Full wwPDB EM Validation Report (i)

Nov 13, 2022 – 06:11 AM EST

PDB ID	:	6WJV
EMDB ID	:	EMD-21701
Title	:	Structure of the Saccharomyces cerevisiae polymerase epsilon holoenzyme
Authors	:	Yuan, Z.; Georgescu, R.; Schauer, G.D.; O'Donnell, M.; Li, H.
Deposited on	:	2020-04-14
Resolution	:	3.50 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 (i) symbol.

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

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

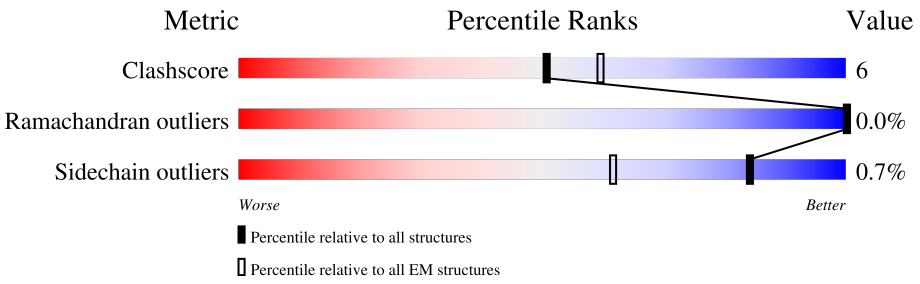
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.50 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	2222	55% 77% 10% 12%
2	2	689	50% 52% 9% 38%
3	3	201	15% 40% • 58%
4	4	196	23% 49% 6% 45%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19593 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 DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1951	14886	9527	2476	2813	70	0	0

- Molecule 2 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	424	3225	2055	545	610	15	0	0

- Molecule 3 is a protein called DNA polymerase epsilon subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	85	652	417	107	126	2	0	0

- Molecule 4 is a protein called DNA polymerase epsilon subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	107	829	521	146	161	1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

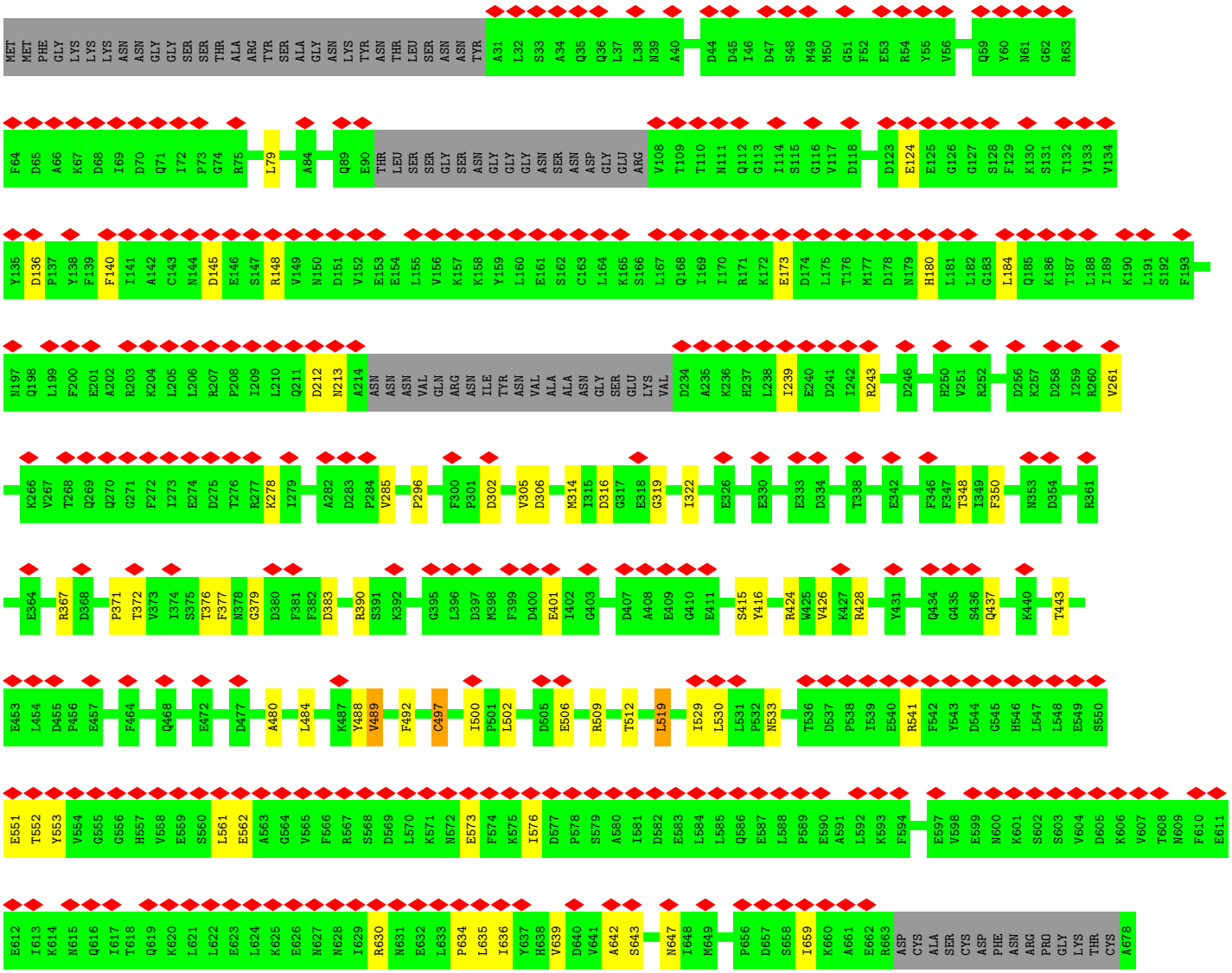
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	1	1	0

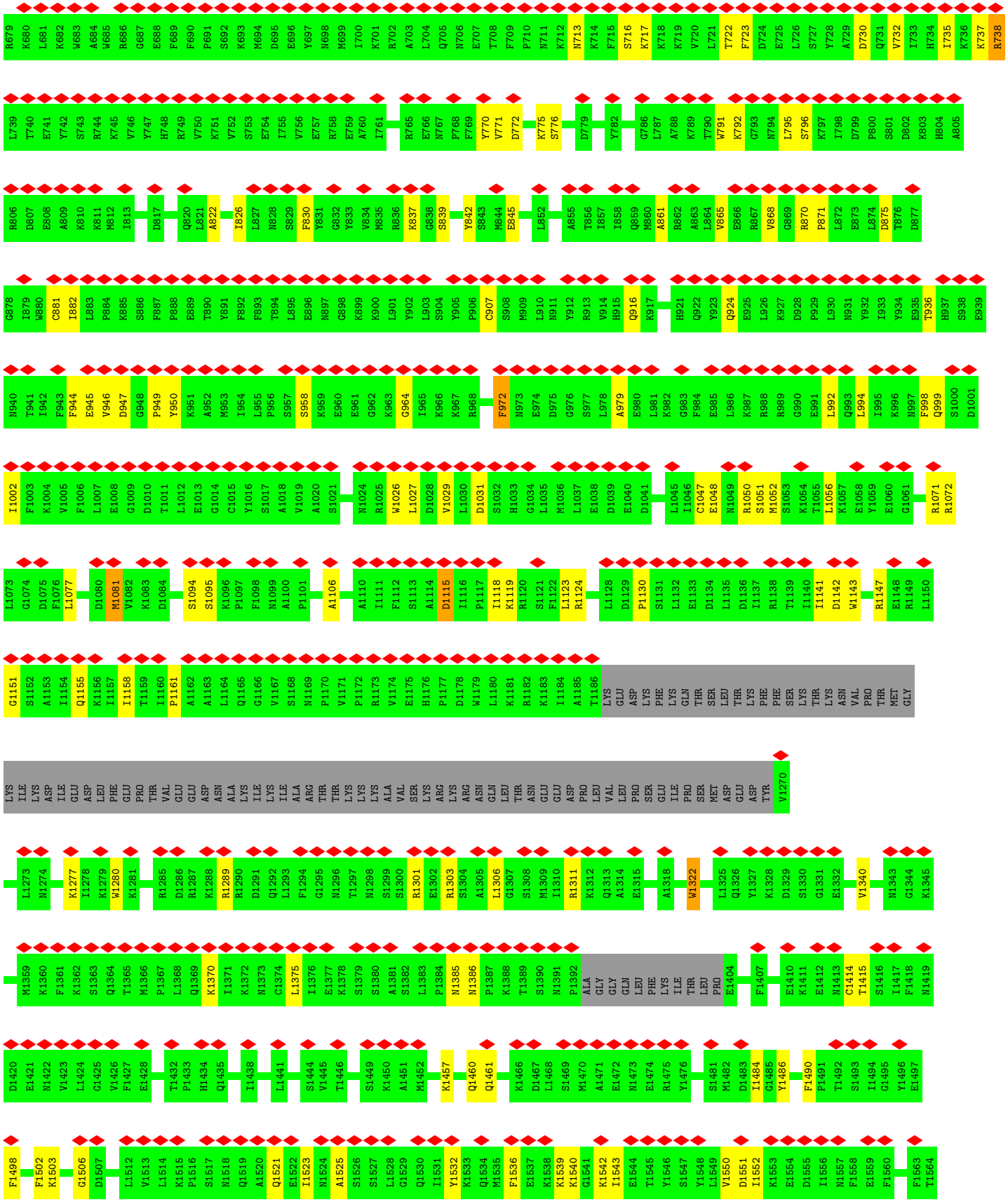
3 Residue-property plots (i)

