Full wwPDB EM Validation Report ⓘ

Feb 3, 2025 – 01:15 PM EST

PDB ID	:	9MHF
EMDB ID	:	EMD-48276
Title	:	Cryo-EM reconstruction of PI3KC3-C1 in complex with Human RAB1A(Q70L)
Authors	:	Cook, A.S.I.; Hurley, J.H.; Chen, M.
Deposited on	:	2024-12-11
Resolution	:	2.73 Å(reported)
Based on initial model	:	.

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

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

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

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

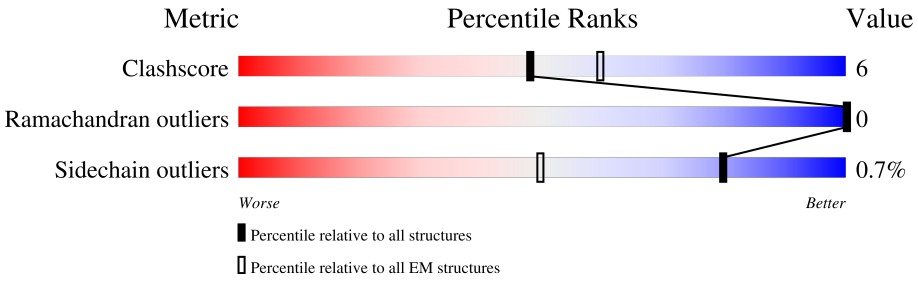
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1409	5% 70% 14% 16%
2	B	887	26% 70%
3	C	492	46% 8% 46%
4	D	450	12% 57% 10% 32%
5	E	226	65% 12% 24%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 17739 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 Phosphoinositide 3-kinase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1179	9403	5993	1637	1726	47	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q99570
A	1359	GLY	-	expression tag	UNP Q99570
A	1360	THR	-	expression tag	UNP Q99570
A	1361	GLU	-	expression tag	UNP Q99570
A	1362	ASN	-	expression tag	UNP Q99570
A	1363	LEU	-	expression tag	UNP Q99570
A	1364	TYR	-	expression tag	UNP Q99570
A	1365	PHE	-	expression tag	UNP Q99570
A	1366	GLN	-	expression tag	UNP Q99570
A	1367	SER	-	expression tag	UNP Q99570
A	1368	GLY	-	expression tag	UNP Q99570
A	1369	MET	-	expression tag	UNP Q99570
A	1370	ALA	-	expression tag	UNP Q99570
A	1371	ALA	-	expression tag	UNP Q99570
A	1372	TRP	-	expression tag	UNP Q99570
A	1373	SER	-	expression tag	UNP Q99570
A	1374	HIS	-	expression tag	UNP Q99570
A	1375	PRO	-	expression tag	UNP Q99570
A	1376	GLN	-	expression tag	UNP Q99570
A	1377	PHE	-	expression tag	UNP Q99570
A	1378	GLU	-	expression tag	UNP Q99570
A	1379	LYS	-	expression tag	UNP Q99570
A	1380	GLY	-	expression tag	UNP Q99570
A	1381	GLY	-	expression tag	UNP Q99570
A	1382	GLY	-	expression tag	UNP Q99570
A	1383	ALA	-	expression tag	UNP Q99570
A	1384	ARG	-	expression tag	UNP Q99570
A	1385	GLY	-	expression tag	UNP Q99570

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1386	GLY	-	expression tag	UNP Q99570
A	1387	SER	-	expression tag	UNP Q99570
A	1388	GLY	-	expression tag	UNP Q99570
A	1389	GLY	-	expression tag	UNP Q99570
A	1390	GLY	-	expression tag	UNP Q99570
A	1391	SER	-	expression tag	UNP Q99570
A	1392	TRP	-	expression tag	UNP Q99570
A	1393	SER	-	expression tag	UNP Q99570
A	1394	HIS	-	expression tag	UNP Q99570
A	1395	PRO	-	expression tag	UNP Q99570
A	1396	GLN	-	expression tag	UNP Q99570
A	1397	PHE	-	expression tag	UNP Q99570
A	1398	GLU	-	expression tag	UNP Q99570
A	1399	LYS	-	expression tag	UNP Q99570
A	1400	GLY	-	expression tag	UNP Q99570
A	1401	PHE	-	expression tag	UNP Q99570
A	1402	ASP	-	expression tag	UNP Q99570
A	1403	TYR	-	expression tag	UNP Q99570
A	1404	LYS	-	expression tag	UNP Q99570
A	1405	ASP	-	expression tag	UNP Q99570
A	1406	ASP	-	expression tag	UNP Q99570
A	1407	ASP	-	expression tag	UNP Q99570
A	1408	ASP	-	expression tag	UNP Q99570
A	1409	LYS	-	expression tag	UNP Q99570

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase catalytic subunit type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	267	Total	C	N	O	S	0	0
			2162	1382	365	399	16		

- Molecule 3 is a protein called Beclin 1-associated autophagy-related key regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	265	Total	C	N	O	S	0	0
			2176	1371	393	401	11		

- Molecule 4 is a protein called Beclin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	305	Total	C	N	O	S	0	0
			2531	1596	431	492	12		

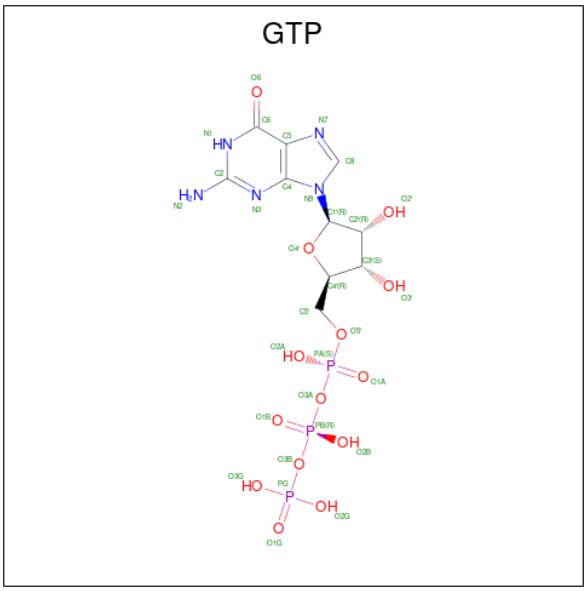
- Molecule 5 is a protein called Ras-related protein Rab-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	172	Total	C	N	O	S	0	0
			1376	878	224	269	5		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	MET	-	expression tag	UNP P62820
E	-19	LYS	-	expression tag	UNP P62820
E	-18	SER	-	expression tag	UNP P62820
E	-17	SER	-	expression tag	UNP P62820
E	-16	HIS	-	expression tag	UNP P62820
E	-15	HIS	-	expression tag	UNP P62820
E	-14	HIS	-	expression tag	UNP P62820
E	-13	HIS	-	expression tag	UNP P62820
E	-12	HIS	-	expression tag	UNP P62820
E	-11	HIS	-	expression tag	UNP P62820
E	-10	GLU	-	expression tag	UNP P62820
E	-9	ASN	-	expression tag	UNP P62820
E	-8	LEU	-	expression tag	UNP P62820
E	-7	TYR	-	expression tag	UNP P62820
E	-6	PHE	-	expression tag	UNP P62820
E	-5	GLN	-	expression tag	UNP P62820
E	-4	SER	-	expression tag	UNP P62820
E	-3	ASN	-	expression tag	UNP P62820
E	-2	ALA	-	expression tag	UNP P62820
E	-1	MET	-	expression tag	UNP P62820
E	0	GLY	-	expression tag	UNP P62820
E	70	LEU	GLN	engineered mutation	UNP P62820

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

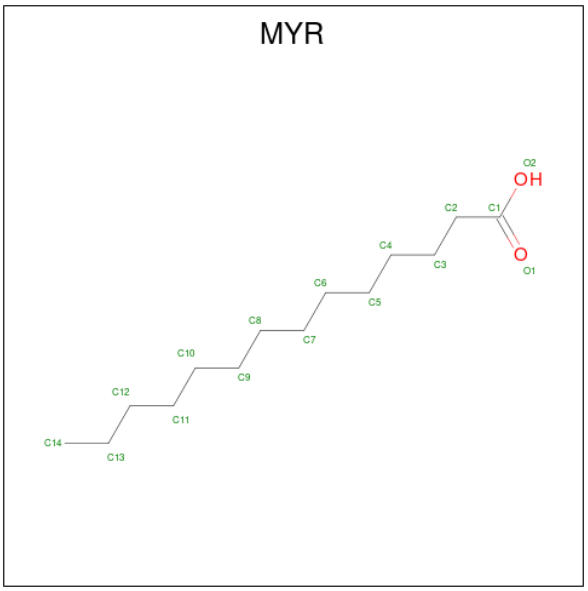


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	E	1	Total	Mg	0
			1	1	

- Molecule 8 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C O 16 14 2	0

- Molecule 9 is water.

