WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Apr 4, 2024 – 11:35 am BST

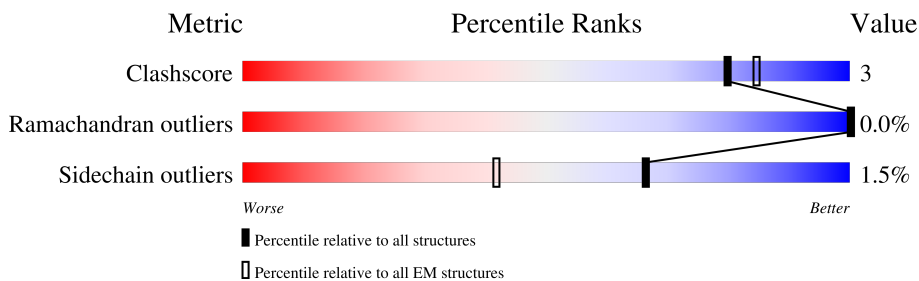|		
PDB ID	:	8RC4
EMDB ID	:	EMD-19047
Title	:	Structure of Integrator-PP2A complex
Authors	:	Fianu, I.; Ochmann, M.; Walshe, J.L.; Cramer, P.
Deposited on	:	2023-12-06
Resolution	:	3.10 Å(reported)
Based on initial model	:	8RBX

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.10 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.
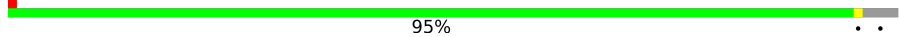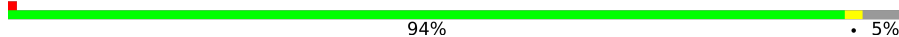
Metric	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.0%
Sidechain outliers		1.5%

Worse ⬛ *Better*

⬛ Percentile relative to all structures

▯ Percentile relative to all EM structures
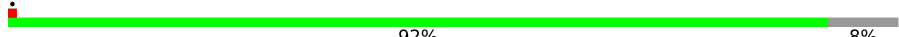
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	p	591	96%
2	q	311	92% 7%
3	r	31	97%
4	a	2192	80% 19%
5	b	1204	86% 13%
6	d	963	84% 15%
7	e	1021	84% 14%
8	f	892	62% 37%

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	g	964	91% · 8%
10	h	995	95% · ·
11	i	658	94% · 5%
12	k	602	96% · ·
13	m	706	44% 77% 23%
14	j	710	92% 8%
15	n	518	27% 97% ·
16	o	451	82% 18%

2 Entry composition ⓘ

There are 18 unique types of molecules in this entry. The entry contains 78273 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	p	580	Total 4437	C 2828	N 753	O 829	S 27	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	-1	SER	-	expression tag	UNP P30153
p	0	ASN	-	expression tag	UNP P30153

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	q	290	Total 2340	C 1481	N 405	O 439	S 15	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	-1	SER	-	expression tag	UNP P67775
q	0	ASN	-	expression tag	UNP P67775
q	88	ASN	ASP	engineered mutation	UNP P67775

- Molecule 3 is a protein called DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	r	31	Total 263	C 161	N 44	O 57	S 1	0	0

- Molecule 4 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	1766	Total 11842	C 7410	N 2168	O 2213	S 51	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-1	SER	-	expression tag	UNP Q8N201
a	0	ASN	-	expression tag	UNP Q8N201

- Molecule 5 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	1051	Total 8099	C 5198	N 1368	O 1471	S 62	0	0

- Molecule 6 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	823	Total 6443	C 4112	N 1099	O 1196	S 36	0	0

- Molecule 7 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	873	Total 6373	C 4050	N 1161	O 1135	S 27	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-1	SER	-	expression tag	UNP Q6P9B9
e	0	ASN	-	expression tag	UNP Q6P9B9

- Molecule 8 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	561	Total 4422	C 2827	N 754	O 815	S 26	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-4	TYR	-	expression tag	UNP Q9UL03
f	-3	PHE	-	expression tag	UNP Q9UL03
f	-2	GLN	-	expression tag	UNP Q9UL03
f	-1	SER	-	expression tag	UNP Q9UL03
f	0	ASN	-	expression tag	UNP Q9UL03

- Molecule 9 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	889	Total 6764	C 4283	N 1173	O 1267	S 41	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-1	SER	-	expression tag	UNP Q9NVH2
g	0	ASN	-	expression tag	UNP Q9NVH2

- Molecule 10 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	h	956	Total 7623	C 4877	N 1297	O 1403	S 46	0	0

- Molecule 11 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	i	626	Total 4871	C 3137	N 792	O 909	S 33	0	0

- Molecule 12 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	589	Total 4411	C 2822	N 768	O 790	S 31	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	-1	SER	-	expression tag	UNP Q5TA45
k	0	ASN	-	expression tag	UNP Q5TA45
k	203	GLN	GLU	engineered mutation	UNP Q5TA45

- Molecule 13 is a protein called Integrator complex subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	m	542	Total 2810	C 1682	N 568	O 560	0	0

- Molecule 14 is a protein called Integrator complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	j	653	Total 3238	C 1932	N 653	O 653	0	0

- Molecule 15 is a protein called Integrator complex subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	n	503	Total 2484	C 1478	N 503	O 503	0	0

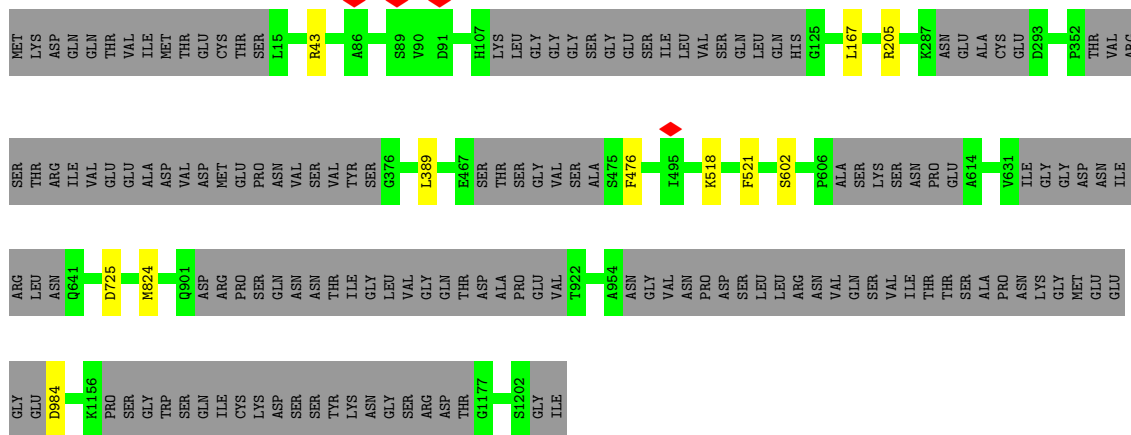- Molecule 16 is a protein called Integrator complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	o	372	Total 1849	C 1105	N 372	O 372	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	-1	SER	-	expression tag	UNP Q96N11
o	0	ASN	-	expression tag	UNP Q96N11

- Molecule 17 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	q	2	Total 2	Mn 2	0

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	k	2	Total 2	Zn 2	0

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: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

Chain p:
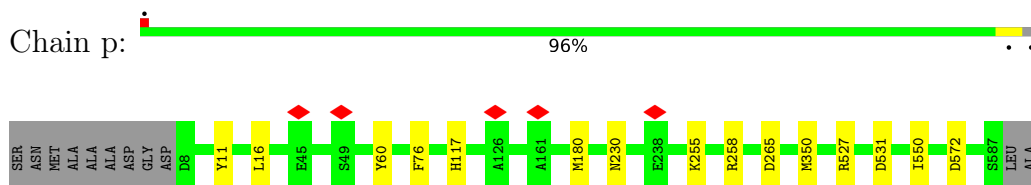
• Molecule 2: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain q:

• Molecule 3: DSS1

Chain r:

• Molecule 4: Integrator complex subunit 1

Chain a:

• Molecule 5: Integrator complex subunit 2
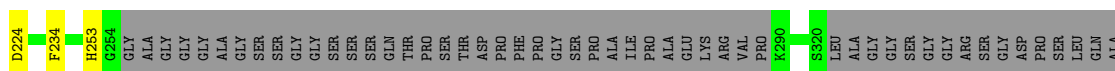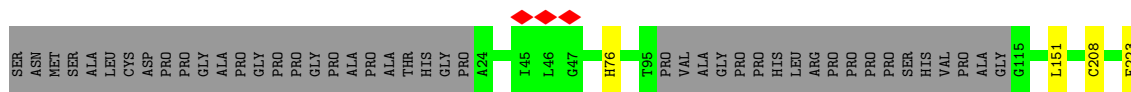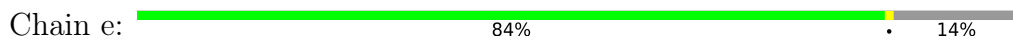
Chain b:

86%   •   13%

• Molecule 6: Integrator complex subunit 4

Chain d:
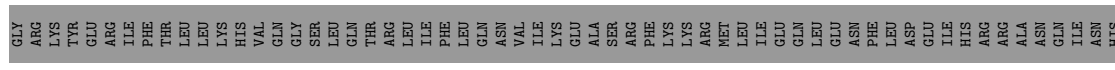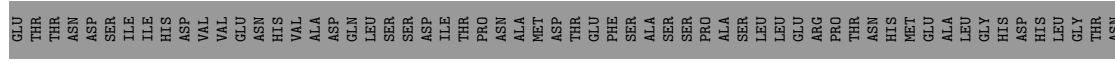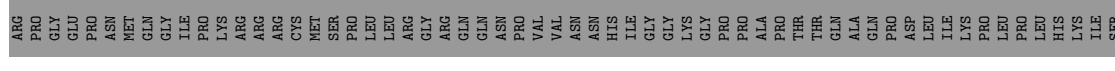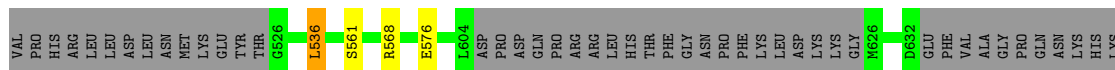

84%   •   15%

GLY ARG LYS LEU VAL SER SER ALA VAL SER PRO SER ILE ILE PRO GLN GLU **D608** L646 L692 M701 H810 D856 N918 SER SER ALA ARG ILE PRO LYS CYS PRO TRP MET GLU GLY GLY GLU MET SER PRO GLN VAL GLU THR SER ILE E943 F948 A961 ARG
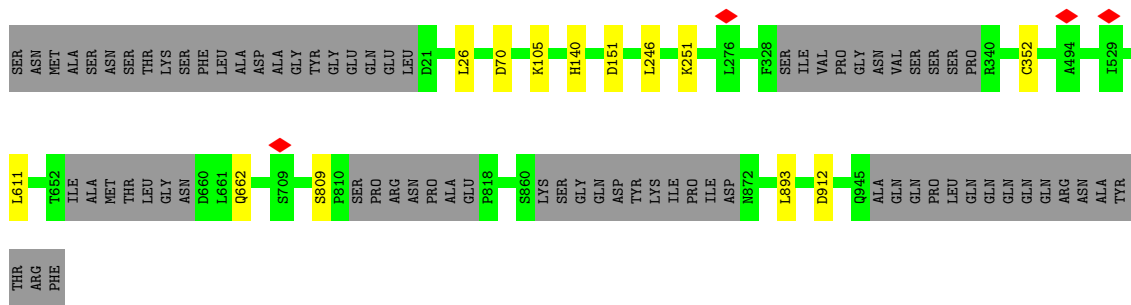
ARG

- Molecule 7: Integrator complex subunit 5

Chain e: 84% • 14%

SER ASN MET SER ALA LEU CYS ASP PRO PRO GLY ALA PRO GLY PRO PRO GLY PRO ALA PRO ALA THR HIS GLY PRO A24 I45 L46 G47 H76 T95 PRO VAL ALA GLY PRO PRO HIS LEU ARG PRO PRO PRO SER HIS VAL PRO ALA GLY G115 L151 C208 F223

D224 F234 H253 G254 GLY ALA GLY GLY ALA GLY SER SER GLY GLY SER SER SER GLN THR PRO SER THR ASP PRO PHE PRO GLY SER PRO ALA ILE PRO ALA GLU LYS ARG VAL PRO K290 S320 LEU ALA GLY GLY SER GLY GLY ARG SER ASP PRO SER LEU GLN ALA

THR V338 L342 F409 M415 PRO ALA SER VAL ILE THR THR GLN GLY LEU ALA VAL P428 L438 G454 GLY SER PRO GLY GLU GLY VAL LEU GLY PRO PRO P466 L470 G515 R527 L647 V709 ASP GLY ASP ASN GLU THR LEU SER VAL VAL SER ALA SER

LEU ALA SER A726 G791 GLY THR GLU C795 P1009 SER PRO SER THR LEU LEU ARG GLN GLY THR

- Molecule 8: Integrator complex subunit 6

Chain f: 62% • 37%

Y-4 R49 S209 P242 SER PRO VAL GLU ASP GLY GLN PRO ASP ILE SER ARG PRO PHE GLY S258 H262 S263 C264 N273 PRO LYS THR GLY V278 N438 R489 SER HIS GLY LEU LEU SER MET ALA TYR ARG ASP PHE GLN LEU LEU GLN GLY ILE ILE SER GLU ASP

VAL PRO HIS LEU LEU ASP LEU ASN MET LYS GLU GLY TYR THR G526 L536 S561 R568 E576 L604 ASP PRO ASP GLN PRO VAL ARG ARG LEU HIS THR PHE GLY ASN PHE LYS LEU ASP LYS LYS GLY M626 D632 GLU PHE VAL ALA GLY PRO GLN ASN LYS HIS LYS

