



## Full wwPDB EM Validation Report ⓘ

Jun 3, 2026 – 10:25 am BST

PDB ID : 9RX5 / pdb\_00009rx5  
EMDB ID : EMD-54358  
Title : VPS34-CII (VPS34 199-REIE-202 to 199-AAAA-202 mutant) bound to RAB5A (Q79L)  
Authors : Spokaite, S.; Ohashi, Y.; Dessus, A.N.; Bourguet, M.; Williams, R.L.  
Deposited on : 2025-07-10  
Resolution : 3.15 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](mailto: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>.

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

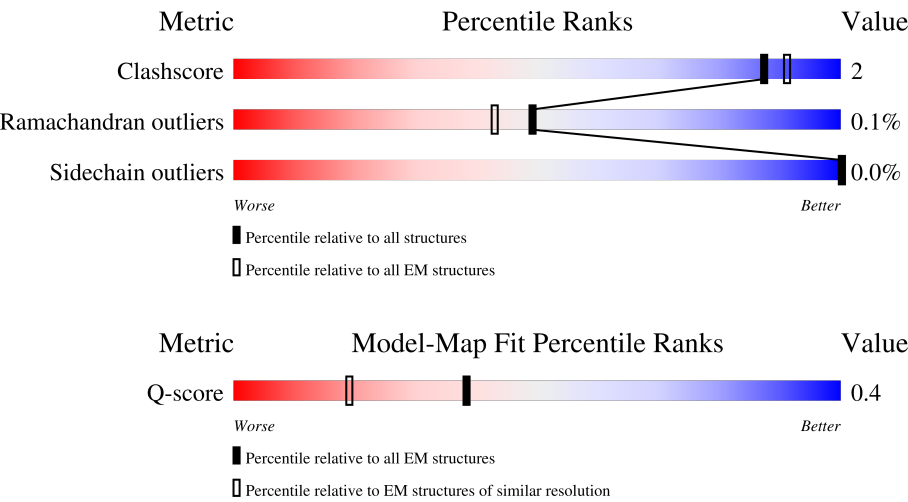
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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) : 2.49

# 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 3.15 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	14486 ( 2.65 - 3.65 )

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  $\geq 3$ , 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  $\leq 5\%$ . 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	887	
2	B	1370	
3	C	450	
4	D	699	

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Mol	Chain	Length	Quality of chain
5	E	212	 75% 6% 20%
5	F	212	 61% 77% 19%

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25422 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 Phosphatidylinositol 3-kinase catalytic subunit type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	810	Total	C	N	O	S	0	0
			6545	4179	1109	1219	38		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	ARG	engineered mutation	UNP Q8NEB9
A	200	ALA	GLU	engineered mutation	UNP Q8NEB9
A	201	ALA	ILE	engineered mutation	UNP Q8NEB9
A	202	ALA	GLU	engineered mutation	UNP Q8NEB9

- Molecule 2 is a protein called Phosphoinositide 3-kinase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1197	Total	C	N	O	S	0	0
			9518	6065	1655	1751	47		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1359	SER	-	expression tag	UNP Q99570
B	1360	ARG	-	expression tag	UNP Q99570
B	1361	PRO	-	expression tag	UNP Q99570
B	1362	THR	-	expression tag	UNP Q99570
B	1363	THR	-	expression tag	UNP Q99570
B	1364	ALA	-	expression tag	UNP Q99570
B	1365	SER	-	expression tag	UNP Q99570
B	1366	GLU	-	expression tag	UNP Q99570
B	1367	ASN	-	expression tag	UNP Q99570
B	1368	LEU	-	expression tag	UNP Q99570
B	1369	TYR	-	expression tag	UNP Q99570
B	1370	PHE	-	expression tag	UNP Q99570
B	1371	GLN	-	expression tag	UNP Q99570

- Molecule 3 is a protein called Beclin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	379	Total	C	N	O	S	0	0
			3119	1964	533	605	17		

- Molecule 4 is a protein called UV radiation resistance associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	423	Total	C	N	O	S	0	0
			3456	2200	615	628	13		

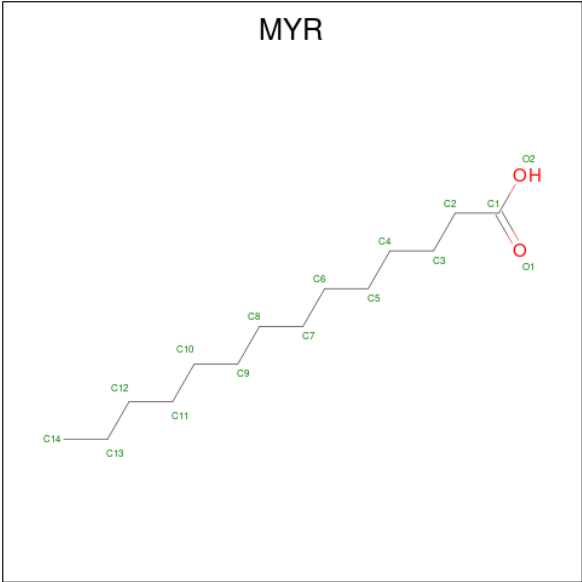
- Molecule 5 is a protein called Ras-related protein Rab-5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	170	Total	C	N	O	S	0	0
			1333	848	226	255	4		
5	F	171	Total	C	N	O	S	0	0
			1340	852	227	257	4		

There are 6 discrepancies between the modelled and reference sequences:

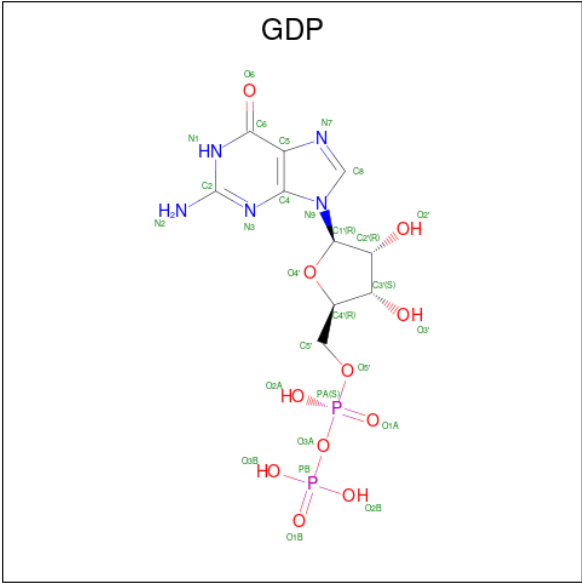
Chain	Residue	Modelled	Actual	Comment	Reference
E	19	SER	CYS	engineered mutation	UNP P20339
E	63	SER	CYS	engineered mutation	UNP P20339
E	79	LEU	GLN	engineered mutation	UNP P20339
F	19	SER	CYS	engineered mutation	UNP P20339
F	63	SER	CYS	engineered mutation	UNP P20339
F	79	LEU	GLN	engineered mutation	UNP P20339

- Molecule 6 is MYRISTIC ACID (CCD ID: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			15	14	1	

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

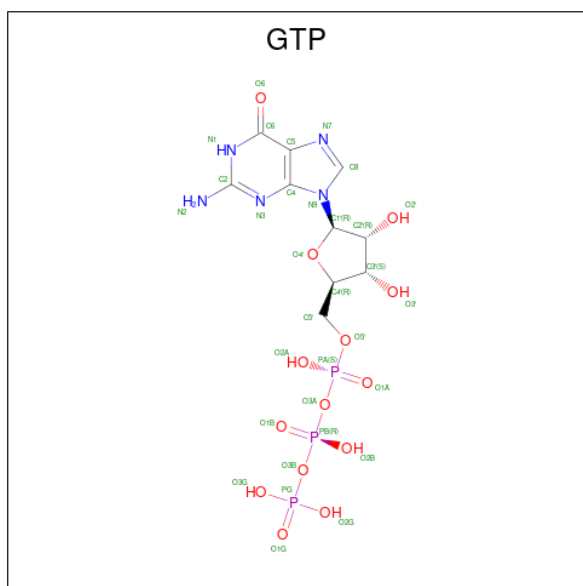
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula:  $Mg$ ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	
8	E	1	Total	Mg	0
			1	1	
8	F	1	Total	Mg	0
			1	1	

