wwPDB EM Validation Summary Report (i)

Oct 12, 2026 – 12:20 PM JST

PDB ID	:	22VF / pdb_000022vf
EMDB ID	:	EMD-68713
Title	:	Cryo-EM structure of DOCK11 complexed with Cdc42(G15A) and Cdc42(Q61L)-GTP
Authors	:	Hisano, T.; Kukimoto-Niino, M.; Shinoda, T.; Katsura, K.; Shirouzu, M.
Deposited on	:	2026-01-25
Resolution	:	3.82 Å(reported)
Based on initial models	:	., 1NF3, 2WM9

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

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

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

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

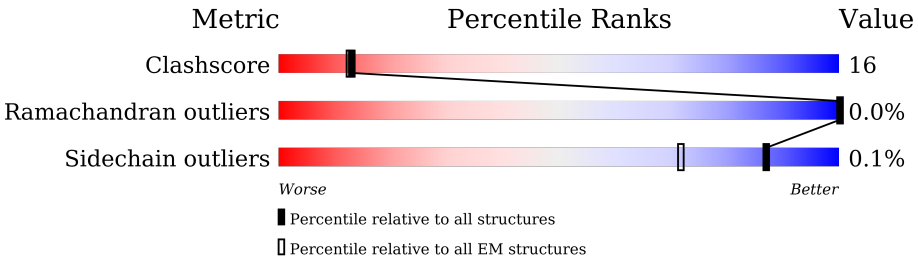
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

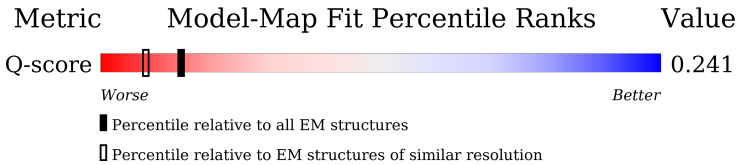
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.82 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9152 (3.32 - 4.32)

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	2079	55% 29% 16%
1	B	2079	55% 28% 16%
2	C	195	58% 33% 9%
2	D	195	58% 33% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	195	6% 79% 11% • 9%
3	F	195	6% 78% 12% • 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 67734 atoms, of which 33916 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 Dedicator of cytokinesis protein 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1743	28368	9071	14225	2389	2606	77	0	0
1	B	1743	28368	9071	14225	2389	2606	77	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q5JSL3
A	-4	GLY	-	expression tag	UNP Q5JSL3
A	-3	SER	-	expression tag	UNP Q5JSL3
A	-2	GLY	-	expression tag	UNP Q5JSL3
A	-1	GLY	-	expression tag	UNP Q5JSL3
A	0	SER	-	expression tag	UNP Q5JSL3
B	-5	GLY	-	expression tag	UNP Q5JSL3
B	-4	GLY	-	expression tag	UNP Q5JSL3
B	-3	SER	-	expression tag	UNP Q5JSL3
B	-2	GLY	-	expression tag	UNP Q5JSL3
B	-1	GLY	-	expression tag	UNP Q5JSL3
B	0	SER	-	expression tag	UNP Q5JSL3

- Molecule 2 is a protein called Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C	177	2678	870	1326	213	262	7	0	0
2	D	177	2678	870	1326	213	262	7	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP P60953

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	SER	-	expression tag	UNP P60953
C	-4	SER	-	expression tag	UNP P60953
C	-3	GLY	-	expression tag	UNP P60953
C	-2	SER	-	expression tag	UNP P60953
C	-1	SER	-	expression tag	UNP P60953
C	0	GLY	-	expression tag	UNP P60953
C	15	ALA	GLY	engineered mutation	UNP P60953
C	188	SER	-	expression tag	UNP P60953
D	-6	GLY	-	expression tag	UNP P60953
D	-5	SER	-	expression tag	UNP P60953
D	-4	SER	-	expression tag	UNP P60953
D	-3	GLY	-	expression tag	UNP P60953
D	-2	SER	-	expression tag	UNP P60953
D	-1	SER	-	expression tag	UNP P60953
D	0	GLY	-	expression tag	UNP P60953
D	15	ALA	GLY	engineered mutation	UNP P60953
D	188	SER	-	expression tag	UNP P60953

- Molecule 3 is a protein called Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	E	177	2775	889	1396	219	265	6	0	0
			Total	C	H	N	O	S		
3	F	177	2775	889	1396	219	265	6	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	GLY	-	expression tag	UNP P60953
E	-5	SER	-	expression tag	UNP P60953
E	-4	SER	-	expression tag	UNP P60953
E	-3	GLY	-	expression tag	UNP P60953
E	-2	SER	-	expression tag	UNP P60953
E	-1	SER	-	expression tag	UNP P60953
E	0	GLY	-	expression tag	UNP P60953
E	61	LEU	GLN	engineered mutation	UNP P60953
E	188	SER	-	expression tag	UNP P60953
F	-6	GLY	-	expression tag	UNP P60953
F	-5	SER	-	expression tag	UNP P60953
F	-4	SER	-	expression tag	UNP P60953
F	-3	GLY	-	expression tag	UNP P60953

Continued on next page...

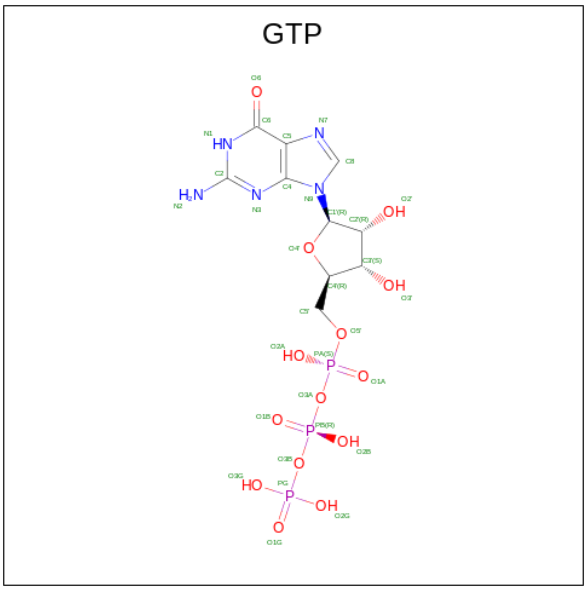
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	SER	-	expression tag	UNP P60953
F	-1	SER	-	expression tag	UNP P60953
F	0	GLY	-	expression tag	UNP P60953
F	61	LEU	GLN	engineered mutation	UNP P60953
F	188	SER	-	expression tag	UNP P60953

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	E	1	1	1	0
4	F	1	1	1	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
5	E	1	43	10	11	5	14	3	0
5	F	1	43	10	11	5	14	3	0

- Molecule 6 is water.

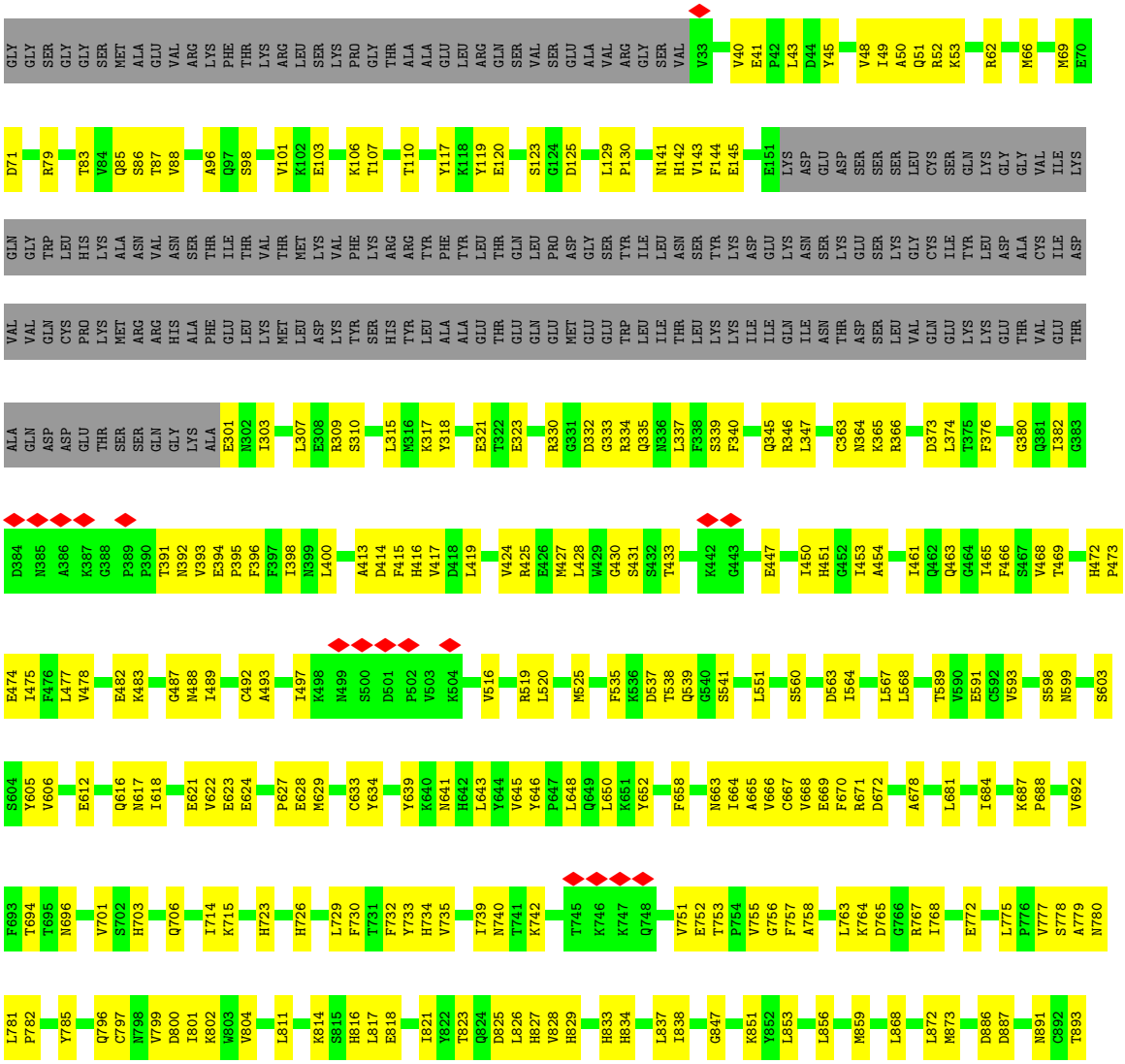
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
6	E	2	2	2	0
			Total	O	
6	F	2	2	2	0