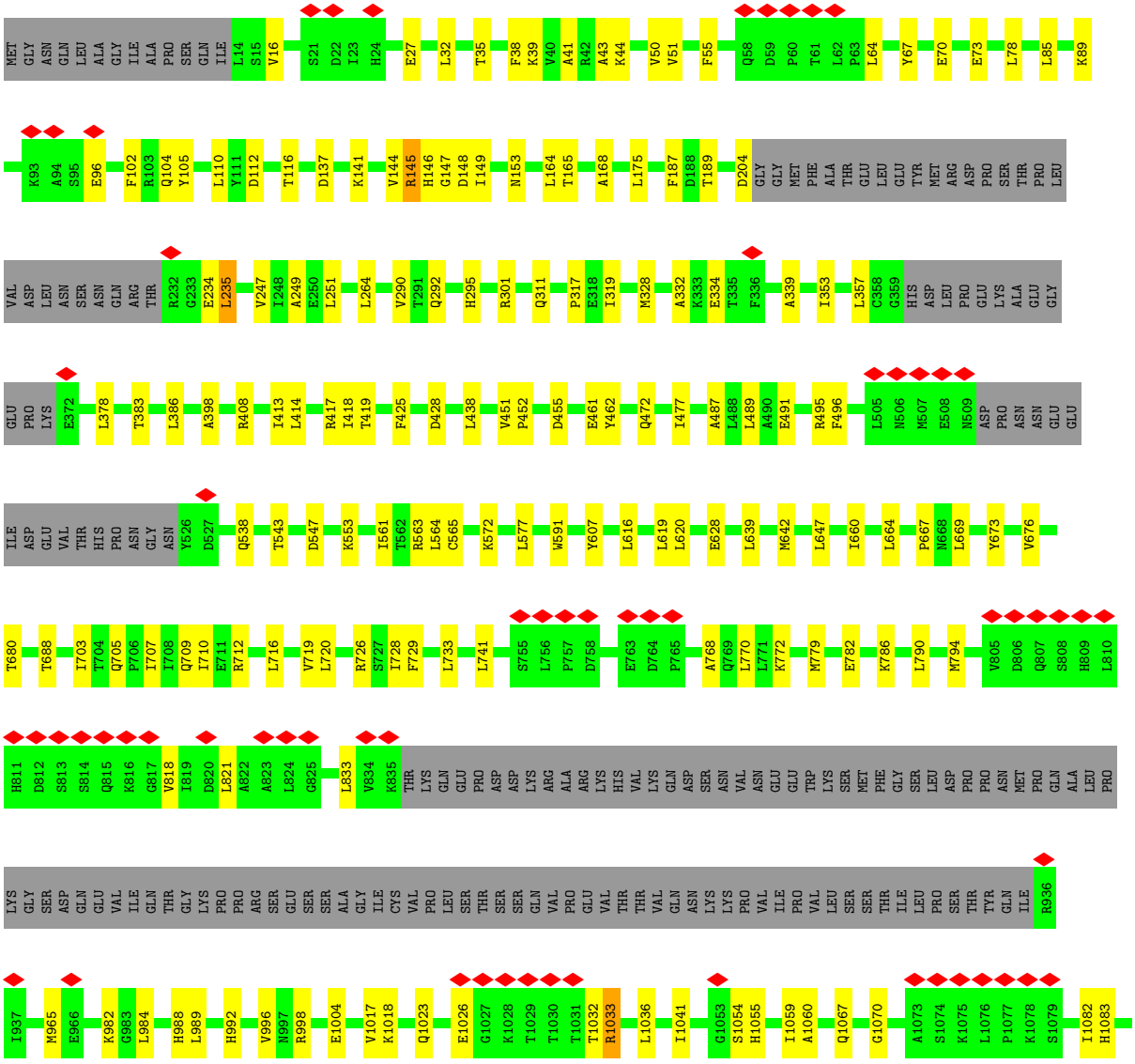
Mol	Chain	Residues	Atoms	AltConf
9	A	3	Total O 3 3	0
9	E	6	Total O 6 6	0

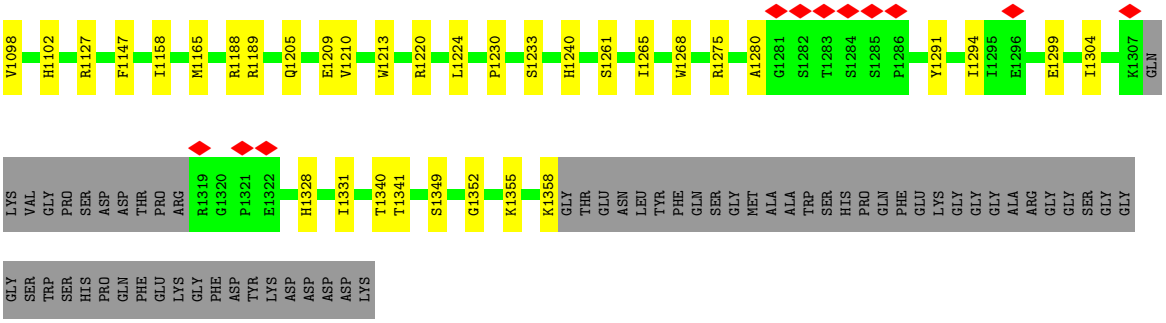
3 Residue-property plots (i)

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: Phosphoinositide 3-kinase regulatory subunit 4

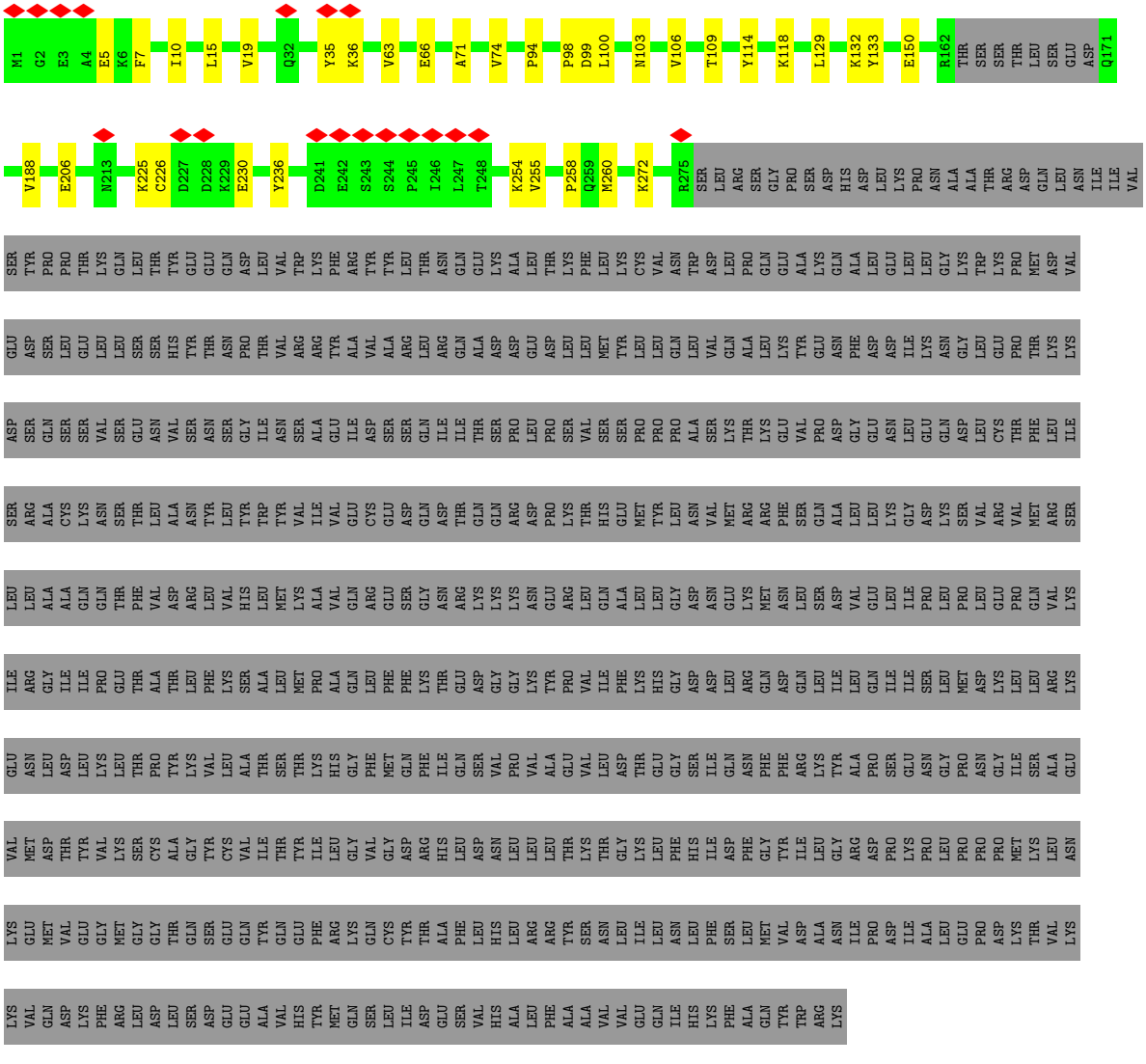
Chain A:





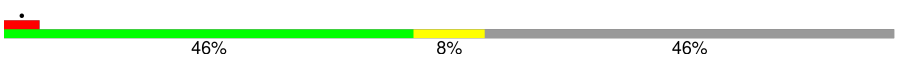
• Molecule 2: Phosphatidylinositol 3-kinase catalytic subunit type 3

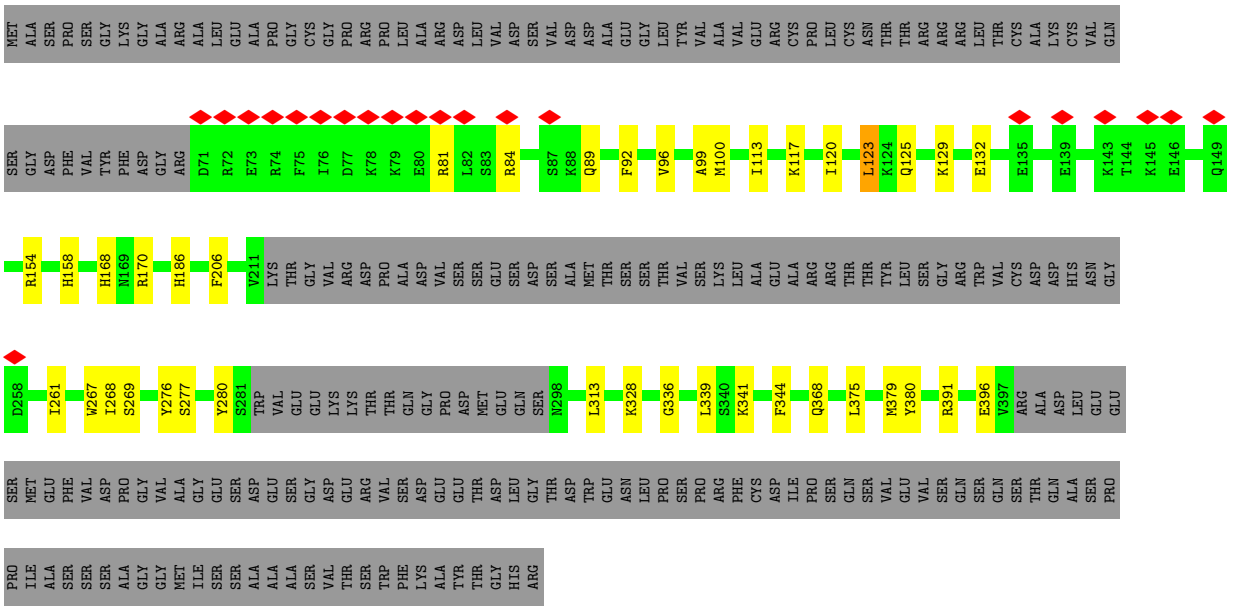
Chain B:



• Molecule 3: Beclin 1-associated autophagy-related key regulator

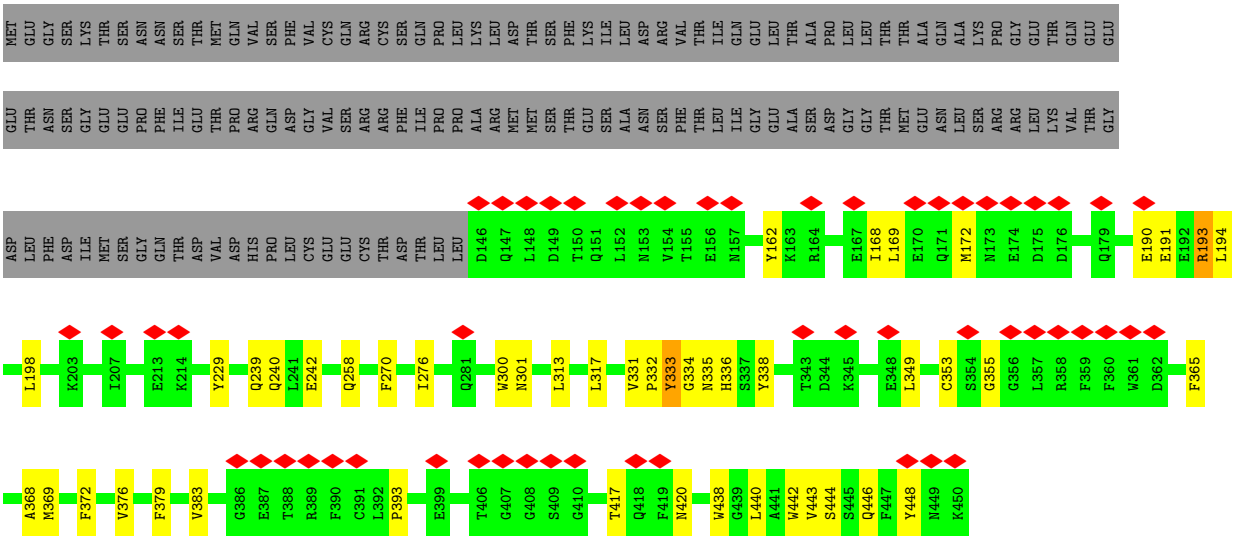
Chain C:





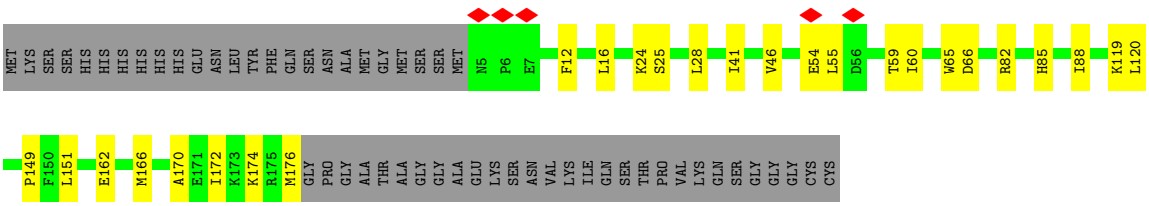
• Molecule 4: Beclin-1

Chain D:



• Molecule 5: Ras-related protein Rab-1A

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	721454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.352	Depositor
Minimum map value	-0.302	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.60	0/9607	0.68	1/13018 (0.0%)
2	B	0.63	0/2215	0.65	0/2988
3	C	0.52	0/2211	0.61	1/2964 (0.0%)
4	D	0.54	0/2580	0.59	0/3471
5	E	0.57	0/1399	0.60	0/1890
All	All	0.59	0/18012	0.65	2/24331 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
3	C	0	2
4	D	0	1
5	E	0	1
All	All	0	10

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	235	LEU	CB-CG-CD2	-6.04	100.74	111.00
3	C	123	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1189	ARG	Sidechain
1	A	301	ARG	Sidechain
1	A	408	ARG	Sidechain
1	A	495	ARG	Sidechain
1	A	712	ARG	Sidechain
1	A	998	ARG	Sidechain
3	C	170	ARG	Sidechain
3	C	391	ARG	Sidechain
4	D	193	ARG	Sidechain
5	E	82	ARG	Sidechain