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	C	1	Total	Zn	0
			1	1	

- Molecule 10 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

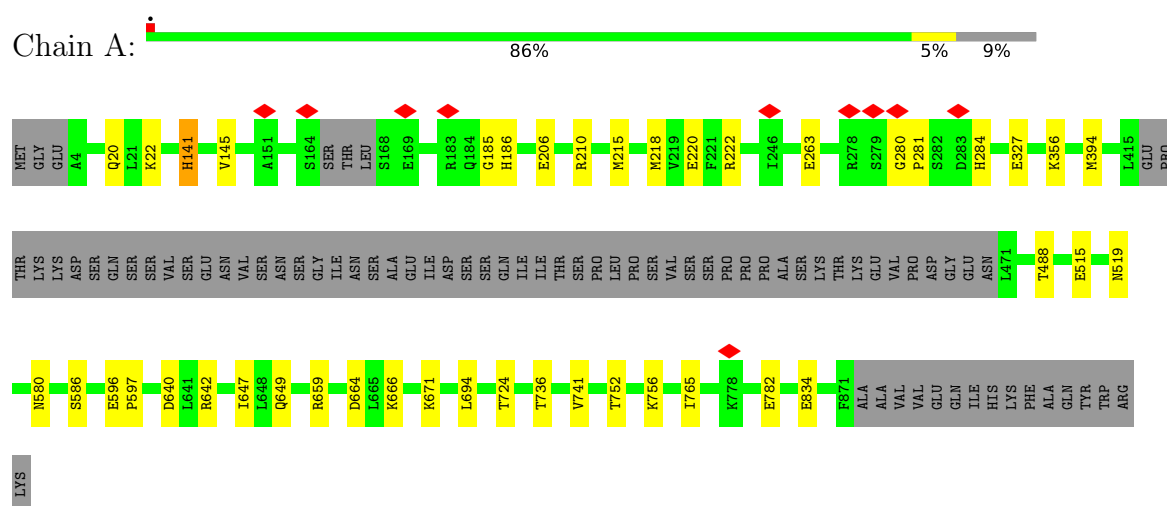


Mol	Chain	Residues	Atoms					AltConf
10	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	F	1	Total	C	N	O	P	0
			32	10	5	14	3	

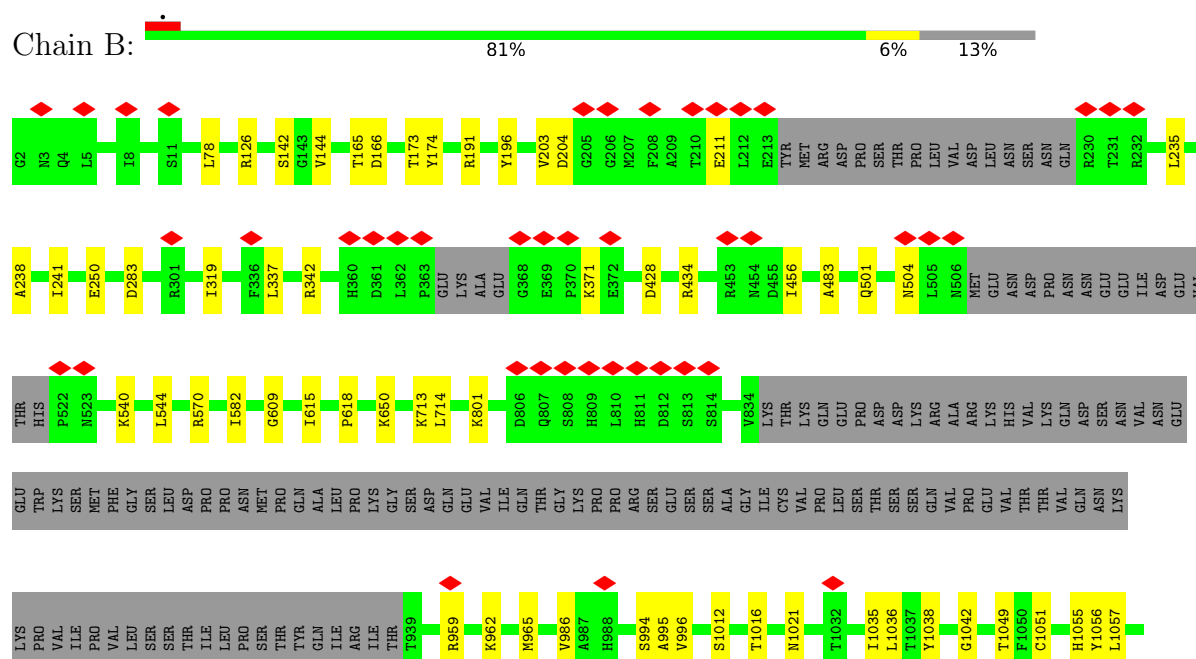
### 3 Residue-property plots

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.

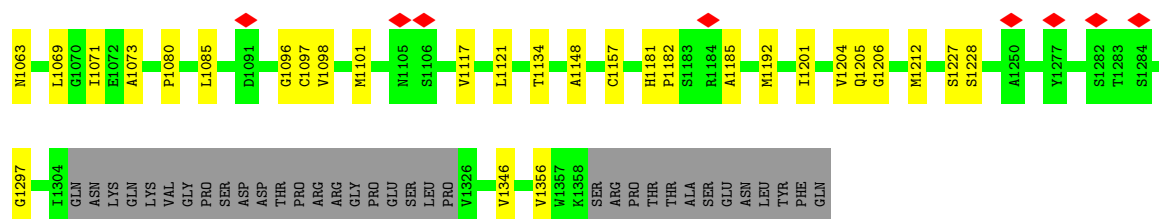
- Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3



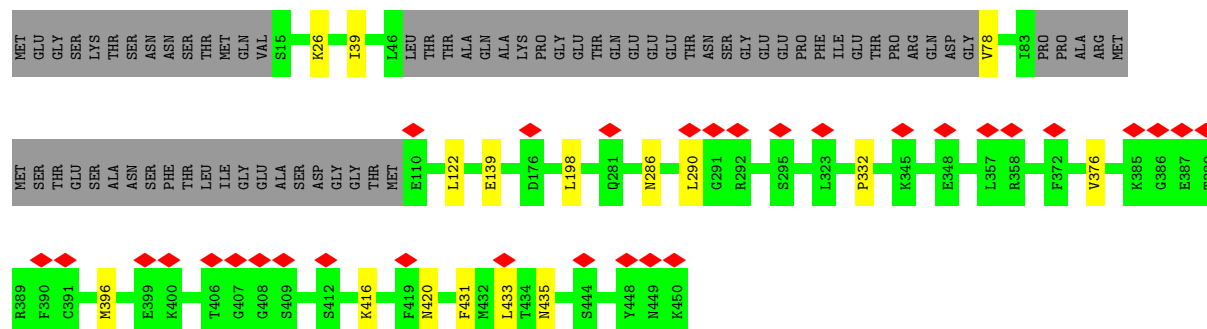
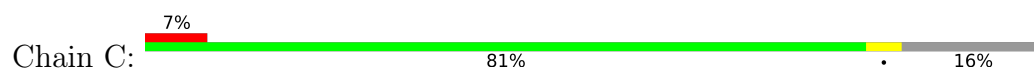
- Molecule 2: Phosphoinositide 3-kinase regulatory subunit 4