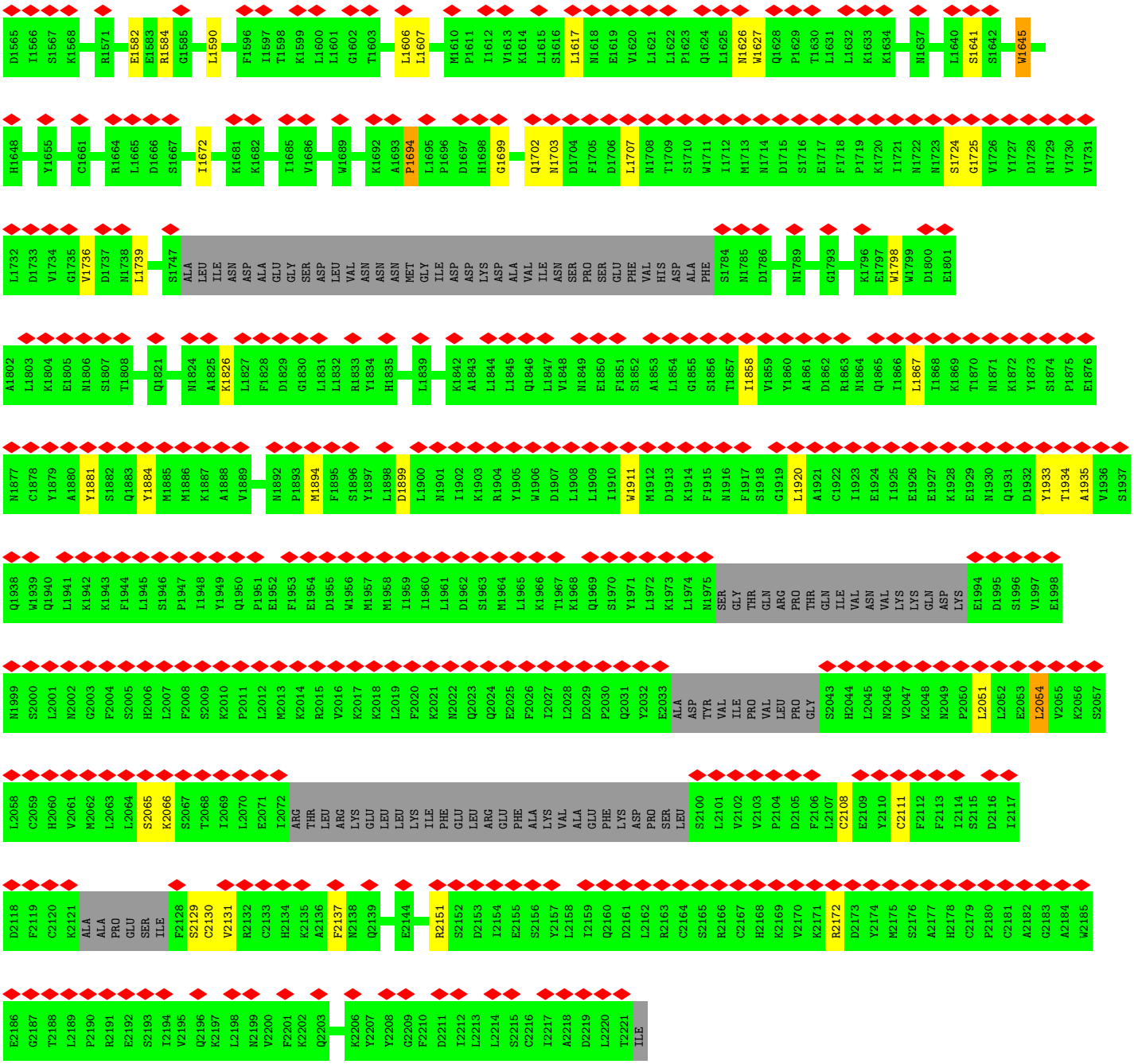
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA polymerase epsilon catalytic subunit A

Chain A:

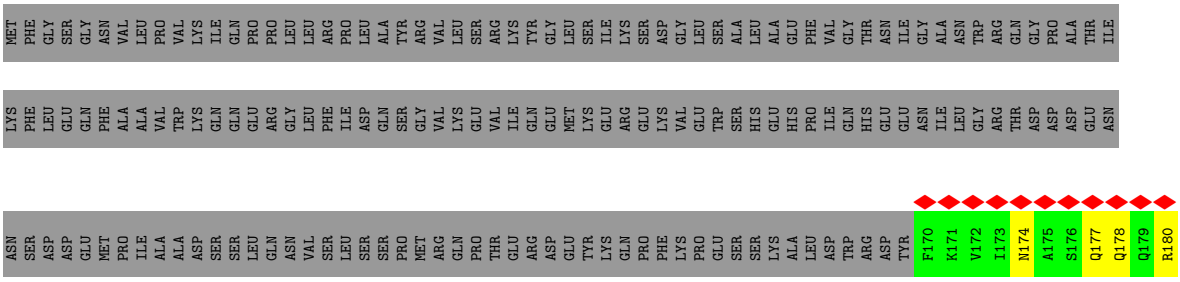



R679 K680 L681 K682 W683 A684 W685 R686 G687 E688 F689 F690 P691 S692 K693 M694 D695 E696 Y697 N698 M699 I700 K701 R702 A703 L704 Q705 N706 E707 T708 F709 P710 N711 K712 N713 K714 F715 S716 K717 K718 K719 V720 L721 T722 F723 D724 E725 L726 S727 Y728 A729 D730 Q731 V732 I733 H734 I735 K736 K737 R738
L739 T740 E741 Y742 S743 R744 K745 V746 Y747 H748 R749 V750 K751 V752 S753 E754 I755 V756 E757 R758 E759 A760 I761 R765 E766 N767 P768 F769 Y770 V771 D772 K775 S776 D779 Y782 G786 L787 A788 K789 T790 W791 K792 G793 N794 L795 S796 K797 I798 D799 P800 S801 D802 K803 H804 A805
R806 D807 E808 A809 K810 K811 M812 I813 D817 Q820 L821 A822 I826 L827 N828 S829 F830 Y831 G832 Y833 V834 M835 R836 K837 G838 S839 Y842 S843 M844 E845 L852 A855 T856 I857 I858 Q859 M860 A861 R862 A863 L864 V865 E866 R867 V868 G869 R870 P871 L872 E873 L874 D875 T876 D877
G878 I879 W880 C881 I882 L883 P884 K885 S886 F887 P888 E889 T890 Y891 F892 F893 T894 L895 E896 N897 G898 K899 K900 L901 Y902 L903 S904 Y905 P906 C907 S908 M909 L910 N911 Y912 R913 V914 H915 Q916 K917 H921 Q922 Y923 Q924 E925 L926 K927 D928 P929 L930 N931 Y932 I933 Y934 E935 T936 H937 S938 E939
N940 T941 I942 F943 F944 E945 V946 D947 G948 P949 Y950 K951 A952 M953 I954 L955 P956 S957 S958 K959 E960 E961 G962 K963 G964 I965 K966 K967 R968 F972 N973 E974 D975 G976 S977 L978 A979 E980 L981 K982 G983 F984 E985 L986 K987 R988 R989 G990 E991 L992 Q993 L994 I995 K996 N997 F998 Q999 S1000 D1001
I1002 F1003 K1004 V1005 F1006 L1007 E1008 G1009 D1010 T1011 L1012 E1013 G1014 C1015 Y1016 S1017 A1018 V1019 A1020 S1021 N1024 R1025 W1026 L1027 D1028 V1029 L1030 D1031 S1032 H1033 G1034 L1035 M1036 L1037 E1038 D1039 E1040 D1041 L1045 I1046 C1047 E1048 N1049 R1050 S1051 M1052 S1053 K1054 T1055 L1056 K1057 E1058 Y1059 E1060 G1061 R1071 R1072
L1073 G1074 D1075 F1076 L1077 D1080 M1081 V1082 K1083 D1084 S1094 S1095 K1096 P1097 F1098 N1099 A1100 P1101 A1106 A1110 I1111 F1112 S1113 A1114 D1115 I1116 P1117 I1118 K1119 R1120 S1121 F1122 L1123 R1124 L1128 D1129 P1130 S1131 L1132 E1133 D1134 L1135 D1136 I1137 R1138 T1139 I1140 I1141 D1142 W1143 R1147 E1148 R1149 L1150
G1151 S1152 A1153 I1154 Q1155 K1156 I1157 I1158 T1159 I1160 P1161 A1162 A1163 L1164 Q1165 G1166 V1167 S1168 N1169 P1170 V1171 P1172 R1173 V1174 E1175 H1176 P1177 D1178 W1179 L1180 K1181 R1182 K1183 I1184 A1185 T1186 LYS GLU ASP LYS PHE LYS GLN THR SER LEU THR LYS PHE PHE SER LYS THR LYS ASN VAL PRO THR MET GLY
LYS ILE LYS ASP ILE GLU ASP LEU PHE GLU PRO THR VAL GLU GLU ASP ASN ALA LYS ILE LYS ILE ALA ARG THR THR LYS LYS LYS ALA VAL SER LYS ARG LYS ARG ASN GLN LEU THR ASN GLU GLU ASP PRO LEU VAL LEU PRO SER GLU ILE PRO SER MET ASP GLU ASP TYR V1270
L1273 N1274 K1277 I1278 K1279 W1280 K1281 R1285 D1286 R1287 K1288 R1289 R1290 D1291 Q1292 L1293 F1294 G1295 N1296 T1297 N1298 S1299 S1300 R1301 E1302 R1303 S1304 A1305 L1306 G1307 S1308 M1309 I1310 R1311 K1312 Q1313 A1314 E1315 A1318 W1322 L1325 Q1326 Y1327 K1328 D1329 S1330 G1331 E1332 V1340 N1343 G1344 K1345
M1359 K1360 F1361 K1362 S1363 Q1364 T1365 M1366 P1367 L1368 Q1369 K1370 I1371 K1372 N1373 C1374 L1375 I1376 E1377 K1378 S1379 S1380 A1381 S1382 L1383 P1384 N1385 N1386 P1387 K1388 T1389 S1390 N1391 P1392 ALA GLY GLY GLN LEU PHE LYS ILE THR LEU PRO E1404 F1407 E1410 K1411 E1412 N1413 C1414 T1415 S1416 I1417 F1418 N1419
D1420 E1421 N1422 V1423 L1424 G1425 V1426 F1427 E1428 T1432 P1433 H1434 Q1435 I1438 L1441 S1444 V1445 T1446 S1449 K1450 A1451 M1452 K1457 Q1460 Q1461 K1466 D1467 L1468 S1469 M1470 A1471 E1472 N1473 E1474 R1475 Y1476 S1481 M1482 D1483 I1484 G1485 Y1486 F1490 P1491 T1492 S1493 I1494 G1495 Y1496 E1497
F1498 F1502 K1503 G1506 D1507 L1512 V1513 L1514 K1515 P1516 S1517 N1518 Q1519 A1520 Q1521 E1522 I1523 N1524 A1525 S1526 S1527 L1528 G1529 Q1530 I1531 Y1532 K1533 Q1534 M1535 F1536 E1537 K1538 K1539 K1540 G1541 K1542 I1543 E1544 T1545 Y1546 S1547 Y1548 L1549 V1550 D1551 I1552 K1553 E1554 D1555 I1556 N1557 F1558 E1559 F1560 F1563 T1564