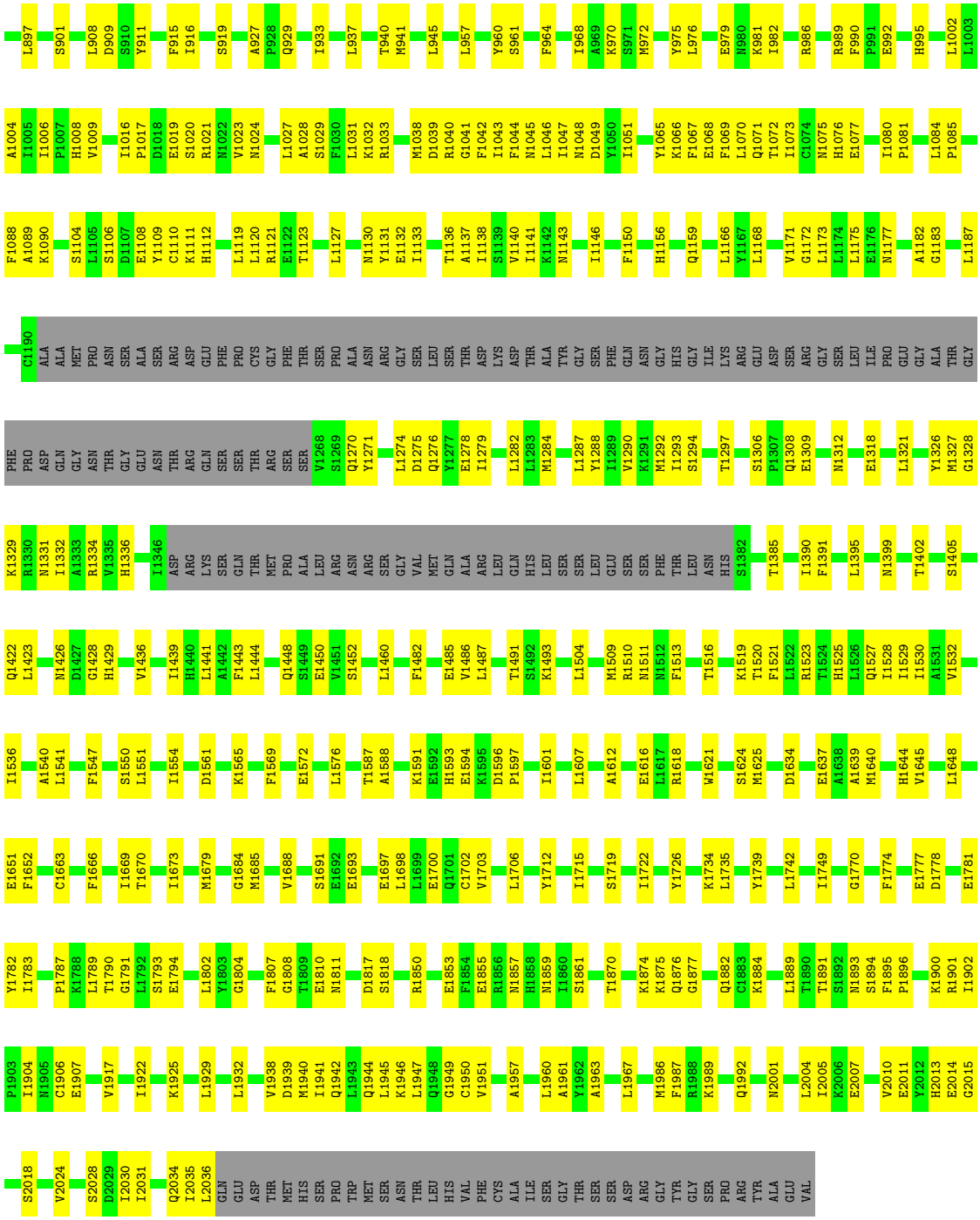
3 Residue-property plots (i)

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: Dedicator of cytokinesis protein 11

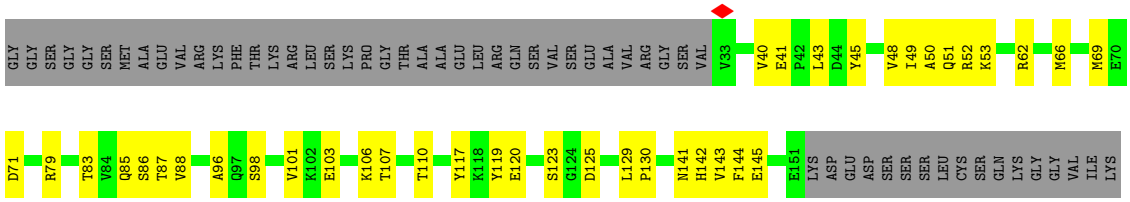
Chain A:

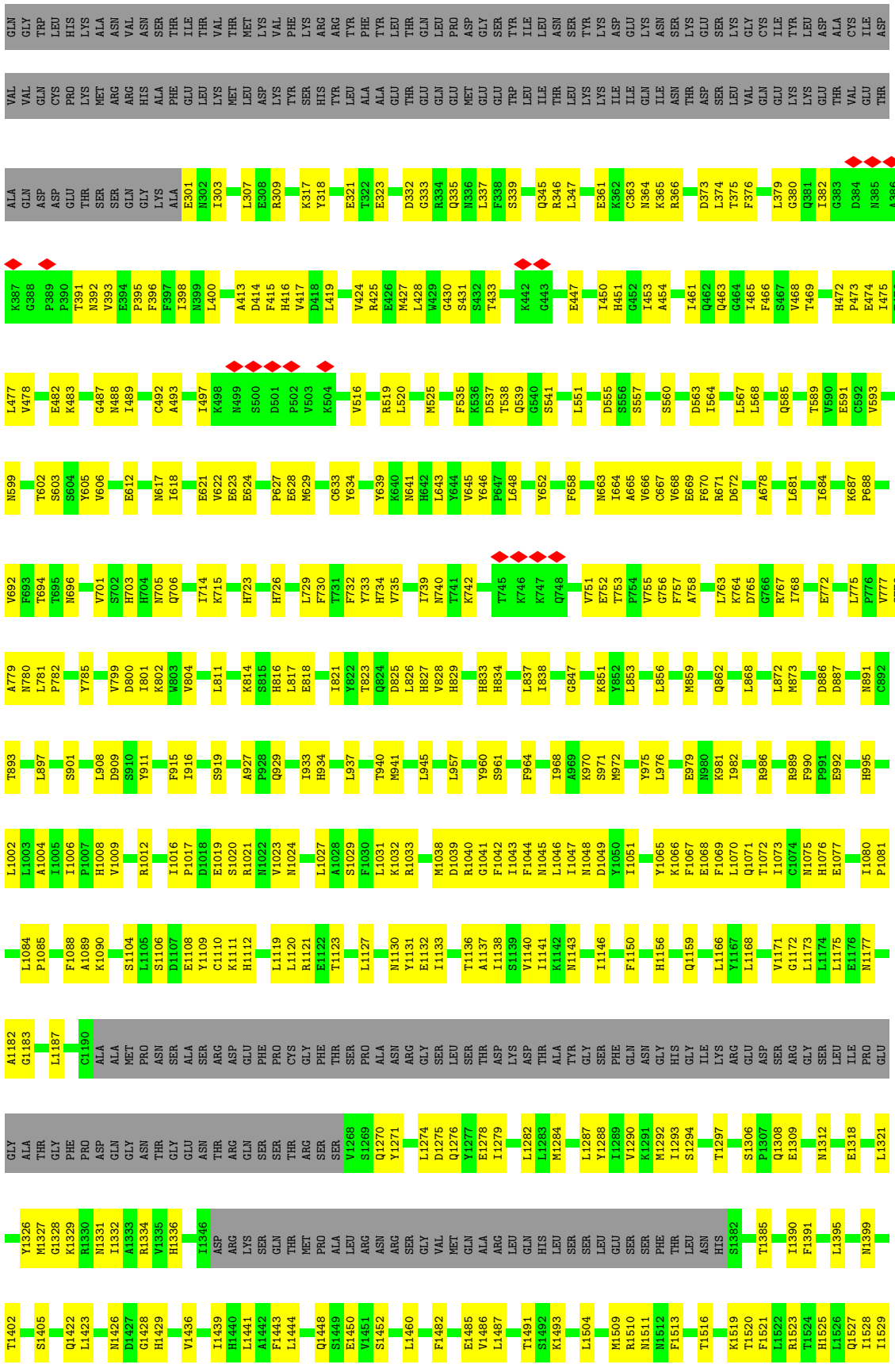


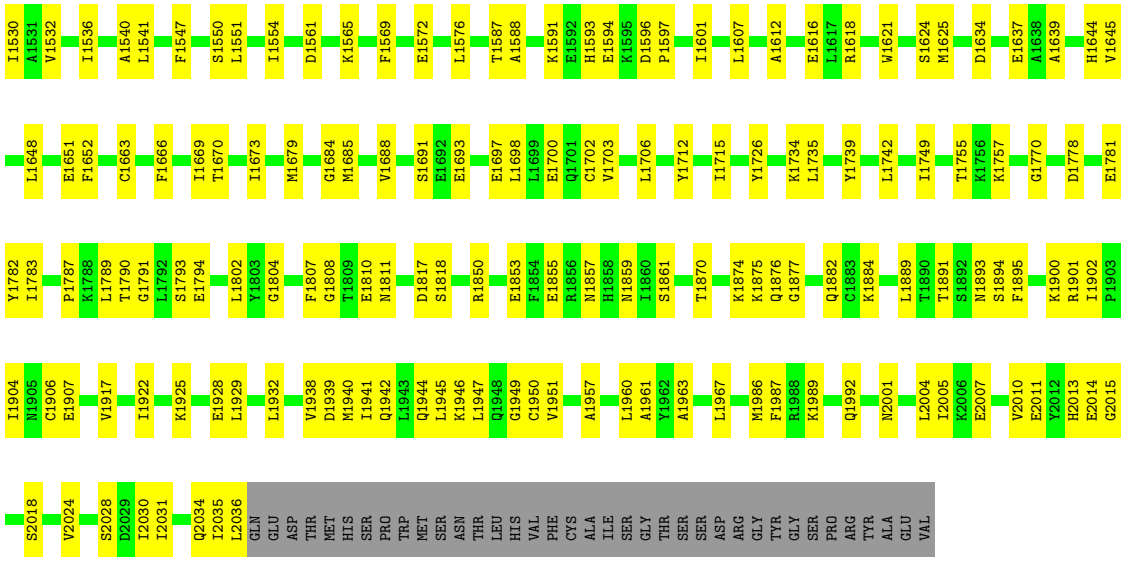


- Molecule 1: Dedicator of cytokinesis protein 11

Chain B:

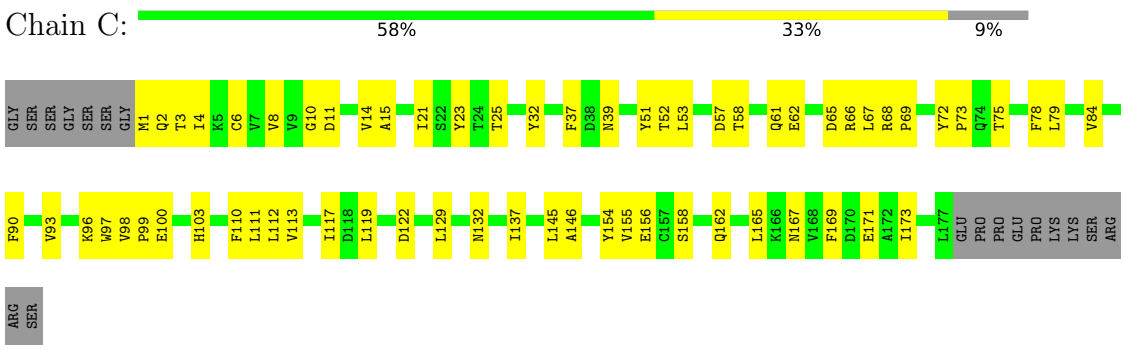



T1402 S1405 Q1422 L1423 N1426 D1427 G1428 H1429 V1436 I1439 H1440 L1441 A1442 F1443 L1444 Q1448 S1449 E1450 V1451 S1452 L1460 F1482 E1485 V1486 L1487 T1491 S1492 K1493 L1504 M1509 R1510 N1511 M1512 F1513 T1516 K1519 T1520 F1521 L1522 R1523 T1524 H1525 L1526 Q1527 I1528 I1529
Y1326 M1327 G1328 K1329 R1330 N1331 I1332 A1333 R1334 V1335 H1336 I1346 ASP ARG LYS SER GLN THR MET PRO ALA LEU ARG ASN ARG SER GLY VAL MET GLN ALA ARG LEU GLN HIS LEU SER SER LEU GLU SER SER PHE THR LEU ASN HIS S1382 T1385 I1390 F1391 L1395 N1399
GLY ALA THR GLY PHE PRO ASP GLN GLY ASN THR GLY GLU ASN THR ARG SER SER V1268 S1269 Q1270 Y1271 L1274 D1275 Q1276 Y1277 E1278 I1279 L1282 L1283 M1284 L1287 Y1288 I1289 V1290 K1291 M1292 I1293 S1294 T1297 S1306 P1307 Q1308 E1309 N1312 E1318 L1321
A1182 G1183 L1187 C1190 ALA ALA MET PRO ASN SER ALA SER ARG ASP GLU PHE PRO CYS GLY PHE THR SER PRO ALA ASN ARG GLY SER LEU SER THR ASP LYS ASP THR ALA TYR GLY SER PHE GLN ASN GLY HIS GLY ILE LYS ARG GLU ASP SER ARG GLY SER LEU ILE PRO GLU
L1084 P1085 F1088 A1089 K1090 S1104 L1105 S1106 D1107 E1108 Y1109 C1110 K1111 H1112 L1119 L1120 R1121 E1122 T1123 L1127 N1130 Y1131 E1132 I1133 T1136 A1137 I1138 S1139 V1140 I1141 K1142 N1143 I1146 F1150 H1156 Q1159 L1166 Y1167 L1168 V1171 G1172 L1173 L1174 L1175 E1176 N1177
L1002 L1003 A1004 I1005 I1006 P1007 H1008 V1009 R1012 I1016 P1017 D1018 E1019 S1020 R1021 N1022 V1023 N1024 L1027 A1028 S1029 F1030 L1031 K1032 R1033 M1038 D1039 R1040 G1041 F1042 I1043 F1044 N1045 L1046 I1047 N1048 D1049 Y1050 I1051 Y1065 K1066 F1067 E1068 F1069 L1070 Q1071 T1072 I1073 C1074 N1075 H1076 E1077 I1080 P1081
T893 L897 S901 L908 D909 S910 Y911 F915 I916 S919 A927 P928 Q929 I933 H934 L937 T940 M941 L945 L957 Y960 S961 F964 I968 A969 K970 S971 M972 Y975 L976 E979 N980 K981 I982 R986 R989 F990 P991 E992 H995
A779 N780 L781 P782 Y785 V799 D800 I801 K802 W803 V804 L811 K814 S815 H816 L817 E818 I821 Y822 T823 Q824 D825 L826 H827 V828 H829 H833 H834 L837 I838 G847 K851 Y852 L853 L856 M859 Q862 L868 L872 M873 D886 D887 N891 C892
V692 F693 T694 T695 N696 V701 S702 H703 H704 N705 Q706 I714 K715 H723 H726 L729 F730 T731 F732 Y733 H734 V735 I739 N740 T741 K742 T745 K746 K747 Q748 V751 E752 T753 P754 V755 G756 F757 A758 L763 K764 D765 G766 R767 I768 E772 L775 P776 V777 S778
N599 T602 S603 S604 Y605 V606 E612 N617 I618 E621 V622 E623 E624 P627 E628 M629 C633 Y634 Y639 K640 N641 H642 L643 Y644 V645 Y646 P647 L648 Y652 F658 N663 I664 A665 V666 C667 V668 E669 F670 R671 D672 A678 L681 I684 K687 P688
L477 V478 E482 K483 G487 N488 I489 C492 A493 I497 K498 N499 S500 D501 P502 V503 K504 V516 R519 L520 M525 F535 K536 D537 T538 Q539 G540 S541 L551 D555 S556 S557 S560 D563 I564 L567 L568 Q585 T589 V590 E591 C592 V593 S598
K387 G388 P389 P390 T391 N392 V393 E394 P395 F396 F397 I398 N399 L400 A413 D414 F415 H416 V417 D418 L419 V424 R425 E426 M427 L428 W429 G430 S431 S432 T433 K442 G443 E447 I450 H451 G452 I453 A454 I461 Q462 Q463 G464 I465 F466 S467 V468 T469 H472 P473 E474 I475 F476
ALA GLN ASP ASP GLU THR SER SER GLN GLY LYS ALA E301 N302 I303 L307 E308 R309 K317 Y318 E321 T322 E323 D332 G333 R334 Q335 N336 L337 F338 S339 Q345 R346 L347 E361 K362 C363 N364 K365 R366 D373 L374 T375 F376 L379 G380 Q381 I382 G383 D384 N385 A386
GLN GLY TRP LEU HIS LYS ALA ASN VAL ASN SER THR ILE THR VAL THR MET LYS VAL PHE LYS ARG ARG TYR PHE TYR LEU THR GLN LEU PRO ASP GLY SER TYR ILE LEU ASN SER TYR LYS ASP GLU LYS ASN SER LYS GLU SER LYS GLY CYS ILE TYR LEU ASP ALA CYS ILE ASP
VAL VAL GLN CYS PRO LYS MET ARG ARG HIS ALA PHE GLU LEU LYS MET LEU ASP LYS TYR SER HIS TYR LEU ALA GLU THR GLU GLN GLU MET GLU GLU TRP LEU ILE THR LEU LYS LYS ILE ILE GLN ILE ASN THR ASP SER LEU VAL GLN GLU LYS LYS GLU THR VAL GLU THR



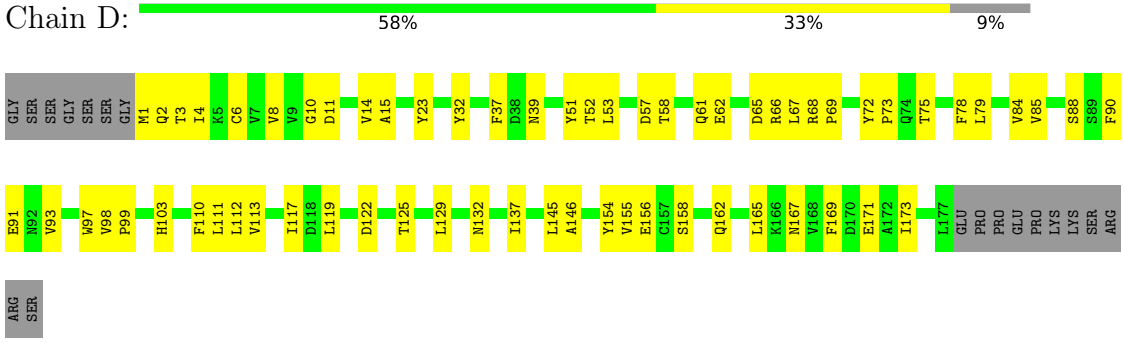
- Molecule 2: Cell division control protein 42 homolog