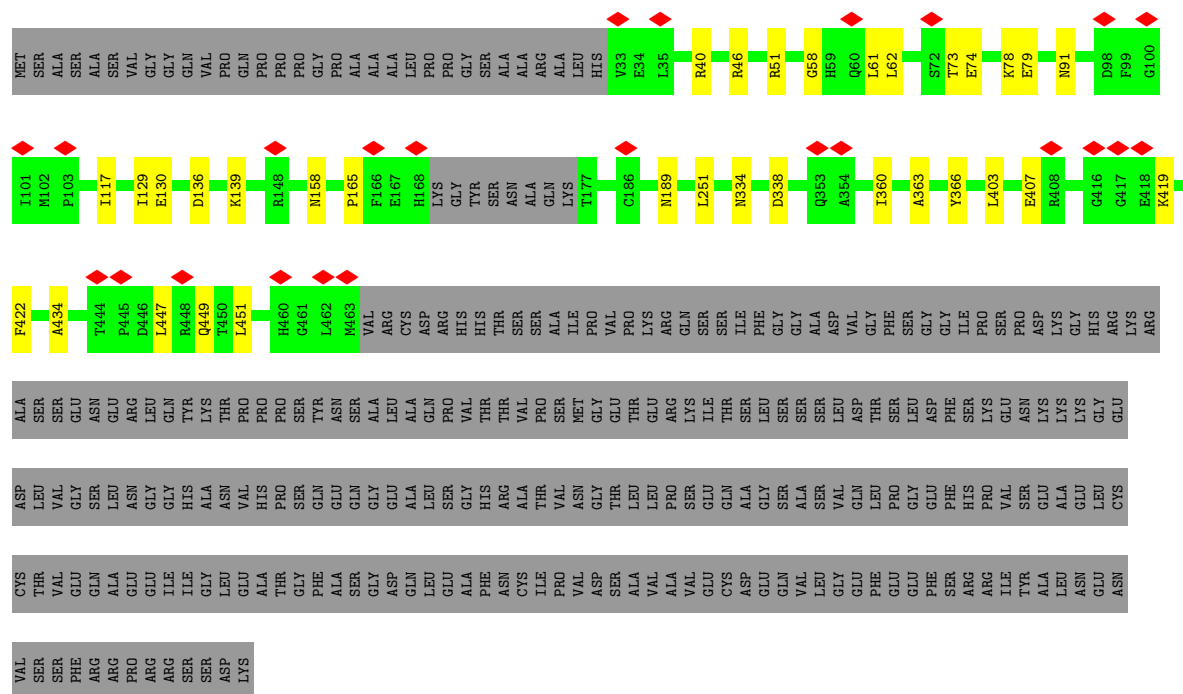




• Molecule 3: Beclin-1

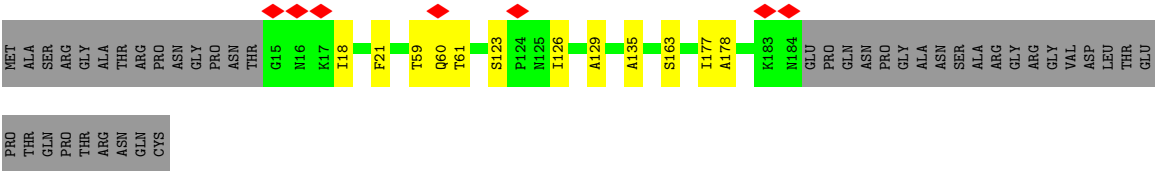


• Molecule 4: UV radiation resistance associated protein

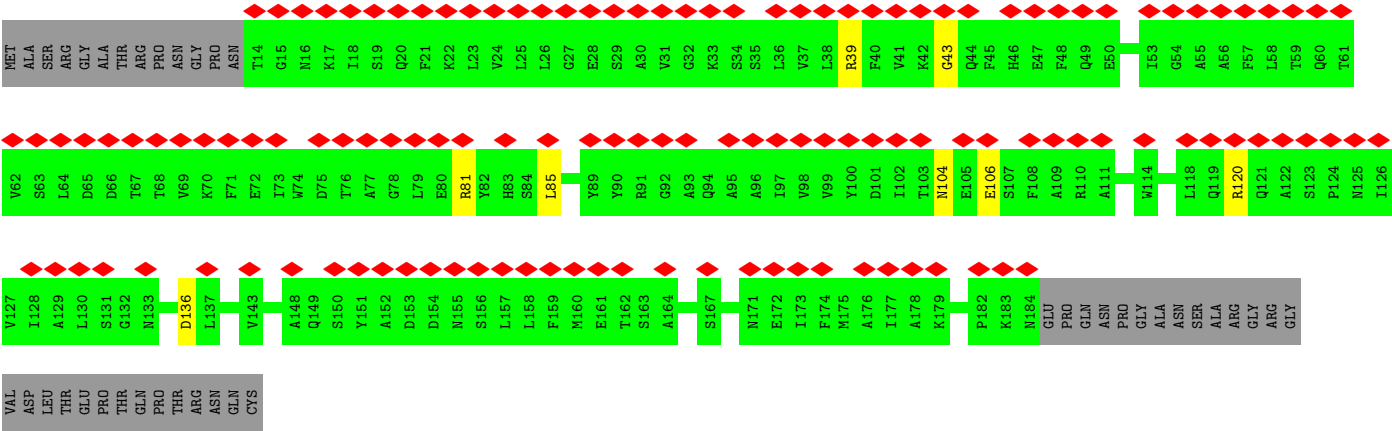
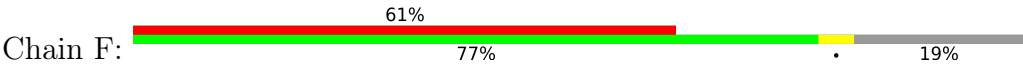


• Molecule 5: Ras-related protein Rab-5A





● Molecule 5: Ras-related protein Rab-5A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155476	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.655	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.14	Depositor
Map size ( $\text{\AA}$ )	350.88, 350.88, 350.88	wwPDB
Map dimensions	408, 408, 408	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.86, 0.86, 0.86	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, GDP, ZN, MYR, 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	0.19	0/6685	0.50	2/9033 (0.0%)
2	B	0.20	0/9726	0.54	6/13182 (0.0%)
3	C	0.16	0/3174	0.41	0/4273
4	D	0.20	0/3518	0.43	0/4737
5	E	0.19	0/1356	0.54	1/1830 (0.1%)
5	F	0.16	0/1363	0.45	0/1840
All	All	0.19	0/25822	0.50	9/34895 (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	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	HIS	CA-C-N	8.43	136.87	121.70
1	A	141	HIS	C-N-CA	8.43	136.87	121.70
2	B	456	ILE	CA-C-N	7.27	134.79	121.70
2	B	456	ILE	C-N-CA	7.27	134.79	121.70
2	B	142	SER	CA-C-N	5.95	132.41	121.70
2	B	142	SER	C-N-CA	5.95	132.41	121.70
5	E	59	THR	N-CA-C	5.43	115.19	108.19
2	B	986	VAL	N-CA-C	-5.36	106.20	111.88
2	B	142	SER	N-CA-C	5.21	116.77	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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	6545	0	6570	23	0
2	B	9518	0	9554	46	0
3	C	3119	0	3042	10	0
4	D	3456	0	3528	19	0
5	E	1333	0	1331	6	0
5	F	1340	0	1337	6	0
6	B	15	0	27	0	0
7	B	28	0	12	0	0
8	B	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	C	1	0	0	0	0
10	E	32	0	12	0	0
10	F	32	0	12	0	0
All	All	25422	0	25425	99	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 2.