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

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

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

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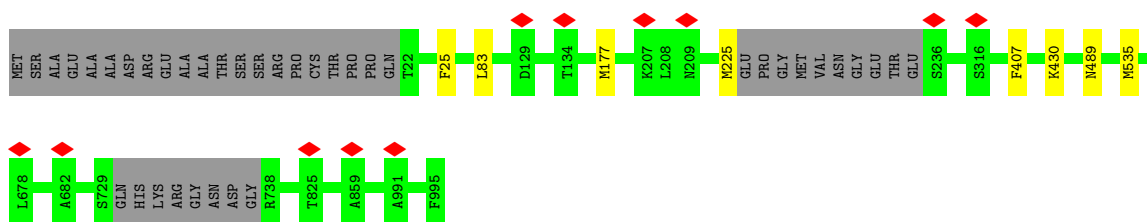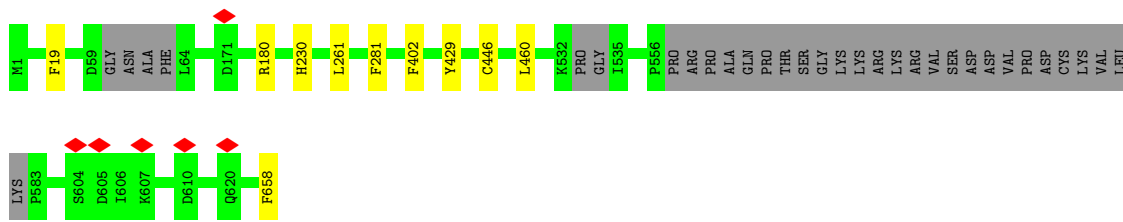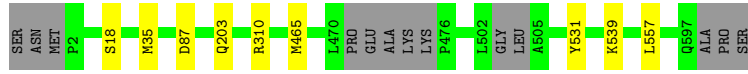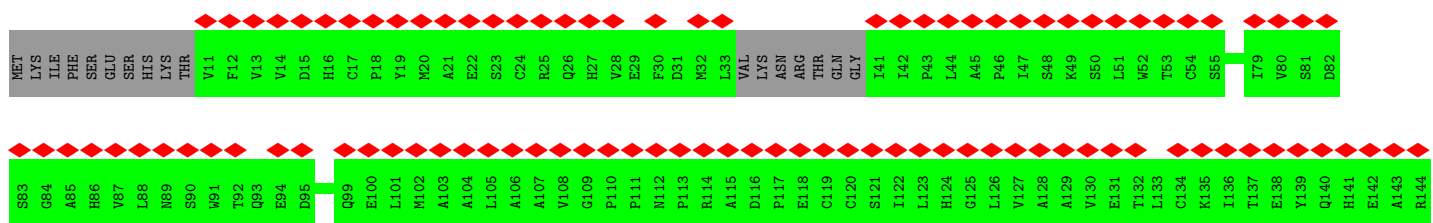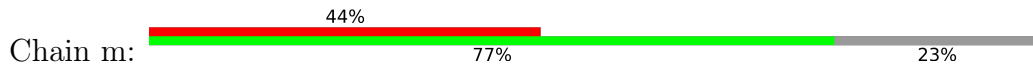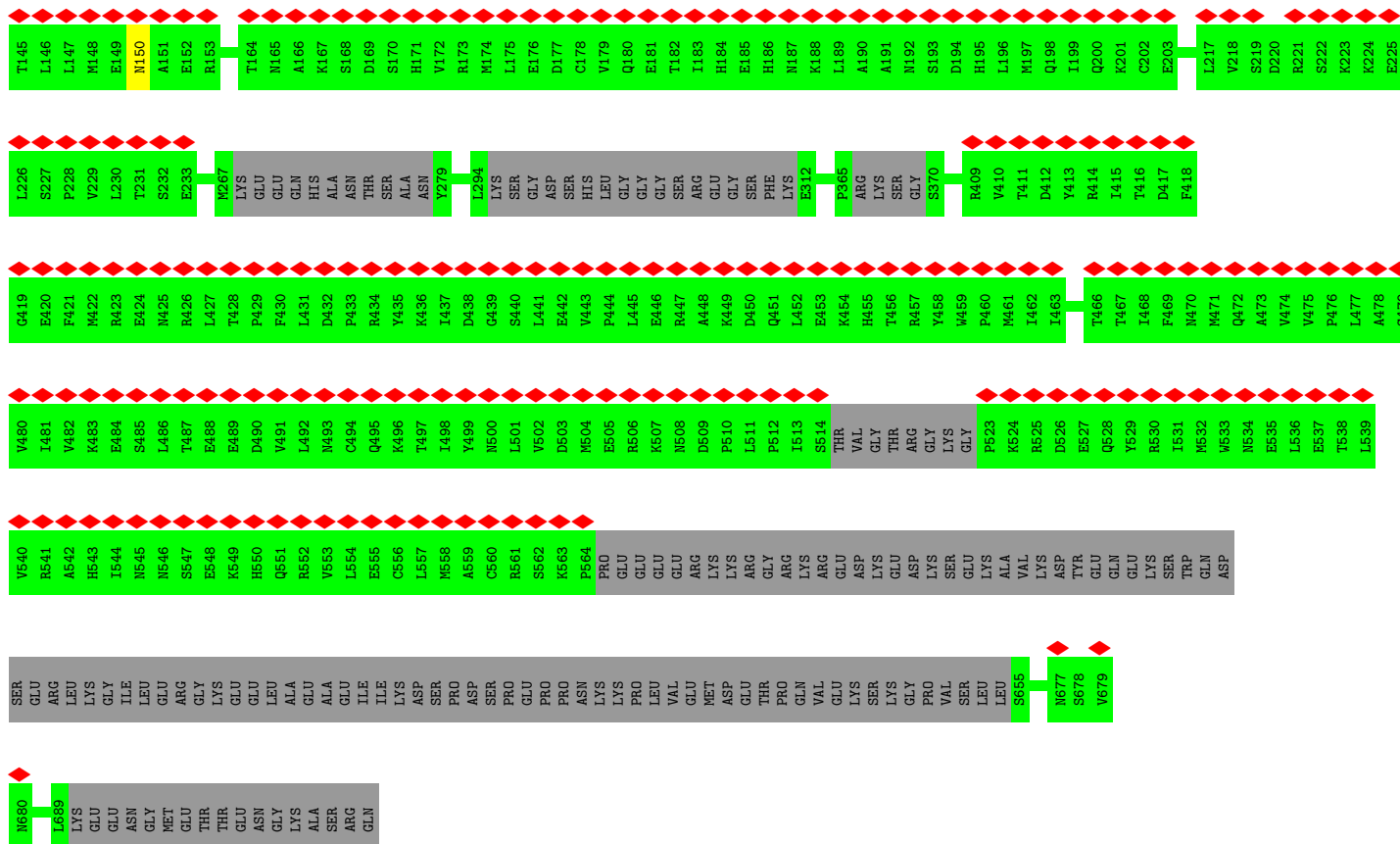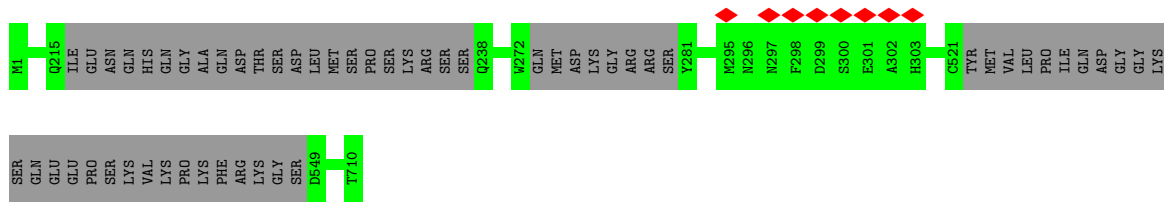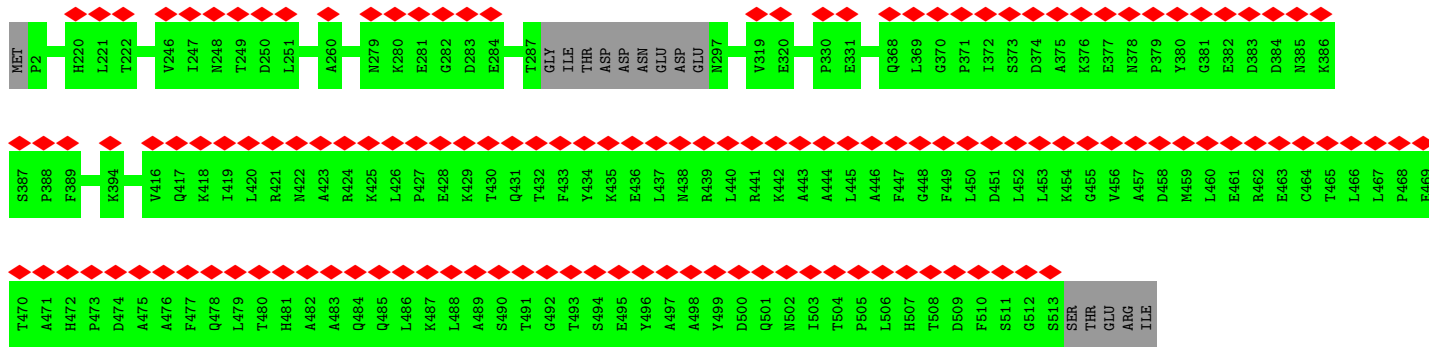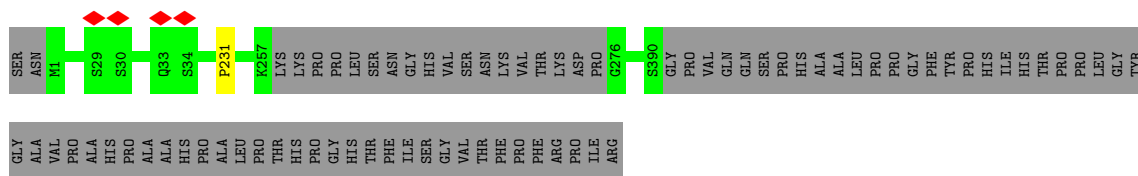
ILE ASN SER ASN

- Molecule 9: Integrator complex subunit 7

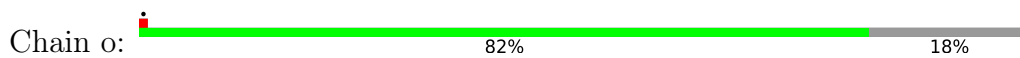Chain g: 91% • 8%

SER ASN MET ALA SER ASN SER THR LYS SER PHE LEU ALA ASP ALA GLY TYR GLY GLU GLN GLN GLU LEU D21 L26 D70 K105 H140 D151 L246 K251 L276 F328 SER ILE VAL PRO GLY ASN VAL SER SER SER PRO R340 C352 A494 I529

L611 T652 ILE ALA MET THR LEU GLY ASN D660 L661 Q662 S709 S809 P810 SER PRO ARG ASN PRO ALA GLU P818 S860 LYS SER GLY GLN ASP TYR LYS ILE PRO ILE ASP N872 L893 D912 Q945 ALA GLN GLN PRO LEU GLN GLN GLN GLN ARG ASN ALA TYR

THR ARG PHE

- Molecule 10: Integrator complex subunit 8

Chain h:　95%

MET SER ALA ALA ALA ALA ASP ARG GLU GLU ALA ALA THR SER SER ARG PRO CYS THR PRO PRO GLN T22 F25 L83 D129 T134 M177 K207 L208 N209 M225 GLU PRO GLY MET VAL ASN GLY GLU THR GLU S236 S316 F407 K430 N489 M535

L678 A682 S729 GLN HIS LYS ARG GLY ASN ASP GLY R738 T825 A859 A991 F995

- Molecule 11: Integrator complex subunit 9

Chain i:　94%　5%

M1 F19 D59 GLY ASN ALA PHE L64 D171 R180 H230 L261 F281 F402 Y429 C446 L460 K532 PRO GLY I535 P556 PRO ARG PRO ALA GLN PRO THR SER GLY LYS LYS ARG LYS ARG VAL SER ASP VAL PRO ASP CYS LYS VAL LEU

LYS P583 S604 D605 I606 K607 D610 Q620 F658

- Molecule 12: Integrator complex subunit 11

Chain k:　96%

SER ASN MET P2 S18 M35 D87 Q203 R310 M465 L470 PRO GLU ALA LYS LYS P476 L502 GLY LEU A505 Y531 K539 L557 Q597 ALA PRO SER

