Full wwPDB EM Validation Report ⓘ

Mar 5, 2025 – 05:25 PM EST

PDB ID	:	9EIJ
EMDB ID	:	EMD-48085
Title	:	Import stalled PINK1 TOM complex, extended TOM20 helix class
Authors	:	Kirk, N.S.; Glukhova, A.
Deposited on	:	2024-11-26
Resolution	:	3.30 Å(reported)
Based on initial models	:	., 7CP9

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:

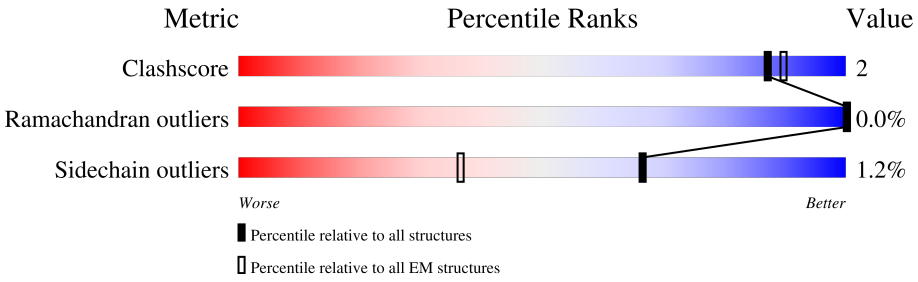
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.30 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.



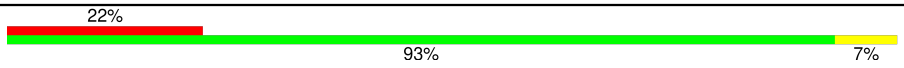
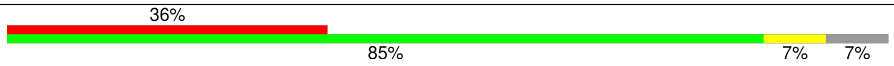
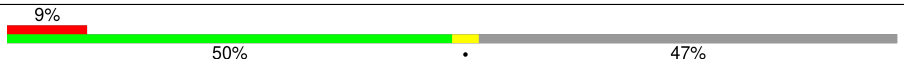
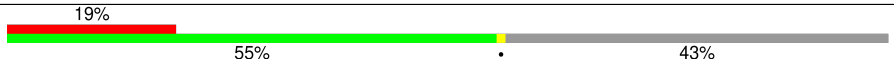
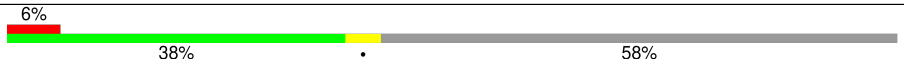
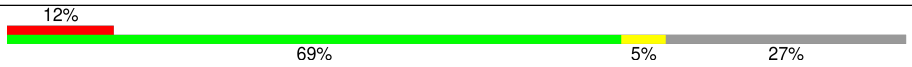
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	D	145	39% 83% 6% 10%
2	E	294	28% 91% 5%
2	F	294	12% 92%
3	I	361	72% 7% 21%
3	J	361	73% 6% 21%
4	K	51	61% 6% 33%
4	L	51	18% 92% 6%
4	Z	51	22% 65% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	N	55	
5	X	55	
6	P	74	
6	V	74	
7	R	142	
7	T	142	
8	B	603	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16970 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 Mitochondrial import receptor subunit TOM20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	130	Total	C	N	O	S	0	0
			1029	655	185	184	5		

- Molecule 2 is a protein called Non-selective voltage-gated ion channel VDAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	284	Total	C	N	O	S	0	0
			2146	1352	357	427	10		
2	F	282	Total	C	N	O	S	0	0
			2131	1342	355	425	9		

- Molecule 3 is a protein called Mitochondrial import receptor subunit TOM40 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	285	Total	C	N	O	S	0	0
			2184	1390	375	409	10		
3	J	285	Total	C	N	O	S	0	0
			2184	1390	375	409	10		

- Molecule 4 is a protein called Mitochondrial import receptor subunit TOM5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	34	Total	C	N	O	S	0	0
			288	190	51	45	2		
4	L	48	Total	C	N	O	S	0	0
			400	263	69	65	3		
4	Z	34	Total	C	N	O	S	0	0
			288	190	51	45	2		

- Molecule 5 is a protein called Mitochondrial import receptor subunit TOM7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	55	Total	C	N	O	S	0	0
			442	294	75	71	2		
5	X	51	Total	C	N	O	S	0	0
			410	272	70	67	1		

- Molecule 6 is a protein called Mitochondrial import receptor subunit TOM6 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	39	Total	C	N	O	0	0
			326	209	63	54		
6	V	42	Total	C	N	O	0	0
			350	225	66	59		

- Molecule 7 is a protein called Mitochondrial import receptor subunit TOM22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	59	Total	C	N	O	S	0	0
			478	309	81	85	3		
7	T	50	Total	C	N	O	S	0	0
			417	271	70	73	3		

- Molecule 8 is a protein called Serine/threonine-protein kinase PINK1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	443	Total	C	N	O	S	0	0
			3411	2172	609	604	26		

There are 22 discrepancies between the modelled and reference sequences:

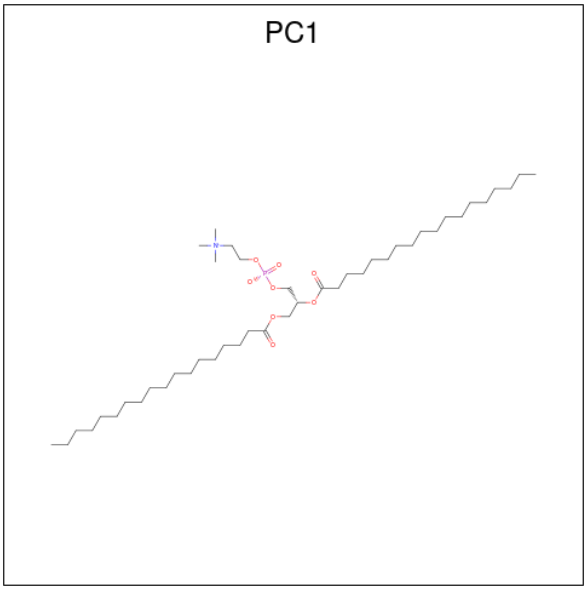
Chain	Residue	Modelled	Actual	Comment	Reference
B	582	ASP	-	expression tag	UNP Q9BXM7
B	583	TYR	-	expression tag	UNP Q9BXM7
B	584	LYS	-	expression tag	UNP Q9BXM7
B	585	ASP	-	expression tag	UNP Q9BXM7
B	586	HIS	-	expression tag	UNP Q9BXM7
B	587	ASP	-	expression tag	UNP Q9BXM7
B	588	GLY	-	expression tag	UNP Q9BXM7
B	589	ASP	-	expression tag	UNP Q9BXM7
B	590	TYR	-	expression tag	UNP Q9BXM7
B	591	LYS	-	expression tag	UNP Q9BXM7
B	592	ASP	-	expression tag	UNP Q9BXM7
B	593	HIS	-	expression tag	UNP Q9BXM7
B	594	ASP	-	expression tag	UNP Q9BXM7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	595	ILE	-	expression tag	UNP Q9BXM7
B	596	ASP	-	expression tag	UNP Q9BXM7
B	597	TYR	-	expression tag	UNP Q9BXM7
B	598	LYS	-	expression tag	UNP Q9BXM7
B	599	ASP	-	expression tag	UNP Q9BXM7
B	600	ASP	-	expression tag	UNP Q9BXM7
B	601	ASP	-	expression tag	UNP Q9BXM7
B	602	ASP	-	expression tag	UNP Q9BXM7
B	603	LYS	-	expression tag	UNP Q9BXM7

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
9	F	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	J	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	N	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	N	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	P	1	Total	C	N	O	P	0
			54	44	1	8	1	

Continued on next page...

Continued from previous page...

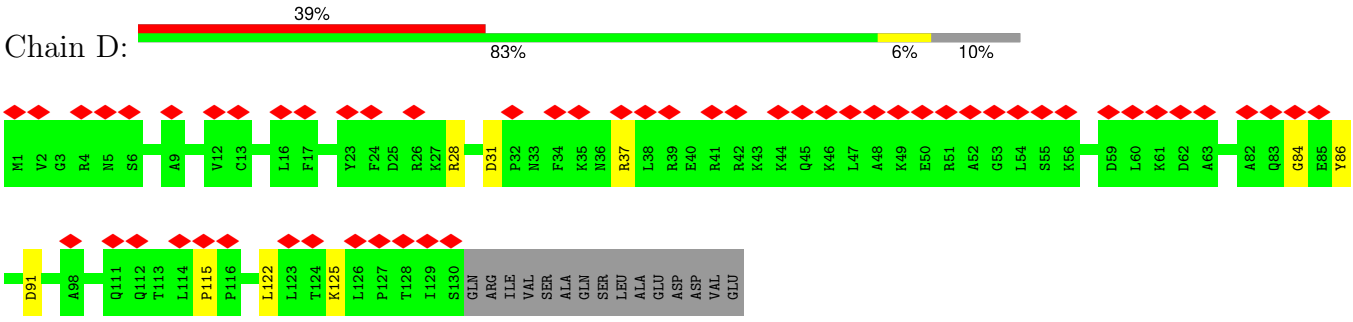
Mol	Chain	Residues	Atoms					AltConf
9	R	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	R	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	T	1	Total	C	N	O	P	0
			54	44	1	8	1	

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.

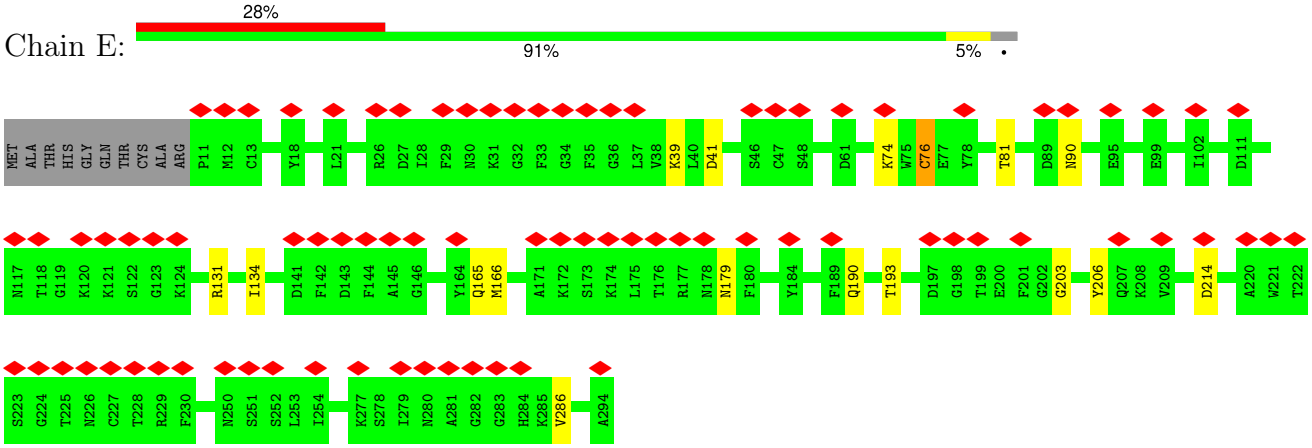
• Molecule 1: Mitochondrial import receptor subunit TOM20 homolog

Chain D:



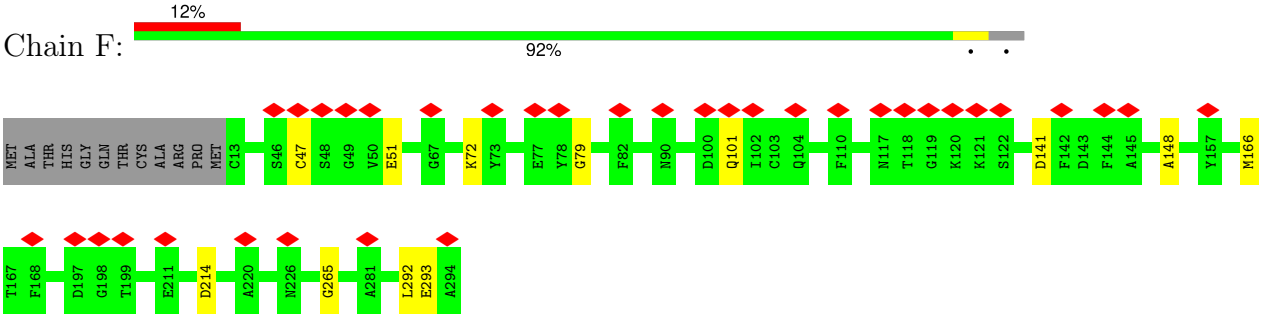
• Molecule 2: Non-selective voltage-gated ion channel VDAC2

Chain E:



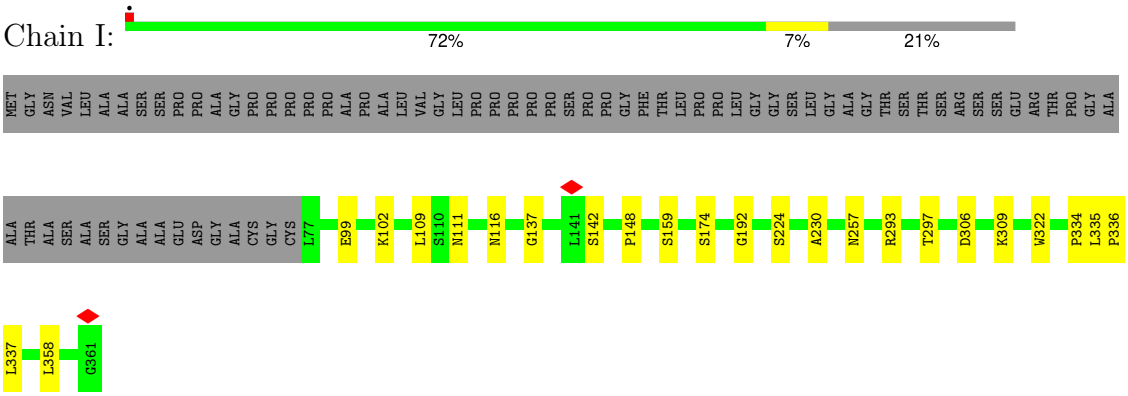
• Molecule 2: Non-selective voltage-gated ion channel VDAC2

Chain F:



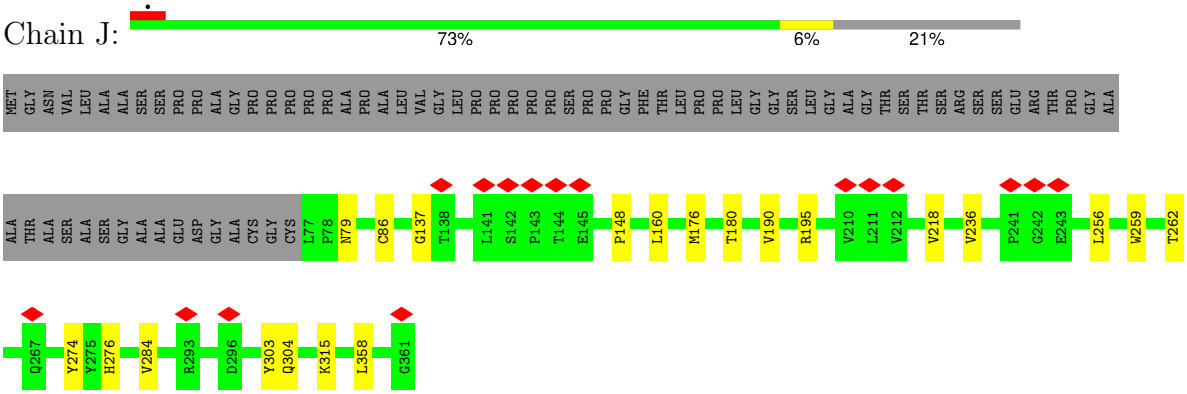
• Molecule 3: Mitochondrial import receptor subunit TOM40 homolog

Chain I:



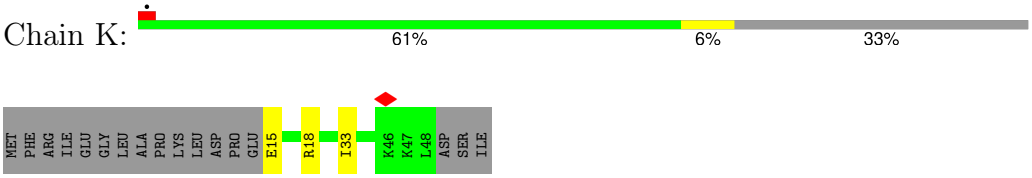
• Molecule 3: Mitochondrial import receptor subunit TOM40 homolog

Chain J:



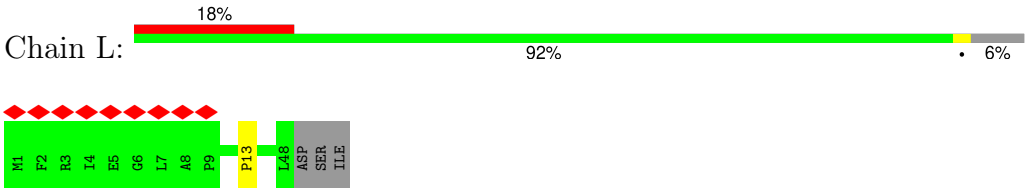
• Molecule 4: Mitochondrial import receptor subunit TOM5 homolog

Chain K:



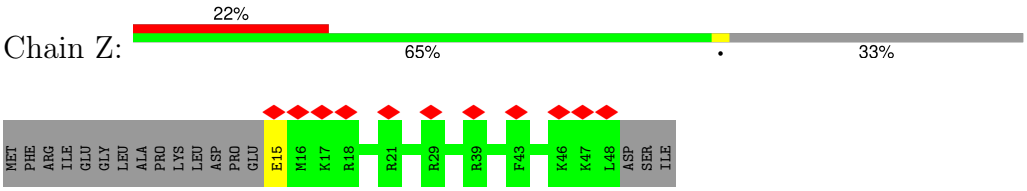
• Molecule 4: Mitochondrial import receptor subunit TOM5 homolog

Chain L:



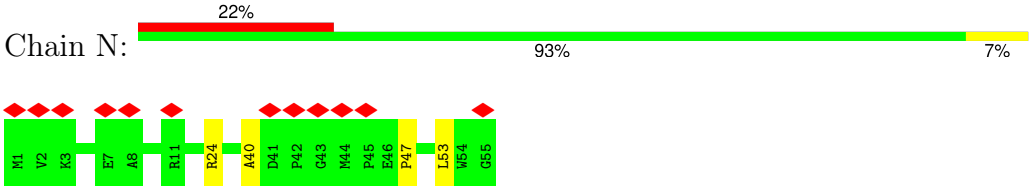
• Molecule 4: Mitochondrial import receptor subunit TOM5 homolog

Chain Z:



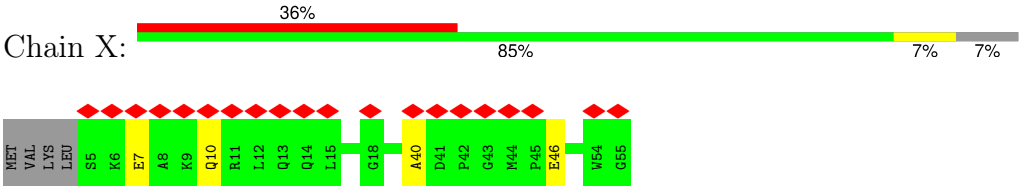
• Molecule 5: Mitochondrial import receptor subunit TOM7 homolog

Chain N:



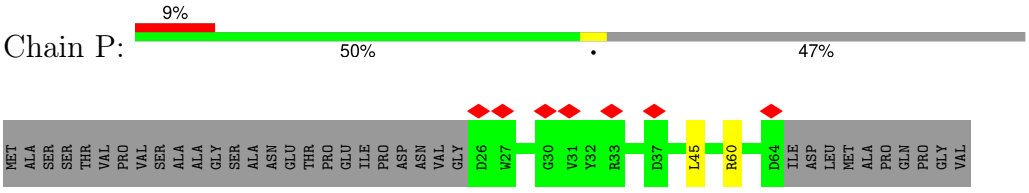
• Molecule 5: Mitochondrial import receptor subunit TOM7 homolog

Chain X:



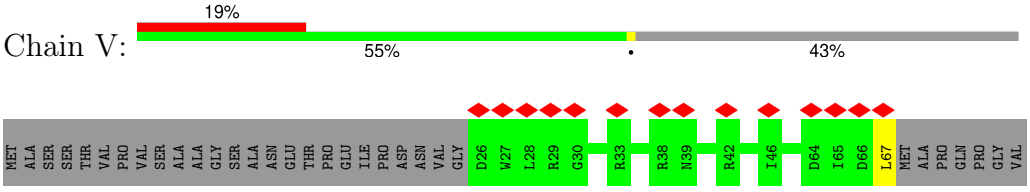
• Molecule 6: Mitochondrial import receptor subunit TOM6 homolog

Chain P:



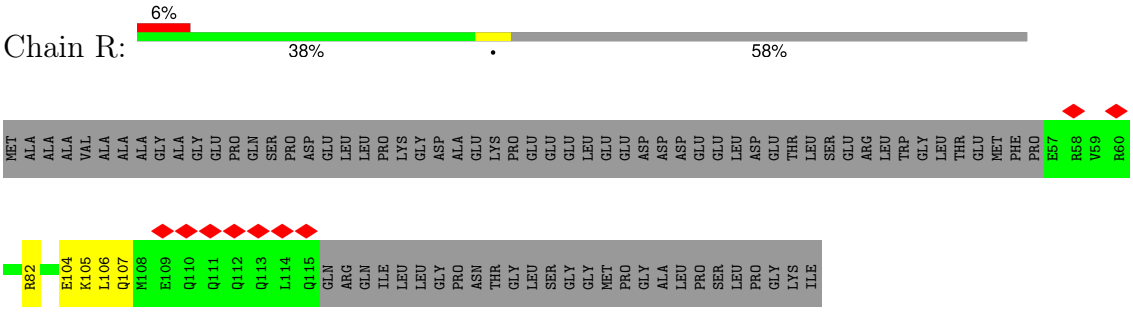
• Molecule 6: Mitochondrial import receptor subunit TOM6 homolog

Chain V:



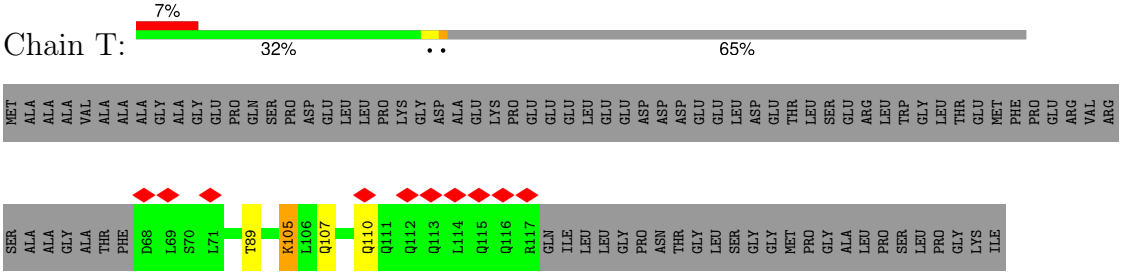
• Molecule 7: Mitochondrial import receptor subunit TOM22 homolog

Chain R:



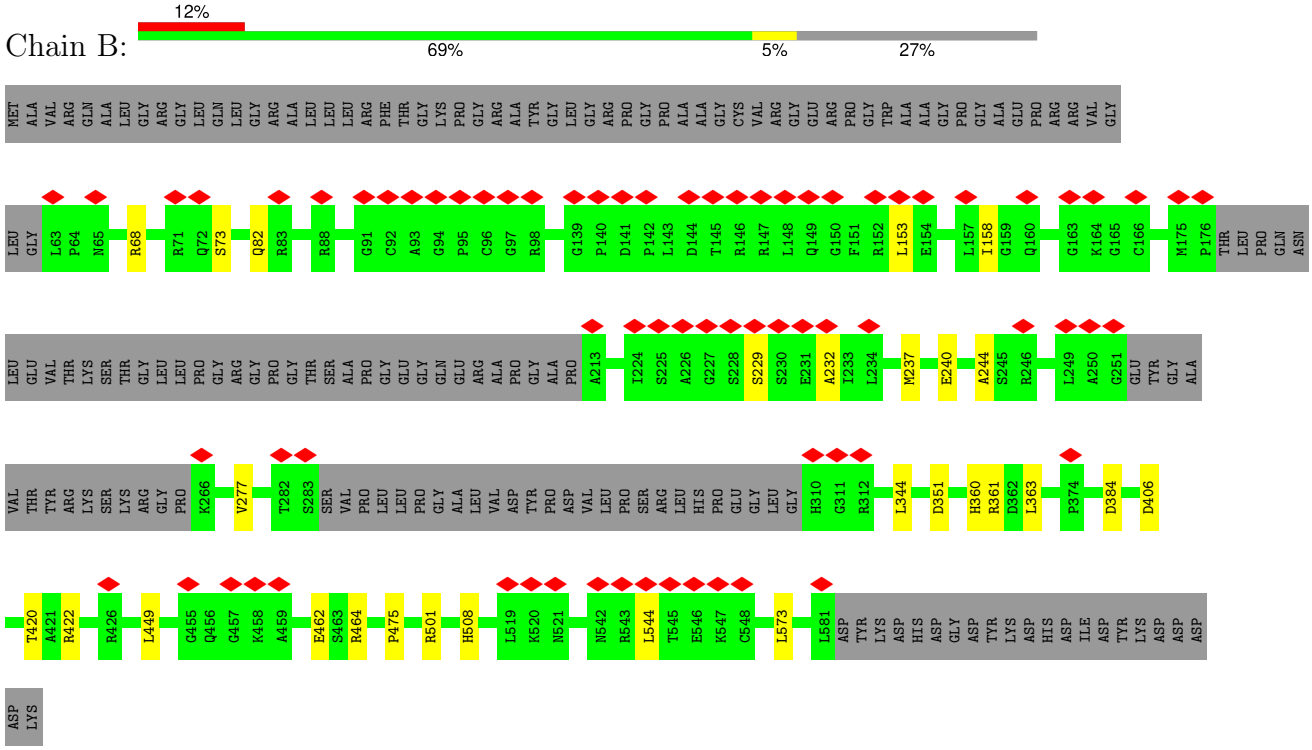
• Molecule 7: Mitochondrial import receptor subunit TOM22 homolog

Chain T:



• Molecule 8: Serine/threonine-protein kinase PINK1, mitochondrial

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	165000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.363	Depositor
Minimum map value	-0.154	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0625	Depositor
Map size (Å)	559.776, 559.776, 559.776	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1662, 1.1662, 1.1662	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1

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	D	0.24	0/1045	0.45	0/1404
2	E	0.25	0/2188	0.51	0/2956
2	F	0.25	0/2172	0.51	0/2935
3	I	0.26	0/2234	0.50	0/3031
3	J	0.25	0/2234	0.51	0/3031
4	K	0.24	0/291	0.49	0/387
4	L	0.25	0/406	0.52	0/542
4	Z	0.24	0/291	0.51	0/387
5	N	0.24	0/454	0.46	0/609
5	X	0.24	0/422	0.42	0/567
6	P	0.24	0/333	0.58	0/450
6	V	0.23	0/357	0.52	0/483
7	R	0.24	0/486	0.48	0/654
7	T	0.25	0/424	0.50	0/570
8	B	0.24	0/3479	0.49	0/4713
All	All	0.25	0/16816	0.50	0/22719

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

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	D	1029	0	1075	4	0
2	E	2146	0	2097	9	0
2	F	2131	0	2080	5	0
3	I	2184	0	2166	11	0
3	J	2184	0	2166	11	0
4	K	288	0	325	2	0
4	L	400	0	443	1	0
4	Z	288	0	325	0	0
5	N	442	0	468	2	0
5	X	410	0	423	2	0
6	P	326	0	320	1	0
6	V	350	0	346	1	0
7	R	478	0	487	4	0
7	T	417	0	428	3	0
8	B	3411	0	3481	16	0
9	F	54	0	88	0	0
9	I	54	0	88	0	0
9	J	54	0	88	0	0
9	N	108	0	176	1	0
9	P	54	0	88	2	0
9	R	108	0	176	2	0
9	T	54	0	88	1	0
All	All	16970	0	17422	64	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 (64) 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)
3:I:334:PRO:HG2	7:R:105:LYS:HE2	1.73	0.69
2:E:165:GLN:OE1	2:E:179:ASN:ND2	2.24	0.67
1:D:31:ASP:OD2	1:D:37:ARG:NH2	2.29	0.65
7:R:104:GLU:OE1	7:R:107:GLN:NE2	2.30	0.63
3:I:257:ASN:ND2	9:P:101:PC1:O14	2.32	0.62
6:P:60:ARG:NH2	9:P:101:PC1:O12	2.34	0.60
8:B:462:GLU:OE2	8:B:464:ARG:NH1	2.35	0.59
8:B:244:ALA:HA	8:B:277:VAL:HB	1.83	0.58
4:K:15:GLU:OE1	4:K:18:ARG:NH1	2.36	0.58
2:E:131:ARG:HB2	2:E:134:ILE:HB	1.87	0.57
8:B:351:ASP:OD2	8:B:501:ARG:NH1	2.33	0.56
2:E:74:LYS:HA	2:E:81:THR:HG23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:24:ARG:NH2	9:N:102:PC1:O32	2.36	0.55
2:F:51:GLU:HB3	2:F:72:LYS:HB2	1.88	0.55
7:T:107:GLN:HA	7:T:110:GLN:HG2	1.90	0.54
8:B:237:MET:HG3	8:B:240:GLU:HB2	1.91	0.52
2:E:131:ARG:HD3	2:E:134:ILE:HD12	1.92	0.52
1:D:91:ASP:OD1	1:D:125:LYS:NZ	2.25	0.51
3:I:99:GLU:O	3:I:102:LYS:NZ	2.30	0.51
3:I:337:LEU:HD22	3:I:358:LEU:HD21	1.92	0.50
2:E:39:LYS:NZ	2:E:41:ASP:OD2	2.43	0.50
8:B:361:ARG:NH1	8:B:406:ASP:O	2.43	0.50
1:D:115:PRO:HD3	8:B:544:LEU:HD13	1.94	0.50
2:E:190:GLN:HB2	2:E:206:TYR:HB3	1.93	0.49
3:I:335:LEU:HB3	3:I:336:PRO:HD2	1.93	0.49
7:T:105:LYS:HB3	7:T:105:LYS:HZ3	1.77	0.49
7:R:82:ARG:NH2	9:R:202:PC1:O32	2.46	0.48
8:B:360:HIS:NE2	8:B:384:ASP:O	2.46	0.48
3:J:137:GLY:HA3	3:J:148:PRO:HD2	1.96	0.48
2:F:79:GLY:HA3	2:F:101:GLN:HG3	1.96	0.47
3:I:224:SER:HA	3:I:230:ALA:HA	1.97	0.46
3:I:322:TRP:CD1	3:I:322:TRP:N	2.83	0.46
8:B:449:LEU:HD11	8:B:475:PRO:HD3	1.97	0.45
2:F:265:GLY:O	2:F:293:GLU:N	2.50	0.44
3:J:160:LEU:H	3:J:180:THR:HG23	1.83	0.44
3:J:256:LEU:HD23	3:J:259:TRP:HE1	1.82	0.44
7:T:89:THR:HG21	9:T:201:PC1:H241	2.00	0.44
8:B:344:LEU:HD11	8:B:508:HIS:CE1	2.53	0.43
2:E:286:VAL:HG11	4:K:33:ILE:HD12	1.99	0.43
3:I:137:GLY:HA3	3:I:148:PRO:HD2	2.00	0.43
3:J:86:CYS:HB3	3:J:262:THR:HG21	1.99	0.43
3:I:109:LEU:HD23	8:B:68:ARG:HD3	2.01	0.43
5:N:40:ALA:HB2	5:N:47:PRO:HD3	1.99	0.43
5:X:7:GLU:OE1	5:X:10:GLN:NE2	2.43	0.43
8:B:344:LEU:HD21	8:B:508:HIS:CE1	2.53	0.43
8:B:420:THR:HG22	8:B:464:ARG:HG3	2.00	0.43
3:I:174:SER:HA	3:I:192:GLY:HA2	2.01	0.43
3:J:218:VAL:HA	3:J:236:VAL:HA	2.01	0.43
4:L:13:PRO:HB3	8:B:573:LEU:HD11	2.01	0.42
2:F:141:ASP:HB2	2:F:148:ALA:HB3	2.01	0.42
1:D:84:GLY:HA2	1:D:86:TYR:CE1	2.55	0.42
2:E:193:THR:HA	2:E:203:GLY:HA2	2.01	0.42
3:J:274:TYR:CE2	3:J:276:HIS:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:284:VAL:HA	3:J:303:TYR:HA	2.01	0.42
3:J:304:GLN:OE1	3:J:315:LYS:HE2	2.20	0.42
3:J:358:LEU:HD22	9:R:201:PC1:H3B2	2.02	0.42
3:J:176:MET:HG2	3:J:190:VAL:HG23	2.02	0.41
8:B:153:LEU:HD11	8:B:158:ILE:HD11	2.02	0.41
7:R:106:LEU:HD13	6:V:67:LEU:HD13	2.02	0.41
5:X:40:ALA:HB2	5:X:46:GLU:HA	2.03	0.41
3:J:79:ASN:HD21	3:J:195:ARG:HB2	1.86	0.40
8:B:229:SER:HB3	8:B:232:ALA:HB3	2.04	0.40
2:E:76:CYS:HA	2:F:47:CYS:HB2	2.03	0.40
3:I:116:ASN:ND2	8:B:82:GLN:OE1	2.54	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	D	128/145 (88%)	121 (94%)	7 (6%)	0	100	100
2	E	282/294 (96%)	271 (96%)	11 (4%)	0	100	100
2	F	280/294 (95%)	263 (94%)	17 (6%)	0	100	100
3	I	283/361 (78%)	277 (98%)	6 (2%)	0	100	100
3	J	283/361 (78%)	275 (97%)	8 (3%)	0	100	100
4	K	32/51 (63%)	32 (100%)	0	0	100	100
4	L	46/51 (90%)	43 (94%)	3 (6%)	0	100	100
4	Z	32/51 (63%)	32 (100%)	0	0	100	100
5	N	53/55 (96%)	52 (98%)	0	1 (2%)	6	29
5	X	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
6	P	37/74 (50%)	37 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	V	40/74 (54%)	39 (98%)	1 (2%)	0	100	100
7	R	57/142 (40%)	57 (100%)	0	0	100	100
7	T	48/142 (34%)	48 (100%)	0	0	100	100
8	B	435/603 (72%)	420 (97%)	15 (3%)	0	100	100
All	All	2085/2753 (76%)	2015 (97%)	69 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	N	53	LEU