- Molecule 2: DNA polymerase epsilon subunit B

Chain 2:



F181 S182 Y183 N184 P185 H186 K187 M188 Q189 F190 I191 F192 V193 P194 ASN LYS LYS GLN ASN GLY LEU GLY GLY ILE ALA GLY F207 L208 P209 D210 I211 E212 D213 K214 V215 Q216 M217 F218 L219 T220 R221 Y222 Y223 L224 T225 N226 D227 R228 V229 M230 R231 N232 E233 ASN PHE GLN ASN SER ASP MET

PHE ASN PRO LEU SER SER MET VAL SER LEU GLN ASN GLU LEU SER ASN THR ASN ARG GLN GLN GLN SER SER SER M266 S267 I268 T269 P270 I271 K272 N273 L274 L275 G276 R277 D278 A279 Q280 N281 F282 L283 L284 L285 G286 L287 L288 N289 K290 N291 F292 K293 G294 N295 W296 S297 L298 L299 E300

P301 S302 G303 S304 V305 E306 I307 D308 I309 S310 Q311 T312 I313 P314 T315 Q316 G317 H318 Y319 Y320 V321 C324 M325 V326 L327 V328 E329 G330 I331 Y332 Y333 S334 V335 G336 N337 K338 F339 H340 V341 T342 S343 M344 T345 L346 P347 P348 G349 E350 R351 R352 E353 I354 T355 L356 E357 T358 I359 G360 N361

L362 D363 L364 L365 G366 I367 HIS GLY ILE SER ASN ASN ASN PHE ILE ALA R378 L379 D380 K381 D382 L383 K384 I385 R386 L387 H388 L389 L390 E391 K392 E393 L394 T395 D396 H397 K398 F399 V400 I401 L402 G403 A404 N405 L406 F407 L408 D409 D410 L411 K412 I413 M414 T415 A416 L417 S418 K419 I420 L421

Q422 K423 L424 N425 D426 D427 P428 P429 T430 L431 L432 I433 W434 Q435 G436 S437 F438 V441 P442 V443 F444 A445 S448 S449 R450 N451 T456 K459 N460 N461 F462 D463 A464 T467 L468 L469 S470 R471 F472 D473 N474 L475 T476 E477 N478 T479 T480 M481 I482 F483 I484 P485 G486 P487 N488

D489 L490 W491 G492 S493 S496 L497 G498 A499 S500 G501 T502 L503 P504 Q505 D506 P507 I508 P509 S510 A511 F512 T513 K514 K515 I516 N517 K518 V519 C520 K521 N522 V523 V524 W525 S526 S527 N528 P529 T530 R531 I532 A533 Y534 L535 S536 Q537 E538 I539 V540 I541 D544 D545 L546 S547 G548 R549 F550

K551 R552 H553 R554 L555 E556 PHE PRO PHE ASN GLU SER GLU ASP VAL TYR THR GLU ASN ASP ASN MET MET SER LYS ASP THR ASP ILE VAL PRO ILE ASP GLU LEU VAL LYS GLU PRO ASP GLN LEU PRO GLN LYS VAL GLN E598 T599 R600 K601 L602 V603 K604 T605 I606 L607 D608 Q609 G610

H611 L612 S613 P614 F615 L616 D617 S618 L619 W624 D625 L626 D627 H628 T629 L630 T631 L632 C633 P634 I635 P636 S637 T638 M639 V640 L641 T644 T645 S646 A647 Q648 F649 D650 L651 T652 Y653 N654 G655 C656 K657 G662 S663 F664 I665 H666 N667 R668 R669 A670 R671 Y672 M673 E674 Y675 V676 P677

S678 S679 K680 K681 T682 I683 Q684 E685 E686 I687 Y688 ILE

- Molecule 3: DNA polymerase epsilon subunit C

Chain 3: 15% 40% 58%

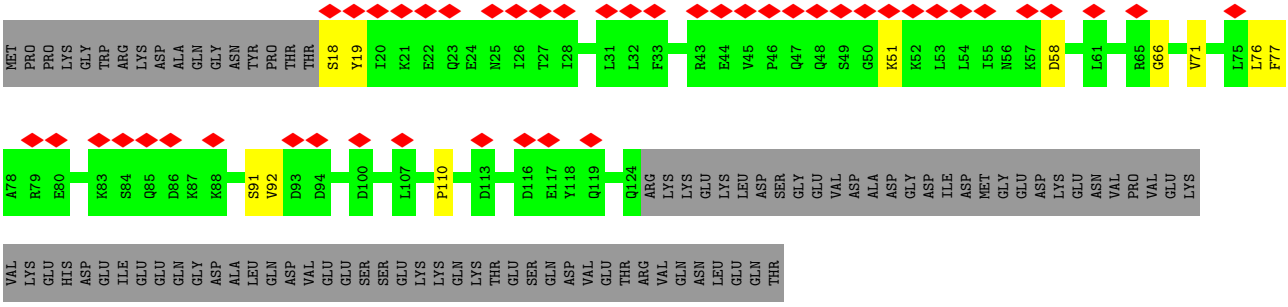
MET SER ASN LEU VAL LYS GLU LYS A9 P10 V11 F12 P13 I14 S15 K18 K19 I20 A21 K22 I29 N32 V33 E43 N48 E51 E52 S53 S61 K62 G63 K64 T65 S66 L67 R68 L69 N72 S73 I74 E75 E76 C77 V78 E79 D82 L87 E88 Q93

LEU LYS LYS ASN SER ALA LEU ASP LYS LYS ARG GLU LEU ASN MET GLN PRO GLY ARG SER ASP GLN GLU VAL VAL ILE GLU GLU PRO GLU LEU HIS GLU ASP ASP GLY VAL GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU VAL SER GLU GLU GLU PRO VAL HIS ASN GLU GLU LEU LEU ASP

ASP SER LYS ASP GLN GLN ASN ASP LYS SER THR ARG SER VAL ALA SER LEU LEU SER ARG PHE GLN TYR LYS SER ALA LEU ASP VAL GLY GLU HIS SER ASP SER SER ASP ILE GLU VAL ASP HIS THR LYS SER THR ASP PRO

- Molecule 4: DNA polymerase epsilon subunit D

Chain 4: 23% 49% 6% 45%


MET PRO PRO LYS GLY TRP ARG LYS ASP ALA GLN GLY ASN TYR PRO THR THR S18 Y19 I20 K21 E22 Q23 E24 N25 I26 T27 I28 L31 L32 F33 R43 E44 V45 P46 Q47 Q48 S49 G50 K51 K52 L53 L54 I55 N56 K57 D58 L61 R65 G66 V71 L75 L76 F77

A78 R79 E80 K83 S84 Q85 D86 K87 K88 S91 V92 D93 D94 D100 L107 P110 D113 D116 E117 Y118 Q119 Q124 ARG LYS LYS GLU LYS LEU ASP SER GLY GLU VAL ASP ALA ASP GLY ASP ILE ASP MET GLY GLU ASP LYS GLU ASN VAL PRO VAL GLU LYS