All (99) 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:22:LYS:HB3	1:A:220:GLU:HB2	1.76	0.66
4:D:40:ARG:HD3	4:D:136:ASP:HA	1.80	0.64
2:B:1204:VAL:HG12	2:B:1206:GLY:H	1.65	0.62
4:D:360:ILE:HD12	4:D:363:ALA:HB3	1.84	0.60
2:B:1148:ALA:HB3	2:B:1157:CYS:HB3	1.85	0.58
4:D:334:ASN:HB2	4:D:338:ASP:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1073:ALA:HA	2:B:1080:PRO:HB3	1.86	0.57
4:D:61:LEU:HB3	4:D:62:LEU:HG	1.85	0.57
3:C:416:LYS:O	3:C:420:ASN:ND2	2.38	0.57
4:D:139:LYS:HB2	4:D:165:PRO:HB3	1.87	0.56
2:B:1035:ILE:HG22	2:B:1036:LEU:HG	1.87	0.55
1:A:666:LYS:HG3	1:A:724:THR:HG23	1.89	0.54
1:A:327:GLU:OE2	1:A:356:LYS:NZ	2.39	0.54
2:B:1049:THR:OG1	2:B:1101:MET:SD	2.63	0.54
1:A:659:ARG:NH1	1:A:664:ASP:OD1	2.41	0.53
2:B:1057:LEU:HD23	2:B:1069:LEU:HD12	1.91	0.52
4:D:46:ARG:NH2	4:D:158:ASN:OD1	2.42	0.52
1:A:647:ILE:HD11	1:A:765:ILE:HD13	1.92	0.52
2:B:1051:CYS:HB2	2:B:1056:TYR:HB2	1.91	0.52
4:D:51:ARG:HD3	4:D:91:ASN:HB3	1.92	0.52
4:D:73:THR:OG1	4:D:74:GLU:N	2.43	0.52
3:C:139:GLU:OE2	5:F:120:ARG:NH2	2.43	0.51
2:B:618:PRO:O	5:F:81:ARG:NH2	2.43	0.51
2:B:1227:SER:OG	2:B:1228:SER:N	2.43	0.51
1:A:206:GLU:OE2	1:A:210:ARG:NH2	2.45	0.50
3:C:26:LYS:HG3	4:D:189:ASN:HB3	1.94	0.50
4:D:403:LEU:HB3	4:D:407:GLU:HB2	1.94	0.50
1:A:580:ASN:HD21	1:A:586:SER:HB2	1.76	0.50
2:B:1055:HIS:O	2:B:1071:ILE:N	2.43	0.49
2:B:1181:HIS:ND1	2:B:1182:PRO:O	2.41	0.49
1:A:515:GLU:O	1:A:519:ASN:ND2	2.43	0.49
5:F:136:ASP:OD1	5:F:136:ASP:N	2.44	0.49
3:C:431:PHE:O	3:C:435:ASN:ND2	2.39	0.48
1:A:141:HIS:O	1:A:218:MET:HA	2.14	0.48
2:B:570:ARG:HH21	2:B:609:GLY:HA3	1.78	0.48
5:E:60:GLN:HB3	5:E:61:THR:HB	1.96	0.47
3:C:290:LEU:HD12	3:C:433:LEU:HD22	1.94	0.47
1:A:20:GLN:HB2	1:A:222:ARG:HD2	1.95	0.47
1:A:694:LEU:HD21	1:A:782:GLU:HG3	1.96	0.47
2:B:174:TYR:HB2	2:B:211:GLU:HG3	1.95	0.47
2:B:1042:GLY:O	2:B:1063:ASN:ND2	2.41	0.47
2:B:1201:ILE:HG12	2:B:1212:MET:HG2	1.96	0.47
2:B:196:TYR:OH	2:B:250:GLU:OE1	2.27	0.47
1:A:488:THR:HG23	1:A:597:PRO:HG2	1.96	0.47
1:A:834:GLU:OE2	2:B:191:ARG:NH2	2.47	0.47
2:B:615:ILE:HG23	5:F:85:LEU:HG	1.97	0.47
3:C:198:LEU:HD13	4:D:251:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:HIS:O	2:B:962:LYS:NZ	2.49	0.46
1:A:596:GLU:OE1	1:A:671:LYS:NZ	2.47	0.46
2:B:173:THR:HG23	2:B:235:LEU:HD23	1.96	0.46
2:B:501:GLN:HA	2:B:504:ASN:HB2	1.96	0.46
1:A:185:GLY:O	2:B:959:ARG:NH1	2.39	0.46
2:B:428:ASP:O	2:B:434:ARG:NH1	2.39	0.46
1:A:145:VAL:HB	1:A:215:MET:HB2	1.97	0.46
2:B:1016:THR:HA	2:B:1038:TYR:O	2.16	0.46
2:B:1021:ASN:HB2	2:B:1035:ILE:HD11	1.97	0.46
5:F:39:ARG:NH1	5:F:43:GLY:O	2.47	0.45
5:E:21:PHE:HE2	5:E:178:ALA:HA	1.82	0.45
2:B:238:ALA:HA	2:B:241:ILE:HD12	1.97	0.45
2:B:1096:GLY:HA3	2:B:1117:VAL:HG22	1.99	0.45
4:D:117:ILE:HB	4:D:129:ILE:HB	1.98	0.45
2:B:1297:GLY:HA3	5:E:18:ILE:HD12	1.99	0.45
2:B:965:MET:HE3	2:B:965:MET:HB3	1.83	0.44
2:B:337:LEU:O	2:B:342:ARG:NH1	2.50	0.44
2:B:540:LYS:HD3	2:B:540:LYS:HA	1.84	0.44
4:D:434:ALA:HB2	4:D:447:LEU:HD21	1.98	0.44
2:B:1185:ALA:HB1	2:B:1205:GLN:HB3	2.00	0.44
3:C:39:ILE:HG23	3:C:122:LEU:HD21	1.99	0.44
4:D:419:LYS:HD3	4:D:422:PHE:HE1	1.83	0.44
4:D:58:GLY:HA2	4:D:61:LEU:HB2	1.99	0.44
3:C:332:PRO:O	4:D:366:TYR:OH	2.36	0.44
1:A:394:MET:SD	1:A:649:GLN:NE2	2.91	0.43
2:B:1192:MET:HE3	2:B:1192:MET:HB3	1.90	0.43
1:A:281:PRO:O	1:A:284:HIS:HB3	2.19	0.43
4:D:78:LYS:HA	4:D:79:GLU:HA	1.73	0.43
2:B:203:VAL:HA	2:B:204:ASP:HA	1.80	0.43
3:C:78:VAL:HG11	4:D:130:GLU:H	1.84	0.43
1:A:640:ASP:OD1	1:A:642:ARG:NH1	2.52	0.42
5:F:104:ASN:ND2	5:F:106:GLU:OE1	2.49	0.42
2:B:78:LEU:HD11	2:B:144:VAL:HG21	2.02	0.42
5:E:129:ALA:HB2	5:E:177:ILE:HD11	2.01	0.42
5:E:135:ALA:HB3	5:E:163:SER:HB2	2.02	0.42
2:B:126:ARG:NH2	2:B:283:ASP:OD2	2.52	0.42
4:D:449:GLN:O	4:D:451:LEU:N	2.53	0.42
2:B:1346:VAL:HG22	2:B:1356:VAL:HG22	2.01	0.42
2:B:483:ALA:HA	2:B:544:LEU:HD21	2.02	0.42
2:B:801:LYS:HE3	2:B:801:LYS:HB3	1.92	0.42
2:B:1097:CYS:HA	2:B:1098:VAL:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1121:LEU:O	2:B:1134:THR:HA	2.20	0.42
5:E:123:SER:HB3	5:E:126:ILE:HG12	2.02	0.42
2:B:165:THR:OG1	2:B:166:ASP:N	2.53	0.41
2:B:371:LYS:HE3	2:B:371:LYS:HB2	1.95	0.41
1:A:752:THR:HG1	1:A:756:LYS:H	1.69	0.41
1:A:280:GLY:HA3	1:A:281:PRO:HD3	1.91	0.41
2:B:713:LYS:HB3	2:B:714:LEU:HD23	2.02	0.41
1:A:736:THR:HG23	1:A:741:VAL:HB	2.03	0.40
2:B:994:SER:OG	2:B:995:ALA:N	2.53	0.40
3:C:376:VAL:HB	3:C:396:MET:HE1	2.02	0.40
2:B:996:VAL:HA	2:B:1012:SER:HA	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	804/887 (91%)	775 (96%)	29 (4%)	0	100	100
2	B	1185/1370 (86%)	1133 (96%)	49 (4%)	3 (0%)	36	64
3	C	373/450 (83%)	367 (98%)	5 (1%)	1 (0%)	36	64
4	D	419/699 (60%)	406 (97%)	13 (3%)	0	100	100
5	E	168/212 (79%)	162 (96%)	6 (4%)	0	100	100
5	F	169/212 (80%)	165 (98%)	4 (2%)	0	100	100
All	All	3118/3830 (81%)	3008 (96%)	106 (3%)	4 (0%)	49	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	319	ILE

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Mol	Chain	Res	Type
3	C	286	ASN
2	B	650	LYS
2	B	582	ILE

### 5.3.2 Protein sidechains ⓘ

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	726/795 (91%)	726 (100%)	0	100	100
2	B	1050/1212 (87%)	1049 (100%)	1 (0%)	88	89
3	C	346/405 (85%)	346 (100%)	0	100	100
4	D	383/607 (63%)	383 (100%)	0	100	100
5	E	142/175 (81%)	142 (100%)	0	100	100
5	F	143/175 (82%)	143 (100%)	0	100	100
All	All	2790/3369 (83%)	2789 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1085	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	88	ASN
1	A	105	GLN
1	A	259	GLN
1	A	264	ASN
1	A	491	ASN
1	A	507	GLN
1	A	545	GLN
1	A	546	GLN

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Mol	Chain	Res	Type
1	A	643	GLN
1	A	814	ASN
2	B	83	ASN
2	B	104	GLN
2	B	138	GLN
2	B	373	ASN
2	B	424	HIS
2	B	457	ASN
2	B	744	HIS
2	B	777	GLN
2	B	988	HIS
3	C	275	HIS
3	C	326	GLN
3	C	420	ASN
4	D	47	ASN
4	D	52	ASN
4	D	181	GLN
4	D	266	HIS
4	D	334	ASN
4	D	456	ASN
5	E	46	HIS
5	E	171	ASN
5	F	20	GLN
5	F	46	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	GDP	B	1402	8	28,30,30	1.15	3 (10%)	44,47,47	1.79	8 (18%)
6	MYR	B	1401	2	14,14,15	0.34	0	13,13,15	0.39	0
10	GTP	E	301	8	30,34,34	0.85	1 (3%)	46,54,54	1.70	11 (23%)
10	GTP	F	301	8	30,34,34	0.83	1 (3%)	46,54,54	1.78	11 (23%)

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
7	GDP	B	1402	8	-	5/16/32/32	0/3/3/3
6	MYR	B	1401	2	-	1/11/12/13	-
10	GTP	E	301	8	-	1/22/38/38	0/3/3/3
10	GTP	F	301	8	-	2/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1402	GDP	C5-C4	3.07	1.47	1.38
7	B	1402	GDP	C6-N1	-2.49	1.34	1.38
10	F	301	GTP	C2-N3	2.26	1.38	1.33
10	E	301	GTP	C2-N3	2.24	1.38	1.33
7	B	1402	GDP	C5-N7	-2.17	1.34	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1402	GDP	C5-C4-N3	-5.97	118.77	128.46
10	F	301	GTP	C5-C4-N3	-5.07	120.23	128.46
10	E	301	GTP	C5-C4-N3	-5.03	120.30	128.46
7	B	1402	GDP	C2-N3-C4	4.76	120.79	112.30
10	F	301	GTP	C2-N3-C4	4.49	120.30	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	301	GTP	C2-N3-C4	4.43	120.19	112.30
7	B	1402	GDP	N9-C4-N3	4.41	134.80	125.94
10	F	301	GTP	PA-O3A-PB	-3.48	120.89	132.83
10	F	301	GTP	PB-O3B-PG	-3.33	121.41	132.83
10	F	301	GTP	N9-C4-N3	3.30	132.57	125.94
10	E	301	GTP	N9-C4-N3	3.27	132.51	125.94
7	B	1402	GDP	PA-O3A-PB	-3.20	121.85	132.83
7	B	1402	GDP	C6-C5-N7	3.20	136.19	130.25
10	E	301	GTP	PA-O3A-PB	-3.02	122.45	132.83
10	F	301	GTP	C2-N1-C6	-2.86	119.89	125.10
10	E	301	GTP	C2-N1-C6	-2.78	120.03	125.10
7	B	1402	GDP	C4-C5-N7	-2.65	106.53	110.72
10	E	301	GTP	N9-C8-N7	-2.50	108.67	113.39
10	F	301	GTP	C5-C6-N1	2.49	119.50	113.19
10	F	301	GTP	N9-C8-N7	-2.47	108.74	113.39
10	E	301	GTP	C5-C6-N1	2.46	119.44	113.19
10	F	301	GTP	C8-N7-C5	2.42	108.63	104.24
10	E	301	GTP	C8-N7-C5	2.41	108.61	104.24
10	F	301	GTP	O6-C6-C5	-2.40	120.24	126.60
10	E	301	GTP	O6-C6-C5	-2.37	120.31	126.60
10	E	301	GTP	PB-O3B-PG	-2.32	124.86	132.83
10	E	301	GTP	C3'-C2'-C1'	2.25	105.71	101.43
10	F	301	GTP	C3'-C2'-C1'	2.18	105.57	101.43
7	B	1402	GDP	C3'-C2'-C1'	2.12	105.44	101.43
7	B	1402	GDP	O6-C6-C5	-2.04	121.19	126.60