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	D	110/123 (89%)	108 (98%)	2 (2%)	54	74
2	E	232/239 (97%)	228 (98%)	4 (2%)	56	74
2	F	230/239 (96%)	227 (99%)	3 (1%)	65	79
3	I	237/288 (82%)	230 (97%)	7 (3%)	36	62
3	J	237/288 (82%)	237 (100%)	0	100	100
4	K	33/48 (69%)	33 (100%)	0	100	100
4	L	45/48 (94%)	45 (100%)	0	100	100
4	Z	33/48 (69%)	32 (97%)	1 (3%)	36	62
5	N	46/46 (100%)	46 (100%)	0	100	100
5	X	42/46 (91%)	42 (100%)	0	100	100
6	P	32/59 (54%)	31 (97%)	1 (3%)	35	61
6	V	35/59 (59%)	35 (100%)	0	100	100
7	R	51/115 (44%)	51 (100%)	0	100	100
7	T	46/115 (40%)	45 (98%)	1 (2%)	47	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	B	360/478 (75%)	357 (99%)	3 (1%)	79 87
All	All	1769/2239 (79%)	1747 (99%)	22 (1%)	66 80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	28	ARG
1	D	122	LEU
2	E	76	CYS
2	E	90	ASN
2	E	166	MET
2	E	214	ASP
2	F	166	MET
2	F	214	ASP
2	F	292	LEU
3	I	111	ASN
3	I	142	SER
3	I	159	SER
3	I	293	ARG
3	I	297	THR
3	I	306	ASP
3	I	309	LYS
6	P	45	LEU
7	T	105	LYS
4	Z	15	GLU
8	B	73	SER
8	B	363	LEU
8	B	422	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	192	HIS

5.3.3 RNA

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)

9 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
9	PC1	R	202	-	53,53,53	0.50	0	59,61,61	0.67	1 (1%)
9	PC1	F	301	-	53,53,53	0.50	0	59,61,61	0.42	0
9	PC1	N	102	-	53,53,53	0.51	0	59,61,61	0.48	0
9	PC1	R	201	-	53,53,53	0.48	0	59,61,61	0.60	1 (1%)
9	PC1	J	401	-	53,53,53	0.50	0	59,61,61	0.65	1 (1%)
9	PC1	P	101	-	53,53,53	0.50	0	59,61,61	0.50	0
9	PC1	N	101	-	53,53,53	0.50	0	59,61,61	0.40	0
9	PC1	T	201	-	53,53,53	0.50	0	59,61,61	0.57	0
9	PC1	I	401	-	53,53,53	0.49	0	59,61,61	0.70	1 (1%)

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
9	PC1	R	202	-	-	14/57/57/57	-
9	PC1	F	301	-	-	13/57/57/57	-
9	PC1	N	102	-	-	8/57/57/57	-
9	PC1	R	201	-	-	9/57/57/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	J	401	-	-	11/57/57/57	-
9	PC1	P	101	-	-	12/57/57/57	-
9	PC1	N	101	-	-	9/57/57/57	-
9	PC1	T	201	-	-	7/57/57/57	-
9	PC1	I	401	-	-	11/57/57/57	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	401	PC1	C2-O21-C21	3.47	126.09	117.80
9	I	401	PC1	C2-O21-C21	3.22	125.51	117.80
9	R	201	PC1	C2-O21-C21	2.74	124.36	117.80
9	R	202	PC1	C3-O31-C31	2.66	126.86	117.12

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	F	301	PC1	C11-O13-P-O12
9	F	301	PC1	C11-O13-P-O14
9	F	301	PC1	C11-O13-P-O11
9	I	401	PC1	C11-O13-P-O12
9	I	401	PC1	C11-O13-P-O14
9	I	401	PC1	C11-O13-P-O11
9	I	401	PC1	O22-C21-O21-C2
9	I	401	PC1	C22-C21-O21-C2
9	J	401	PC1	C1-O11-P-O12
9	J	401	PC1	C1-O11-P-O14
9	J	401	PC1	C1-O11-P-O13
9	J	401	PC1	C2-C1-O11-P
9	J	401	PC1	O22-C21-O21-C2
9	J	401	PC1	C22-C21-O21-C2
9	N	101	PC1	C1-O11-P-O12
9	N	102	PC1	C12-C11-O13-P
9	P	101	PC1	C12-C11-O13-P
9	R	202	PC1	C2-C3-O31-C31
9	T	201	PC1	O32-C31-O31-C3
9	T	201	PC1	C32-C31-O31-C3
9	R	202	PC1	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	R	202	PC1	C32-C31-O31-C3
9	F	301	PC1	O21-C2-C3-O31
9	R	202	PC1	C31-C32-C33-C34
9	R	202	PC1	C2C-C2D-C2E-C2F
9	J	401	PC1	C27-C28-C29-C2A
9	F	301	PC1	C2C-C2D-C2E-C2F
9	J	401	PC1	C35-C36-C37-C38
9	F	301	PC1	C2A-C2B-C2C-C2D
9	F	301	PC1	C3A-C3B-C3C-C3D
9	R	202	PC1	C28-C29-C2A-C2B
9	P	101	PC1	C28-C29-C2A-C2B
9	R	201	PC1	C27-C28-C29-C2A
9	F	301	PC1	C32-C33-C34-C35
9	I	401	PC1	C24-C25-C26-C27
9	R	201	PC1	C2B-C2C-C2D-C2E
9	N	102	PC1	C31-C32-C33-C34
9	N	101	PC1	C35-C36-C37-C38
9	T	201	PC1	C1-C2-C3-O31
9	R	202	PC1	C36-C37-C38-C39
9	J	401	PC1	O11-C1-C2-O21
9	R	201	PC1	C3B-C3C-C3D-C3E
9	F	301	PC1	C1-C2-C3-O31
9	J	401	PC1	C31-C32-C33-C34
9	P	101	PC1	O11-C1-C2-O21
9	T	201	PC1	O21-C2-C3-O31
9	J	401	PC1	O11-C1-C2-C3
9	N	101	PC1	O11-C1-C2-C3
9	F	301	PC1	C23-C24-C25-C26
9	N	101	PC1	O11-C1-C2-O21
9	F	301	PC1	C12-C11-O13-P
9	I	401	PC1	C12-C11-O13-P
9	R	202	PC1	C12-C11-O13-P
9	N	102	PC1	C32-C33-C34-C35
9	R	201	PC1	C28-C29-C2A-C2B
9	N	102	PC1	O13-C11-C12-N
9	R	202	PC1	O13-C11-C12-N
9	F	301	PC1	C24-C25-C26-C27
9	P	101	PC1	O11-C1-C2-C3
9	N	102	PC1	C2A-C2B-C2C-C2D
9	R	202	PC1	C2B-C2C-C2D-C2E
9	N	101	PC1	C1-O11-P-O14
9	N	101	PC1	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	R	202	PC1	C11-O13-P-O14
9	P	101	PC1	C2-C1-O11-P
9	R	201	PC1	C31-C32-C33-C34
9	R	201	PC1	O21-C2-C3-O31
9	P	101	PC1	C2-C3-O31-C31
9	N	101	PC1	C25-C26-C27-C28
9	F	301	PC1	C28-C29-C2A-C2B
9	R	201	PC1	C39-C3A-C3B-C3C
9	R	201	PC1	C3-C2-O21-C21
9	P	101	PC1	C33-C34-C35-C36
9	R	201	PC1	C2D-C2E-C2F-C2G
9	N	102	PC1	C34-C35-C36-C37
9	T	201	PC1	C32-C33-C34-C35
9	N	102	PC1	C25-C26-C27-C28
9	P	101	PC1	C2A-C2B-C2C-C2D
9	I	401	PC1	C3C-C3D-C3E-C3F
9	I	401	PC1	C39-C3A-C3B-C3C
9	R	202	PC1	C3D-C3E-C3F-C3G
9	P	101	PC1	C38-C39-C3A-C3B
9	T	201	PC1	O21-C21-C22-C23
9	I	401	PC1	O21-C21-C22-C23
9	P	101	PC1	O21-C21-C22-C23
9	N	101	PC1	O21-C2-C3-O31
9	N	102	PC1	O21-C2-C3-O31
9	R	202	PC1	C3-C2-O21-C21
9	P	101	PC1	O22-C21-C22-C23
9	N	101	PC1	O21-C21-C22-C23
9	T	201	PC1	O22-C21-C22-C23
9	P	101	PC1	C2C-C2D-C2E-C2F
9	I	401	PC1	O22-C21-C22-C23
9	R	202	PC1	C37-C38-C39-C3A

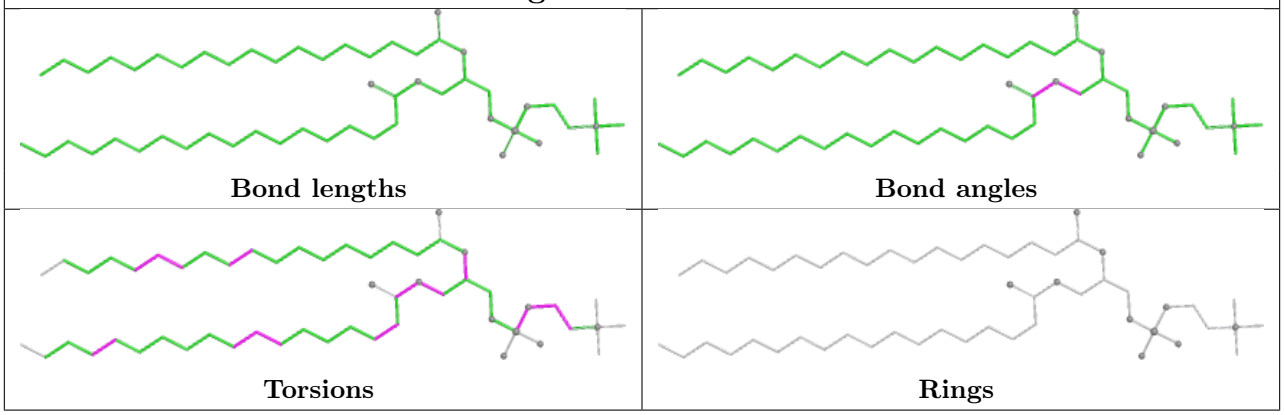
There are no ring outliers.

5 monomers are involved in 6 short contacts:

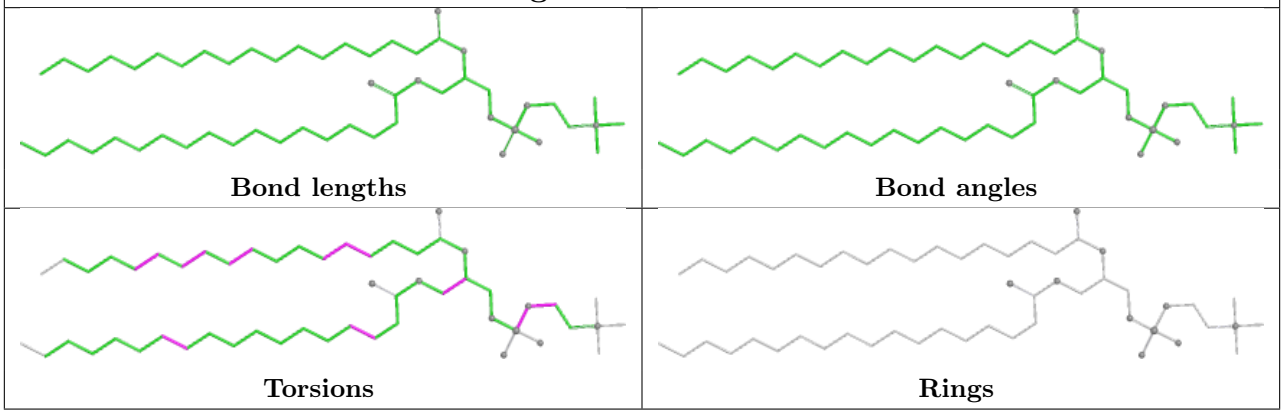
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	202	PC1	1	0
9	N	102	PC1	1	0
9	R	201	PC1	1	0
9	P	101	PC1	2	0
9	T	201	PC1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