- Molecule 13: Integrator complex subunit 13

Chain m:　44%　77%　23%

MET LYS ILE PHE GLU SER HIS LYS THR V11 F12 V13 V14 D15 H16 C17 P18 Y19 M20 A21 E22 S23 C24 R25 Q26 H27 V28 E29 F30 D31 M32 L33 VAL LYS ASN ARG THR GLN GLY I41 I42 P43 L44 A45 P46 I47 S48 K49 S50 L51 W52 T53 C54 S55 I79 V80 S81 D82

S83 G84 A85 H86 V87 L88 N89 S90 W91 T92 Q93 E94 D95 Q99 E100 L101 M102 A103 A104 L105 A106 A107 V108 G109 P110 M112 P113 R114 A115 D116 P117 E118 C119 C120 S121 I122 L123 H124 G125 L126 V127 A128 A129 V130 E131 T132 L133 C134 K135 I136 T137 E138 Y139 Q140 H141 E142 A143 R144

• Molecule 14: Integrator complex subunit 10

Chain j:

92% 8%

• Molecule 15: Integrator complex subunit 14

Chain n:

27%

97%

• Molecule 16: Integrator complex subunit 15

Chain o:

82%　　　　18%

SER ASN M1 S29 S30 Q33 S34 P231 K257 LYS LYS PRO PRO LEU SER ASN GLY HIS VAL SER ASN LYS VAL THR LYS ASP PRO G276 S390 GLY PRO VAL GLN GLN SER PRO HIS ALA ALA LEU PRO PRO GLY PHE TYR PRO HIS ILE HIS THR PRO PRO LEU GLY TYR

GLY ALA VAL PRO ALA HIS PRO ALA ALA HIS PRO ALA LEU PRO THR HIS PRO GLY HIS THR PHE ILE SER GLY VAL THR PHE PRO PHE ARG PRO ILE ARG

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2335349	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40.49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.00502	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	p	0.33	0/4511	0.56	2/6136 (0.0%)
2	q	0.41	0/2397	0.63	2/3250 (0.1%)
3	r	0.37	0/267	0.66	0/362
4	a	0.27	0/11994	0.55	6/16391 (0.0%)
5	b	0.31	0/8242	0.55	2/11212 (0.0%)
6	d	0.28	0/6568	0.57	5/8919 (0.1%)
7	e	0.32	0/6520	0.56	3/8895 (0.0%)
8	f	0.30	0/4531	0.56	1/6154 (0.0%)
9	g	0.29	0/6874	0.52	2/9324 (0.0%)
10	h	0.30	0/7768	0.51	0/10530
11	i	0.29	0/4990	0.56	0/6802
12	k	0.28	0/4508	0.58	0/6119
13	m	0.24	0/2809	0.47	0/3897
14	j	0.24	0/3234	0.38	0/4505
15	n	0.25	0/2482	0.46	0/3453
16	o	0.25	0/1847	0.40	0/2576
All	All	0.30	0/79542	0.54	23/108525 (0.0%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	q	253	ASP	CB-CG-OD2	10.07	127.36	118.30
4	a	1282	ASP	CB-CG-OD2	8.65	126.08	118.30
7	e	151	LEU	CA-CB-CG	7.66	132.91	115.30
7	e	438	LEU	CA-CB-CG	7.04	131.50	115.30
1	p	16	LEU	CA-CB-CG	6.70	130.70	115.30
4	a	989	LEU	CA-CB-CG	6.63	130.55	115.30
8	f	536	LEU	CA-CB-CG	6.36	129.92	115.30
6	d	548	LEU	CA-CB-CG	6.08	129.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	389	LEU	CA-CB-CG	6.02	129.15	115.30
2	q	166	LEU	CA-CB-CG	5.96	129.00	115.30
6	d	856	ASP	CB-CG-OD1	5.94	123.64	118.30
6	d	701	MET	CB-CG-SD	5.87	130.02	112.40
6	d	429	LEU	CA-CB-CG	5.77	128.56	115.30
7	e	470	LEU	CA-CB-CG	5.67	128.34	115.30
4	a	2051	MET	CG-SD-CE	-5.64	91.18	100.20
9	g	611	LEU	CA-CB-CG	5.63	128.25	115.30
6	d	701	MET	CA-CB-CG	5.47	122.60	113.30
4	a	1508	LEU	CA-CB-CG	5.35	127.60	115.30
4	a	1446	VAL	CG1-CB-CG2	-5.26	102.48	110.90
9	g	246	LEU	CA-CB-CG	5.20	127.26	115.30
4	a	1173	LEU	CB-CG-CD2	5.13	119.72	111.00
5	b	167	LEU	CA-CB-CG	5.04	126.89	115.30
1	p	550	ILE	CG1-CB-CG2	-5.01	100.37	111.40

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	p	4437	0	4508	0	0
2	q	2340	0	2248	0	0
3	r	263	0	229	0	0
4	a	11842	0	10065	0	0
5	b	8099	0	8211	0	0
6	d	6443	0	6483	0	0
7	e	6373	0	6187	0	0
8	f	4422	0	4393	0	0
9	g	6764	0	6747	0	0
10	h	7623	0	7779	0	0
11	i	4871	0	4849	0	0
12	k	4411	0	4248	0	0
13	m	2810	0	1353	0	0
14	j	3238	0	1433	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	n	2484	0	1104	0	0
16	o	1849	0	811	0	0
17	q	2	0	0	0	0
18	k	2	0	0	0	0
All	All	78273	0	70648	0	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 3.

There are no clashes within the asymmetric unit.

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	p	578/591 (98%)	567 (98%)	11 (2%)	0	100	100
2	q	288/311 (93%)	273 (95%)	15 (5%)	0	100	100
3	r	29/31 (94%)	29 (100%)	0	0	100	100
4	a	1734/2192 (79%)	1682 (97%)	51 (3%)	1 (0%)	51	83
5	b	1031/1204 (86%)	983 (95%)	48 (5%)	0	100	100
6	d	813/963 (84%)	791 (97%)	22 (3%)	0	100	100
7	e	857/1021 (84%)	824 (96%)	33 (4%)	0	100	100
8	f	551/892 (62%)	535 (97%)	16 (3%)	0	100	100
9	g	879/964 (91%)	847 (96%)	32 (4%)	0	100	100
10	h	950/995 (96%)	927 (98%)	23 (2%)	0	100	100
11	i	618/658 (94%)	588 (95%)	30 (5%)	0	100	100
12	k	583/602 (97%)	540 (93%)	42 (7%)	1 (0%)	47	79
13	m	528/706 (75%)	491 (93%)	36 (7%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	j	645/710 (91%)	626 (97%)	19 (3%)	0	100	100
15	n	499/518 (96%)	466 (93%)	33 (7%)	0	100	100
16	o	368/451 (82%)	347 (94%)	20 (5%)	1 (0%)	41	73
All	All	10951/12809 (86%)	10516 (96%)	431 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	k	310	ARG
16	o	231	PRO
4	a	566	LYS
13	m	150	ASN

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	p	487/514 (95%)	474 (97%)	13 (3%)	44	74
2	q	255/276 (92%)	253 (99%)	2 (1%)	81	92
3	r	28/28 (100%)	27 (96%)	1 (4%)	35	67
4	a	931/1909 (49%)	915 (98%)	16 (2%)	60	83
5	b	894/1072 (83%)	885 (99%)	9 (1%)	76	90
6	d	709/845 (84%)	700 (99%)	9 (1%)	69	87
7	e	630/814 (77%)	621 (99%)	9 (1%)	67	86
8	f	491/801 (61%)	482 (98%)	9 (2%)	59	82
9	g	733/842 (87%)	722 (98%)	11 (2%)	65	85
10	h	859/896 (96%)	851 (99%)	8 (1%)	78	91
11	i	555/600 (92%)	545 (98%)	10 (2%)	59	82
12	k	443/522 (85%)	435 (98%)	8 (2%)	59	82
13	m	31/639 (5%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	7046/9758 (72%)	6941 (98%)	105 (2%)	66	85

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	p	11	TYR
1	p	60	TYR
1	p	76	PHE
1	p	117	HIS
1	p	180	MET
1	p	230	ASN
1	p	255	LYS
1	p	258	ARG
1	p	265	ASP
1	p	350	MET
1	p	527	ARG
1	p	531	ASP
1	p	572	ASP
2	q	6	PHE
2	q	178	ASP
3	r	1053	GLN
4	a	974	TYR
4	a	977	ARG
4	a	996	LEU
4	a	1084	ASP
4	a	1107	LEU
4	a	1144	SER
4	a	1223	MET
4	a	1282	ASP
4	a	1373	ARG
4	a	1444	ARG
4	a	1534	CYS
4	a	1840	HIS
4	a	1997	MET
4	a	2000	SER
4	a	2073	MET
4	a	2171	MET
5	b	43	ARG
5	b	205	ARG
5	b	476	PHE
5	b	518	LYS
5	b	521	PHE