Chain C:



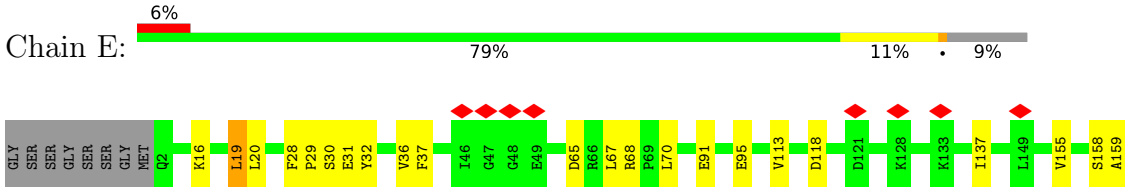
- Molecule 2: Cell division control protein 42 homolog

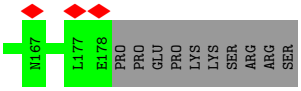
Chain D:



- Molecule 3: Cell division control protein 42 homolog

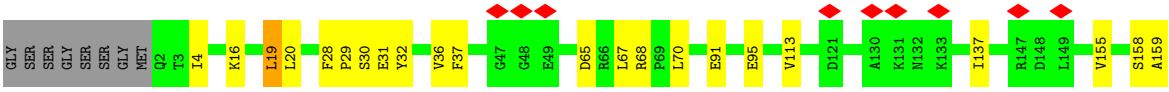
Chain E:

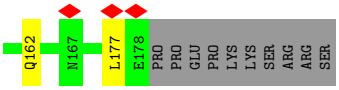




- Molecule 3: Cell division control protein 42 homolog

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	141956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.799	Depositor
Minimum map value	-0.272	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.077	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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: GTP, 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	0.22	0/14457	0.40	0/19534
1	B	0.22	0/14457	0.40	0/19534
2	C	0.20	0/1382	0.43	0/1891
2	D	0.20	0/1382	0.42	0/1891
3	E	0.17	0/1409	0.57	0/1919
3	F	0.17	0/1409	0.58	0/1919
All	All	0.22	0/34496	0.42	0/46688

There are no bond length outliers.

There are no bond angle outliers.

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	14143	14225	14221	488	0
1	B	14143	14225	14221	492	0
2	C	1352	1326	1328	57	0
2	D	1352	1326	1328	54	0
3	E	1379	1396	1394	15	0
3	F	1379	1396	1395	16	0
4	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
5	E	32	11	12	4	0
5	F	32	11	12	3	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
All	All	33818	33916	33911	1107	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 16.

The worst 5 of 1107 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:B:827:HIS:HB2	1:B:859:MET:HE1	1.51	0.92
1:A:827:HIS:HB2	1:A:859:MET:HE1	1.51	0.91
1:B:665:ALA:HB3	1:B:735:VAL:HG21	1.53	0.90
1:A:665:ALA:HB3	1:A:735:VAL:HG21	1.53	0.90
1:B:1783:ILE:HD11	1:B:1889:LEU:HD11	1.55	0.87

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	1735/2079 (84%)	1646 (95%)	89 (5%)	0	100 100
1	B	1735/2079 (84%)	1647 (95%)	88 (5%)	0	100 100
2	C	175/195 (90%)	166 (95%)	9 (5%)	0	100 100
2	D	175/195 (90%)	166 (95%)	9 (5%)	0	100 100
3	E	175/195 (90%)	167 (95%)	7 (4%)	1 (1%)	21 55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	175/195 (90%)	167 (95%)	7 (4%)	1 (1%)	21	55
All	All	4170/4938 (84%)	3959 (95%)	209 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	30	SER
3	F	30	SER

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	1586/1875 (85%)	1586 (100%)	0	100	100
1	B	1586/1875 (85%)	1586 (100%)	0	100	100
2	C	149/172 (87%)	149 (100%)	0	100	100
2	D	149/172 (87%)	149 (100%)	0	100	100
3	E	157/172 (91%)	156 (99%)	1 (1%)	78	79
3	F	157/172 (91%)	156 (99%)	1 (1%)	78	79
All	All	3784/4438 (85%)	3782 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	19	LEU
3	F	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	585	GLN
1	B	1045	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	39	ASN
1	B	703	HIS
1	B	740	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	GTP	E	202	4	30,34,34	0.81	1 (3%)	46,54,54	1.78	11 (23%)
5	GTP	F	202	4	30,34,34	0.83	1 (3%)	46,54,54	1.79	10 (21%)

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	GTP	E	202	4	-	1/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	F	202	4	-	1/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	202	GTP	C2-N3	2.21	1.38	1.33
5	E	202	GTP	C2-N3	2.14	1.38	1.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	202	GTP	C5-C4-N3	-5.04	120.29	128.46
5	E	202	GTP	C5-C4-N3	-4.99	120.37	128.46
5	E	202	GTP	C2-N3-C4	4.50	120.32	112.30
5	F	202	GTP	C2-N3-C4	4.50	120.32	112.30
5	F	202	GTP	PB-O3B-PG	-4.04	118.97	132.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	202	GTP	PB-O3A-PA-O2A
5	F	202	GTP	PB-O3A-PA-O2A

There are no ring outliers.

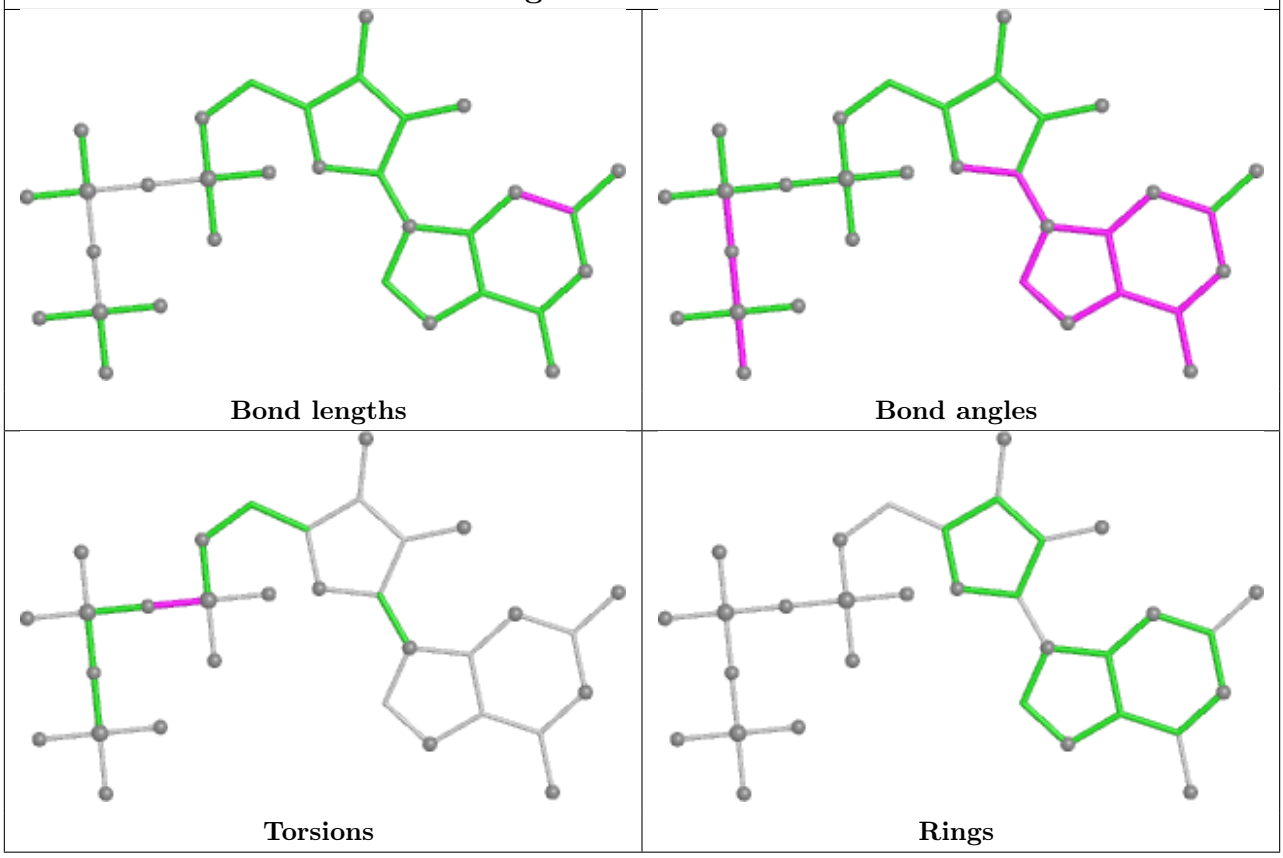
2 monomers are involved in 7 short contacts:

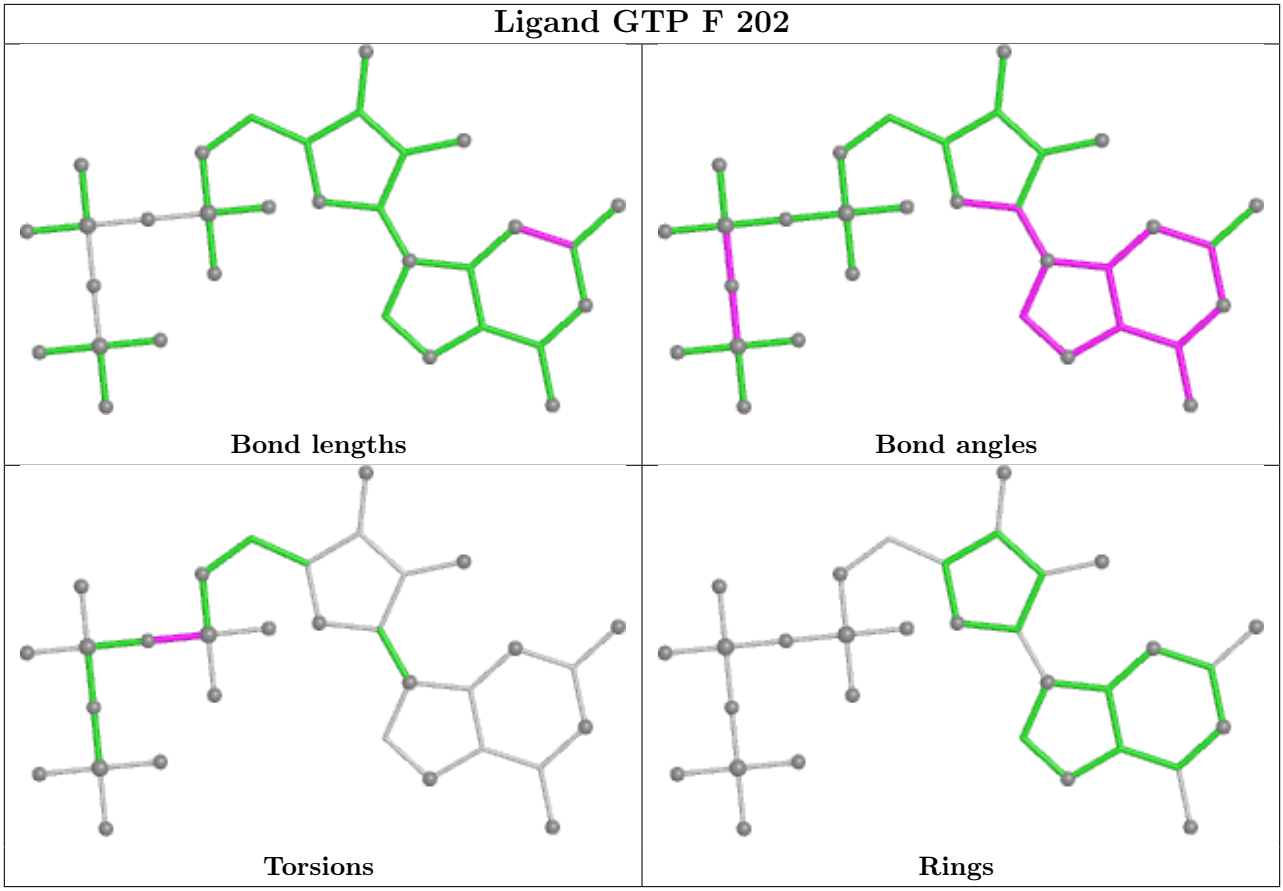
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	202	GTP	4	0
5	F	202	GTP	3	0

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 GTP E 202





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.

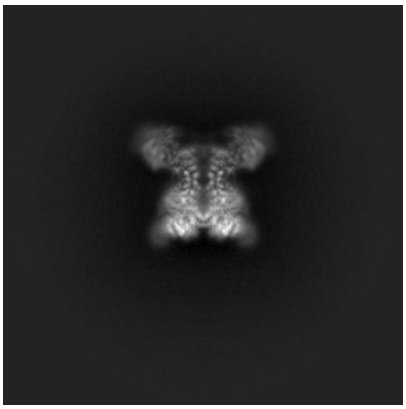
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-68713. These allow visual inspection of the internal detail of the map and identification of artifacts.

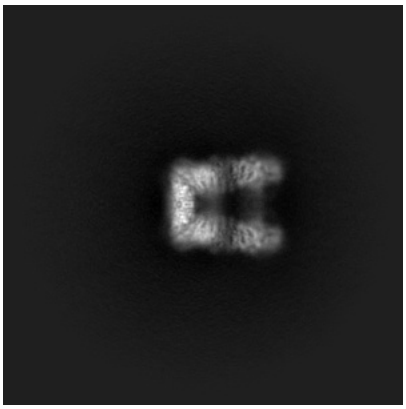
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

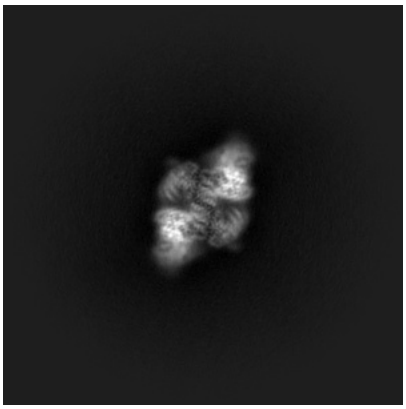
6.1.1 Primary map



X

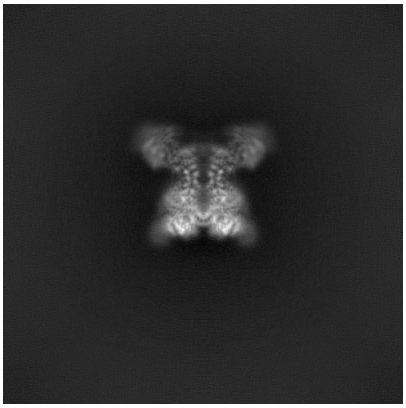


Y

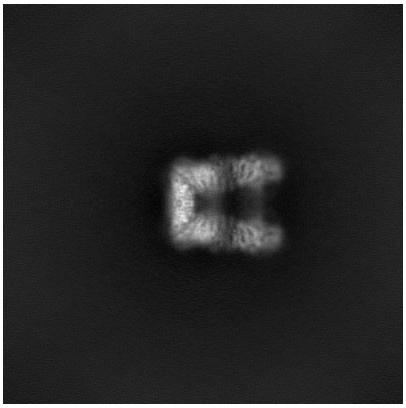


Z

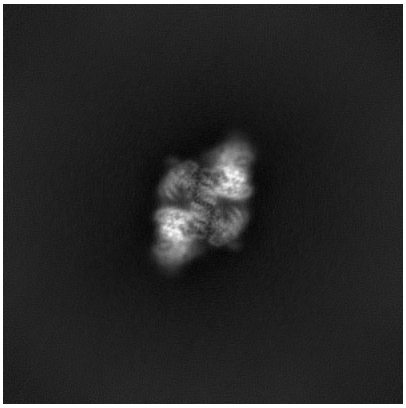
6.1.2 Raw map



X



Y

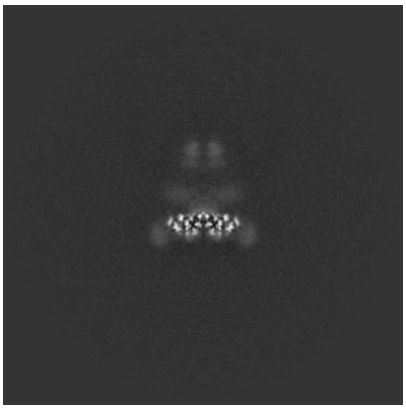


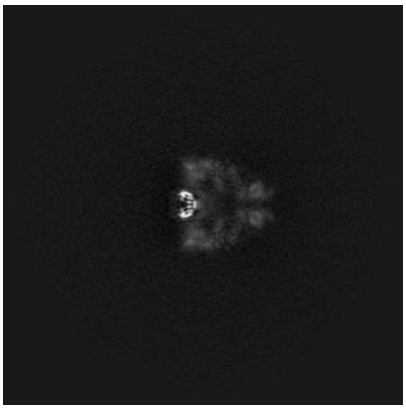
Z

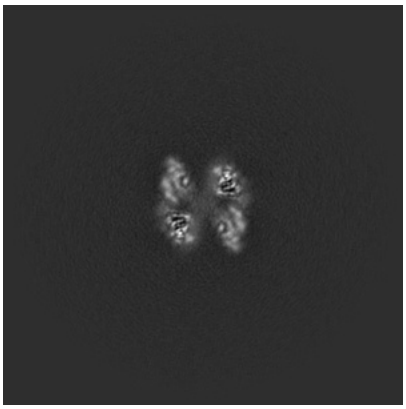
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

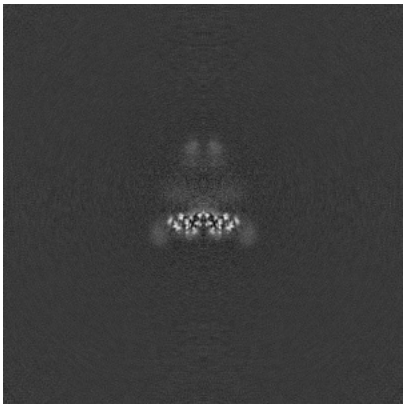
6.2.1 Primary map

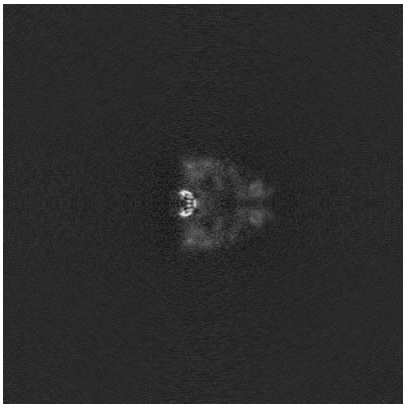

X Index: 200


Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200


Y Index: 200

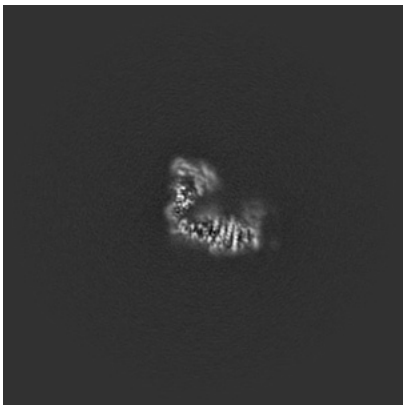
Z Index: 200

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

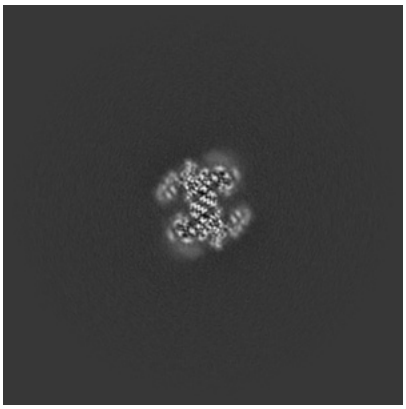
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 228