There are no chirality outliers.

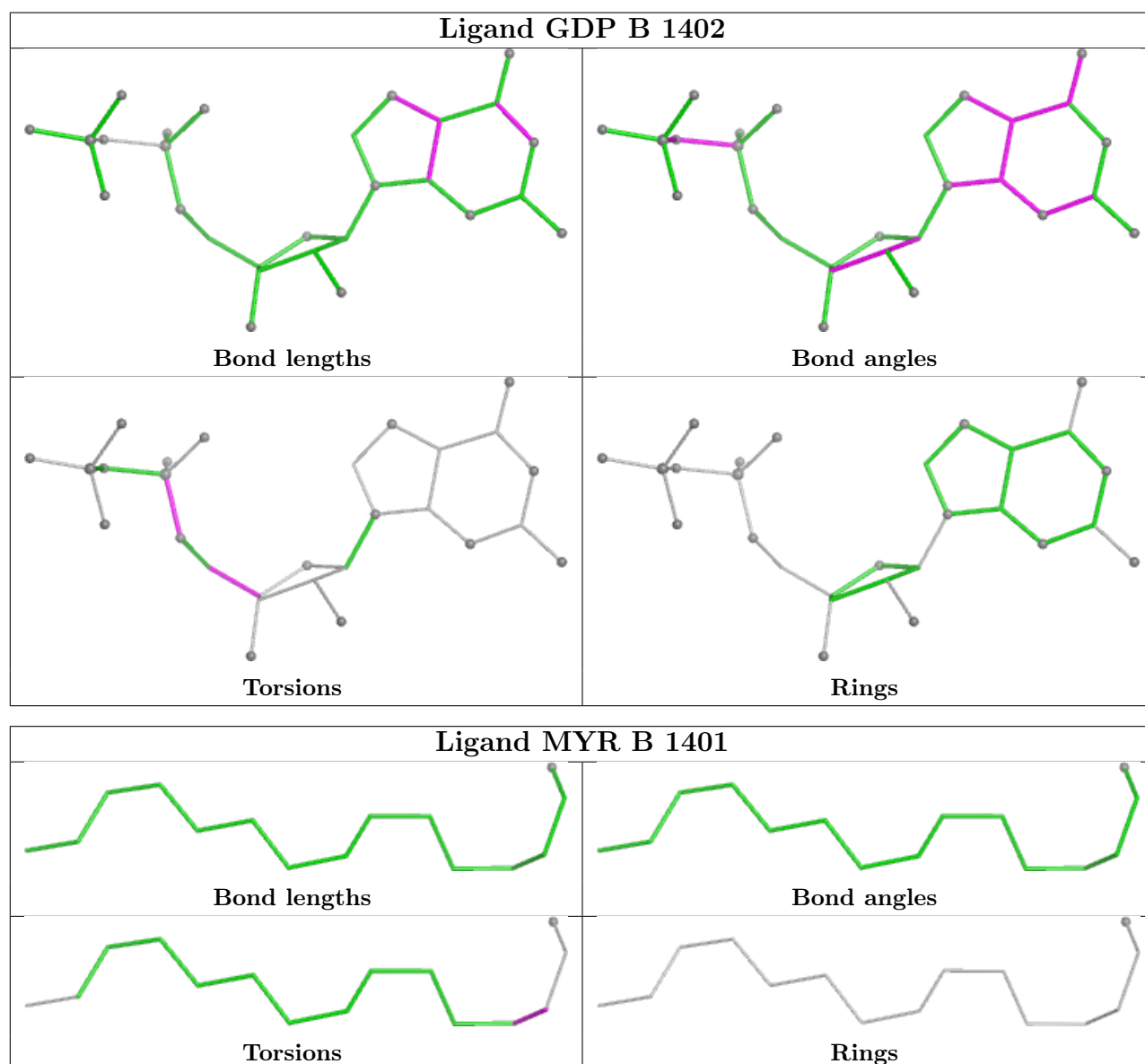
All (9) torsion outliers are listed below:

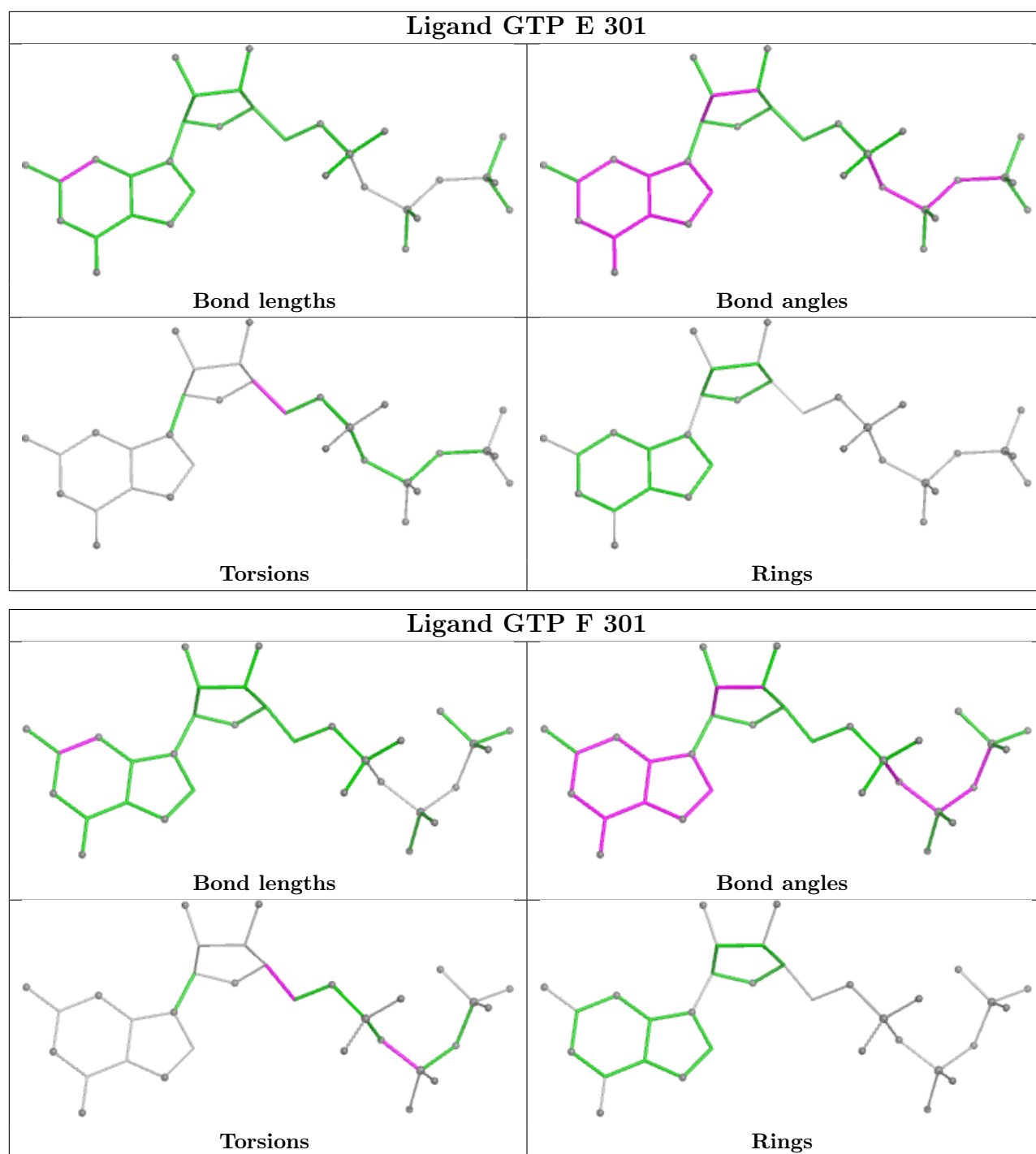
Mol	Chain	Res	Type	Atoms
6	B	1401	MYR	C1-C2-C3-C4
7	B	1402	GDP	C5'-O5'-PA-O3A
7	B	1402	GDP	C5'-O5'-PA-O2A
7	B	1402	GDP	O4'-C4'-C5'-O5'
7	B	1402	GDP	C3'-C4'-C5'-O5'
7	B	1402	GDP	C5'-O5'-PA-O1A
10	F	301	GTP	PA-O3A-PB-O2B
10	F	301	GTP	O4'-C4'-C5'-O5'
10	E	301	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.