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	9403	0	9455	115	0
2	B	2162	0	2145	28	0
3	C	2176	0	2229	35	0
4	D	2531	0	2448	37	0
5	E	1376	0	1372	15	0
6	A	32	0	12	0	0
6	E	32	0	12	3	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
8	A	16	0	27	0	0
9	A	3	0	0	1	0
9	E	6	0	0	2	0
All	All	17739	0	17700	201	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 (201) 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:1017:VAL:HG21	1:A:1059:ILE:HG21	1.70	0.74
1:A:153:ASN:OD1	9:A:2101:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:270:PHE:HB3	4:D:440:LEU:HD11	1.70	0.73
1:A:477:ILE:HD12	2:B:99:ASP:HB3	1.72	0.72
1:A:1188:ARG:HH21	1:A:1205:GLN:HE22	1.36	0.72
1:A:965:MET:HG3	2:B:188:VAL:HG21	1.73	0.71
6:E:1000:GTP:O3G	9:E:1101:HOH:O	2.09	0.70
1:A:85:LEU:HB3	1:A:165:THR:HG22	1.73	0.69
1:A:982:LYS:HG3	1:A:984:LEU:HG	1.76	0.68
1:A:1210:VAL:HB	1:A:1224:LEU:HD12	1.77	0.66
1:A:703:ILE:HD12	1:A:719:VAL:HG23	1.78	0.65
1:A:591:TRP:CD2	1:A:628:GLU:HG2	2.32	0.64
1:A:1004:GLU:OE2	1:A:1054:SER:HB3	1.98	0.64
3:C:261:ILE:HG23	3:C:375:LEU:HD12	1.81	0.63
4:D:379:PHE:O	4:D:383:VAL:HG23	1.99	0.62
2:B:63:VAL:HG22	2:B:106:VAL:HG12	1.81	0.61
3:C:81:ARG:HA	3:C:84:ARG:HD2	1.82	0.60
3:C:277:SER:HA	3:C:280:TYR:CD1	2.38	0.59
4:D:331:VAL:HG11	4:D:338:TYR:CE1	2.37	0.59
1:A:561:ILE:HD11	1:A:577:LEU:HD11	1.84	0.58
1:A:78:LEU:HD11	1:A:144:VAL:HG11	1.85	0.58
1:A:149:ILE:HG22	1:A:247:VAL:HG21	1.85	0.58
4:D:383:VAL:HG13	4:D:442:TRP:CE2	2.38	0.58
4:D:444:SER:O	4:D:448:TYR:HB3	2.04	0.58
1:A:707:ILE:O	1:A:710:ILE:HG23	2.04	0.57
1:A:147:GLY:CA	1:A:235:LEU:HD21	2.34	0.57
1:A:353:ILE:HG21	1:A:378:LEU:HD22	1.86	0.56
1:A:1224:LEU:HD22	1:A:1268:TRP:CE3	2.40	0.56
1:A:728:ILE:HD13	1:A:779:MET:HA	1.86	0.56
1:A:145:ARG:HB3	1:A:235:LEU:HD23	1.88	0.55
1:A:1158:ILE:O	1:A:1165:MET:HA	2.07	0.55
3:C:123:LEU:HB3	4:D:194:LEU:CD2	2.36	0.55
1:A:1340:THR:HG23	1:A:1341:THR:H	1.72	0.55
1:A:292:GLN:O	1:A:295:HIS:HB2	2.06	0.55
1:A:319:ILE:HG12	1:A:357:LEU:HD23	1.89	0.55
3:C:113:ILE:HG22	3:C:117:LYS:HE3	1.89	0.55
1:A:332:ALA:O	2:B:255:VAL:HG13	2.07	0.54
5:E:24:LYS:HE2	9:E:1102:HOH:O	2.06	0.54
1:A:110:LEU:HD11	1:A:251:LEU:HD13	1.88	0.54
1:A:821:LEU:HB2	2:B:226:CYS:SG	2.48	0.54
3:C:277:SER:HA	3:C:280:TYR:HD1	1.71	0.54
3:C:186:HIS:HE1	4:D:258:GLN:HE21	1.56	0.54
4:D:372:PHE:O	4:D:376:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:VAL:HG13	2:B:129:LEU:HD21	1.90	0.53
4:D:300:TRP:CD1	4:D:355:GLY:HA2	2.42	0.53
4:D:383:VAL:HG13	4:D:442:TRP:CD2	2.43	0.53
1:A:782:GLU:HG3	1:A:786:LYS:HE3	1.91	0.53
1:A:148:ASP:OD1	1:A:168:ALA:HB2	2.08	0.53
1:A:676:VAL:HG13	1:A:716:LEU:HD23	1.90	0.53
1:A:818:VAL:HG13	2:B:225:LYS:HG3	1.92	0.52
1:A:1036:LEU:HB3	1:A:1082:ILE:HD11	1.89	0.52
1:A:1291:TYR:CD1	1:A:1304:ILE:HD13	2.45	0.52
3:C:158:HIS:HD2	4:D:229:TYR:CE2	2.27	0.52
3:C:154:ARG:HG2	3:C:158:HIS:CE1	2.44	0.52
3:C:280:TYR:CE2	3:C:344:PHE:HD2	2.28	0.52
5:E:25:SER:OG	6:E:1000:GTP:O2B	2.27	0.52
4:D:317:LEU:HD22	4:D:443:VAL:HG21	1.90	0.51
1:A:27:GLU:HG3	1:A:44:LYS:HE2	1.93	0.51
3:C:261:ILE:HD11	3:C:379:MET:SD	2.49	0.51
1:A:414:LEU:HD23	1:A:418:ILE:HD12	1.92	0.51
1:A:451:VAL:HG22	1:A:496:PHE:CE1	2.45	0.51
4:D:369:MET:HE1	4:D:417:THR:HG23	1.92	0.51
3:C:336:GLY:HA2	4:D:301:ASN:HB3	1.92	0.50
3:C:129:LYS:O	3:C:132:GLU:HG2	2.11	0.50
5:E:46:VAL:HG22	5:E:65:TRP:HE3	1.77	0.50
1:A:1328:HIS:ND1	1:A:1349:SER:HB2	2.27	0.50
3:C:123:LEU:HB3	4:D:194:LEU:HD21	1.94	0.49
4:D:349:LEU:HB3	4:D:368:ALA:HA	1.93	0.49
2:B:225:LYS:HE2	2:B:230:GLU:OE2	2.12	0.49
1:A:821:LEU:HD11	2:B:10:ILE:HD11	1.95	0.49
1:A:1036:LEU:HB3	1:A:1082:ILE:CD1	2.43	0.49
1:A:16:VAL:HG22	1:A:39:LYS:HB3	1.95	0.49
3:C:368:GLN:HB3	3:C:380:TYR:CE2	2.48	0.49
1:A:438:LEU:HD11	1:A:489:LEU:HD11	1.94	0.49
3:C:168:HIS:CD2	4:D:240:GLN:HE21	2.31	0.48
1:A:707:ILE:HG22	1:A:709:GLN:H	1.78	0.48
3:C:96:VAL:O	3:C:100:MET:HG2	2.13	0.48
3:C:261:ILE:HG21	3:C:375:LEU:HB2	1.95	0.48
5:E:16:LEU:HD23	5:E:88:ILE:HB	1.95	0.48
3:C:89:GLN:HE21	4:D:162:TYR:HE2	1.59	0.48
3:C:158:HIS:CD2	4:D:229:TYR:CE2	3.01	0.48
1:A:89:LYS:HB3	1:A:102:PHE:HB2	1.94	0.48
1:A:790:LEU:O	1:A:794:MET:HG3	2.14	0.48
4:D:239:GLN:HA	4:D:242:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:LEU:O	2:B:98:PRO:HD3	2.13	0.48
1:A:642:MET:HG2	1:A:647:LEU:HD12	1.96	0.47
5:E:162:GLU:O	5:E:166:MET:HG2	2.14	0.47
3:C:268:ILE:HD11	4:D:332:PRO:O	2.14	0.47
4:D:393:PRO:HG3	4:D:438:TRP:CD1	2.49	0.47
1:A:38:PHE:CE1	1:A:55:PHE:HB2	2.50	0.47
1:A:1041:ILE:HD12	1:A:1067:GLN:HG3	1.96	0.47
1:A:992:HIS:CE1	1:A:1018:LYS:HD2	2.50	0.47
1:A:1328:HIS:HD1	1:A:1349:SER:HB2	1.79	0.47
2:B:36:LYS:NZ	4:D:198:LEU:HD21	2.30	0.47
3:C:339:LEU:HD13	3:C:344:PHE:HA	1.96	0.47
1:A:1265:ILE:HD12	1:A:1280:ALA:HB2	1.97	0.47
1:A:1294:ILE:HD13	1:A:1299:GLU:HA	1.96	0.47
1:A:175:LEU:HD21	1:A:187:PHE:HE2	1.80	0.46
1:A:487:ALA:HA	1:A:564:LEU:HD21	1.98	0.46
1:A:984:LEU:HD12	1:A:1358:LYS:HE3	1.96	0.46
1:A:137:ASP:OD1	1:A:141:LYS:HE2	2.16	0.46
1:A:703:ILE:HG22	1:A:705:GLN:H	1.79	0.46
5:E:119:LYS:O	5:E:149:PRO:HD2	2.16	0.46
1:A:413:ILE:HG23	1:A:417:ARG:HD2	1.98	0.46
1:A:664:LEU:HB3	1:A:720:LEU:HD22	1.98	0.46
1:A:105:TYR:HD1	2:B:260:MET:CE	2.29	0.46
2:B:19:VAL:HG21	2:B:100:LEU:HD11	1.98	0.46
1:A:146:HIS:CD2	1:A:164:LEU:HG	2.51	0.45
1:A:339:ALA:HB2	2:B:258:PRO:HB3	1.98	0.45
5:E:12:PHE:HA	5:E:85:HIS:ND1	2.31	0.45
1:A:1026:GLU:HG3	1:A:1026:GLU:O	2.17	0.45
1:A:1230:PRO:HG2	1:A:1233:SER:HB3	1.97	0.45
1:A:1240:HIS:HA	1:A:1261:SER:HB2	1.99	0.45
4:D:194:LEU:C	4:D:194:LEU:HD23	2.36	0.45
1:A:616:LEU:HD23	1:A:619:LEU:HD12	1.99	0.45
1:A:833:LEU:HD11	2:B:7:PHE:HB2	1.99	0.45
2:B:132:LYS:HE3	2:B:133:TYR:CZ	2.52	0.45
1:A:688:THR:HG22	3:C:100:MET:HE2	1.99	0.45
4:D:333:TYR:O	4:D:334:GLY:C	2.55	0.45
2:B:206:GLU:HG3	5:E:41:ILE:HD12	1.99	0.45
1:A:70:GLU:O	1:A:73:GLU:HG3	2.17	0.44
1:A:249:ALA:HB2	1:A:290:VAL:HG11	1.99	0.44
1:A:591:TRP:CG	1:A:628:GLU:HG2	2.52	0.44
1:A:1261:SER:HA	1:A:1331:ILE:HG23	1.99	0.44
5:E:170:ALA:O	5:E:174:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:THR:HG23	2:B:150:GLU:HA	1.99	0.44
1:A:1070:GLY:HA3	1:A:1083:HIS:CE1	2.52	0.44
1:A:1275:ARG:HH11	1:A:1275:ARG:HG2	1.82	0.44
2:B:114:TYR:O	2:B:118:LYS:HB3	2.18	0.44
1:A:1102:HIS:HD2	1:A:1147:PHE:CZ	2.36	0.44
4:D:353:CYS:SG	4:D:365:PHE:CD2	3.10	0.44
1:A:565:CYS:HB3	1:A:607:TYR:CD2	2.53	0.44
2:B:36:LYS:HZ1	4:D:198:LEU:HD21	1.83	0.44
5:E:172:ILE:O	5:E:176:MET:HG2	2.18	0.44
2:B:206:GLU:HG3	5:E:41:ILE:HG23	2.00	0.44
4:D:168:ILE:O	4:D:172:MET:HG2	2.18	0.44
1:A:547:ASP:O	1:A:553:LYS:HE2	2.18	0.43
1:A:988:HIS:CD2	1:A:1355:LYS:HE2	2.53	0.43
1:A:1033:ARG:HD3	3:C:396:GLU:O	2.18	0.43
1:A:639:LEU:HD13	1:A:660:ILE:HD11	2.00	0.43
3:C:120:ILE:HD11	4:D:191:GLU:HB2	2.00	0.43
1:A:1209:GLU:HA	1:A:1224:LEU:O	2.18	0.43
1:A:461:GLU:O	2:B:272:LYS:HE2	2.19	0.43
1:A:16:VAL:HG12	1:A:41:ALA:HB2	2.00	0.43
1:A:35:THR:HG21	1:A:189:THR:HB	2.01	0.43
1:A:620:LEU:HD21	1:A:642:MET:HE1	2.01	0.43
3:C:123:LEU:HB3	4:D:194:LEU:HD22	2.00	0.43
4:D:276:ILE:HD11	4:D:313:LEU:HD22	2.01	0.43
1:A:1213:TRP:CH2	1:A:1220:ARG:HG3	2.54	0.43
3:C:99:ALA:HB3	4:D:169:LEU:HD13	2.01	0.43
5:E:120:LEU:HD11	5:E:151:LEU:HD13	2.01	0.42
1:A:538:GLN:HE22	1:A:572:LYS:HD3	1.84	0.42
3:C:206:PHE:CD2	3:C:313:LEU:HD13	2.54	0.42
1:A:425:PHE:O	1:A:428:ASP:HB2	2.19	0.42
1:A:989:LEU:HD21	1:A:1032:THR:HB	2.01	0.42
1:A:741:LEU:HD22	1:A:770:LEU:HD21	2.01	0.42
1:A:996:VAL:HG23	1:A:1352:GLY:HA2	2.01	0.42
4:D:417:THR:O	4:D:420:ASN:HB3	2.20	0.42
4:D:442:TRP:CZ2	4:D:446:GLN:HG3	2.55	0.42
1:A:64:LEU:HA	1:A:67:TYR:HD2	1.85	0.42
1:A:729:PHE:CE2	1:A:733:LEU:HD22	2.54	0.42
1:A:491:GLU:OE2	1:A:563:ARG:HD2	2.20	0.42
3:C:328:LYS:HA	3:C:328:LYS:HD2	1.91	0.42
1:A:1055:HIS:O	1:A:1070:GLY:HA2	2.19	0.42
4:D:190:GLU:HG3	4:D:193:ARG:HH21	1.85	0.42
1:A:768:ALA:O	1:A:772:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:GLU:HG3	2:B:103:ASN:HD21	1.85	0.42
1:A:146:HIS:HD2	1:A:164:LEU:HG	1.84	0.42
1:A:667:PRO:HB2	1:A:726:ARG:HD2	2.01	0.42
2:B:71:ALA:HB3	2:B:94:PRO:HG2	2.01	0.42
5:E:54:GLU:OE2	5:E:59:THR:HG22	2.19	0.42
1:A:112:ASP:O	1:A:116:THR:HG23	2.21	0.41
1:A:741:LEU:HD13	1:A:770:LEU:HD23	2.03	0.41
1:A:1060:ALA:HB1	1:A:1098:VAL:HB	2.02	0.41
3:C:92:PHE:O	3:C:96:VAL:HG23	2.21	0.41
1:A:43:ALA:HB3	1:A:50:VAL:HG23	2.02	0.41
2:B:35:TYR:CB	3:C:125:GLN:HE22	2.32	0.41
4:D:335:ASN:HB2	4:D:336:HIS:CD2	2.56	0.41
1:A:419:THR:HG22	1:A:462:TYR:HE2	1.85	0.41
3:C:261:ILE:O	3:C:269:SER:HA	2.21	0.41
5:E:55:LEU:HB3	5:E:60:ILE:HD12	2.03	0.41
6:E:1000:GTP:O3G	6:E:1000:GTP:O2B	2.38	0.41
1:A:175:LEU:HD21	1:A:187:PHE:CE2	2.56	0.41
1:A:472:GLN:OE1	1:A:543:THR:HG23	2.21	0.41
1:A:1291:TYR:HD1	1:A:1304:ILE:HD13	1.84	0.41
1:A:386:LEU:HD22	1:A:398:ALA:HB1	2.02	0.41
1:A:452:PRO:HG2	1:A:455:ASP:OD2	2.21	0.41
2:B:36:LYS:HA	2:B:36:LYS:HE2	2.03	0.41
2:B:74:VAL:CG2	2:B:94:PRO:HD3	2.51	0.41
3:C:158:HIS:HD2	4:D:229:TYR:CD2	2.39	0.41
1:A:32:LEU:HD12	1:A:51:VAL:HG13	2.03	0.41
1:A:669:LEU:HD22	1:A:673:TYR:CZ	2.56	0.41
1:A:1127:ARG:HE	1:A:1127:ARG:HB3	1.55	0.41
1:A:334:GLU:HG2	2:B:254:LYS:HE3	2.03	0.40
1:A:965:MET:HE3	1:A:965:MET:HB3	2.02	0.40
3:C:276:TYR:N	3:C:276:TYR:CD1	2.87	0.40
3:C:280:TYR:CD2	3:C:341:LYS:HG3	2.56	0.40
1:A:1023:GLN:O	1:A:1026:GLU:HG2	2.21	0.40
1:A:680:THR:HG22	1:A:710:ILE:O	2.21	0.40
5:E:28:LEU:HD22	5:E:66:ASP:HB2	2.03	0.40
1:A:383:THR:HA	1:A:386:LEU:HG	2.03	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	1167/1409 (83%)	1116 (96%)	51 (4%)	0	100	100
2	B	263/887 (30%)	249 (95%)	14 (5%)	0	100	100
3	C	259/492 (53%)	256 (99%)	3 (1%)	0	100	100
4	D	303/450 (67%)	298 (98%)	5 (2%)	0	100	100
5	E	170/226 (75%)	168 (99%)	2 (1%)	0	100	100
All	All	2162/3464 (62%)	2087 (96%)	75 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1040/1238 (84%)	1030 (99%)	10 (1%)	73	84
2	B	238/799 (30%)	236 (99%)	2 (1%)	79	88
3	C	246/434 (57%)	245 (100%)	1 (0%)	89	94
4	D	275/405 (68%)	274 (100%)	1 (0%)	89	94
5	E	152/194 (78%)	152 (100%)	0	100	100
All	All	1951/3070 (64%)	1937 (99%)	14 (1%)	80	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	GLU
1	A	104	GLN
1	A	145	ARG
1	A	204	ASP
1	A	234	GLU
1	A	264	LEU
1	A	311	GLN
1	A	317	PRO
1	A	328	MET
1	A	1033	ARG
2	B	5	GLU
2	B	236	TYR
3	C	267	TRP
4	D	333	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	1102	HIS
1	A	1205	GLN
3	C	158	HIS
3	C	168	HIS
3	C	186	HIS
3	C	338	ASN
3	C	377	ASN
4	D	275	HIS
4	D	301	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
8	MYR	A	2003	-	15,15,15	0.66	0	15,15,15	0.72	1 (6%)
6	GTP	E	1000	7	29,34,34	1.34	2 (6%)	35,54,54	1.38	4 (11%)
6	GTP	A	2001	7	29,34,34	1.43	3 (10%)	35,54,54	1.54	6 (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
8	MYR	A	2003	-	-	2/13/13/13	-
6	GTP	E	1000	7	-	2/18/38/38	0/3/3/3
6	GTP	A	2001	7	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1000	GTP	C5-C6	-4.60	1.38	1.47
6	A	2001	GTP	C5-C6	-4.39	1.38	1.47
6	A	2001	GTP	C5-C4	-2.67	1.36	1.43
6	A	2001	GTP	C2'-C3'	-2.24	1.47	1.53
6	E	1000	GTP	C5-C4	-2.13	1.37	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2001	GTP	C8-N7-C5	4.35	109.96	102.55
6	E	1000	GTP	C8-N7-C5	3.67	108.81	102.55
6	E	1000	GTP	O2A-PA-O3A	3.00	115.38	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1000	GTP	C5-C6-N1	3.00	119.79	114.07
6	A	2001	GTP	C4'-O4'-C1'	-2.95	107.22	109.92
6	A	2001	GTP	C5-C6-N1	2.90	119.61	114.07
6	A	2001	GTP	O2B-PB-O3B	2.84	114.95	107.27
6	A	2001	GTP	C2-N1-C6	-2.75	120.07	125.11
6	E	1000	GTP	C2-N1-C6	-2.68	120.21	125.11
6	A	2001	GTP	O4'-C1'-N9	2.57	112.16	108.75
8	A	2003	MYR	O1-C1-C2	-2.05	116.60	123.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2001	GTP	C5'-O5'-PA-O1A
6	A	2001	GTP	C5'-O5'-PA-O3A
6	A	2001	GTP	C5'-O5'-PA-O2A
6	A	2001	GTP	C4'-C5'-O5'-PA
6	E	1000	GTP	PA-O3A-PB-O2B
8	A	2003	MYR	O1-C1-C2-C3
8	A	2003	MYR	O2-C1-C2-C3
6	E	1000	GTP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1000	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.