VAL LYS GLU HIS ASP GLU ILE GLU GLU GLN GLY ASP ALA LEU GLN ASP VAL GLU GLU SER SER GLU LYS LYS GLN LYS THR GLU SER GLN ASP VAL GLU THR ARG VAL GLN ASN LEU GLU GLN THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	187298	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 ($e^-/Å^2$)	60	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	0.223	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	263.424, 263.424, 263.424	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.029, 1.029, 1.029	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.47	4/15201 (0.0%)	0.73	15/20663 (0.1%)
2	2	0.44	0/3286	0.80	7/4467 (0.2%)
3	3	0.42	0/660	0.60	0/891
4	4	0.54	1/839 (0.1%)	0.74	0/1132
All	All	0.47	5/19986 (0.0%)	0.74	22/27153 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1161	PRO	N-CD	-8.85	1.35	1.47
4	4	110	PRO	N-CD	-7.39	1.37	1.47
1	A	1645	TRP	CB-CG	-6.58	1.38	1.50
1	A	497	CYS	CB-SG	-5.92	1.72	1.81
1	A	489	VAL	CB-CG1	-5.36	1.41	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1884	TYR	CA-CB-CG	8.09	128.78	113.40
2	2	403	GLY	N-CA-C	7.99	133.07	113.10
1	A	1707	LEU	CA-CB-CG	7.95	133.59	115.30
1	A	1933	TYR	CA-CB-CG	7.02	126.75	113.40
2	2	662	GLY	N-CA-C	6.39	129.09	113.10
1	A	1881	TYR	CA-CB-CG	6.19	125.17	113.40
1	A	1826	LYS	C-N-CA	6.17	137.12	121.70
1	A	1694	PRO	C-N-CA	6.12	137.00	121.70
2	2	534	TYR	C-N-CA	5.72	136.00	121.70
2	2	336	GLY	N-CA-C	-5.63	99.03	113.10
2	2	403	GLY	C-N-CA	5.57	135.62	121.70
1	A	2054	LEU	CA-CB-CG	5.55	128.06	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	334	SER	CA-C-O	-5.49	108.57	120.10
1	A	1375	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	1322	TRP	CA-CB-CG	5.35	123.87	113.70
1	A	1894	MET	C-N-CA	5.35	135.07	121.70
1	A	1703	ASN	C-N-CA	5.27	134.87	121.70
1	A	1115	ASP	CB-CG-OD2	5.24	123.01	118.30
2	2	346	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	1920	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	1386	ASN	N-CA-C	5.09	124.75	111.00
1	A	519	LEU	CA-CB-CG	5.09	127.01	115.30