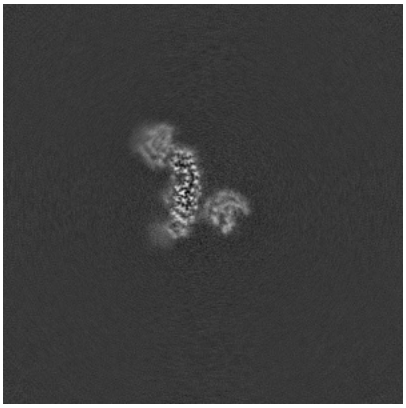


Y Index: 183



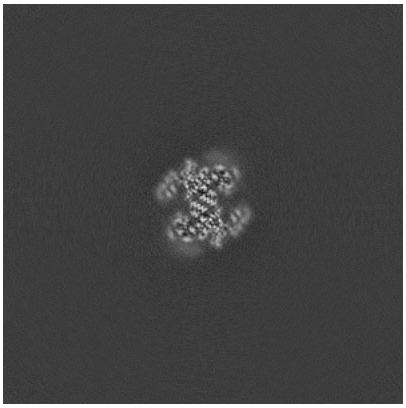
Z Index: 180

6.3.2 Raw map



X Index: 172

Y Index: 183



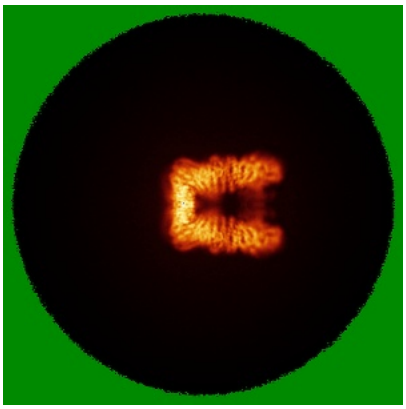
Z Index: 180

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

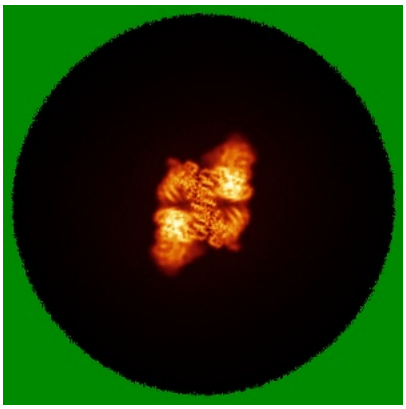
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X

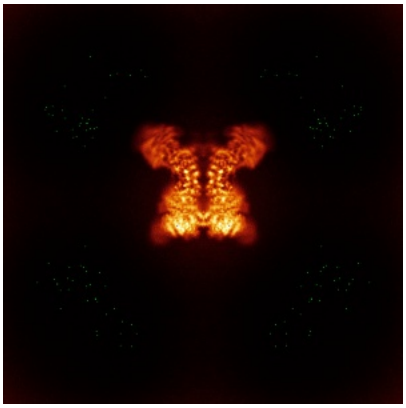


Y

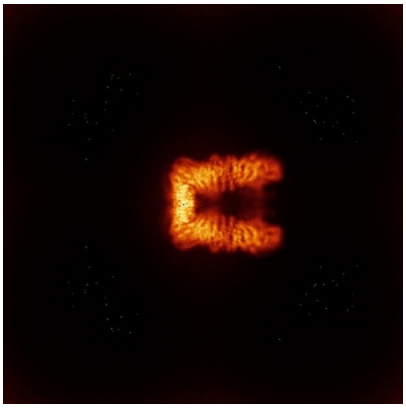


Z

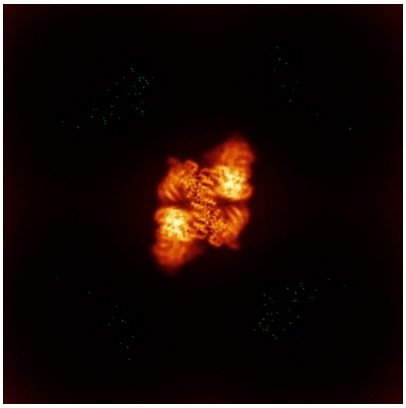
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

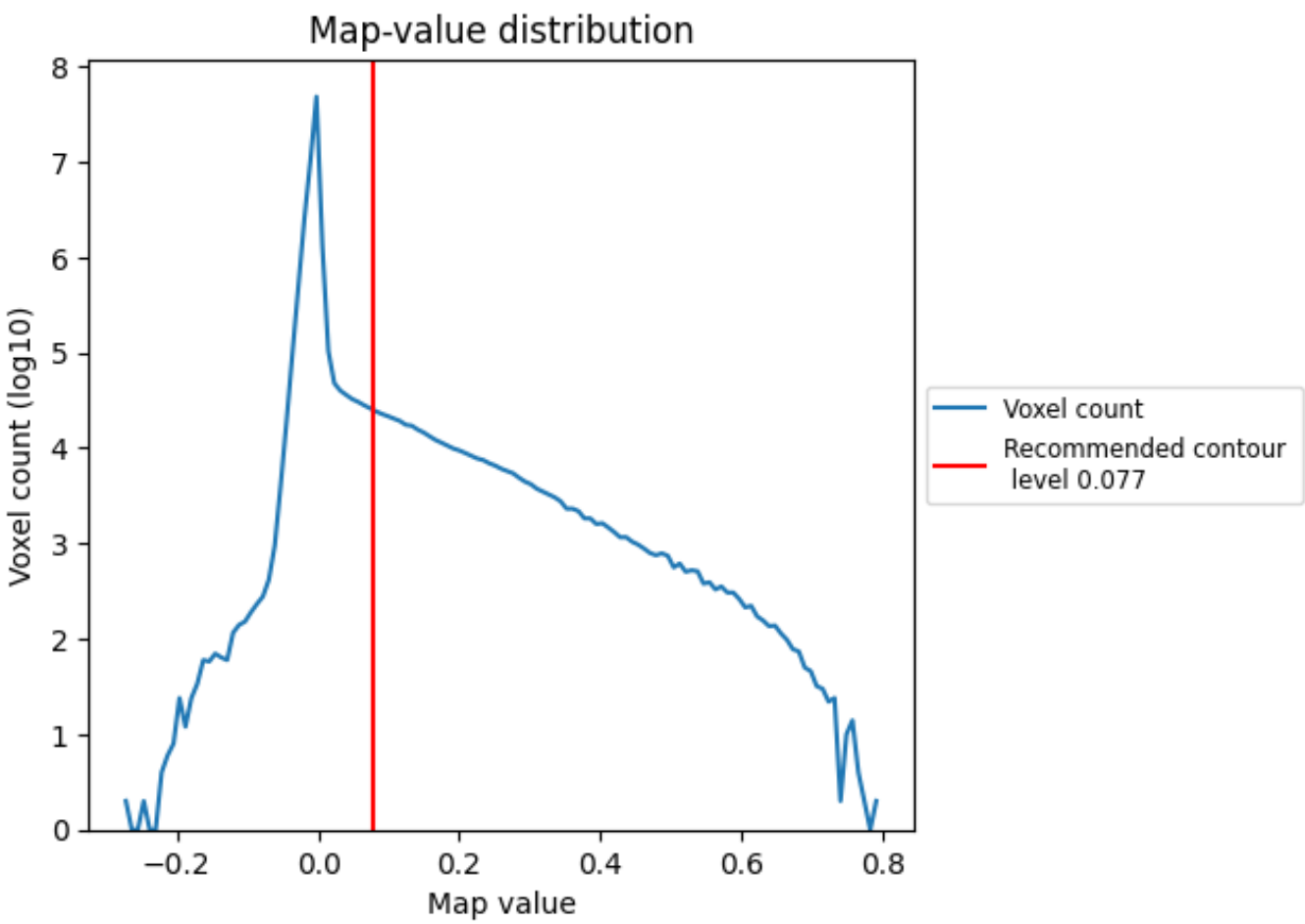
6.6 Mask visualisation (i)