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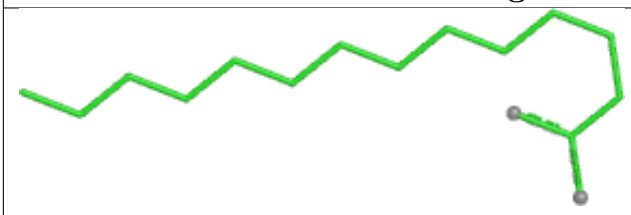
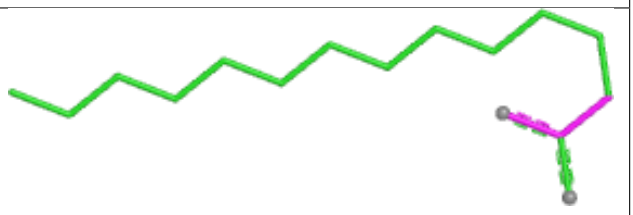
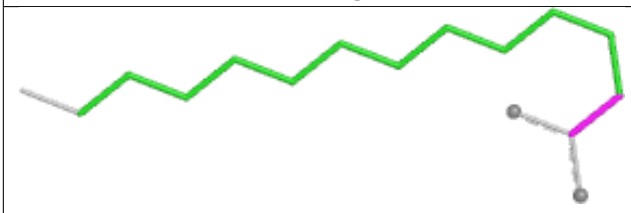