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	14886	0	13968	179	0
2	2	3225	0	3134	43	0
3	3	652	0	664	4	0
4	4	829	0	842	10	0
5	A	1	0	0	0	0
All	All	19593	0	18608	226	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.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:VAL:HG13	1:A:1301:ARG:NH1	1.48	1.26
1:A:1115:ASP:OD1	1:A:1118:ILE:CG1	1.99	1.08
1:A:1540:LYS:HA	1:A:1543:ILE:HG22	1.32	1.05
1:A:306:ASP:OD1	1:A:1301:ARG:NH1	1.93	1.00
1:A:1115:ASP:OD1	1:A:1118:ILE:HG12	1.60	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1540:LYS:HA	1:A:1543:ILE:CG2	1.98	0.93
1:A:305:VAL:HG13	1:A:1301:ARG:HH11	1.25	0.92
2:2:497:LEU:HD22	2:2:501:GLY:HA3	1.50	0.92
1:A:1115:ASP:CG	1:A:1118:ILE:HG12	1.90	0.92
1:A:1115:ASP:OD1	1:A:1118:ILE:CB	2.19	0.90
1:A:305:VAL:CG1	1:A:1301:ARG:NH1	2.33	0.89
1:A:1115:ASP:OD2	1:A:1118:ILE:CG1	2.21	0.88
2:2:497:LEU:CD2	2:2:501:GLY:HA3	2.05	0.86
1:A:639:VAL:HG12	1:A:946:VAL:HG22	1.57	0.86
1:A:1115:ASP:OD1	1:A:1118:ILE:HB	1.74	0.86
1:A:1115:ASP:CG	1:A:1118:ILE:CG1	2.44	0.85
1:A:1540:LYS:CA	1:A:1543:ILE:HG22	2.05	0.85
1:A:1115:ASP:OD2	1:A:1118:ILE:HG12	1.76	0.84
1:A:770:TYR:CE2	1:A:771:VAL:HG13	2.13	0.83
1:A:1115:ASP:N	1:A:1289:ARG:NH2	2.25	0.82
1:A:296:PRO:HD3	1:A:1301:ARG:HH22	1.44	0.81
1:A:1115:ASP:H	1:A:1289:ARG:NH2	1.77	0.81
1:A:1582:GLU:OE2	3:3:33:VAL:CB	2.28	0.80
1:A:1641:SER:O	1:A:1645:TRP:HB2	1.82	0.78
1:A:1115:ASP:H	1:A:1289:ARG:NH1	1.83	0.77
1:A:861:ALA:O	1:A:865:VAL:HG23	1.85	0.77
1:A:1115:ASP:H	1:A:1289:ARG:HH12	1.33	0.77
1:A:305:VAL:HG13	1:A:1301:ARG:HH12	1.45	0.76
1:A:285:VAL:HG23	1:A:316:ASP:OD2	1.85	0.75
1:A:79:LEU:HG	1:A:261:VAL:HG23	1.67	0.75
1:A:1115:ASP:H	1:A:1289:ARG:CZ	2.04	0.71
1:A:285:VAL:HG13	1:A:371:PRO:HA	1.73	0.70
1:A:1303:ARG:O	1:A:1303:ARG:HG3	1.89	0.70
1:A:1118:ILE:HG21	1:A:1289:ARG:NE	2.07	0.70
1:A:1115:ASP:OD2	1:A:1118:ILE:HG13	1.90	0.69
1:A:261:VAL:HG13	1:A:497:CYS:SG	2.32	0.68
1:A:1027:LEU:O	1:A:1031:ASP:HB2	1.93	0.68
1:A:1306:LEU:CD2	1:A:1311:ARG:HH11	2.07	0.68
1:A:1550:VAL:HG12	1:A:1552:ILE:HG13	1.77	0.67
2:2:497:LEU:HD22	2:2:501:GLY:CA	2.25	0.66
1:A:1306:LEU:HD23	1:A:1311:ARG:HH11	1.60	0.66
1:A:770:TYR:CD2	1:A:771:VAL:HG13	2.30	0.66
1:A:519:LEU:HD11	1:A:830:PHE:CE1	2.33	0.64
1:A:907:CYS:SG	1:A:945:GLU:HA	2.38	0.64
1:A:999:GLN:HA	1:A:1002:ILE:HG22	1.78	0.64
2:2:497:LEU:C	2:2:497:LEU:HD12	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1484:ILE:CD1	1:A:1550:VAL:HG22	2.28	0.63
1:A:305:VAL:CG1	1:A:1301:ARG:HH11	2.06	0.61
1:A:1115:ASP:CG	1:A:1118:ILE:HG13	2.21	0.61
1:A:296:PRO:CD	1:A:1301:ARG:HH22	2.13	0.60
1:A:999:GLN:HA	1:A:1002:ILE:CG2	2.31	0.59
1:A:1484:ILE:HD12	1:A:1550:VAL:HG22	1.83	0.59
2:2:435:GLN:OE1	2:2:435:GLN:HA	2.01	0.59
1:A:519:LEU:HD11	1:A:830:PHE:HE1	1.66	0.59
1:A:1539:LYS:O	1:A:1543:ILE:HG22	2.03	0.58
2:2:654:ASN:ND2	2:2:656:CYS:SG	2.77	0.57
1:A:305:VAL:CG2	1:A:1301:ARG:HD2	2.35	0.57
1:A:1026:TRP:HA	1:A:1029:VAL:HG12	1.87	0.57
1:A:1550:VAL:HG12	1:A:1552:ILE:CG1	2.35	0.56
1:A:1002:ILE:HD11	1:A:1158:ILE:HD11	1.87	0.56
1:A:443:THR:HG21	1:A:480:ALA:HB1	1.87	0.56
1:A:659:ILE:HG21	1:A:845:GLU:HG2	1.88	0.56
1:A:1151:GLY:O	1:A:1155:GLN:HB2	2.05	0.56
1:A:791:TRP:O	1:A:795:LEU:HB2	2.05	0.56
3:3:67:LEU:HD13	4:4:51:LYS:H	1.70	0.55
1:A:1503:LYS:HE3	1:A:1506:GLY:HA3	1.88	0.55
1:A:1736:VAL:HG11	1:A:1739:LEU:HD13	1.88	0.54
1:A:972:PHE:HA	1:A:979:ALA:H	1.72	0.54
1:A:999:GLN:CA	1:A:1002:ILE:HG22	2.38	0.54
1:A:561:LEU:HD22	1:A:871:PRO:HG2	1.90	0.53
1:A:881:CYS:SG	1:A:882:ILE:N	2.80	0.53
1:A:1414:CYS:SG	1:A:1415:THR:N	2.82	0.53
1:A:1115:ASP:N	1:A:1289:ARG:HH12	2.05	0.53
4:4:91:SER:OG	4:4:92:VAL:N	2.42	0.53
1:A:998:PHE:O	1:A:1002:ILE:HG22	2.09	0.52
2:2:286:GLY:HA3	2:2:298:LEU:CD1	2.39	0.52
1:A:305:VAL:HG22	1:A:1301:ARG:HD2	1.91	0.52
2:2:497:LEU:HD23	2:2:501:GLY:HA3	1.89	0.52
1:A:822:ALA:O	1:A:826:ILE:HG13	2.09	0.52
1:A:140:PHE:HB2	1:A:243:ARG:HB2	1.92	0.52
1:A:1303:ARG:HB2	1:A:1460:GLN:HG2	1.92	0.52
2:2:520:CYS:SG	2:2:521:LYS:N	2.83	0.52
1:A:180:HIS:HA	1:A:184:LEU:HB3	1.91	0.52
1:A:1858:ILE:HA	1:A:1867:LEU:HB3	1.92	0.52
2:2:669:ARG:HH12	2:2:687:ILE:HG13	1.74	0.52
1:A:2131:VAL:HG12	1:A:2131:VAL:O	2.09	0.52
1:A:1277:LYS:HB2	4:4:76:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:663:SER:OG	2:2:664:PHE:N	2.42	0.51
1:A:285:VAL:CG1	1:A:371:PRO:HA	2.39	0.51
1:A:1523:ILE:HG23	1:A:1525:ALA:H	1.75	0.51
4:4:76:LEU:HD12	4:4:77:PHE:CD2	2.45	0.51
1:A:1143:TRP:O	1:A:1147:ARG:HB2	2.10	0.51
1:A:296:PRO:HD3	1:A:1301:ARG:NH2	2.22	0.51
1:A:145:ASP:HB3	1:A:148:ARG:HB2	1.93	0.50
1:A:500:ILE:HD11	1:A:519:LEU:HD23	1.92	0.50
2:2:406:LEU:CD2	2:2:417:LEU:HD13	2.42	0.50
1:A:839:SER:HB2	1:A:842:TYR:HB2	1.93	0.50
2:2:402:LEU:HA	2:2:672:TYR:HB2	1.94	0.50
1:A:213:ASN:ND2	1:A:239:ILE:O	2.45	0.50
1:A:1303:ARG:O	1:A:1303:ARG:CG	2.57	0.50
2:2:286:GLY:HA3	2:2:298:LEU:HD11	1.93	0.50
1:A:314:MET:HA	1:A:319:GLY:HA2	1.94	0.49
1:A:261:VAL:CG1	1:A:497:CYS:SG	3.00	0.49
1:A:1536:PHE:O	1:A:1540:LYS:N	2.45	0.49
4:4:18:SER:OG	4:4:19:TYR:N	2.45	0.49
1:A:958:SER:H	1:A:964:GLY:HA2	1.78	0.49
1:A:1899:ASP:OD1	1:A:1899:ASP:N	2.46	0.49
1:A:1094:SER:HA	1:A:1141:ILE:HA	1.95	0.49
1:A:562:GLU:OE2	1:A:870:ARG:NH2	2.46	0.48
1:A:348:THR:HG23	1:A:348:THR:O	2.13	0.48
2:2:178:GLN:O	2:2:180:ARG:NH1	2.46	0.48
1:A:136:ASP:OD1	1:A:136:ASP:N	2.47	0.48
1:A:552:THR:OG1	1:A:553:TYR:N	2.46	0.48
1:A:636:ILE:HB	1:A:950:TYR:HB2	1.96	0.48
2:2:266:MET:HG3	2:2:267:SER:N	2.29	0.48
2:2:669:ARG:HH12	2:2:687:ILE:CG1	2.27	0.48
3:3:87:LEU:HD11	4:4:66:GLY:HA2	1.95	0.48
1:A:1115:ASP:OD1	1:A:1118:ILE:HG13	2.07	0.48
1:A:415:SER:OG	1:A:416:TYR:N	2.47	0.47
1:A:2172:ARG:NH2	2:2:291:ASN:O	2.47	0.47
4:4:76:LEU:CD1	4:4:77:PHE:CD2	2.97	0.47
4:4:58:ASP:OD1	4:4:58:ASP:N	2.47	0.47
1:A:376:THR:OG1	1:A:377:PHE:N	2.48	0.47
1:A:1072:ARG:NH1	1:A:1106:ALA:O	2.48	0.47
1:A:124:GLU:OE2	1:A:278:LYS:NZ	2.47	0.47
1:A:1539:LYS:HA	1:A:1542:LYS:HB2	1.96	0.47
1:A:635:LEU:HD12	1:A:949:PRO:HB3	1.97	0.47
1:A:639:VAL:HG12	1:A:946:VAL:CG2	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ALA:O	1:A:647:ASN:ND2	2.47	0.47
1:A:730:ASP:N	1:A:730:ASP:OD1	2.47	0.47
1:A:792:LYS:O	1:A:796:SER:HB3	2.15	0.47
1:A:713:ASN:OD1	1:A:713:ASN:N	2.48	0.47
1:A:426:VAL:O	1:A:437:GLN:NE2	2.48	0.47
1:A:322:ILE:HG12	1:A:350:PHE:HB2	1.97	0.47
2:2:664:PHE:HD1	2:2:670:ALA:HA	1.80	0.47
1:A:1124:ARG:HD3	1:A:1130:PRO:HA	1.97	0.46
1:A:1724:SER:HB2	1:A:1911:TRP:H	1.80	0.46
1:A:306:ASP:O	1:A:390:ARG:NH1	2.48	0.46
1:A:1486:TYR:HB3	1:A:1502:PHE:HB3	1.98	0.46
1:A:1536:PHE:O	1:A:1540:LYS:CB	2.64	0.46
1:A:771:VAL:O	1:A:775:LYS:HB2	2.15	0.46
1:A:1048:GLU:OE2	1:A:1050:ARG:NH2	2.48	0.46
1:A:484:LEU:O	1:A:488:TYR:HB2	2.16	0.46
1:A:305:VAL:HG22	1:A:1301:ARG:CD	2.46	0.46
1:A:424:ARG:NH2	1:A:509:ARG:O	2.49	0.46
1:A:1385:ASN:HB3	1:A:1699:GLY:HA3	1.98	0.46
1:A:1490:PHE:HB2	1:A:1498:PHE:HB2	1.98	0.46
2:2:231:ARG:NH2	2:2:350:GLU:OE2	2.48	0.46
2:2:286:GLY:CA	2:2:298:LEU:HD11	2.46	0.46
1:A:1694:PRO:HD3	2:2:442:PRO:HG2	1.98	0.46
1:A:1550:VAL:HG11	1:A:1552:ILE:HD11	1.98	0.46
2:2:367:ILE:HD12	2:2:381:LYS:HE3	1.98	0.46
2:2:514:LYS:HE2	2:2:518:LYS:HE3	1.98	0.45
1:A:243:ARG:HA	1:A:533:ASN:HD21	1.82	0.45
1:A:1521:GLN:O	1:A:1627:TRP:NE1	2.46	0.45
2:2:496:SER:OG	2:2:497:LEU:N	2.50	0.45
1:A:772:ASP:O	1:A:776:SER:HB3	2.17	0.45
2:2:654:ASN:OD1	2:2:654:ASN:N	2.49	0.45
1:A:907:CYS:SG	1:A:944:PHE:O	2.74	0.45
1:A:947:ASP:OD1	1:A:947:ASP:N	2.47	0.45
1:A:994:LEU:O	1:A:998:PHE:HB2	2.17	0.45
1:A:1306:LEU:HD21	1:A:1311:ARG:HH11	1.82	0.45
1:A:1617:LEU:O	2:2:451:ASN:ND2	2.49	0.44
2:2:676:VAL:HG21	2:2:679:SER:HB3	1.99	0.44
1:A:173:GLU:HB3	1:A:529:ILE:HA	1.98	0.44
2:2:428:PRO:HB2	2:2:478:ASN:HD21	1.82	0.44
3:3:20:ILE:HB	4:4:71:VAL:HG11	1.99	0.44
2:2:554:ARG:NH1	2:2:556:GLU:O	2.51	0.44
1:A:716:SER:OG	1:A:717:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ILE:O	1:A:738:ARG:NH1	2.50	0.44
1:A:1322:TRP:HA	1:A:1340:VAL:HA	1.99	0.44
1:A:372:THR:O	1:A:372:THR:HG22	2.18	0.43
1:A:1370:LYS:HA	1:A:1370:LYS:HD2	1.82	0.43
1:A:1702:GLN:HA	2:2:499:ALA:HB1	1.99	0.43
2:2:312:THR:HB	2:2:555:LEU:HD21	2.00	0.43
1:A:367:ARG:HD3	1:A:401:GLU:HB2	2.00	0.43
1:A:428:ARG:HD3	1:A:512:THR:HB	2.00	0.43
1:A:722:THR:HG22	1:A:723:PHE:N	2.33	0.43
1:A:1077:LEU:HB3	1:A:1081:MET:HE1	1.99	0.43
1:A:1095:SER:HB3	1:A:1142:ASP:HA	1.99	0.43
1:A:305:VAL:HG21	1:A:1301:ARG:HD2	2.00	0.43
1:A:1672:ILE:HG23	1:A:1798:TRP:HH2	1.82	0.43
1:A:1626:ASN:N	1:A:1626:ASN:OD1	2.51	0.43
2:2:355:THR:HG23	2:2:356:LEU:HG	2.00	0.43
2:2:529:PRO:O	2:2:629:THR:OG1	2.37	0.43
1:A:243:ARG:HG3	1:A:530:LEU:HD21	1.99	0.43
1:A:1457:LYS:O	1:A:1461:GLN:NE2	2.52	0.43
1:A:643:SER:OG	1:A:647:ASN:ND2	2.52	0.43
2:2:174:ASN:HB2	2:2:177:GLN:HB2	2.01	0.43
2:2:355:THR:HG21	2:2:635:ILE:HG22	1.99	0.43
1:A:1280:TRP:HE3	4:4:76:LEU:HD21	1.84	0.43
1:A:1532:TYR:O	1:A:1536:PHE:HB2	2.18	0.43
1:A:2108:CYS:SG	1:A:2137:PHE:HE1	2.42	0.43
1:A:732:VAL:HA	1:A:735:ILE:HB	2.01	0.43
1:A:634:PRO:HB2	1:A:882:ILE:HB	2.01	0.42
1:A:924:GLN:HG2	1:A:936:THR:HB	2.01	0.42
1:A:502:LEU:HD22	1:A:506:GLU:HG3	2.00	0.42
1:A:541:ARG:NE	1:A:551:GLU:OE1	2.48	0.42
1:A:576:ILE:H	1:A:576:ILE:HG13	1.65	0.42
1:A:1724:SER:OG	1:A:1725:GLY:N	2.53	0.42
1:A:1119:LYS:O	1:A:1123:LEU:CB	2.67	0.42
1:A:2051:LEU:HA	1:A:2054:LEU:HG	2.01	0.42
1:A:1606:LEU:HB3	1:A:1607:LEU:H	1.76	0.41
1:A:573:GLU:O	1:A:870:ARG:NH1	2.50	0.41
1:A:875:ASP:N	1:A:875:ASP:OD1	2.54	0.41
1:A:1584:ARG:HD3	1:A:1584:ARG:HA	1.88	0.41
1:A:2065:SER:OG	1:A:2066:LYS:N	2.53	0.41
2:2:406:LEU:HD12	2:2:406:LEU:C	2.40	0.41
1:A:379:GLY:HA2	1:A:383:ASP:HB3	2.01	0.41
1:A:489:VAL:HG12	1:A:492:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:477:GLU:O	2:2:522:ASN:ND2	2.52	0.41
2:2:478:ASN:OD1	2:2:478:ASN:N	2.53	0.41
1:A:302:ASP:HB2	1:A:305:VAL:HG12	2.02	0.41
1:A:1303:ARG:NH2	1:A:1306:LEU:HD13	2.35	0.41
1:A:1934:THR:OG1	1:A:1935:ALA:N	2.51	0.41
1:A:1056:LEU:HD11	1:A:1071:ARG:HG3	2.02	0.41
1:A:2151:ARG:HA	1:A:2151:ARG:HD3	1.88	0.41
1:A:576:ILE:HG23	1:A:868:VAL:HA	2.01	0.41
1:A:992:LEU:HD12	1:A:992:LEU:HA	1.95	0.41
1:A:1051:SER:OG	1:A:1052:MET:N	2.54	0.41
2:2:305:VAL:HG12	2:2:306:GLU:N	2.36	0.41
1:A:2129:SER:OG	1:A:2130:CYS:N	2.54	0.40
2:2:497:LEU:C	2:2:497:LEU:CD1	2.88	0.40
1:A:865:VAL:HG13	1:A:881:CYS:SG	2.62	0.40
2:2:437:SER:HB2	2:2:485:PRO:HA	2.01	0.40
2:2:327:LEU:HG	2:2:347:PRO:HD3	2.02	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	1929/2222 (87%)	1802 (93%)	127 (7%)	0	100	100
2	2	414/689 (60%)	370 (89%)	43 (10%)	1 (0%)	47	81
3	3	83/201 (41%)	80 (96%)	3 (4%)	0	100	100
4	4	105/196 (54%)	96 (91%)	9 (9%)	0	100	100
All	All	2531/3308 (76%)	2348 (93%)	182 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	434	TRP