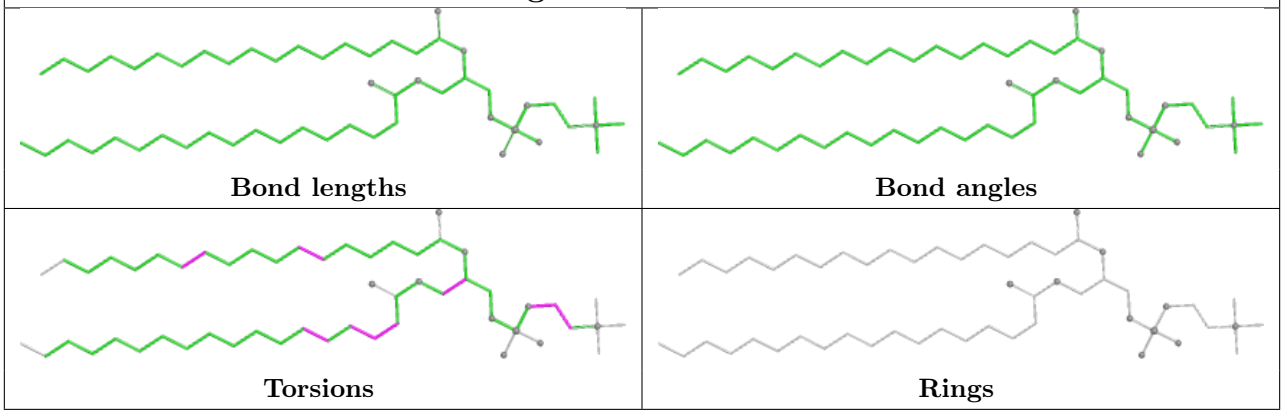
Ligand PC1 R 202



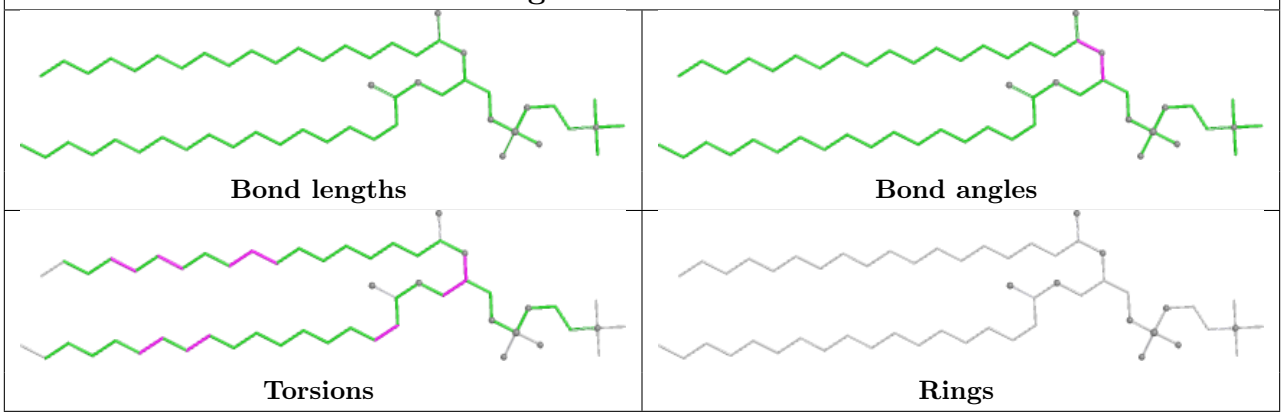
Ligand PC1 F 301



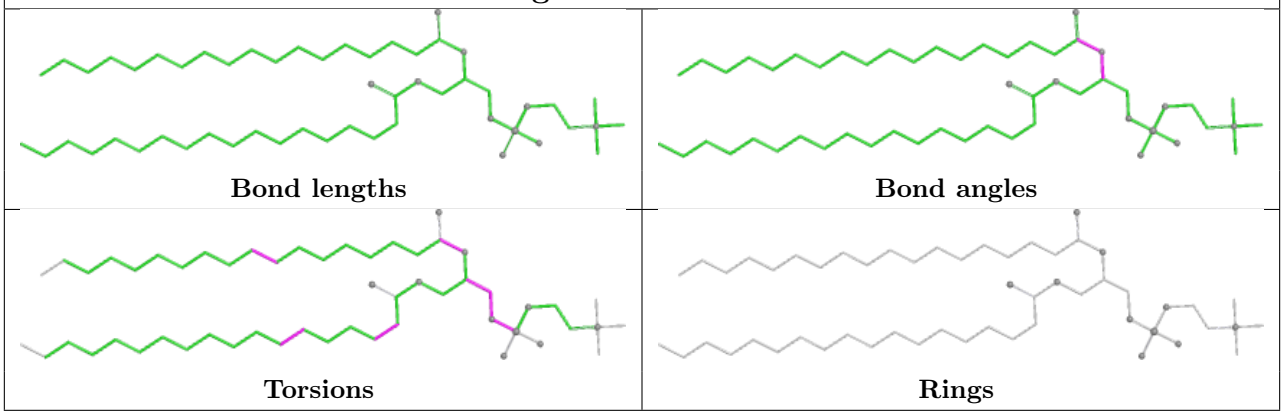
Ligand PC1 N 102



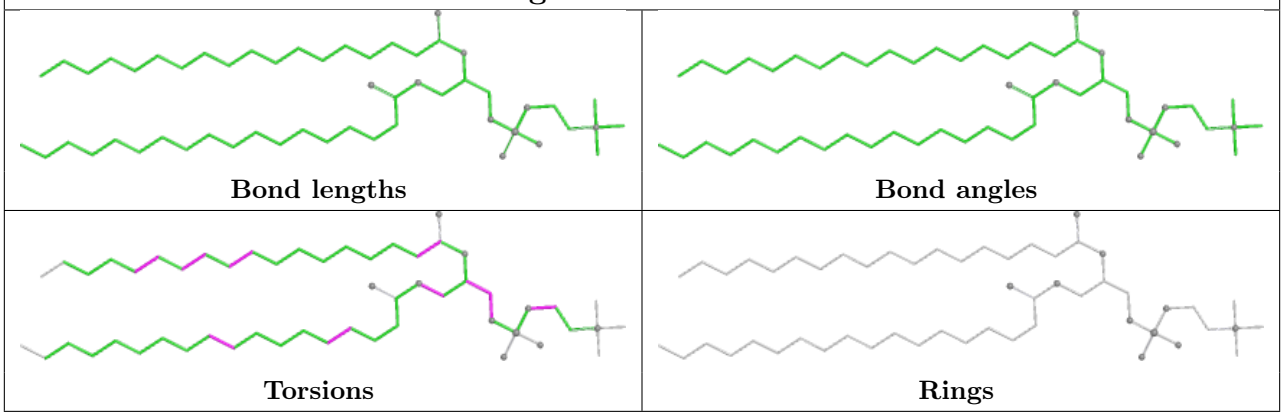
Ligand PC1 R 201



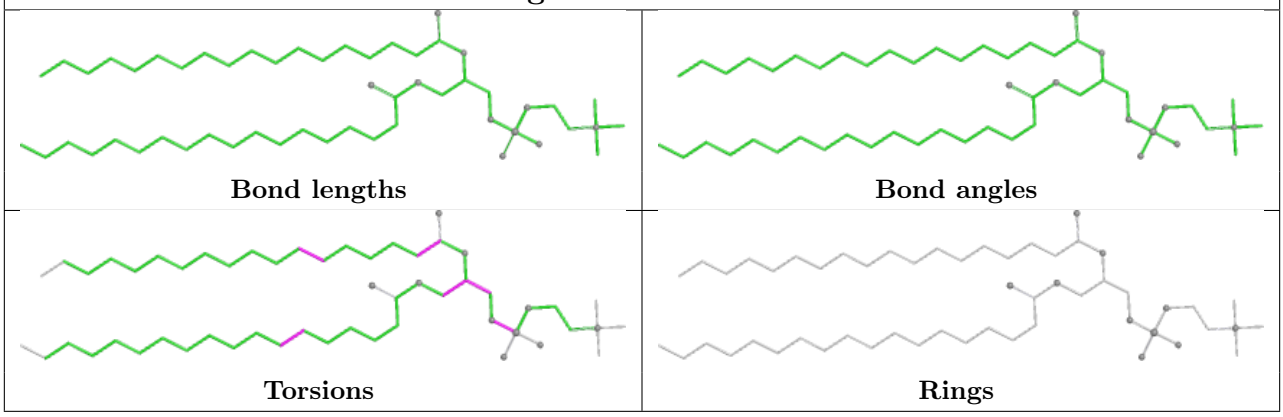
Ligand PC1 J 401



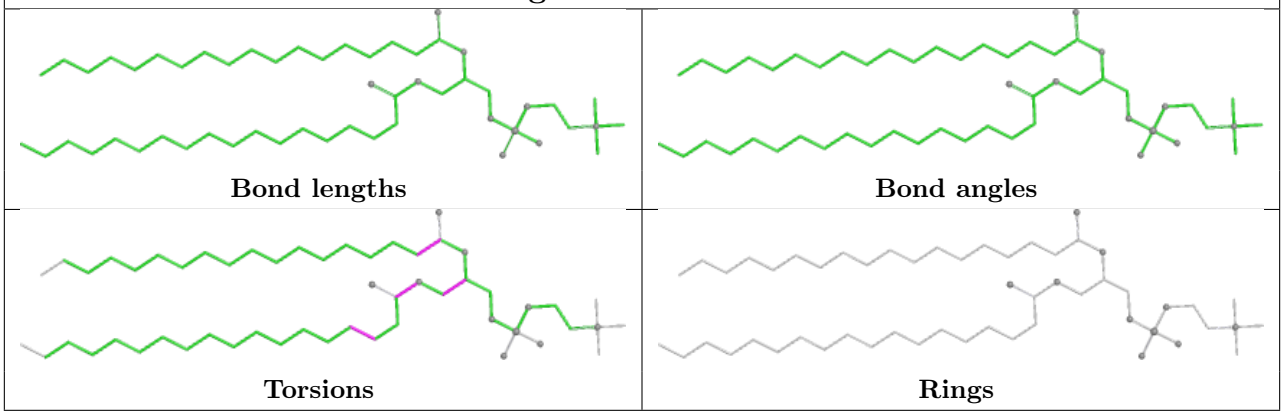
Ligand PC1 P 101

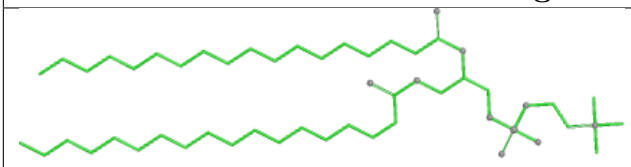
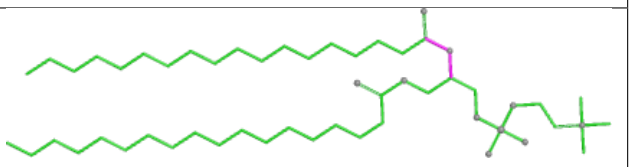
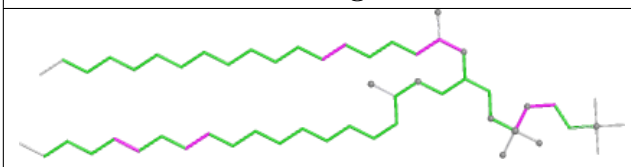
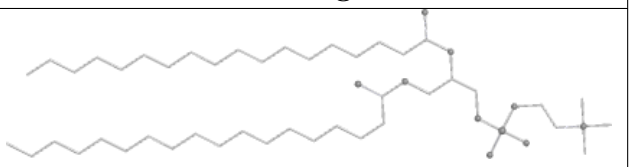


Ligand PC1 N 101



Ligand PC1 T 201



Ligand PC1 I 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

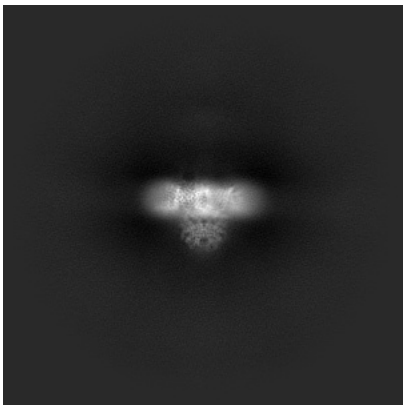
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48085. These allow visual inspection of the internal detail of the map and identification of artifacts.