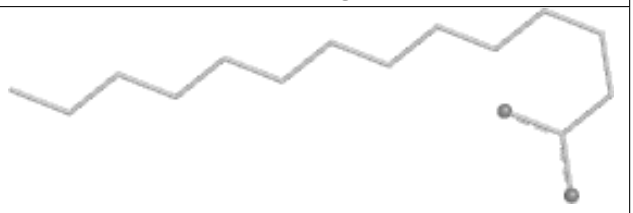
Bond lengths



Bond angles

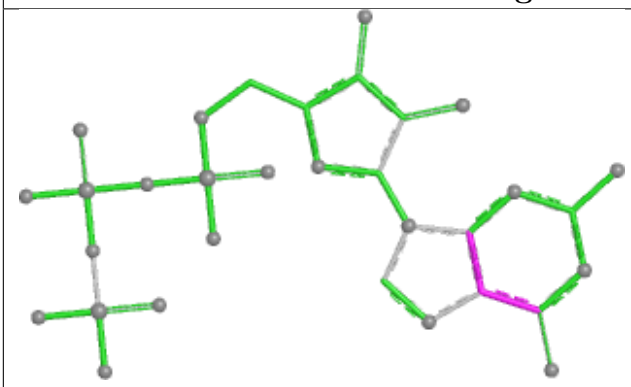


Torsions

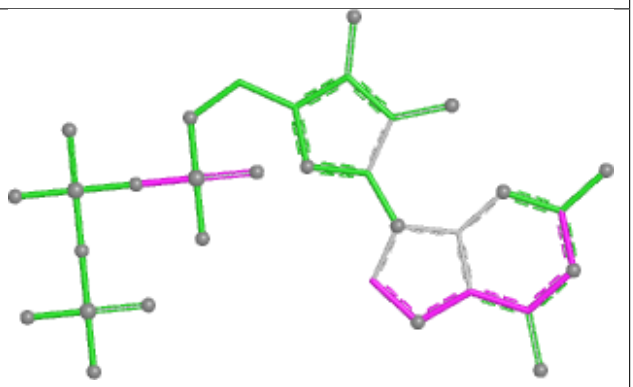


Rings

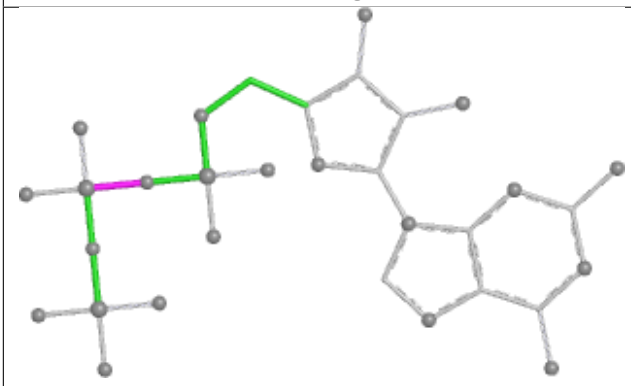
Ligand GTP E 1000



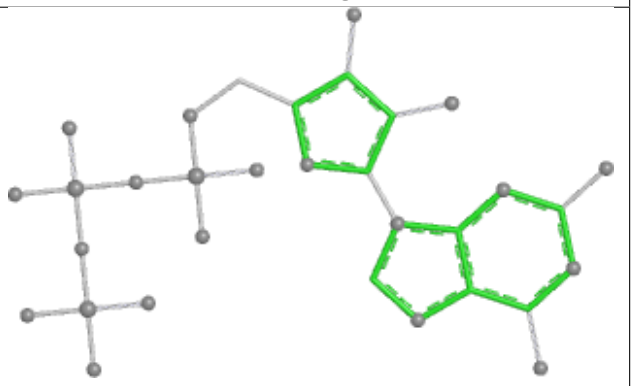
Bond lengths



Bond angles

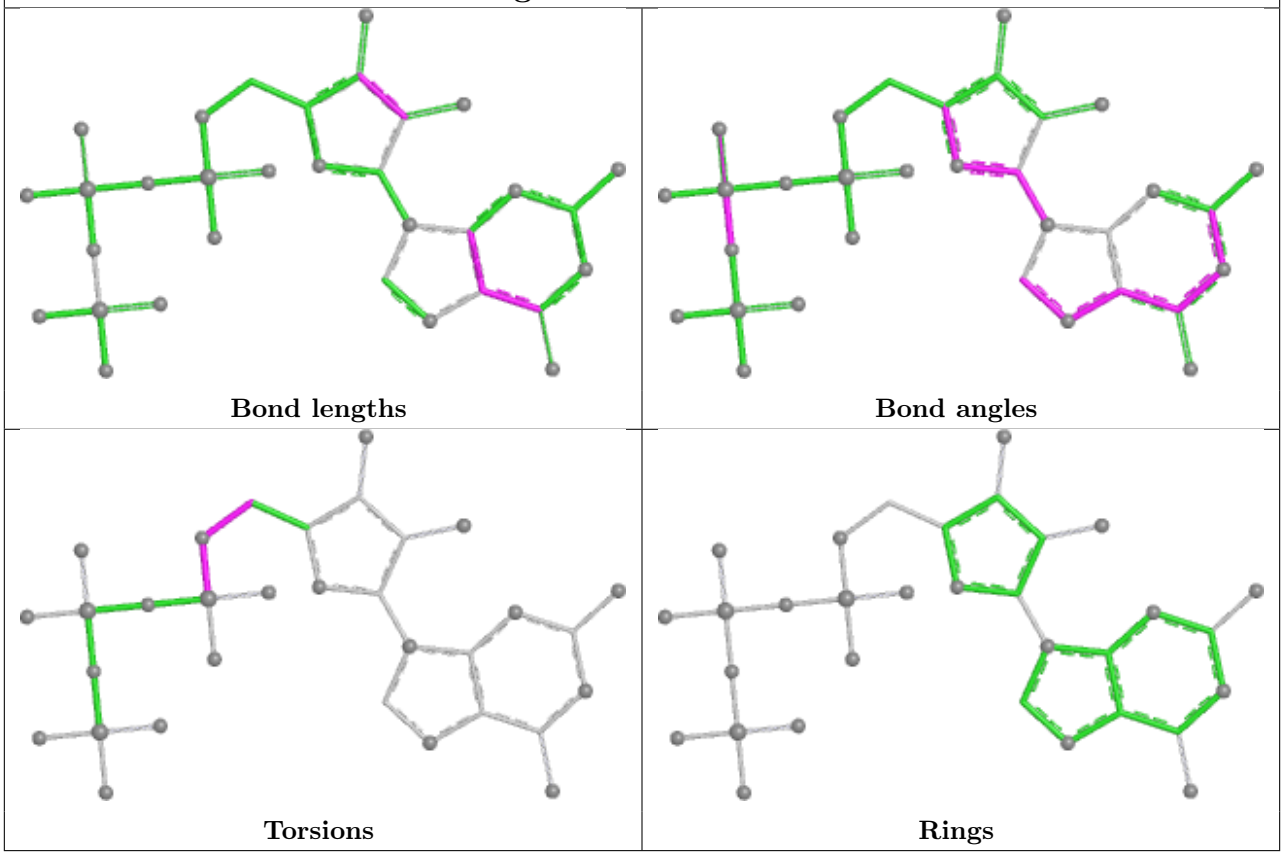


Torsions



Rings

Ligand GTP A 2001



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.

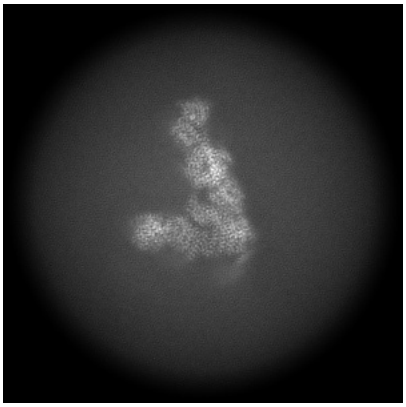
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48276. These allow visual inspection of the internal detail of the map and identification of artifacts.

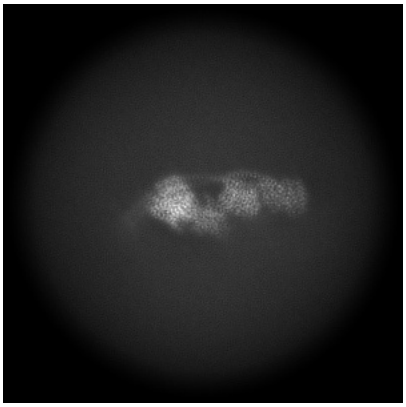
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

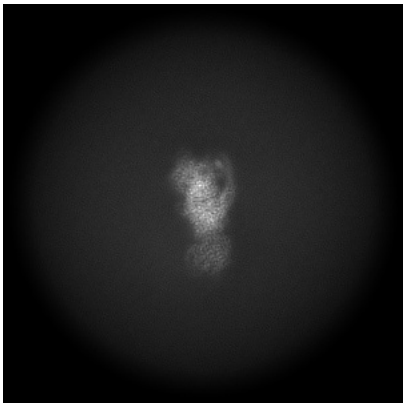
6.1.1 Primary map



X



Y

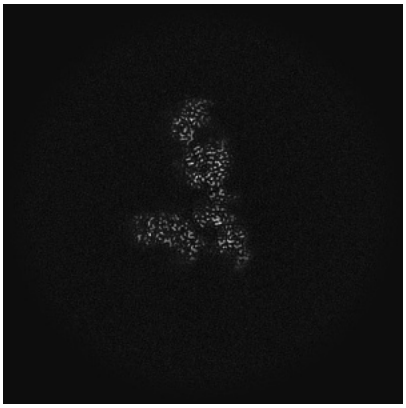


Z

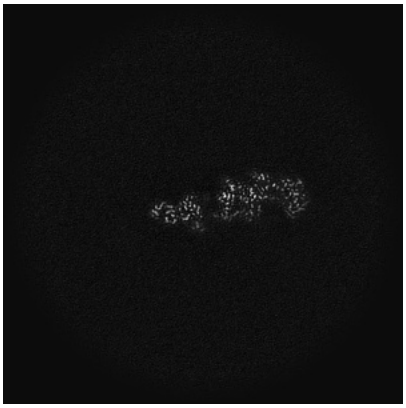
The images above show the map projected in three orthogonal directions.

6.2 Central slices

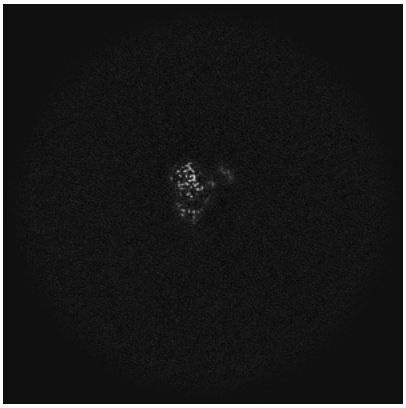
6.2.1 Primary map



X Index: 200



Y Index: 200

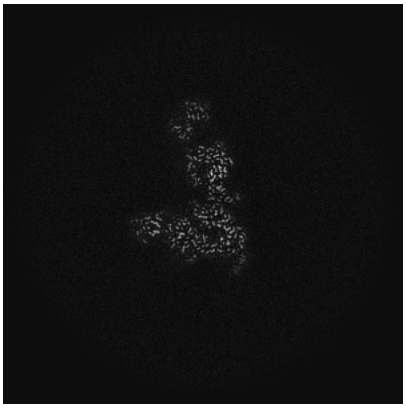


Z Index: 200

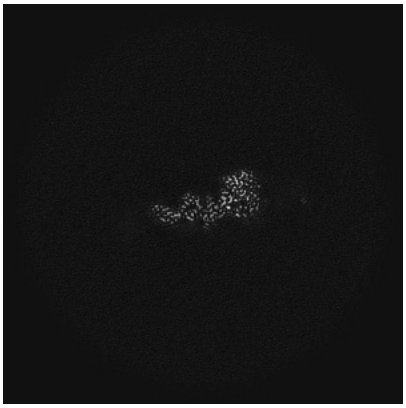
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

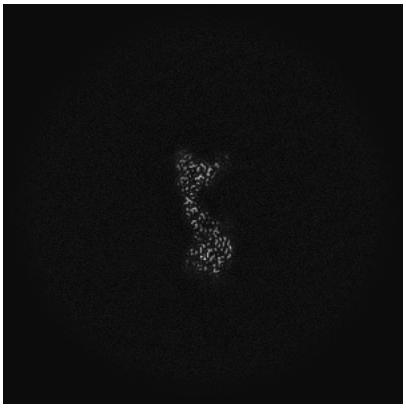
6.3.1 Primary map



X Index: 197



Y Index: 210

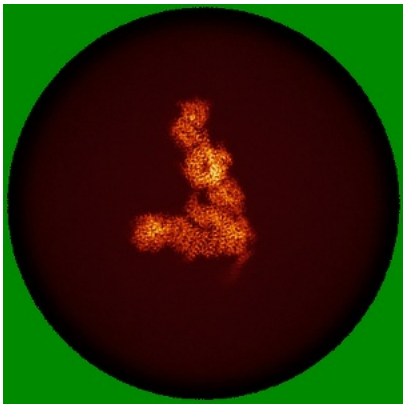


Z Index: 171

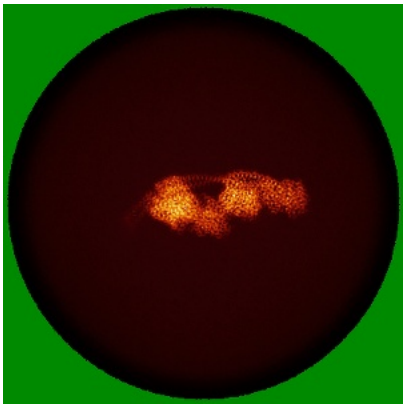
The images above show the largest variance slices of the map in three orthogonal directions.