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

7 Map analysis (i)

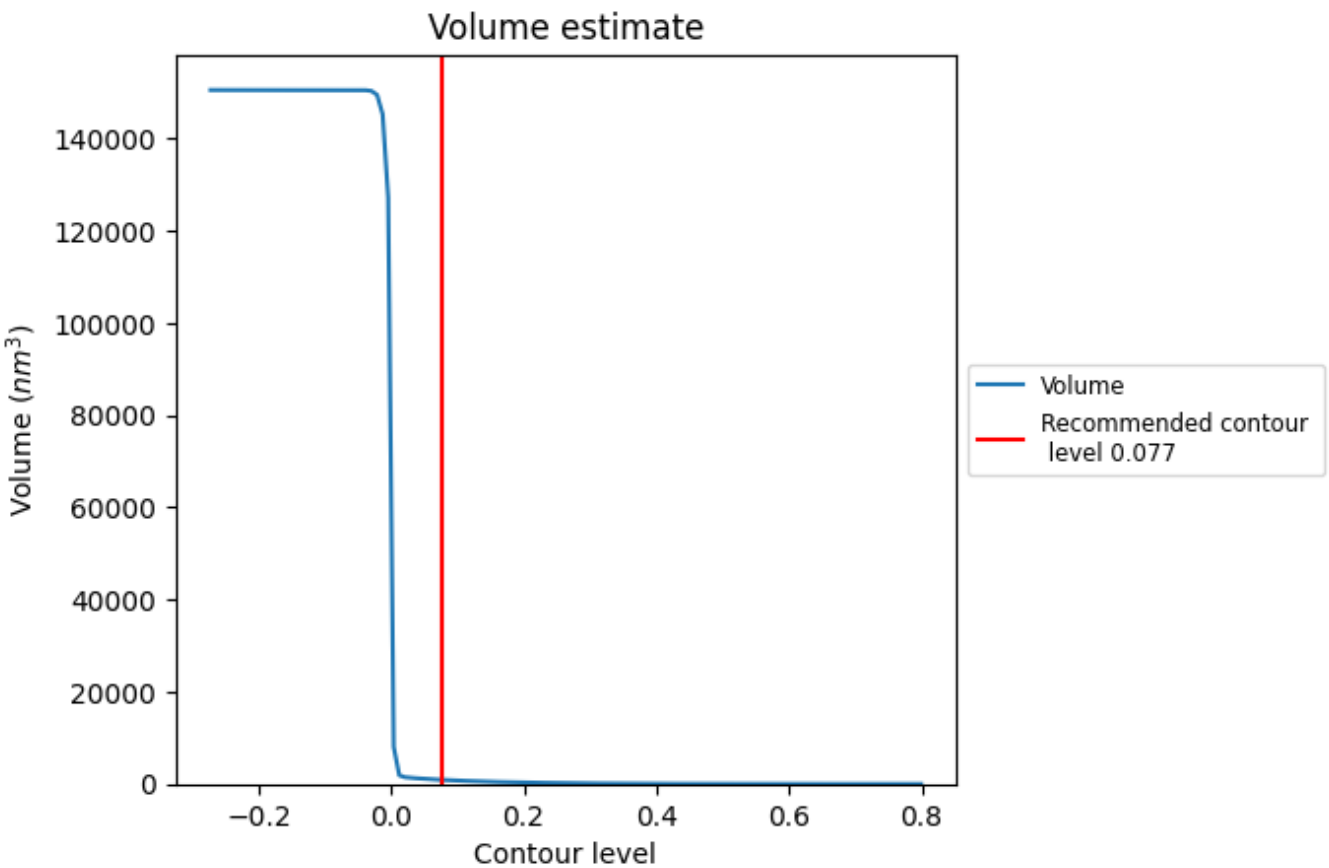
This section contains the results of statistical analysis of the map.

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.

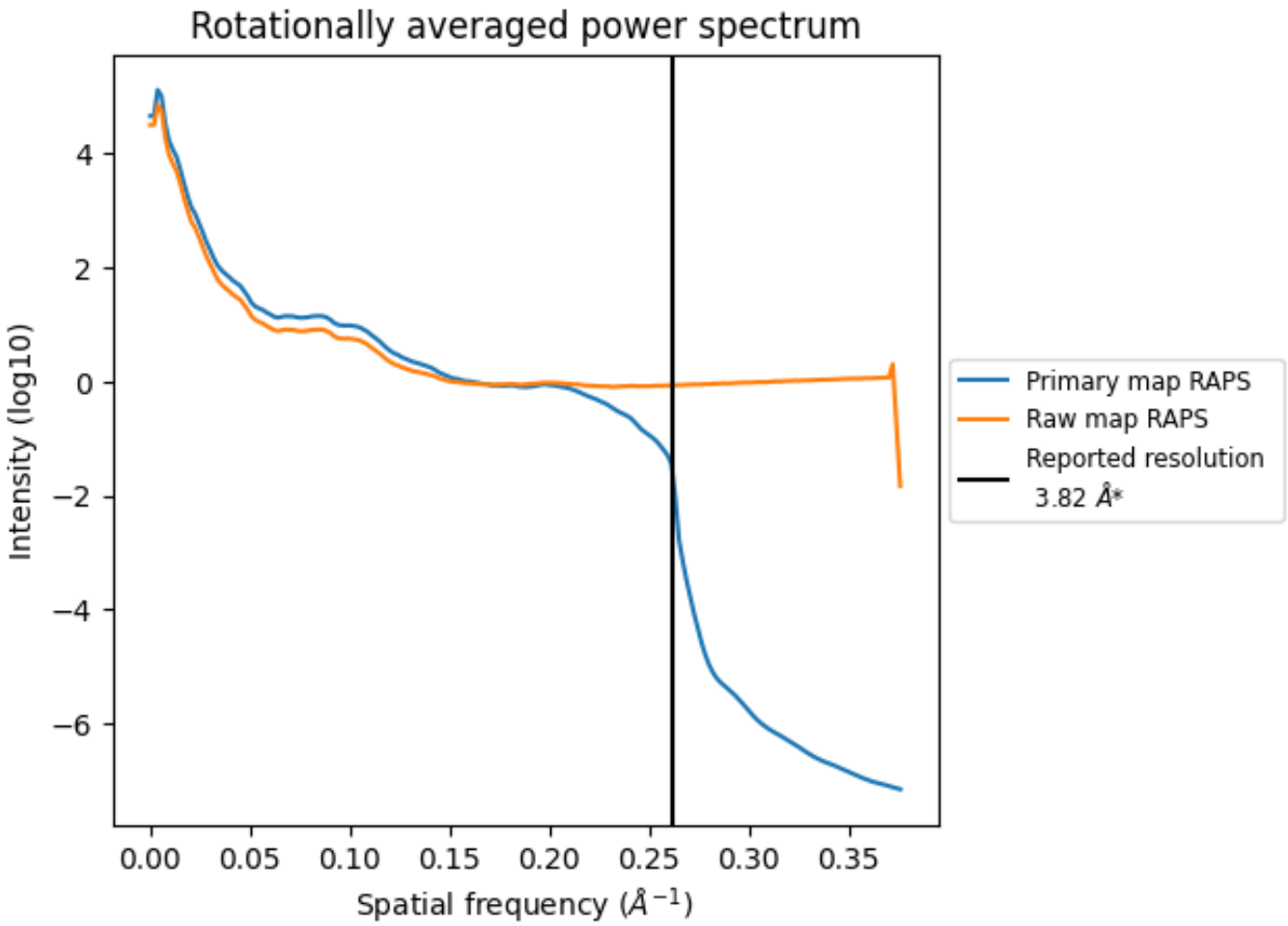
7.2 Volume estimate (i)



The volume at the recommended contour level is 894 nm^3; this corresponds to an approximate mass of 808 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)

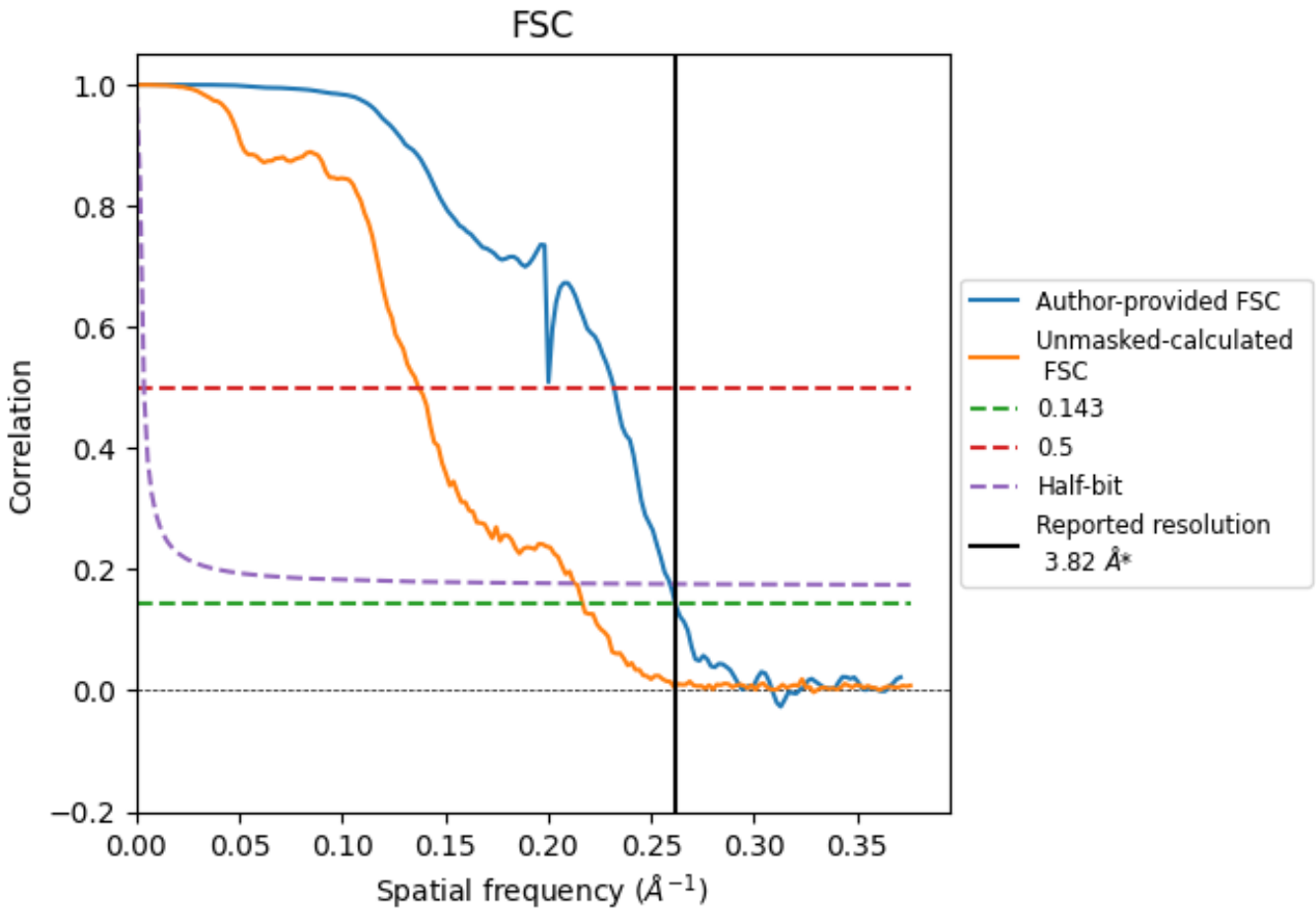


*Reported resolution corresponds to spatial frequency of 0.262 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.262 Å^{-1}