## 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.

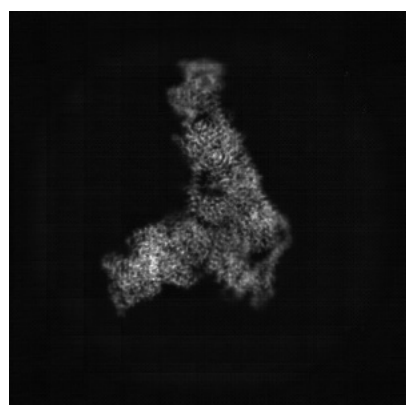
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54358. These allow visual inspection of the internal detail of the map and identification of artifacts.

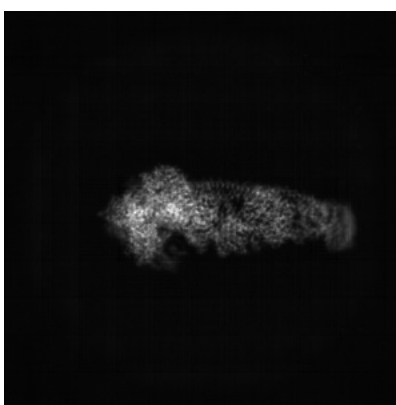
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

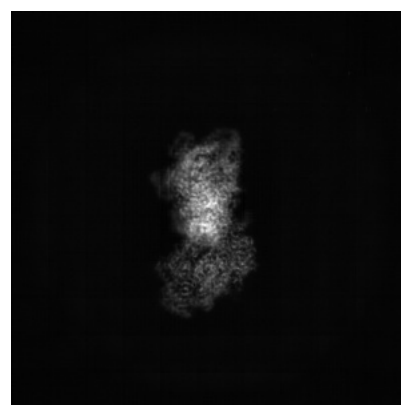
#### 6.1.1 Primary map



X



Y



Z

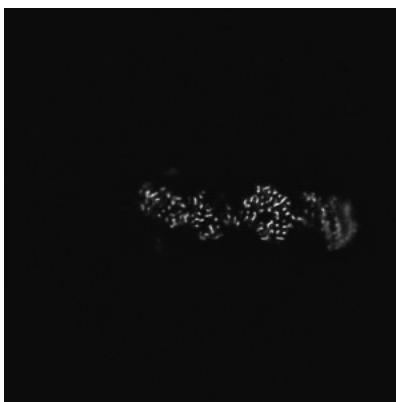
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 204



Y Index: 204

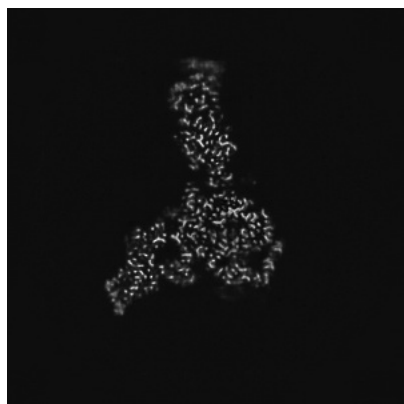


Z Index: 204

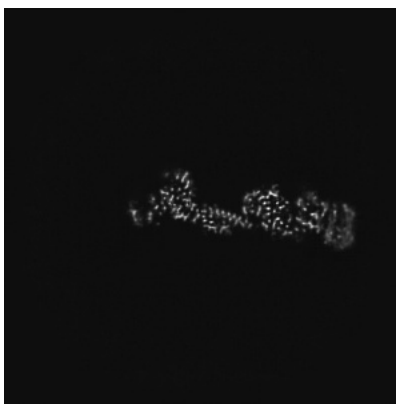
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 201



Y Index: 189

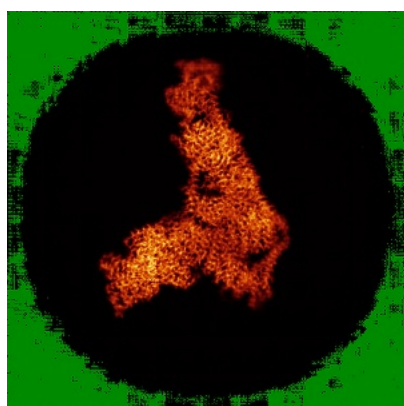


Z Index: 147

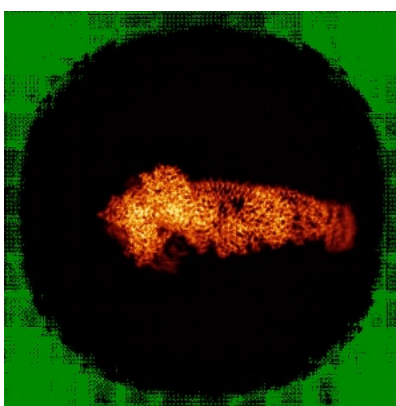
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

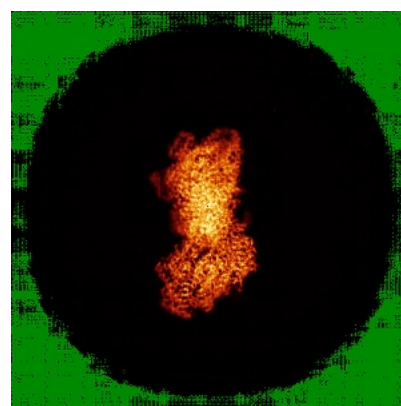
### 6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

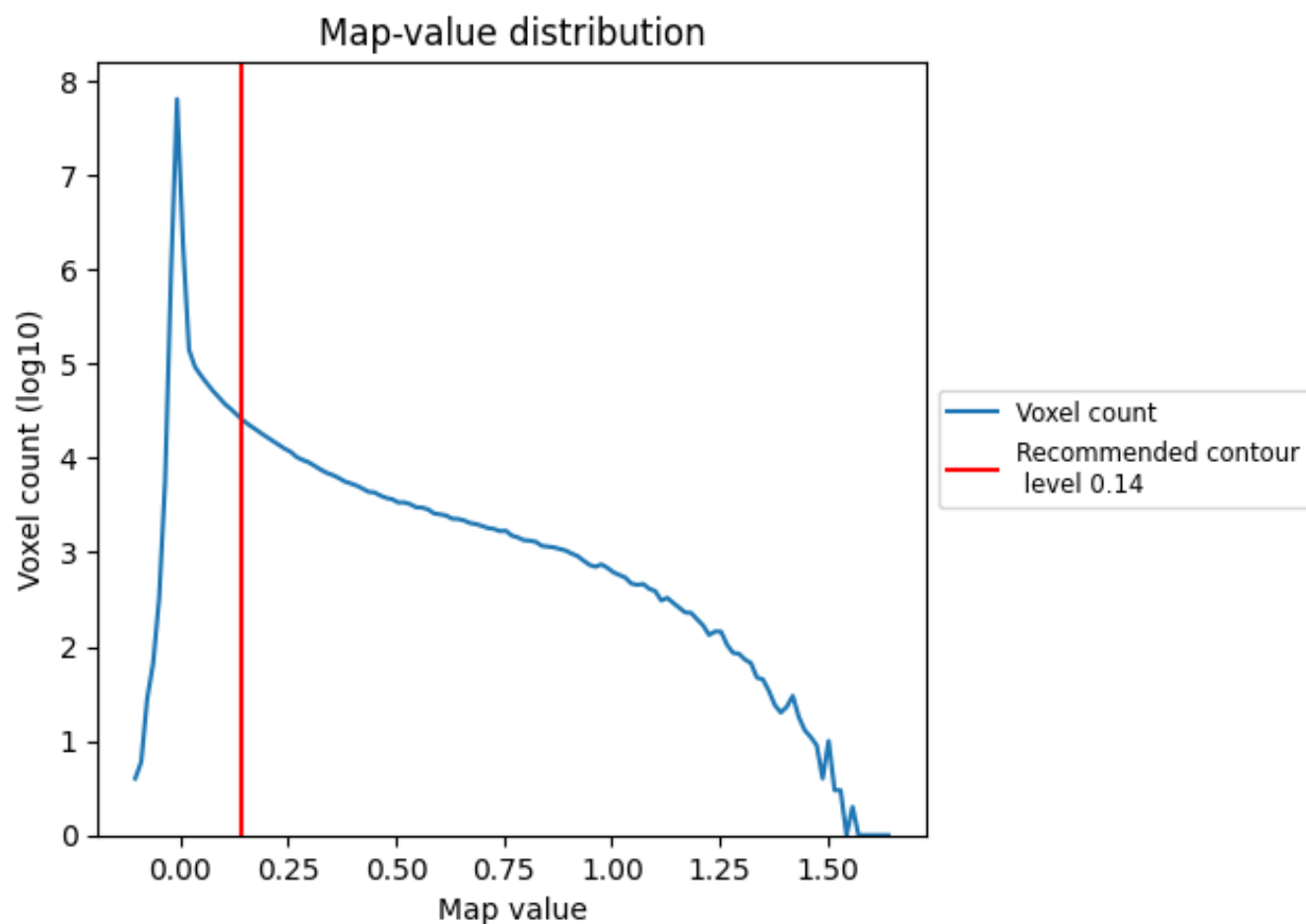
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