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

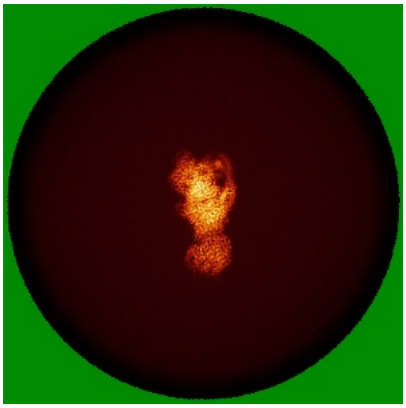
6.4.1 Primary map



X



Y



Z

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

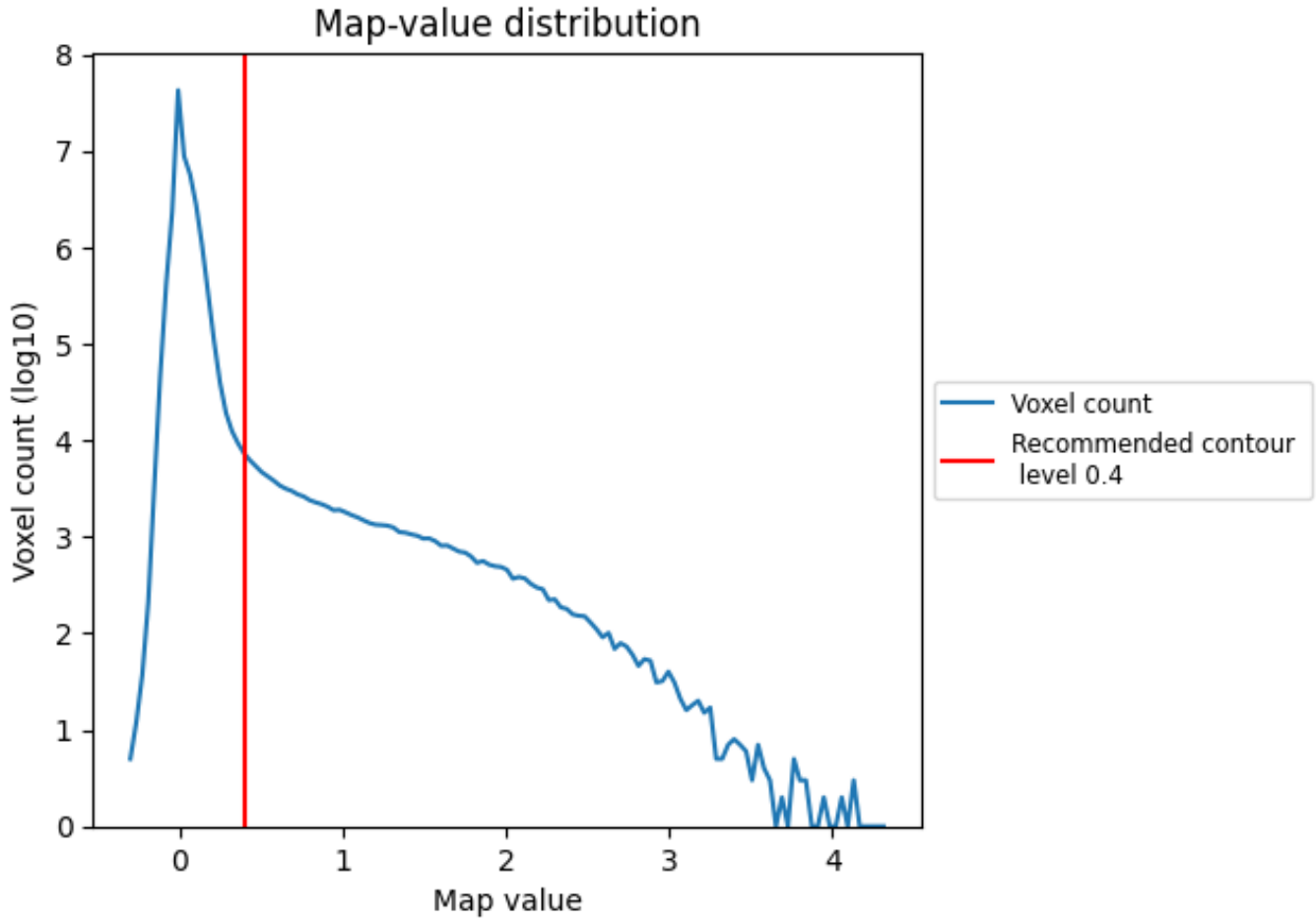
6.6 Mask visualisation (i)

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

7 Map analysis

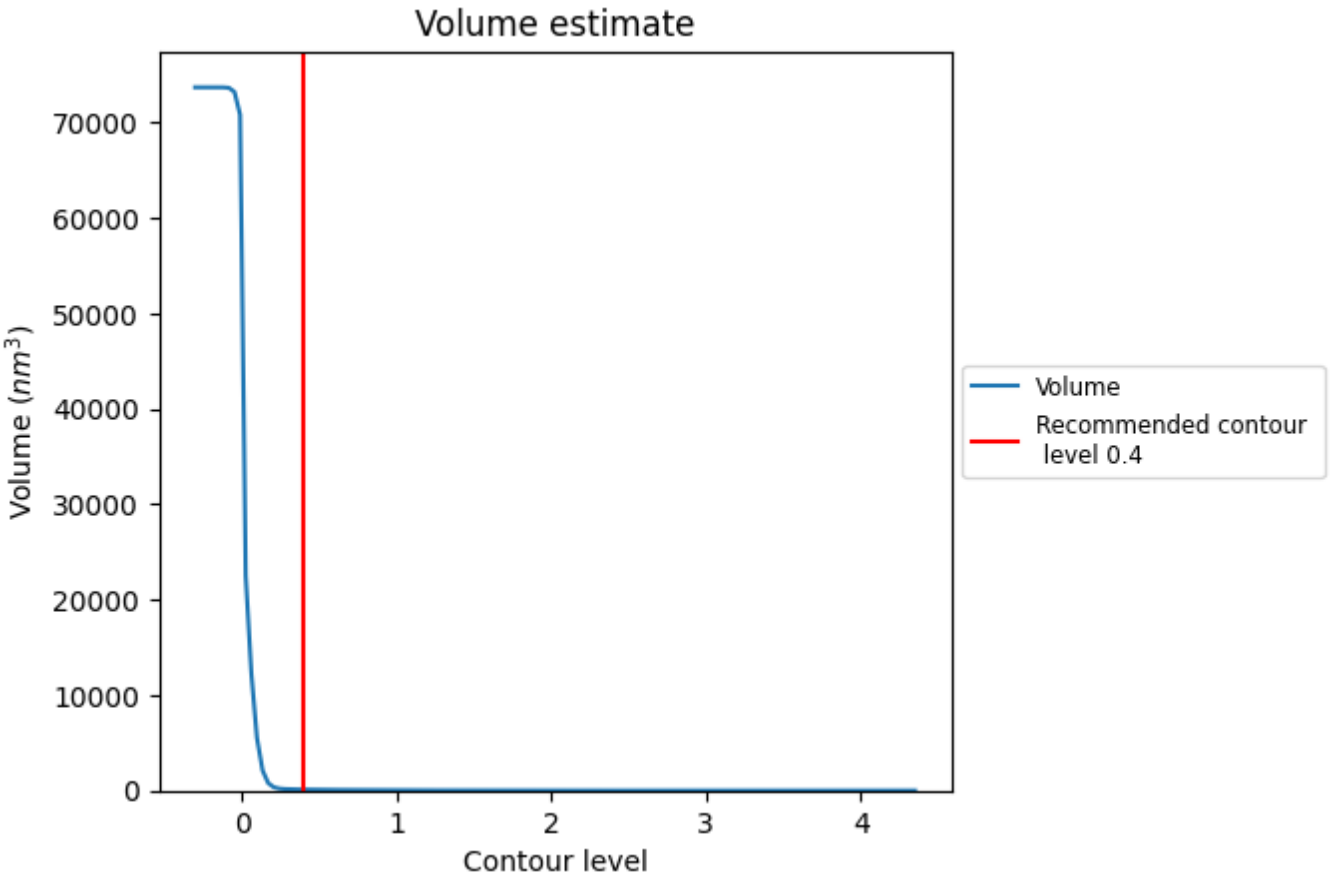
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

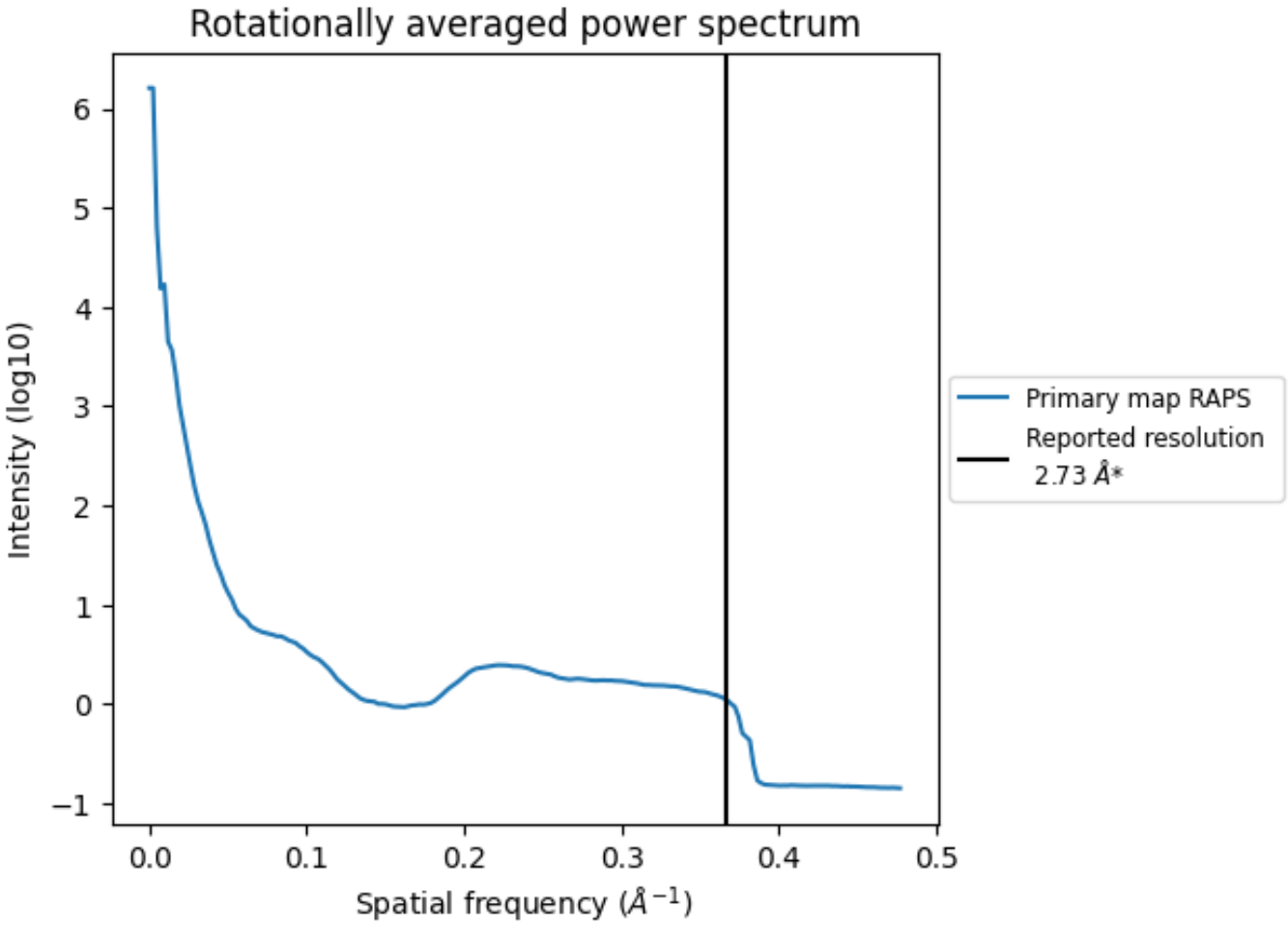
7.2 Volume estimate



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 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 0.366 Å^{-1}