8.2 Resolution estimates (i)

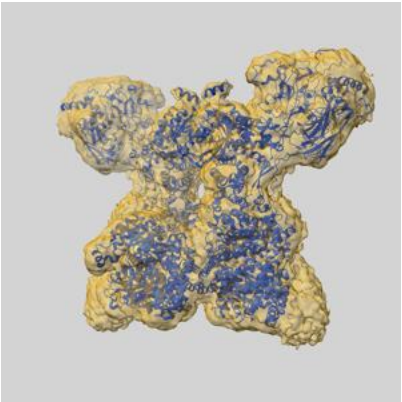
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	3.82	4.31	3.86
Unmasked-calculated*	4.61	7.29	4.69

*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 4.61 differs from the reported value 3.82 by more than 10 %

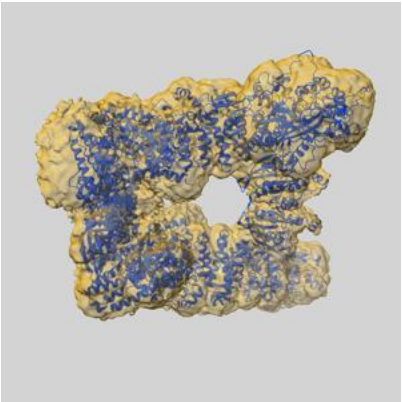
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-68713 and PDB model 22VF. Per-residue inclusion information can be found in section 3 on page 8.

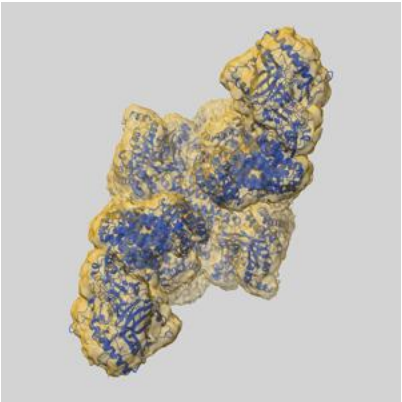
9.1 Map-model overlay (i)



X



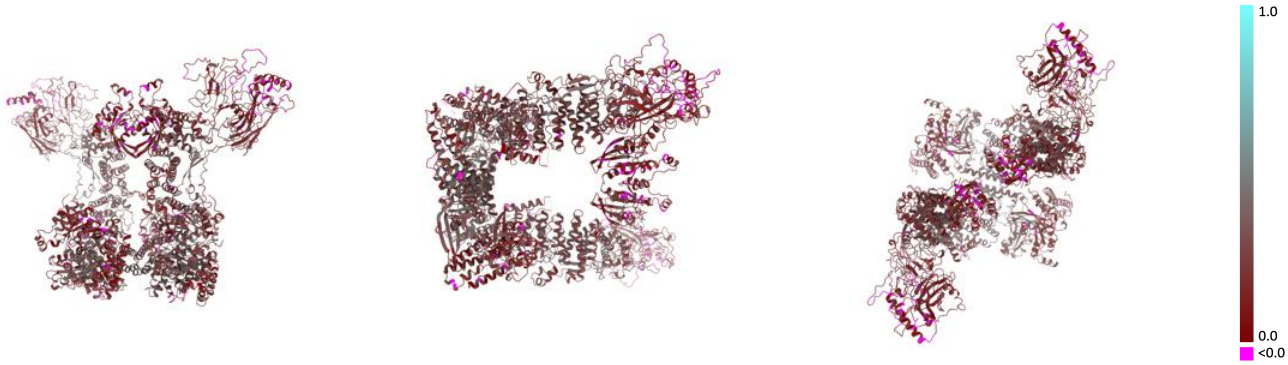
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.077 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.

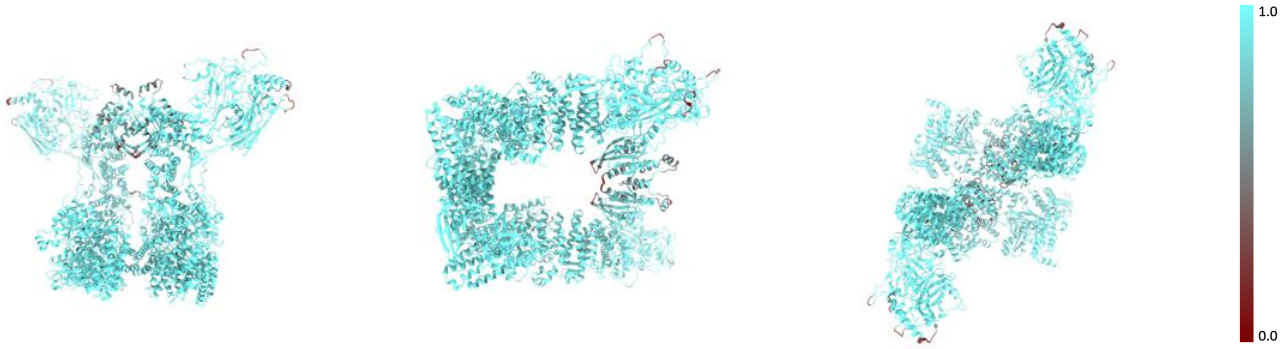
9.2 Q-score mapped to coordinate model (i)



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.

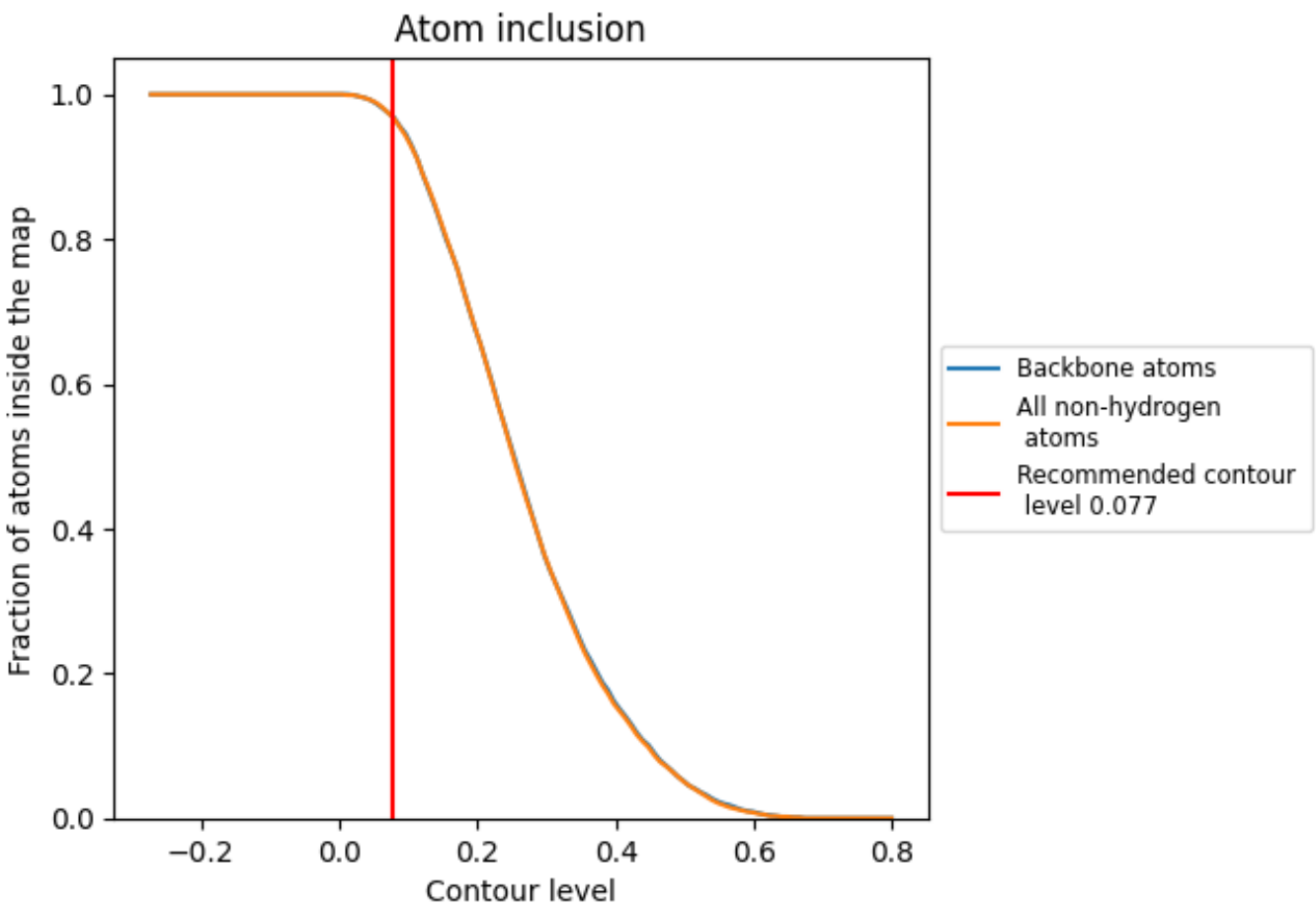
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.077).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9690	0.2410
A	0.9830	0.2540
B	0.9820	0.2550
C	0.9940	0.1990
D	0.9940	0.2010
E	0.8030	0.1420
F	0.8130	0.1490