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Mol	Chain	Res	Type
5	b	602	SER
5	b	725	ASP
5	b	824	MET
5	b	984	ASP
6	d	51	ASP
6	d	111	MET
6	d	132	ASP
6	d	385	ASP
6	d	479	LYS
6	d	646	LEU
6	d	692	LEU
6	d	810	HIS
6	d	948	PHE
7	e	76	HIS
7	e	208	CYS
7	e	223	PHE
7	e	224	ASP
7	e	234	PHE
7	e	253	HIS
7	e	342	LEU
7	e	409	PHE
7	e	527	ARG
8	f	49	ARG
8	f	209	SER
8	f	262	HIS
8	f	264	CYS
8	f	438	ASN
8	f	536	LEU
8	f	561	SER
8	f	568	ARG
8	f	576	GLU
9	g	26	LEU
9	g	70	ASP
9	g	105	LYS
9	g	140	HIS
9	g	151	ASP
9	g	251	LYS
9	g	352	CYS
9	g	662	GLN
9	g	809	SER
9	g	893	LEU
9	g	912	ASP

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Mol	Chain	Res	Type
10	h	25	PHE
10	h	83	LEU
10	h	177	MET
10	h	225	MET
10	h	407	PHE
10	h	430	LYS
10	h	489	ASN
10	h	535	MET
11	i	19	PHE
11	i	180	ARG
11	i	230	HIS
11	i	261	LEU
11	i	281	PHE
11	i	402	PHE
11	i	429	TYR
11	i	446	CYS
11	i	460	LEU
11	i	658	PHE
12	k	18	SER
12	k	35	MET
12	k	87	ASP
12	k	203	GLN
12	k	465	MET
12	k	531	TYR
12	k	539	LYS
12	k	557	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	p	479	HIS
1	p	520	HIS
10	h	170	GLN
11	i	389	GLN
11	i	418	ASN

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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7　Other polymers ⓘ

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-19047. 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 ⓘ
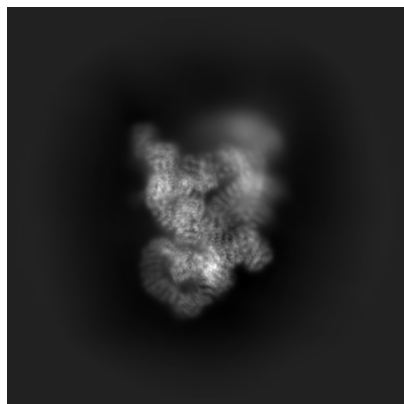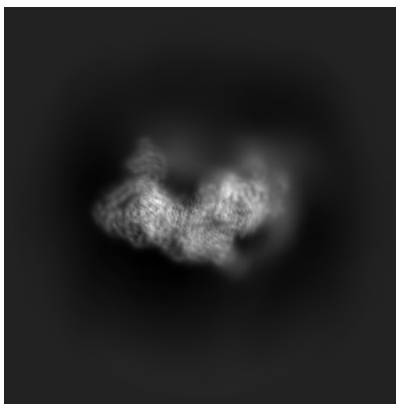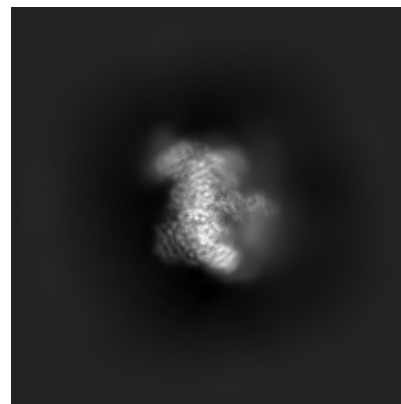
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

| X | Y | Z |
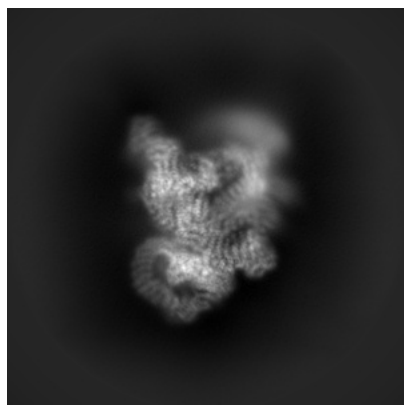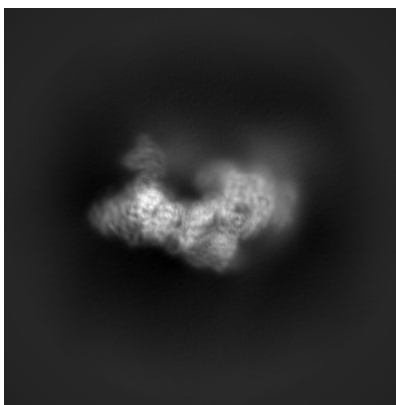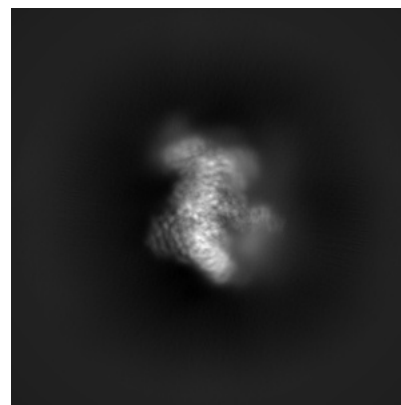
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
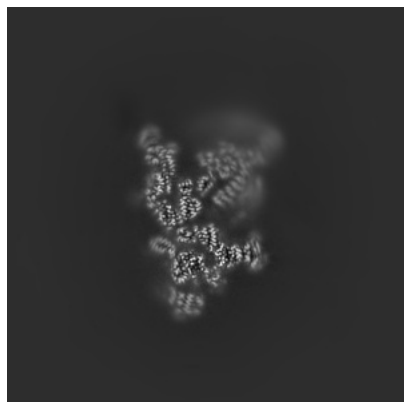
6.2.1   Primary map
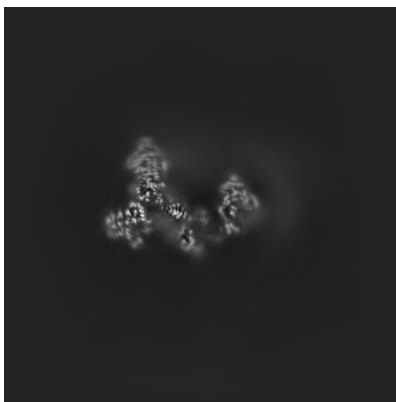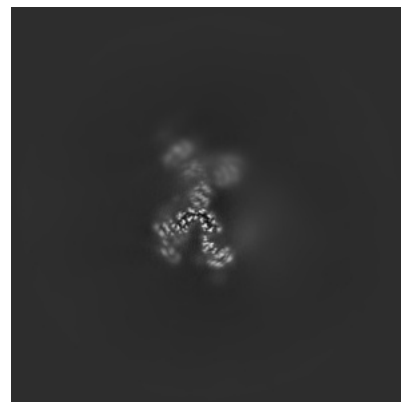
| X Index: 240 | Y Index: 240 | Z Index: 240 |