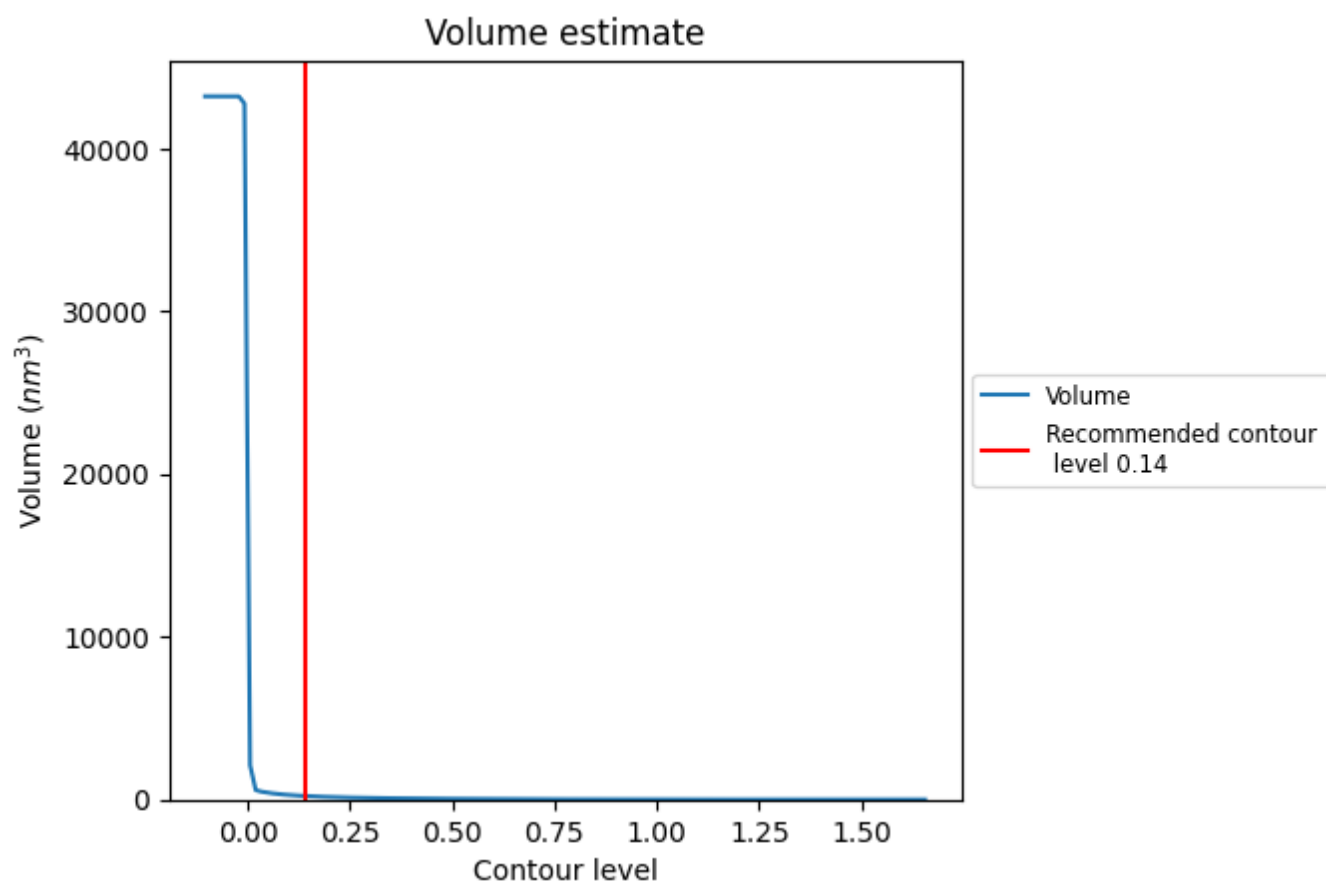
This section contains the results of statistical analysis of the map.

### 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.

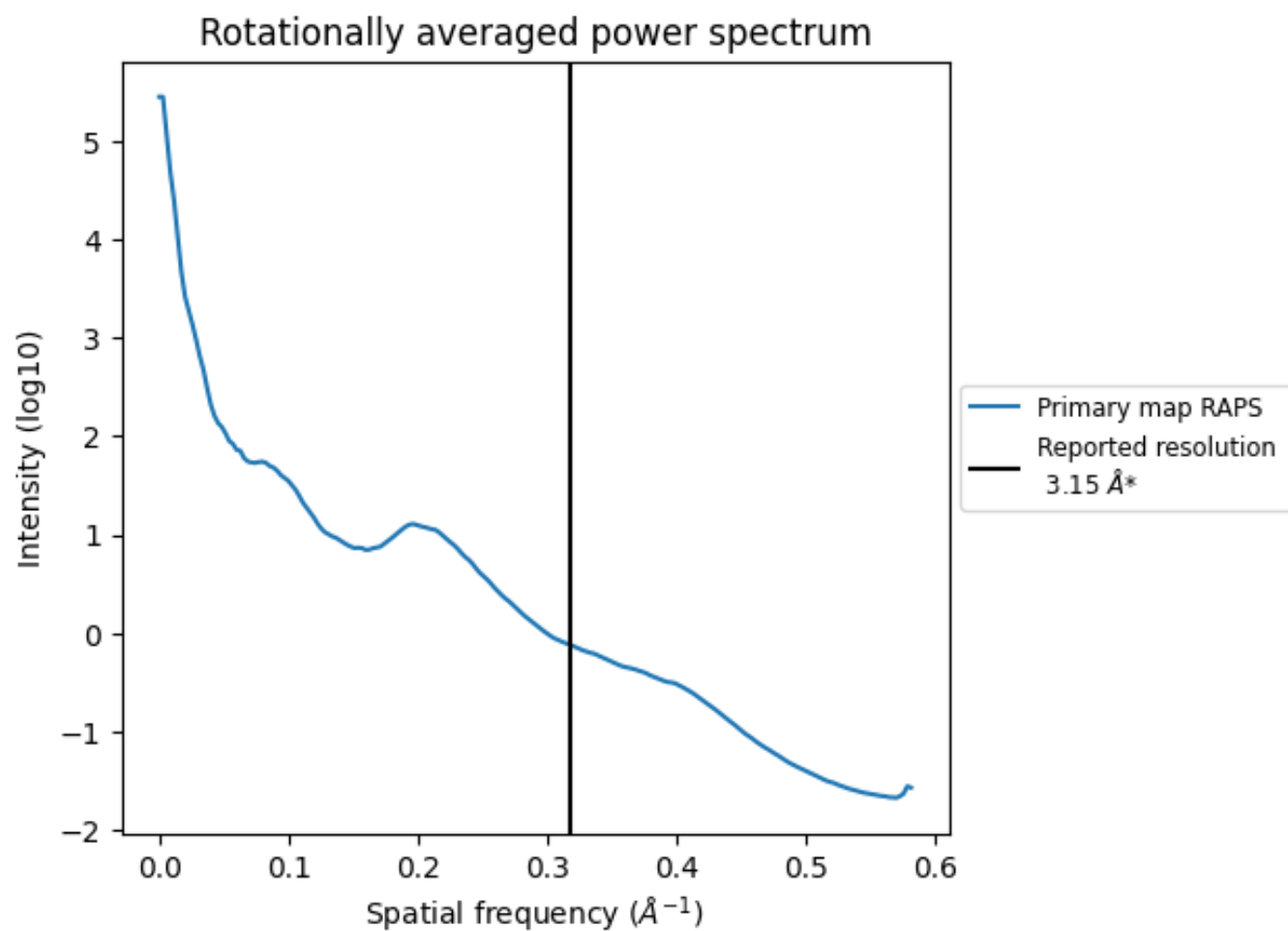
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm<sup>3</sup>; this corresponds to an approximate mass of 198 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.317 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