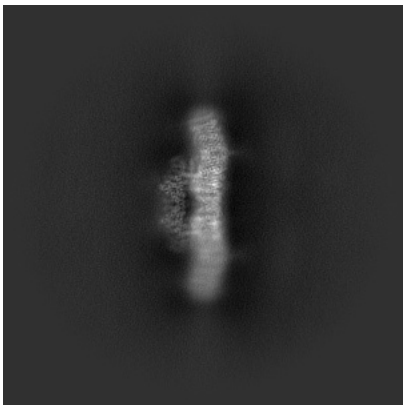
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

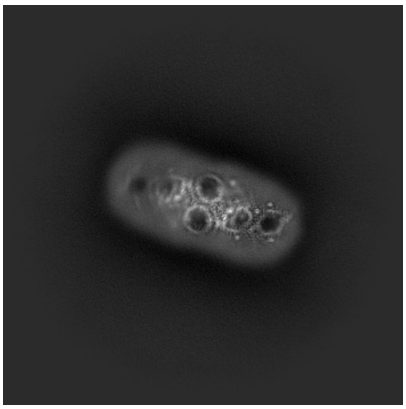
6.1.1 Primary map



X

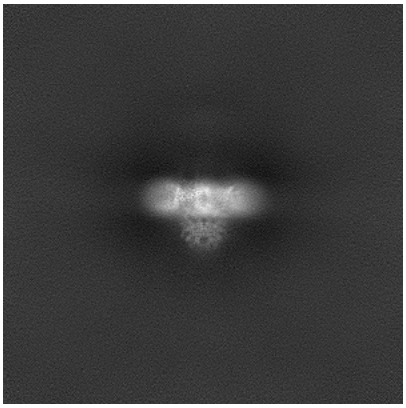


Y

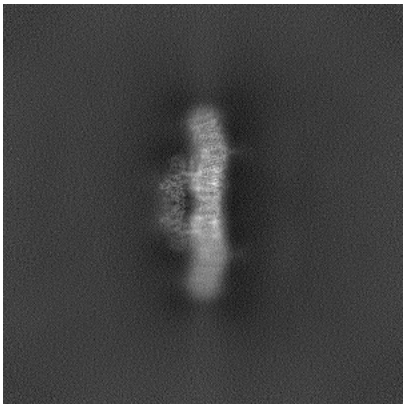


Z

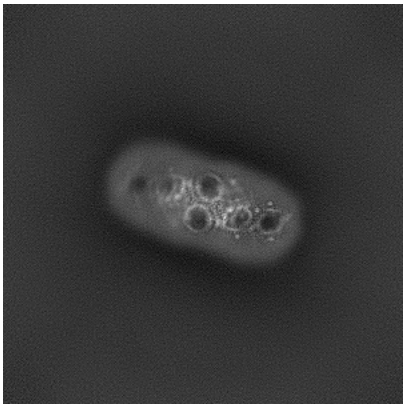
6.1.2 Raw map



X



Y



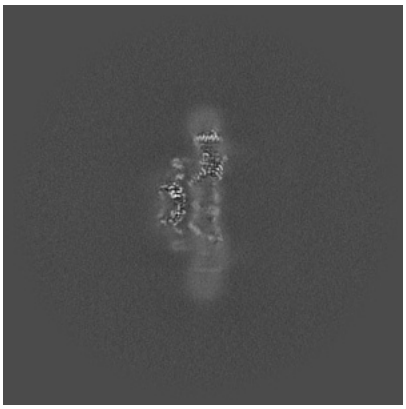
Z

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

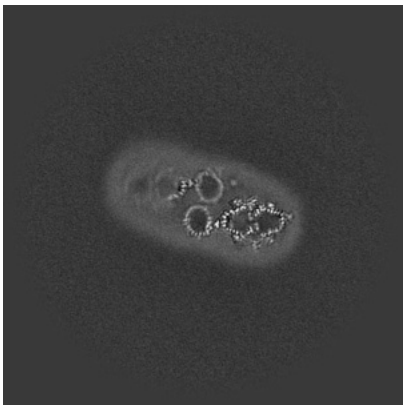
6.2 Central slices (i)

6.2.1 Primary map

X Index: 240

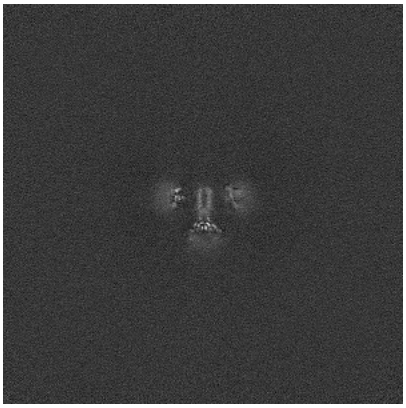


Y Index: 240

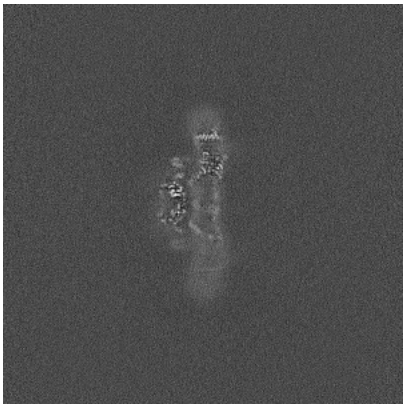


Z Index: 240

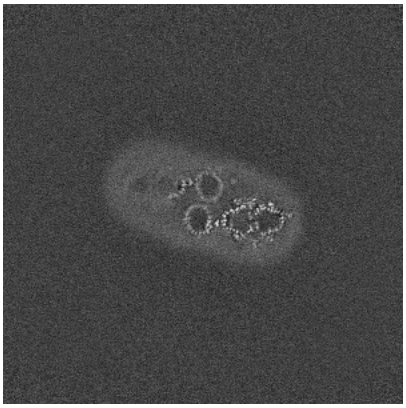
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

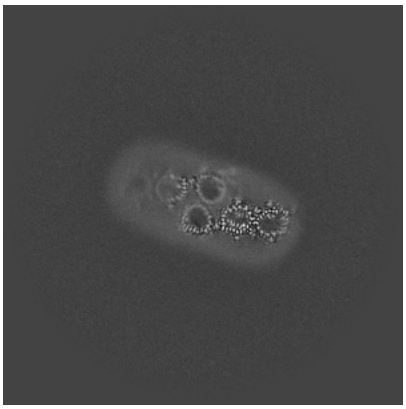
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

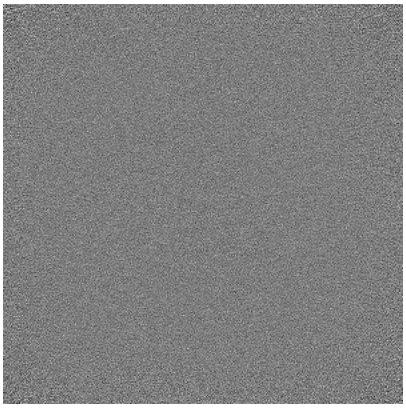
X Index: 265

Y Index: 233

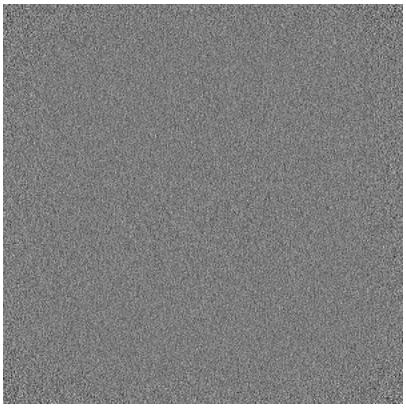


Z Index: 252

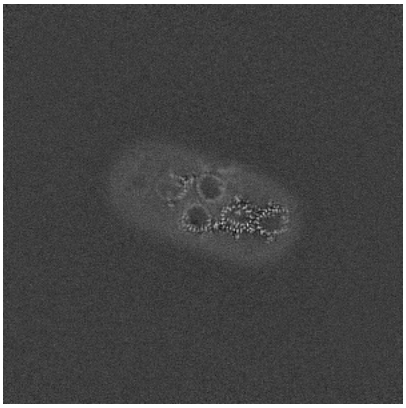
6.3.2 Raw map



X Index: 0



Y Index: 0

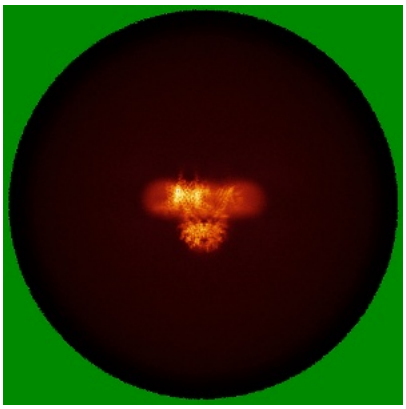


Z Index: 253

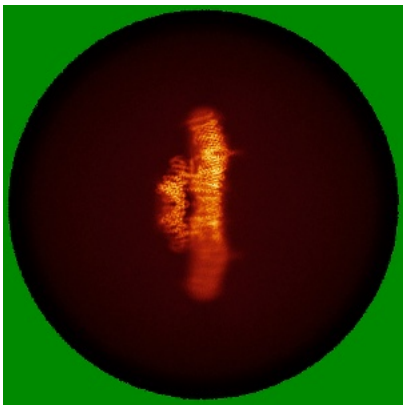
The images above show the largest variance slices of the map in three orthogonal directions.

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

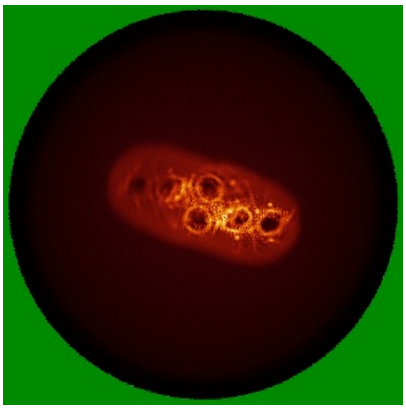
6.4.1 Primary map



X

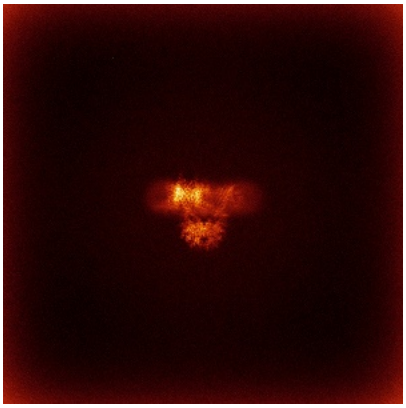


Y

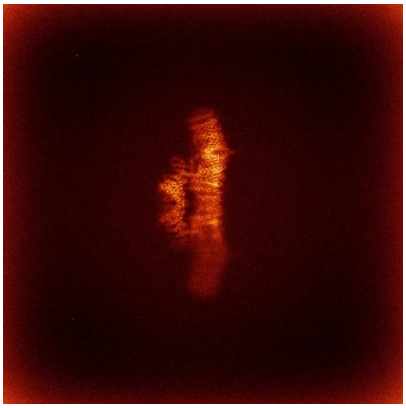


Z

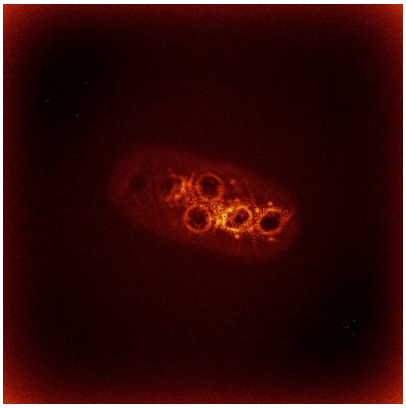
6.4.2 Raw map



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 0.0625. 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.