6.2.2   Raw map
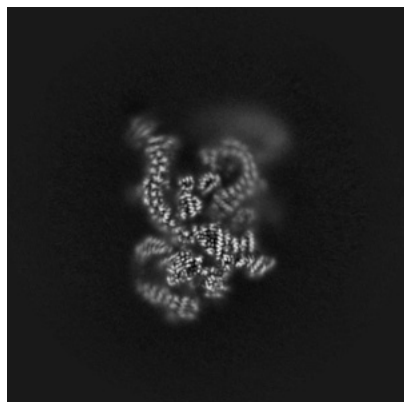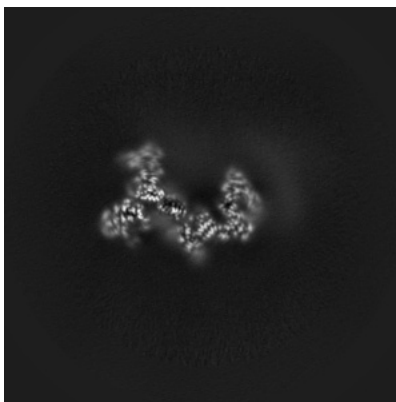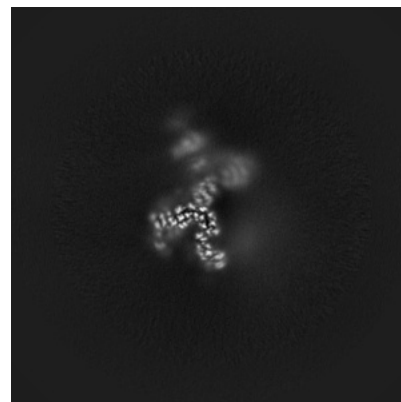
| X Index: 240 | Y Index: 240 | Z Index: 240 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
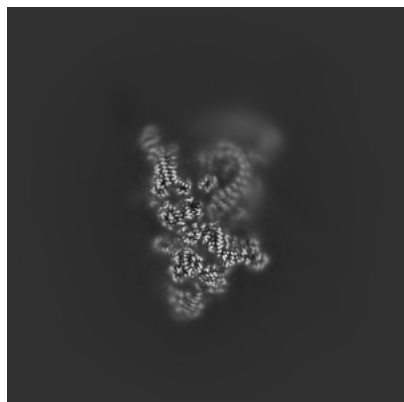
X Index: 235	Y Index: 245	Z Index: 177
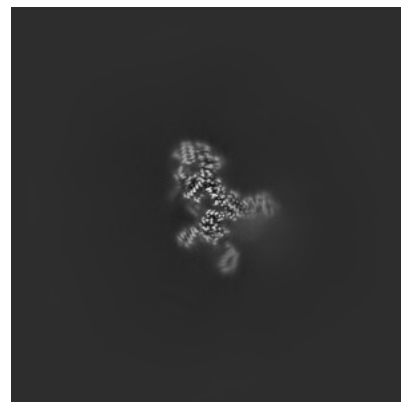
6.3.2 Raw map
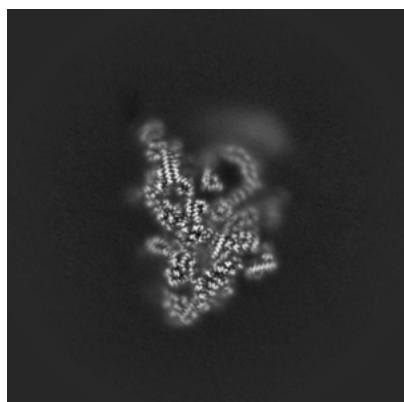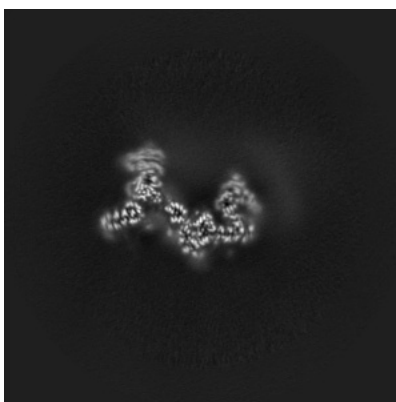
X Index: 230	Y Index: 236	Z Index: 175
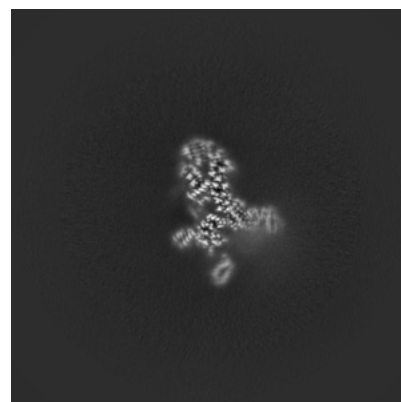
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
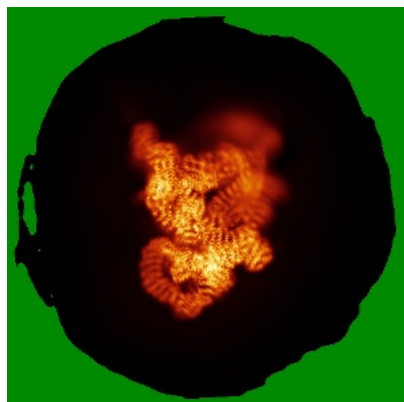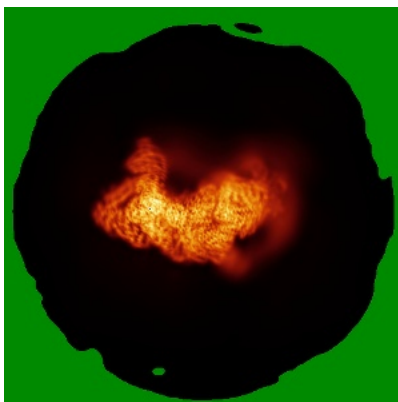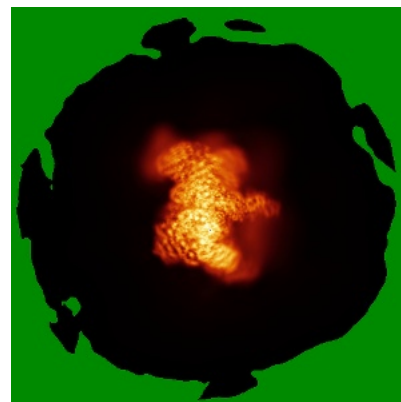
X Y Z

6.4.2 Raw map

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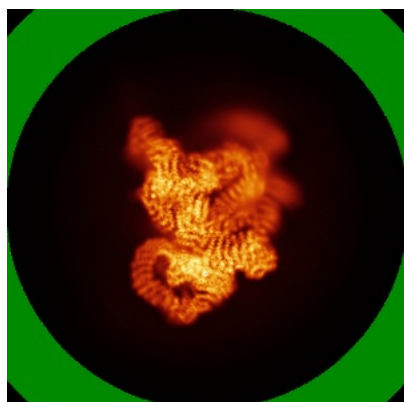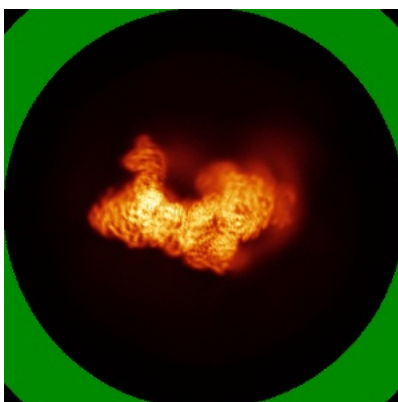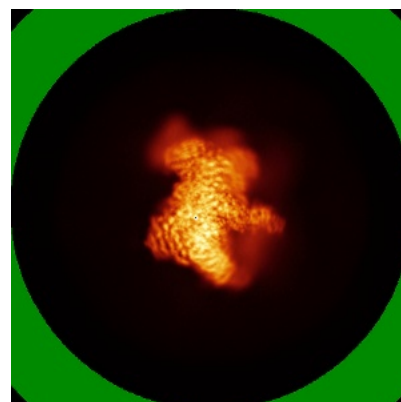
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.00502. 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
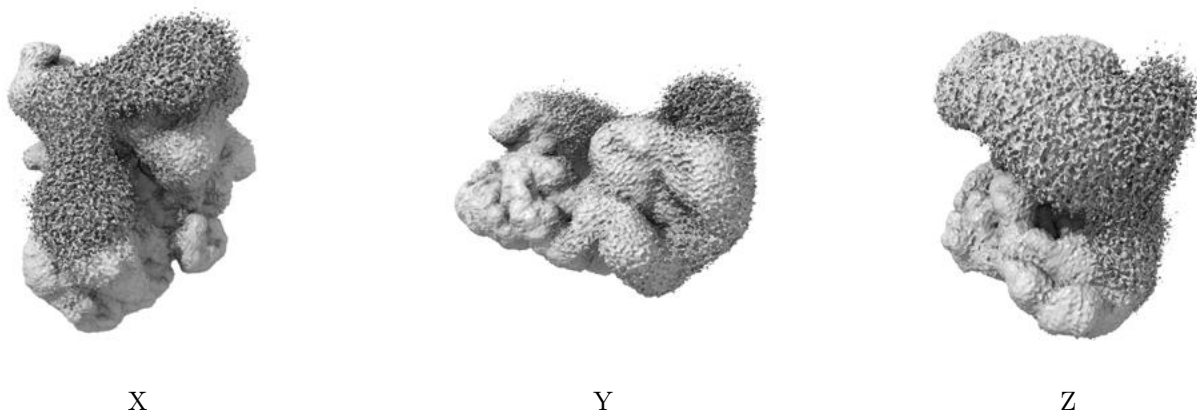
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6　Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1　emd_19047_msk_1.map ⓘ

X　　　　　　　　　　　Y　　　　　　　　　　　Z
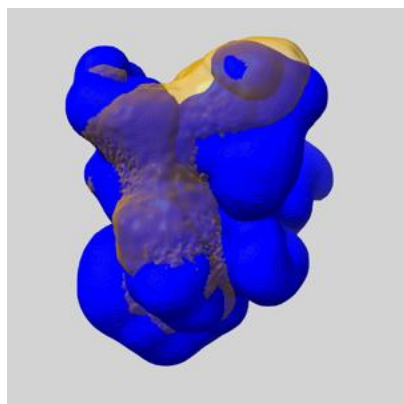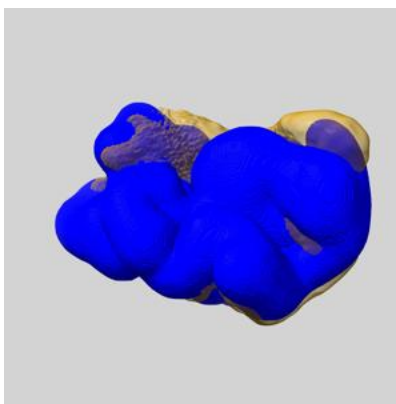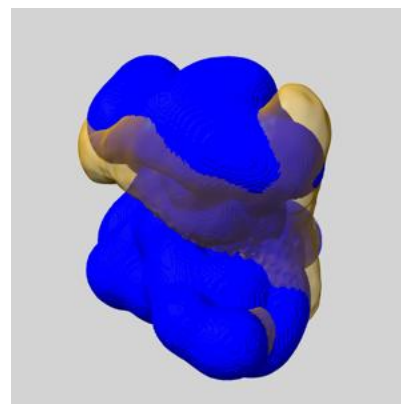
7 Map analysis ⓘ