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	1522/2014 (76%)	1510 (99%)	12 (1%)	81	91
2	2	351/629 (56%)	349 (99%)	2 (1%)	86	94
3	3	72/185 (39%)	71 (99%)	1 (1%)	67	85
4	4	91/173 (53%)	91 (100%)	0	100	100
All	All	2036/3001 (68%)	2021 (99%)	15 (1%)	84	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	ASP
1	A	630	ARG
1	A	737	LYS
1	A	738	ARG
1	A	837	LYS
1	A	916	GLN
1	A	972	PHE
1	A	1047	CYS
1	A	1081	MET
1	A	1551	ASP
1	A	1590	LEU
1	A	2111	CYS
2	2	277	ARG
2	2	669	ARG
3	3	43	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	ASN

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Mol	Chain	Res	Type
1	A	437	GLN
1	A	533	ASN
1	A	647	ASN
1	A	794	ASN
1	A	997	ASN
1	A	1155	GLN
1	A	1176	HIS
1	A	1461	GLN
1	A	1789	ASN
1	A	1838	ASN
1	A	2199	ASN
2	2	174	ASN
2	2	517	ASN
2	2	537	GLN
4	4	72	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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

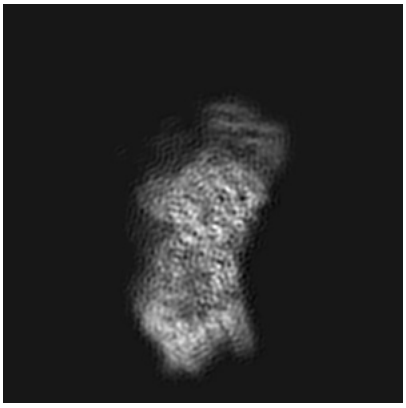
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21701. These allow visual inspection of the internal detail of the map and identification of artifacts.

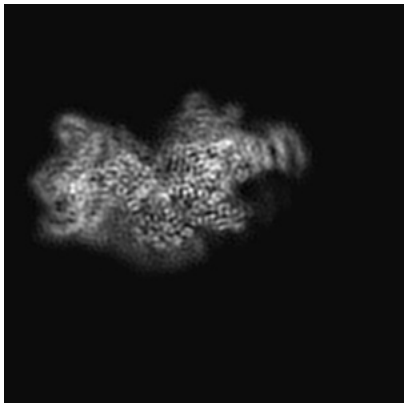
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

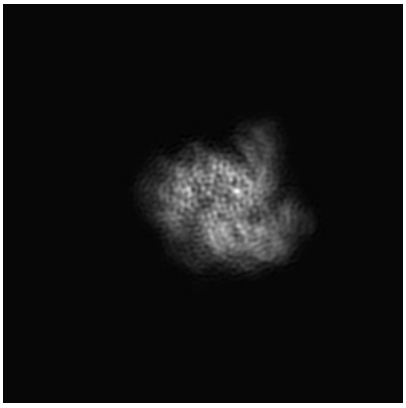
6.1.1 Primary map



X



Y



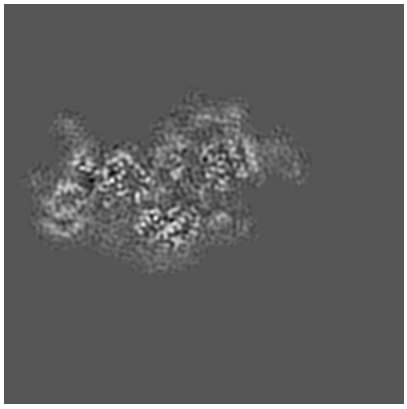
Z

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

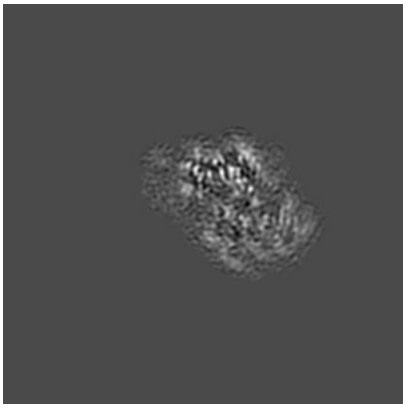
6.2 Central slices (i)

6.2.1 Primary map

X Index: 128



Y Index: 128



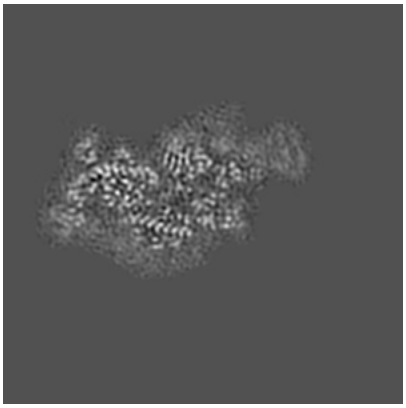
Z Index: 128

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

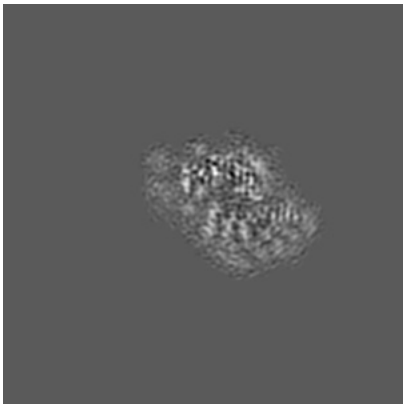
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 150



Y Index: 136



Z Index: 125

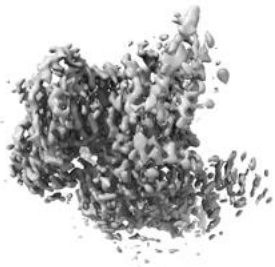
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