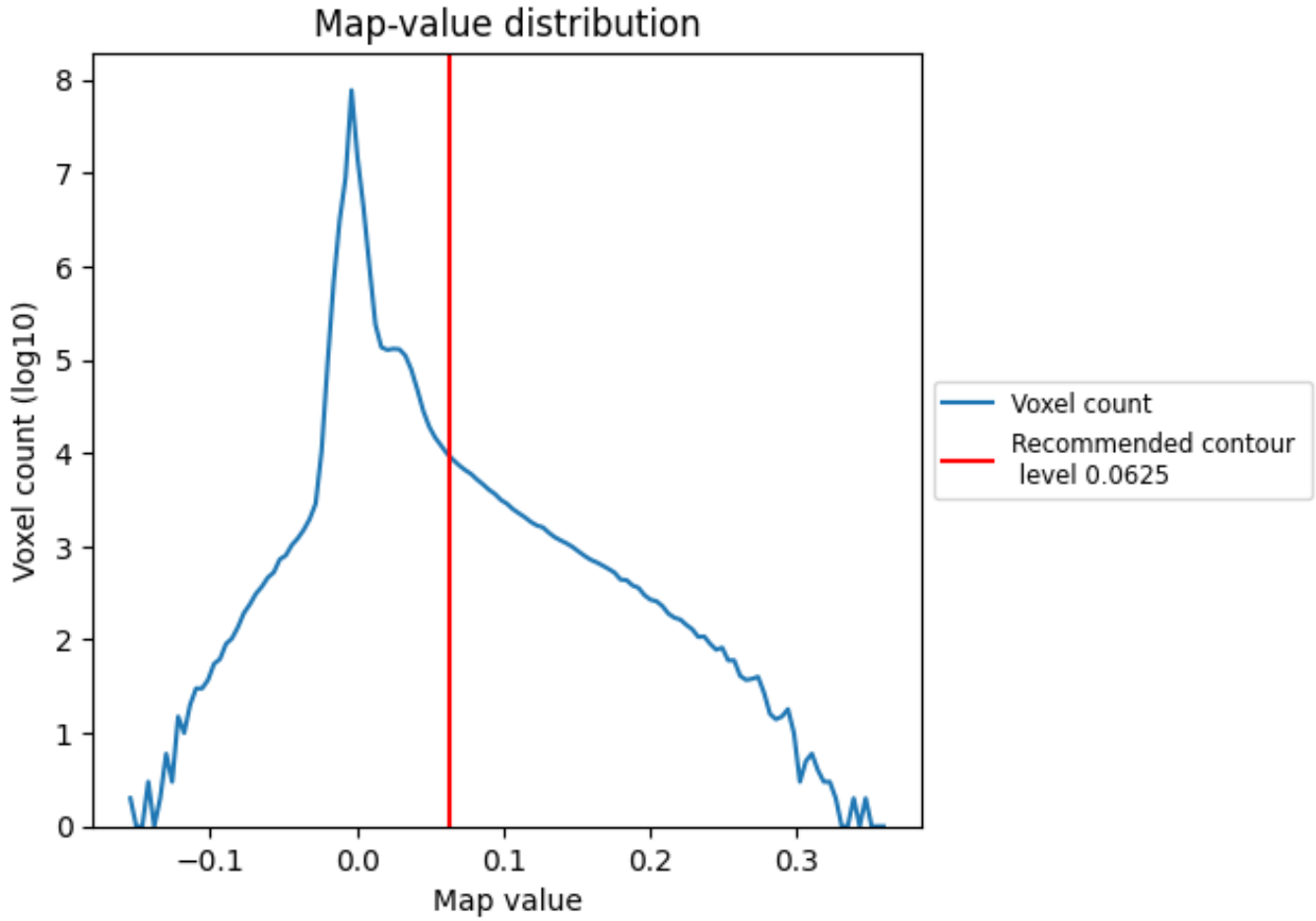
6.6 Mask visualisation (i)

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

7 Map analysis

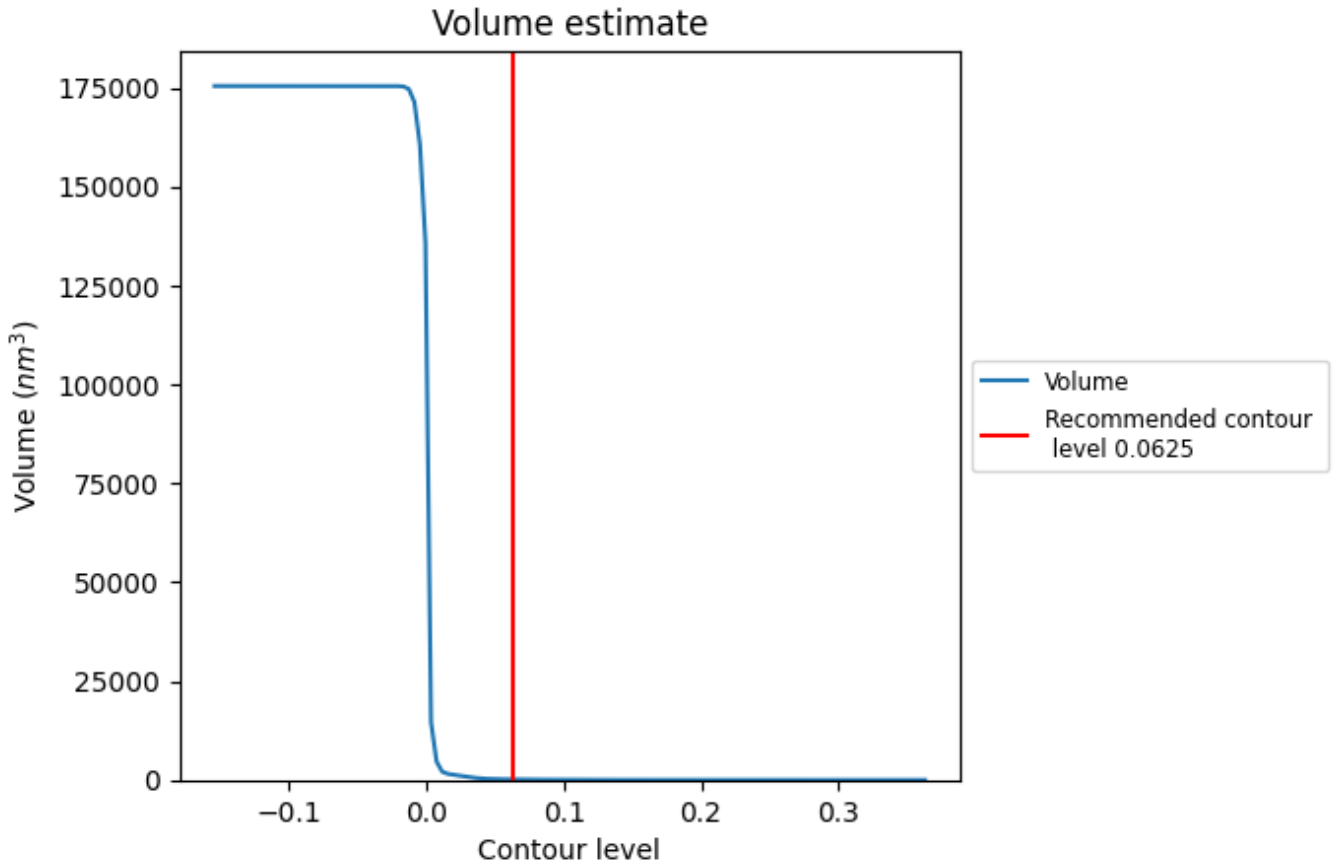
This section contains the results of statistical analysis of the map.

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.

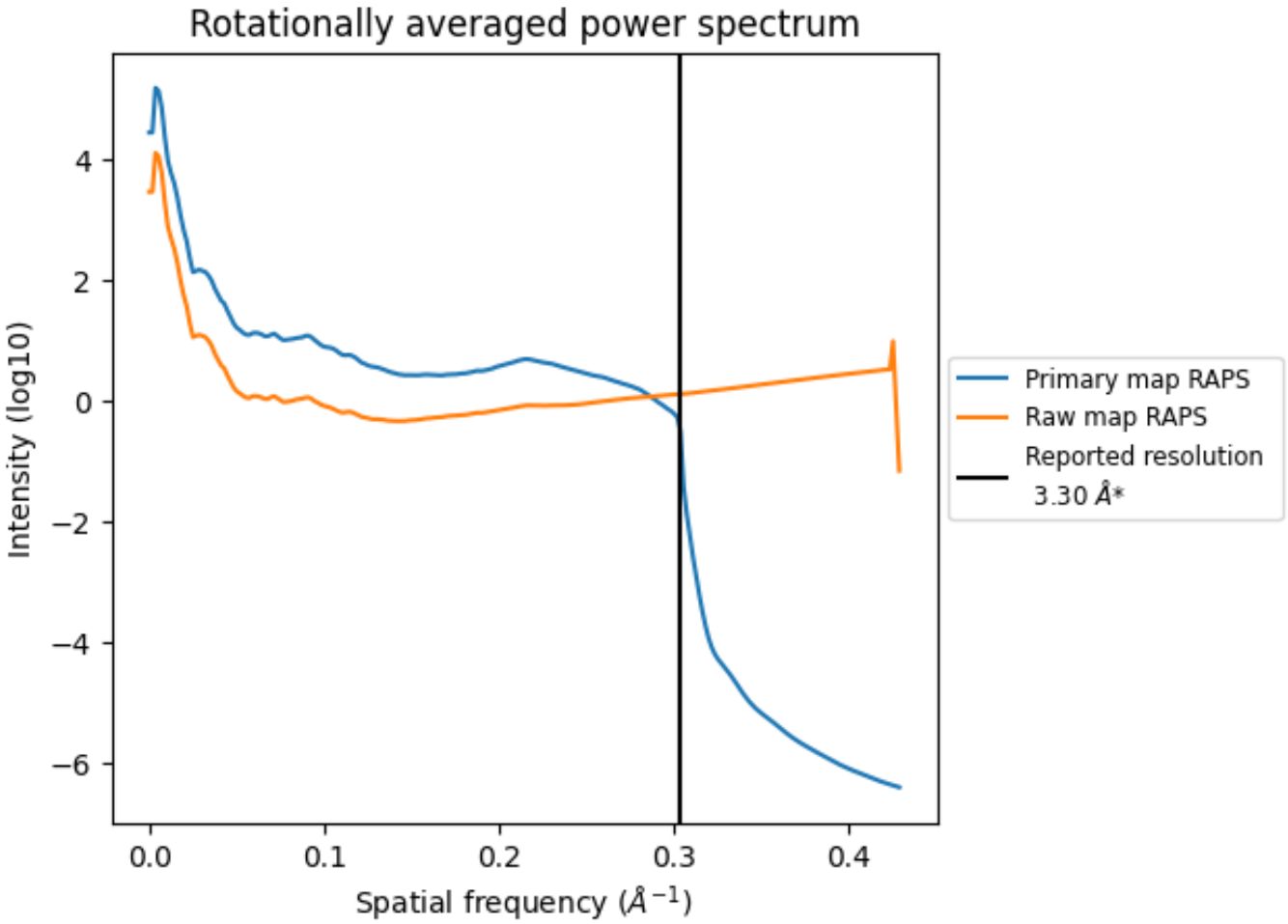
7.2 Volume estimate



The volume at the recommended contour level is 137 nm^3; this corresponds to an approximate mass of 123 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)