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 ⓘ
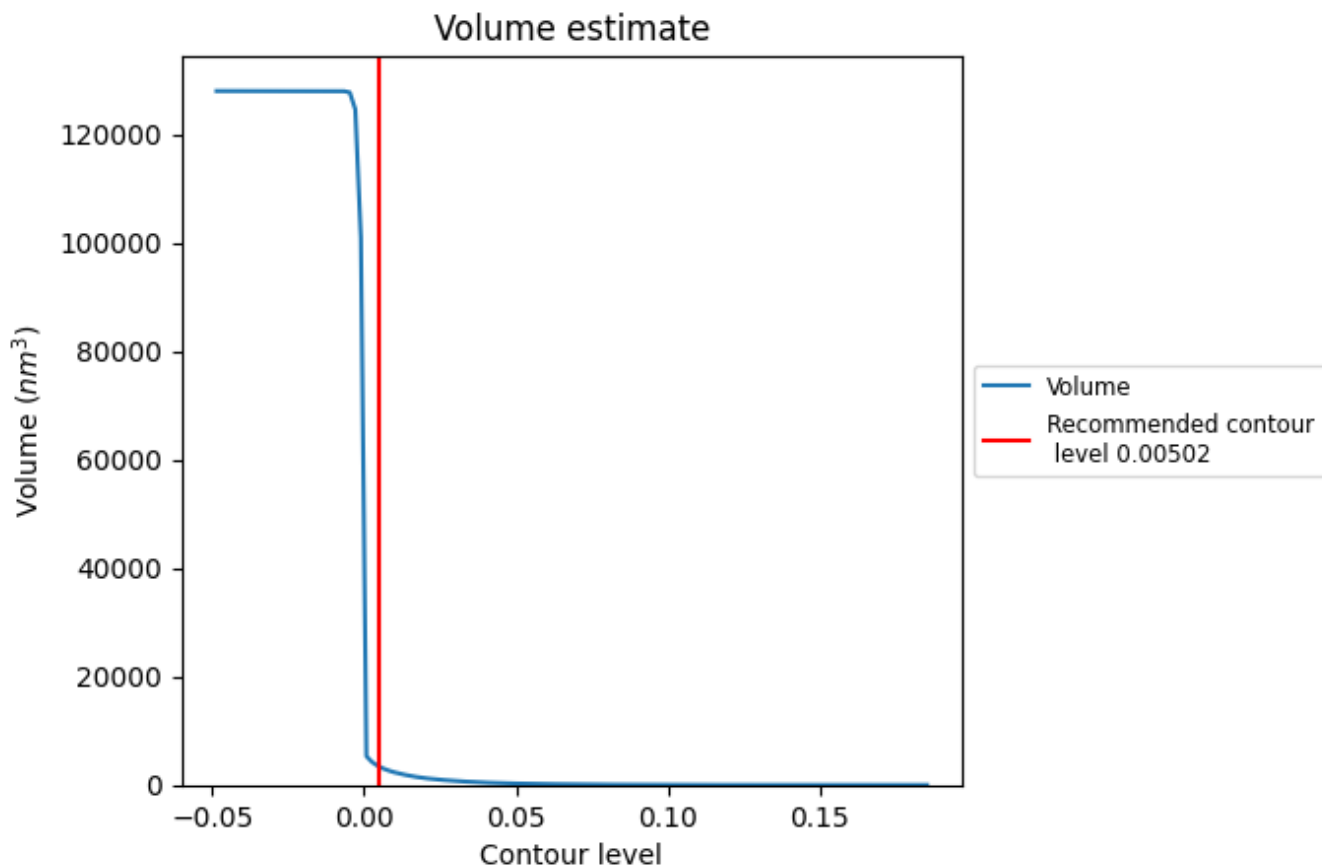
The volume at the recommended contour level is 3389 nm^3; this corresponds to an approximate mass of 3061 kDa.

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 ⓘ
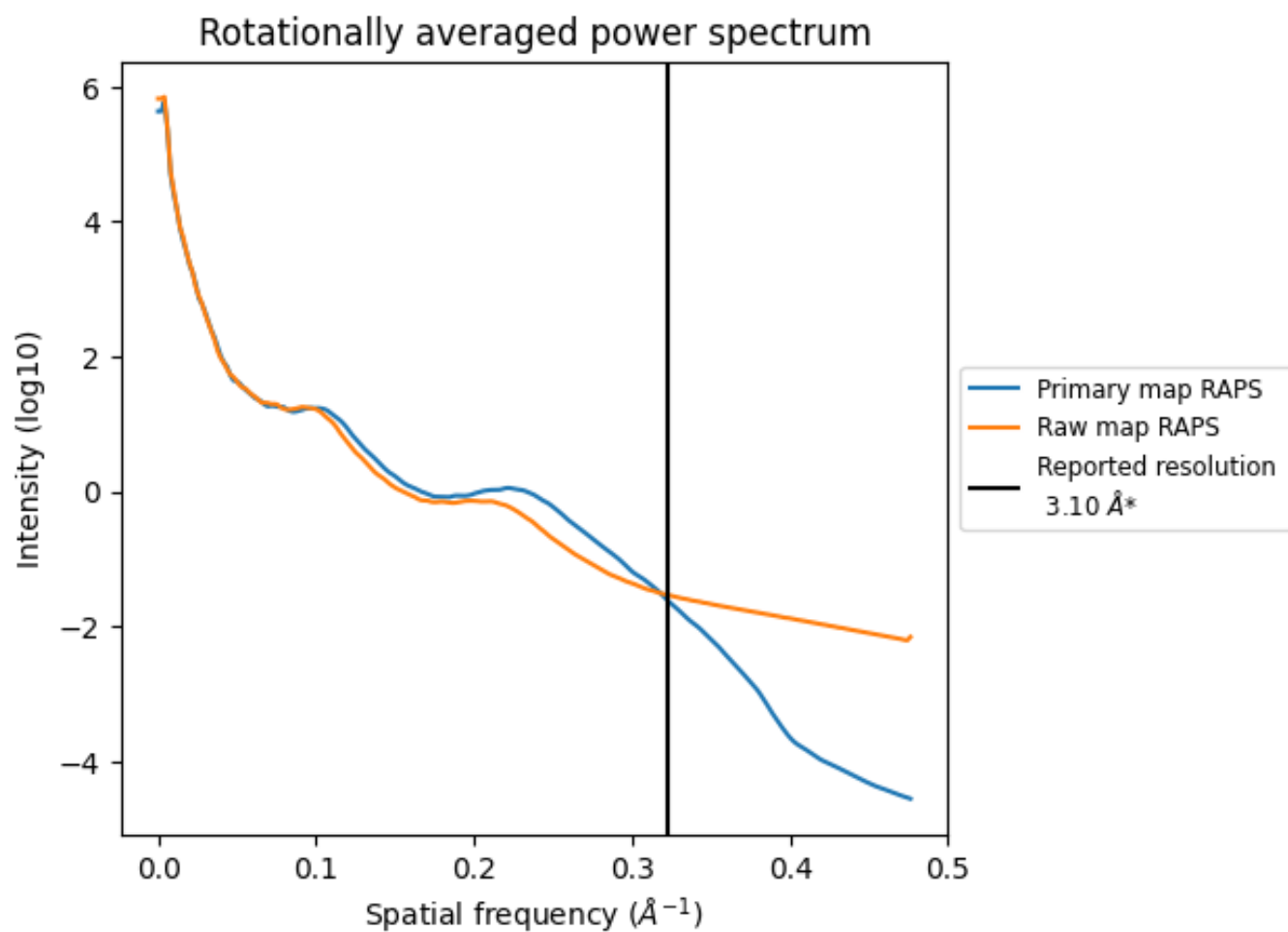
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 ⓘ
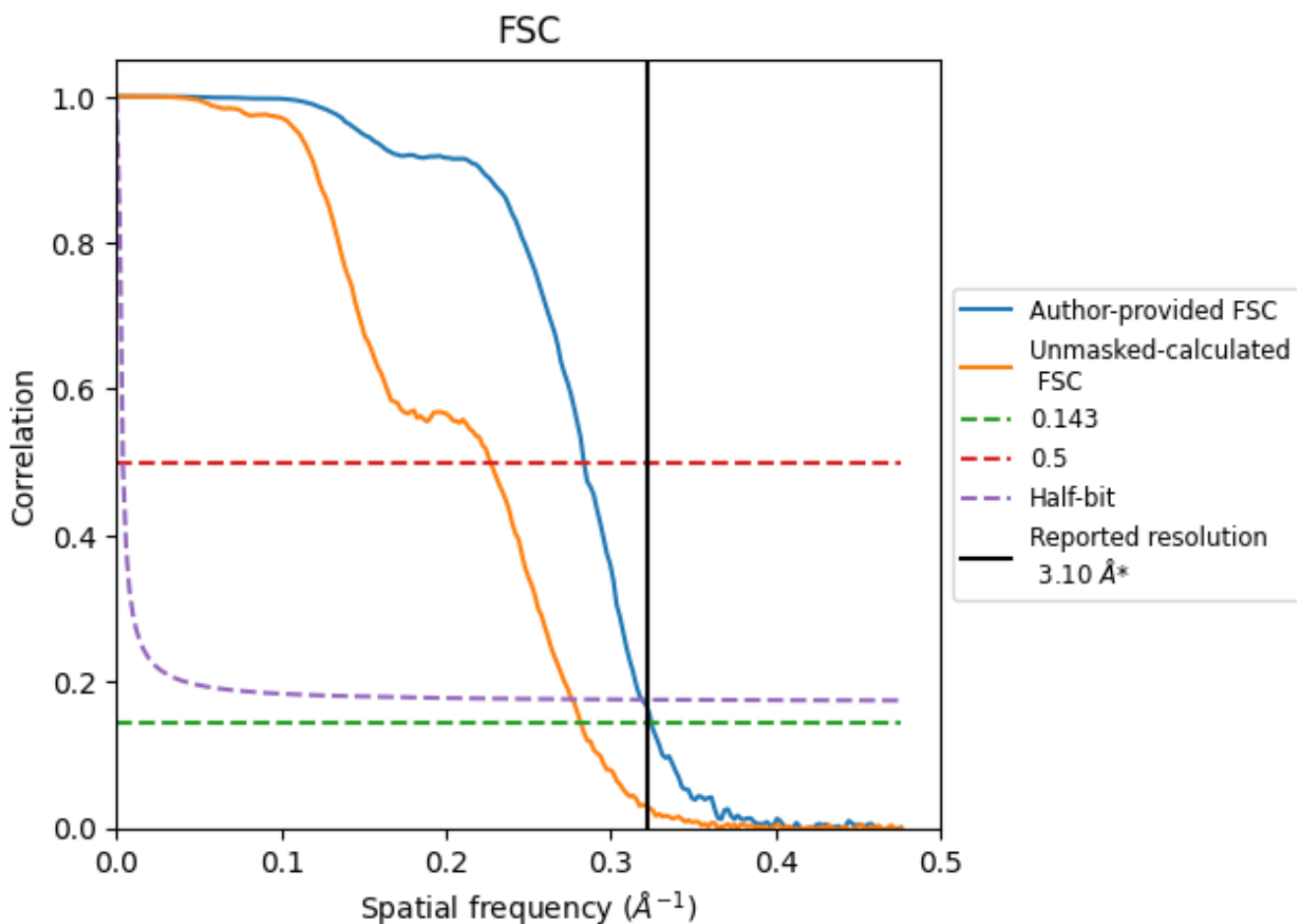
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.52	3.13
Unmasked-calculated*	3.55	4.41	3.62

