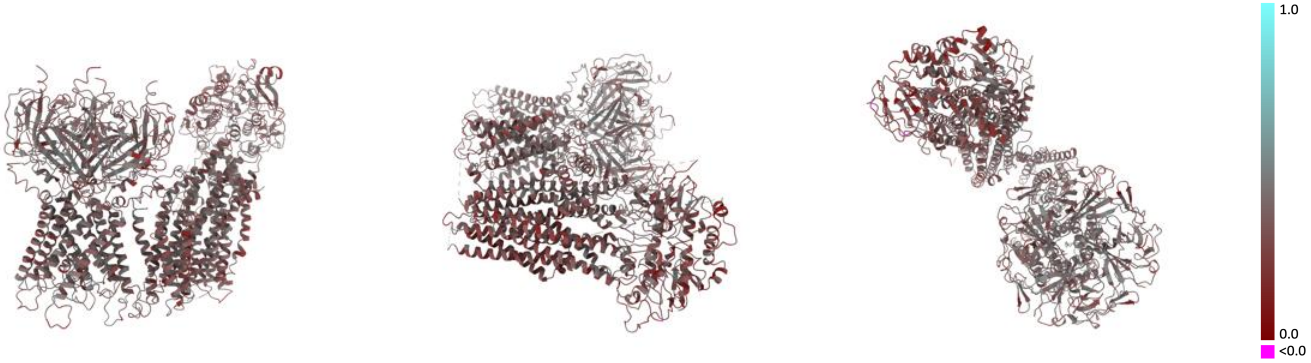
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

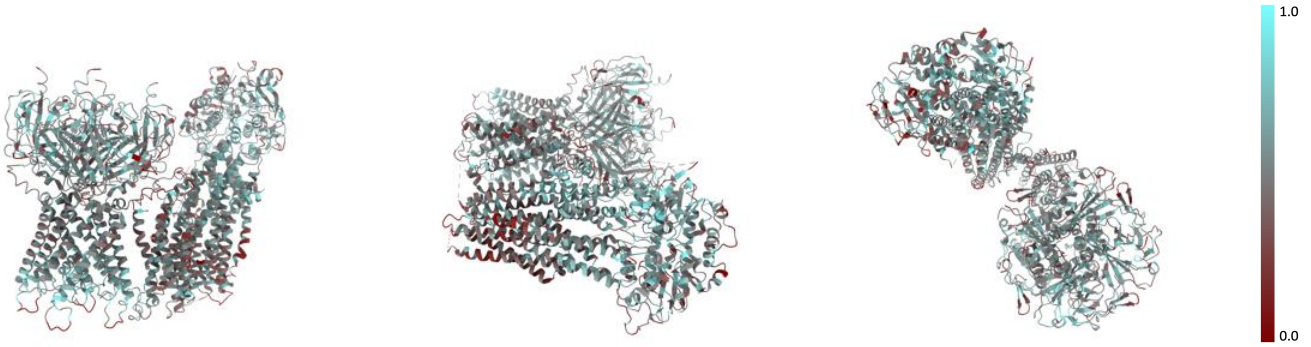
9.2 Q-score mapped to coordinate model (i)



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.

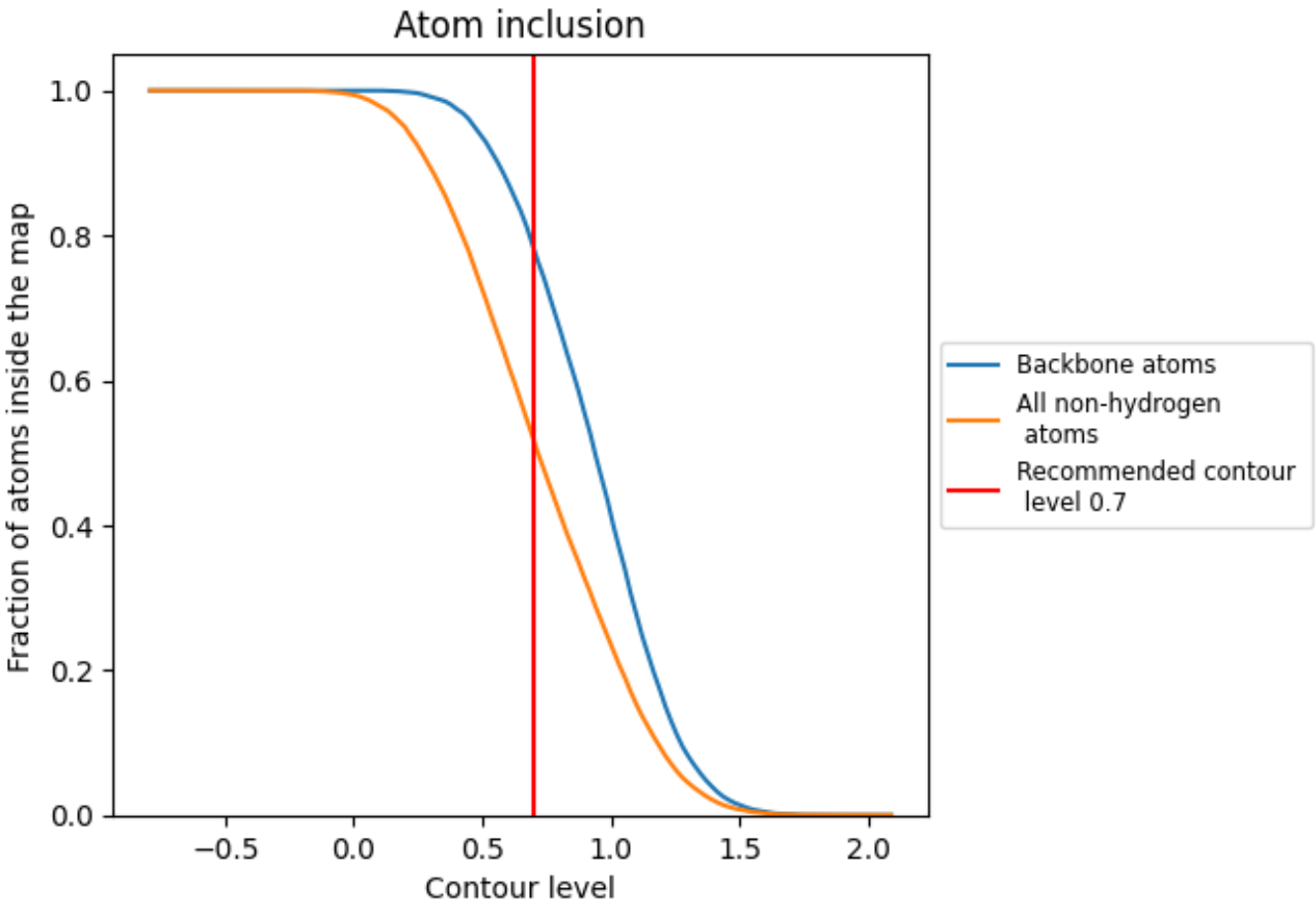
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 52% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5169	0.3590
A	0.5446	0.3960
B	0.5305	0.3810
C	0.5228	0.3880
D	0.5349	0.3780
E	0.5019	0.3340