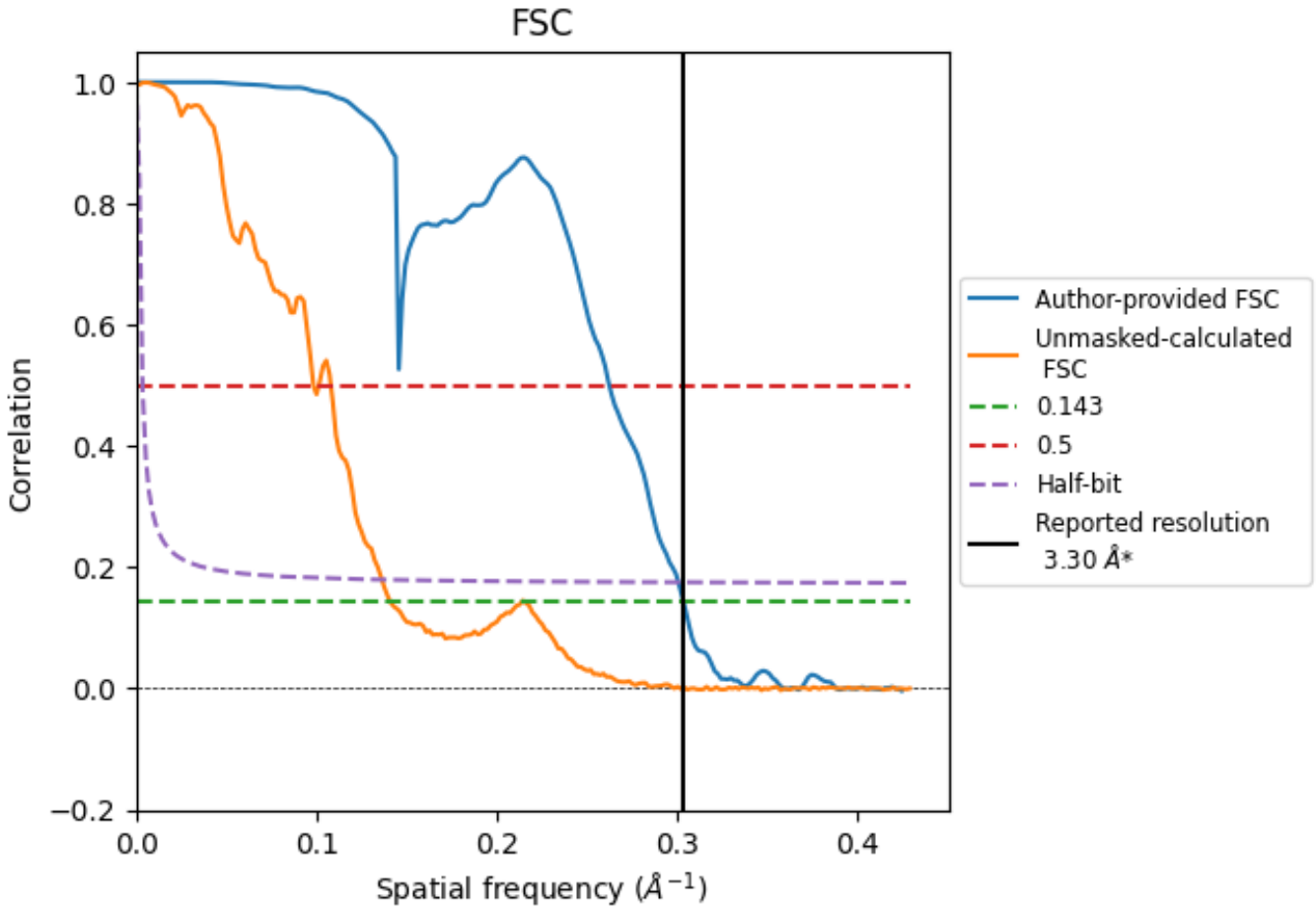


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8.2 Resolution estimates (i)

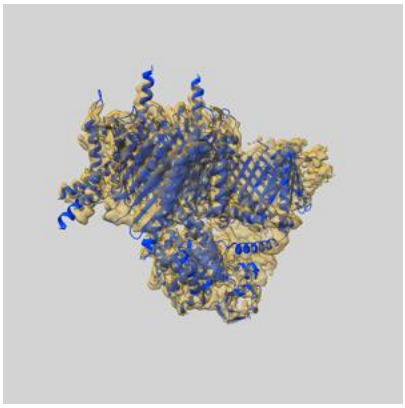
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.81	3.33
Unmasked-calculated*	7.10	10.18	7.34

*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 7.10 differs from the reported value 3.3 by more than 10 %

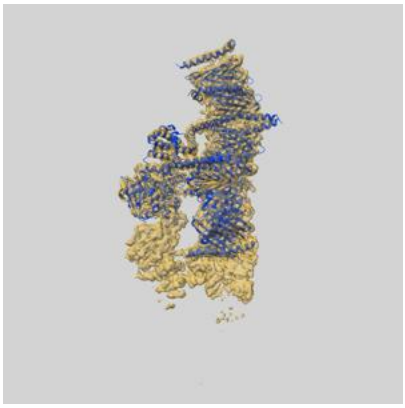
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48085 and PDB model 9EIJ. Per-residue inclusion information can be found in section 3 on page 8.

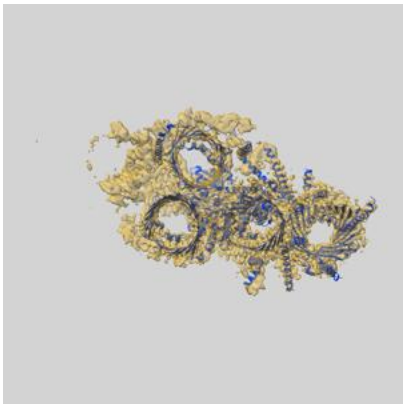
9.1 Map-model overlay



X



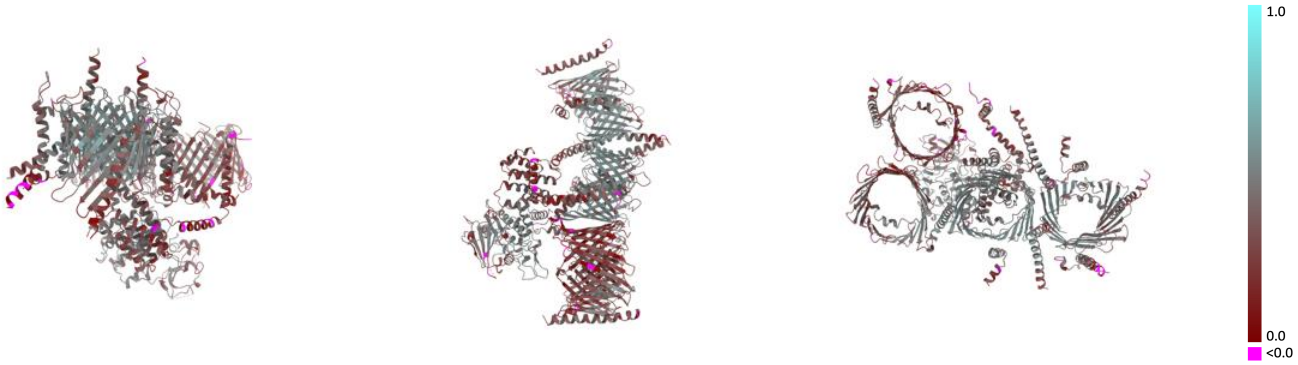
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0625 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.

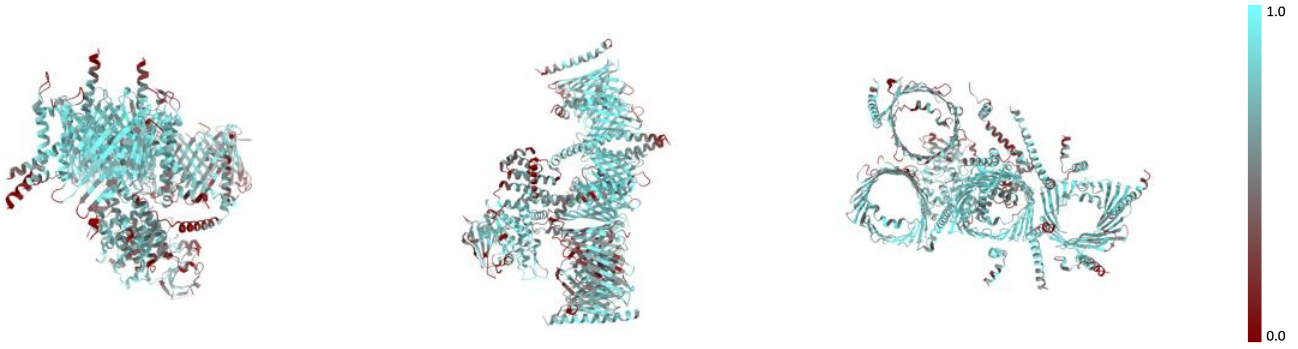
9.2 Q-score mapped to coordinate model (i)



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.

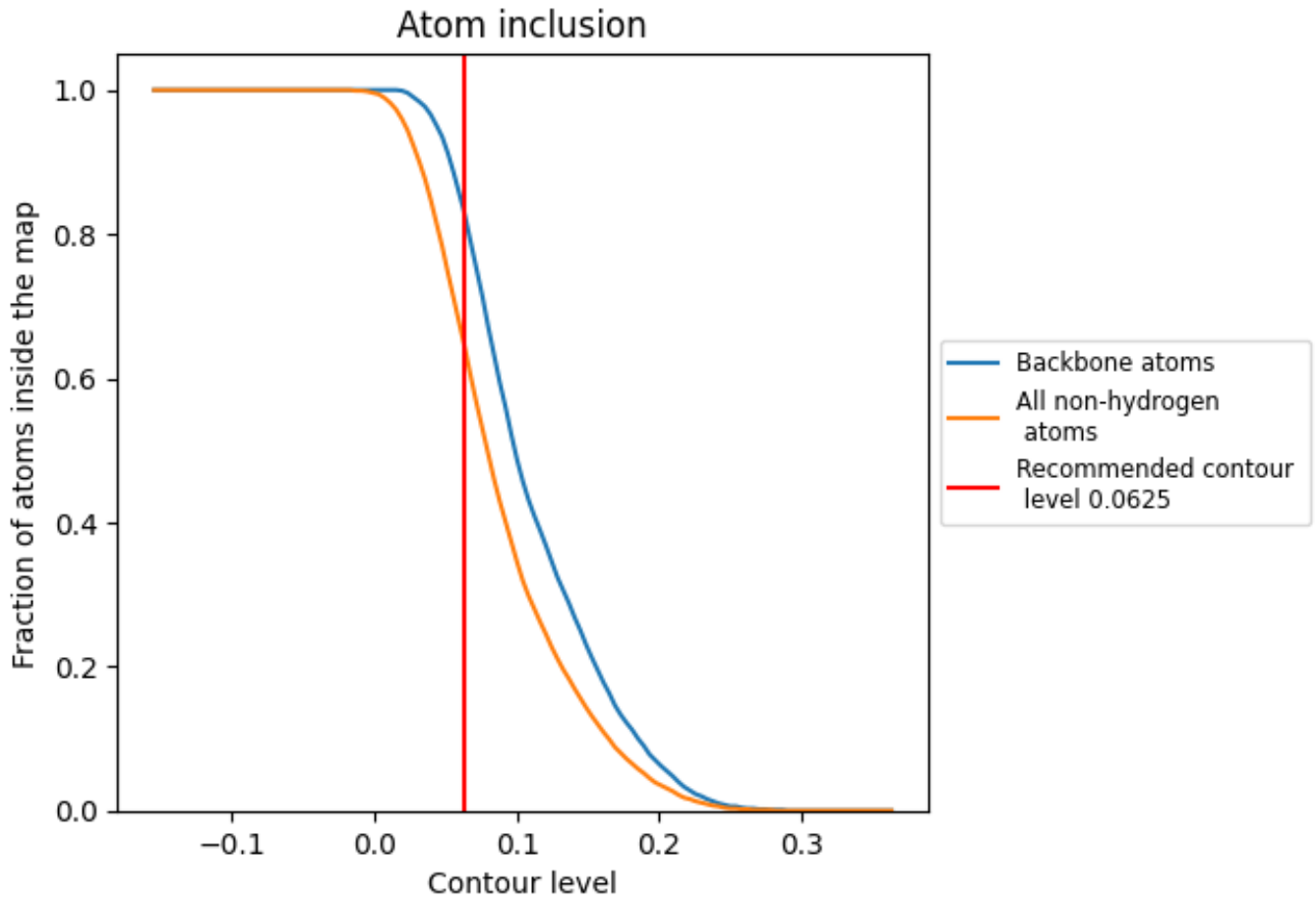
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0625).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 65% 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 (0.0625) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6530	0.3790
B	0.6910	0.4270
D	0.4100	0.2440
E	0.5060	0.2430
F	0.6490	0.3340
I	0.8360	0.5100
J	0.7430	0.4520
K	0.7460	0.3560
L	0.6580	0.4020
N	0.5960	0.3820
P	0.6970	0.3720
R	0.6450	0.3770
T	0.5920	0.4070
V	0.5370	0.3320
X	0.4740	0.2790
Z	0.5050	0.2450