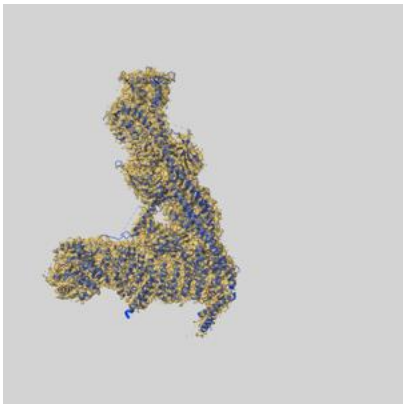
8 Fourier-Shell correlation (i)

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

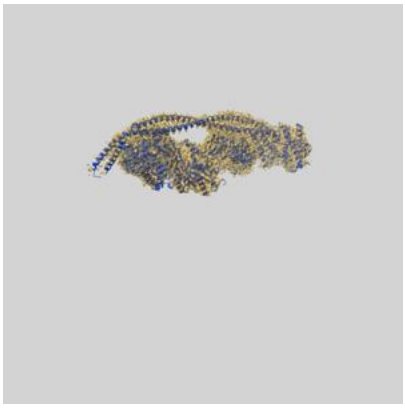
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48276 and PDB model 9MHF. Per-residue inclusion information can be found in section 3 on page 8.

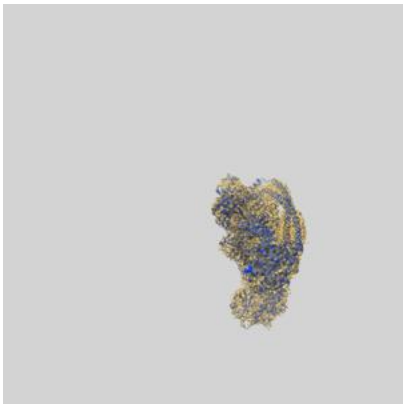
9.1 Map-model overlay



X



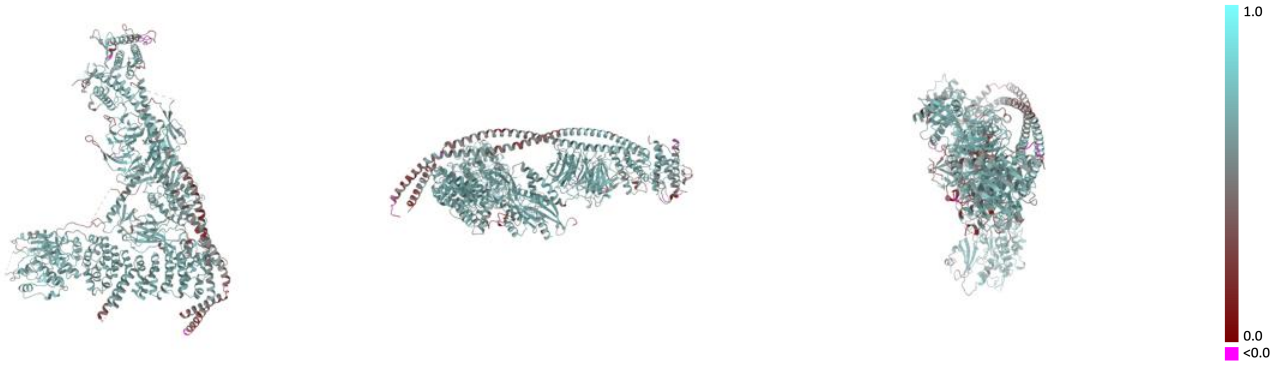
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

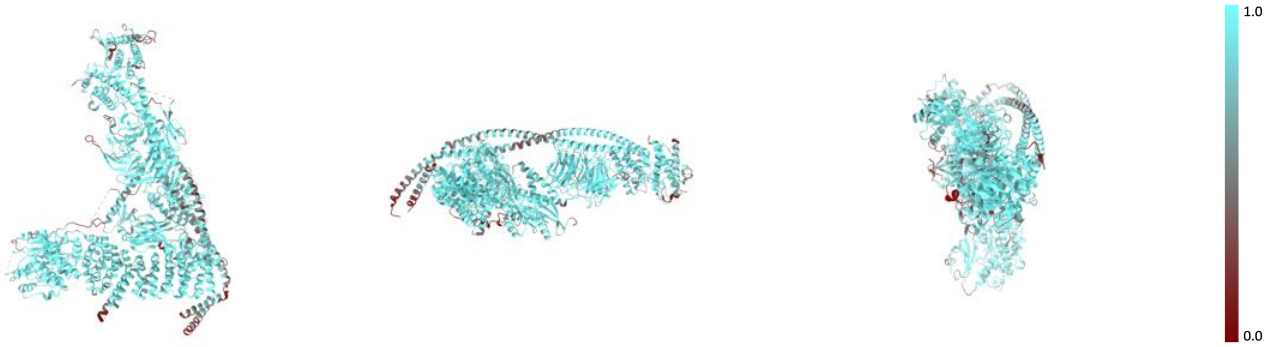
9.2 Q-score mapped to coordinate model (i)



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.

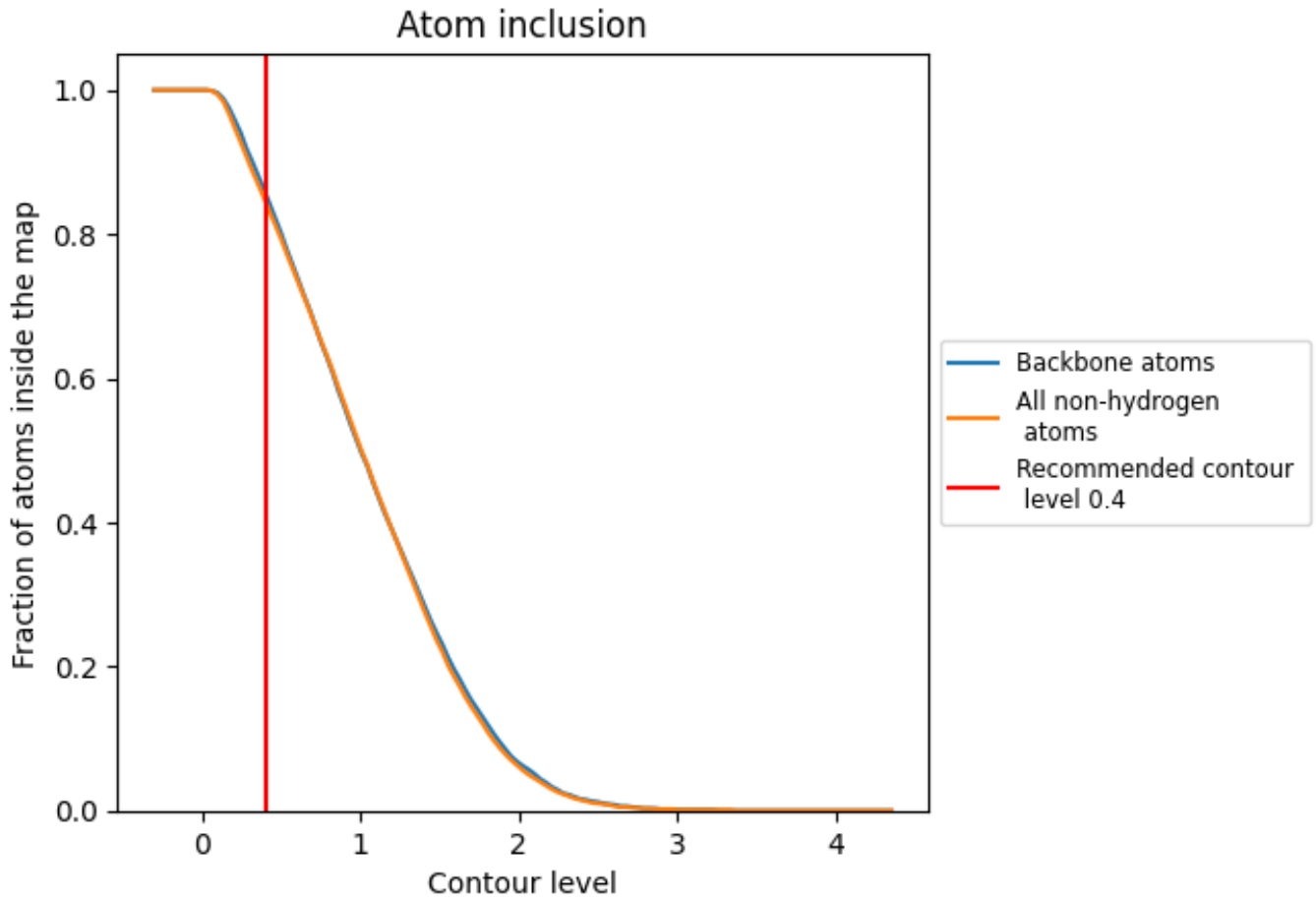
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.5880
A	0.8810	0.6110
B	0.8800	0.6240
C	0.7860	0.5310
D	0.7210	0.4990
E	0.8960	0.6290