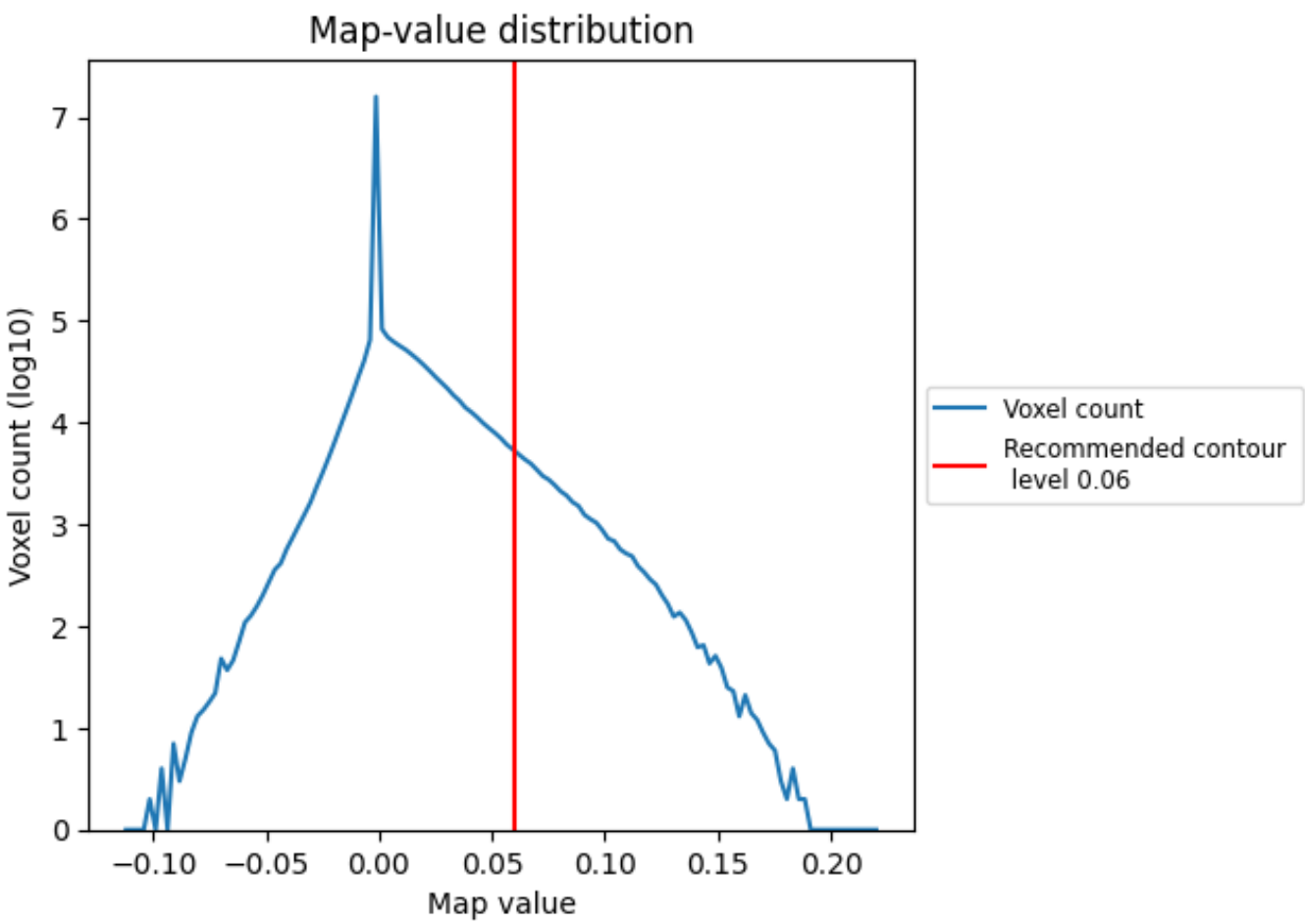
6.5 Mask visualisation (i)

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

7 Map analysis (i)

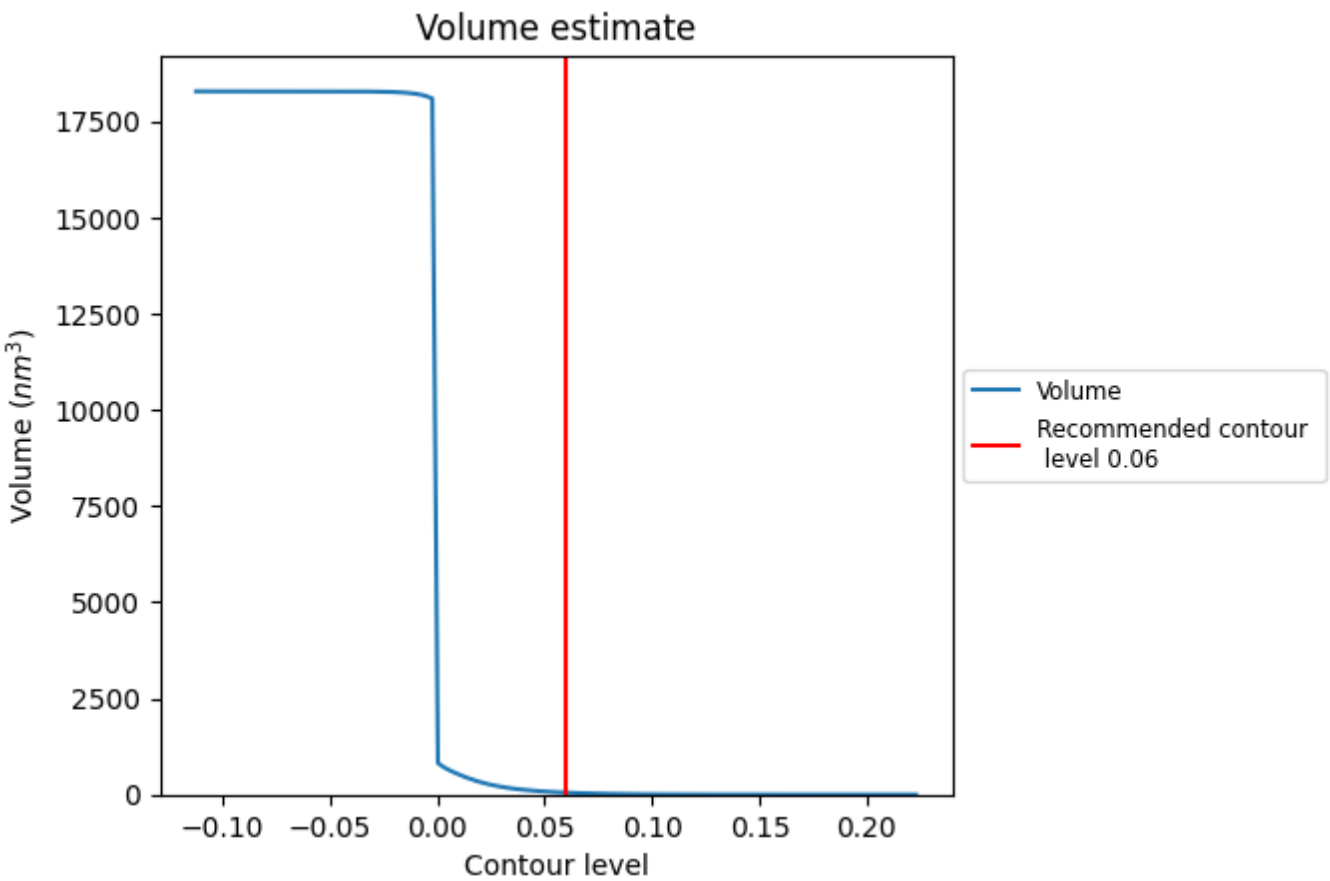
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