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

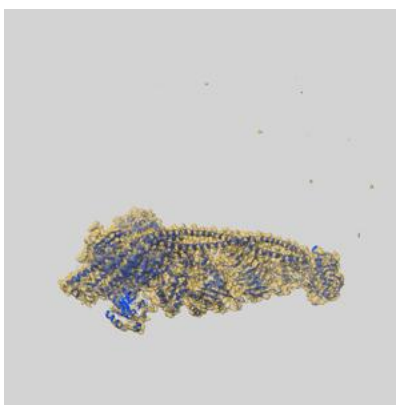
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54358 and PDB model 9RX5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

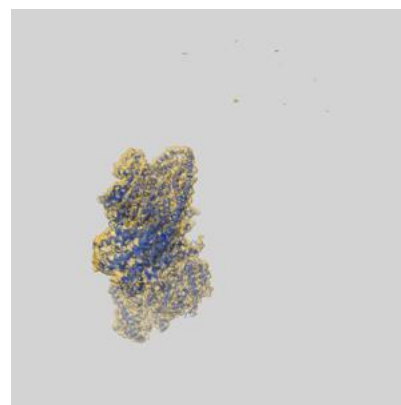
### 9.1 Map-model overlay [i](#)



X



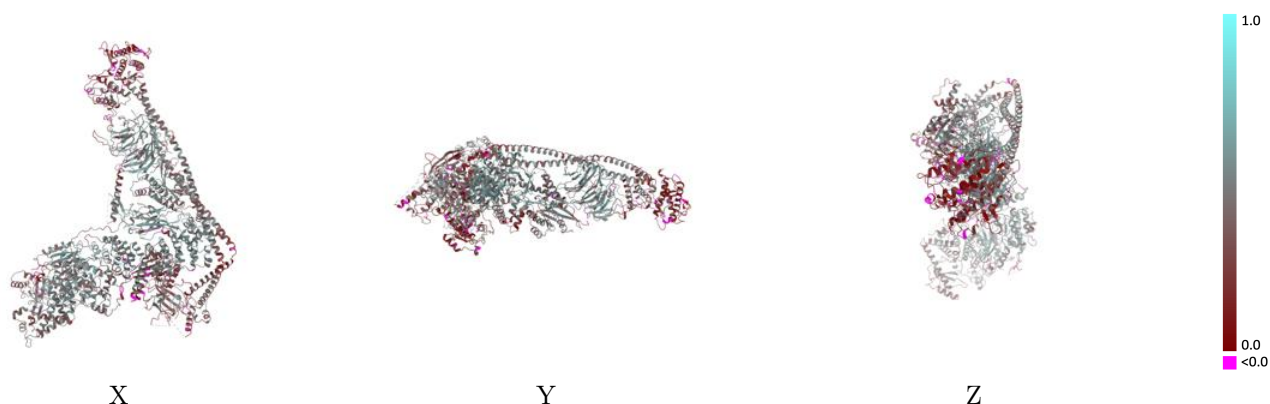
Y



Z

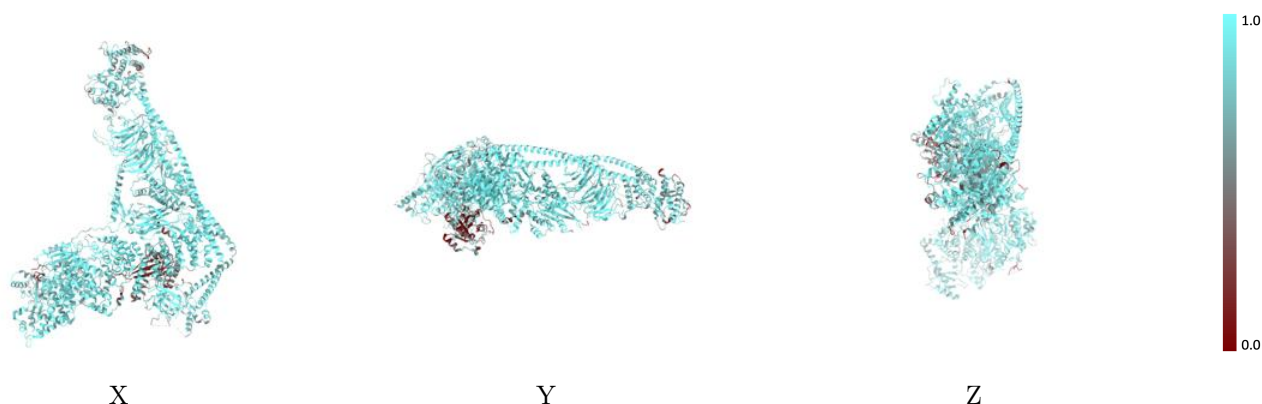
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



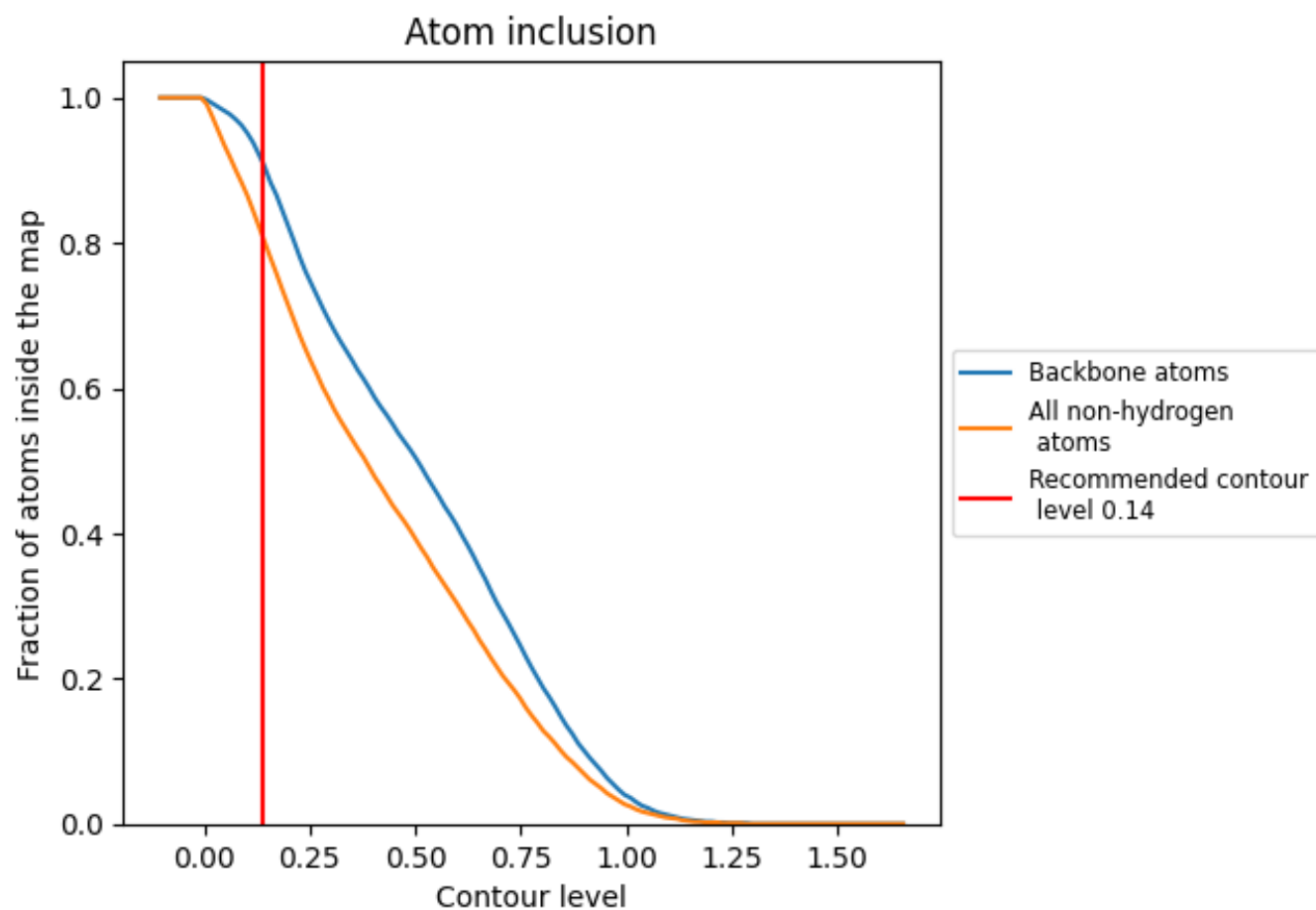
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.14).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 81% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8060</div>	<div><div></div>0.4000</div>
A	<div><div></div>0.8510</div>	<div><div></div>0.4480</div>
B	<div><div></div>0.8690</div>	<div><div></div>0.4590</div>
C	<div><div></div>0.7520</div>	<div><div></div>0.2660</div>
D	<div><div></div>0.7940</div>	<div><div></div>0.3360</div>
E	<div><div></div>0.8630</div>	<div><div></div>0.4300</div>
F	<div><div></div>0.2630</div>	<div><div></div>0.1990</div>

1.0

0.0

<0.0