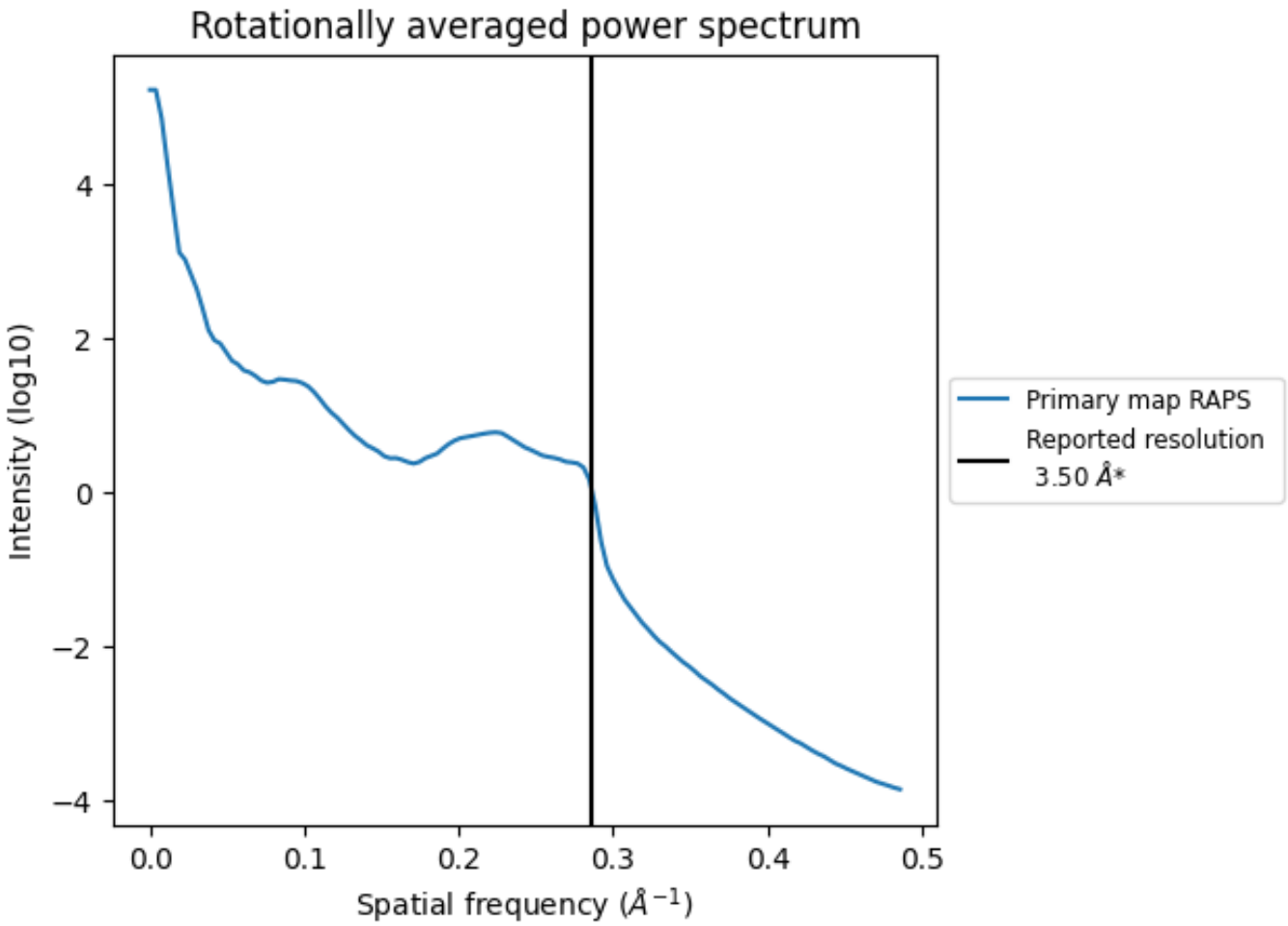
7.2 Volume estimate (i)



The volume at the recommended contour level is 50 nm^3; this corresponds to an approximate mass of 45 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 0.286 Å^{-1}

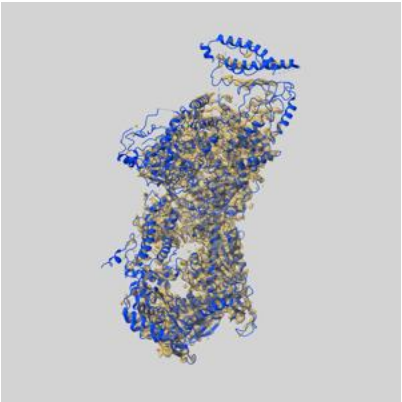
8 Fourier-Shell correlation (i)

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

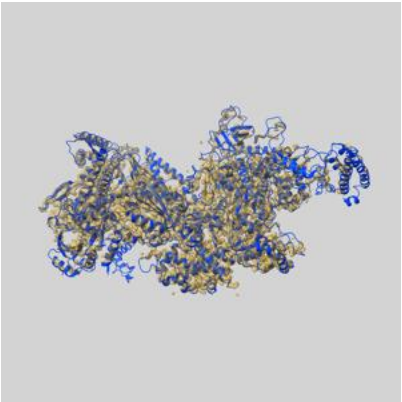
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21701 and PDB model 6WJV. Per-residue inclusion information can be found in section 3 on page 4.

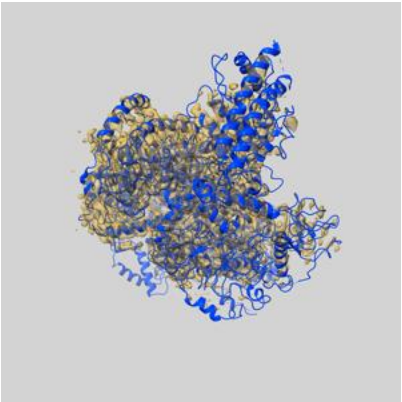
9.1 Map-model overlay (i)



X



Y



Z

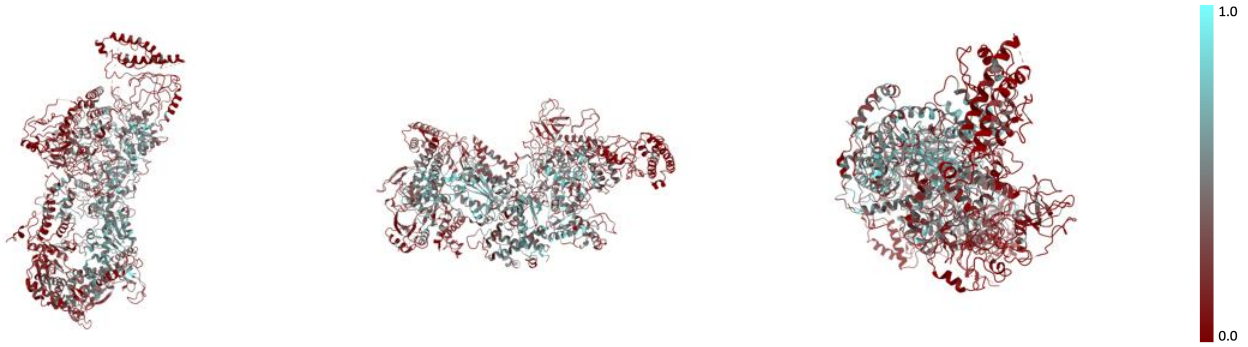
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

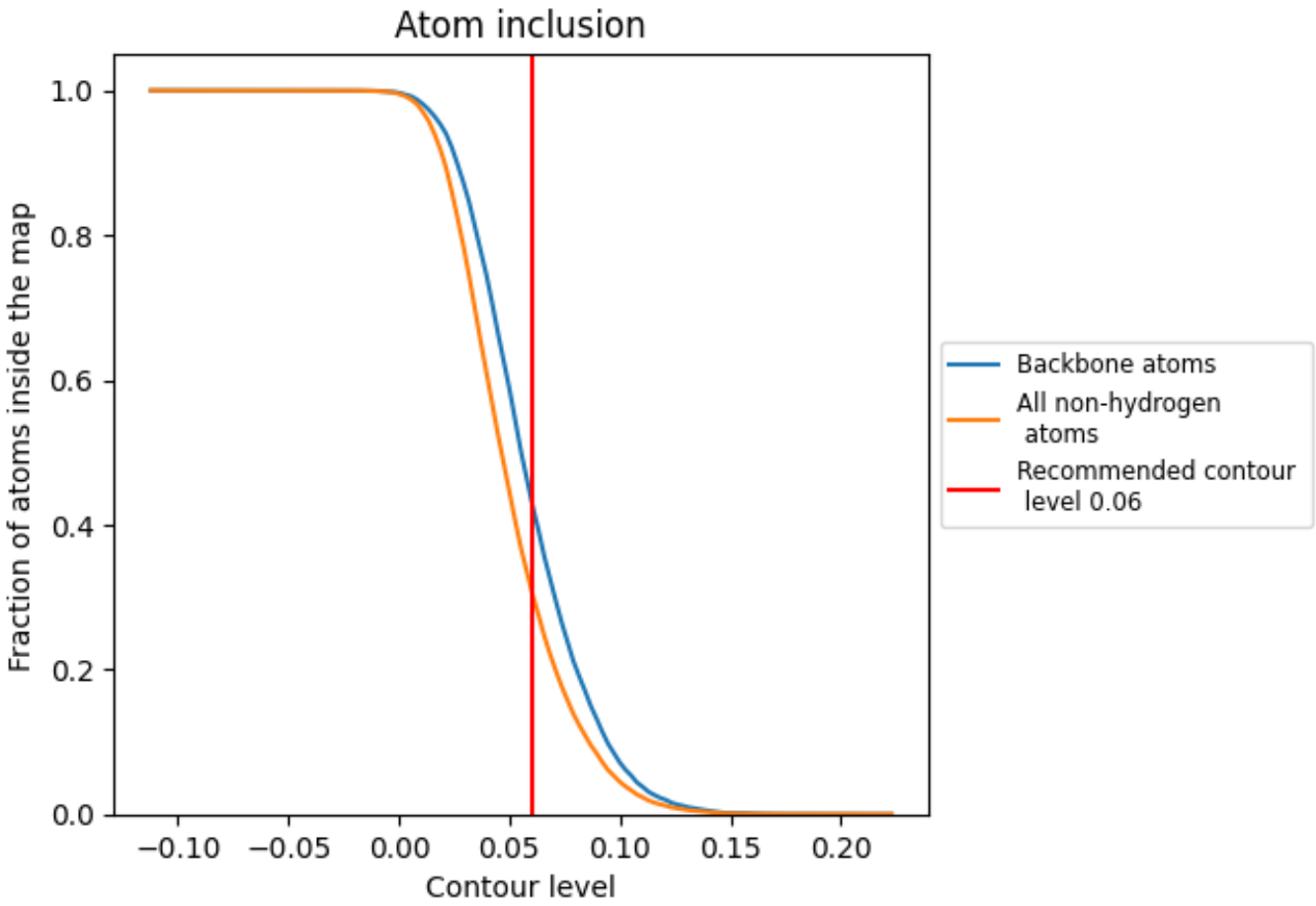
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 43% of all backbone atoms, 31% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3085	0.3490
2	0.2000	0.3340
3	0.4405	0.3700
4	0.4347	0.3910
A	0.3192	0.3490