*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 3.55 differs from the reported value 3.1 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19047 and PDB model 8RC4. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)
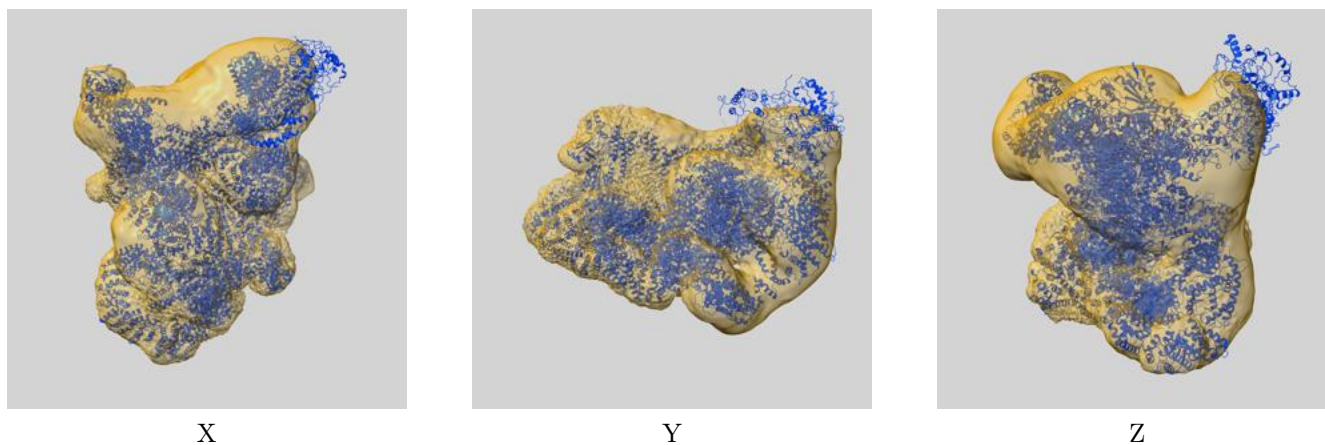
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.00502 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 ⓘ

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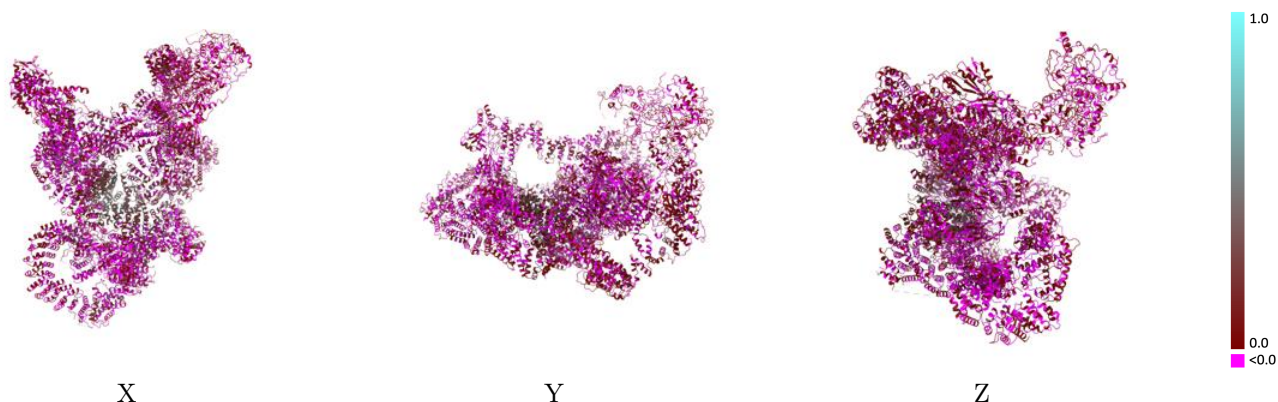
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
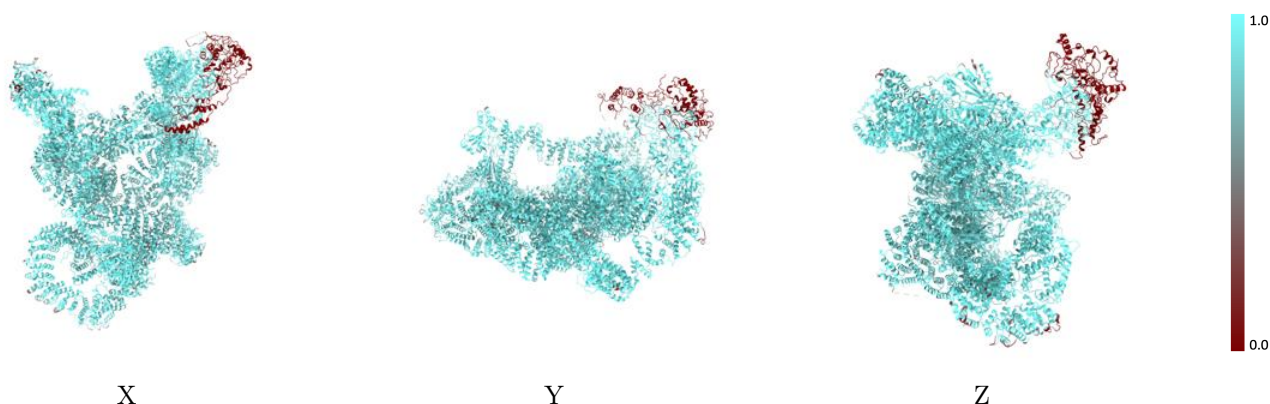
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00502).

9.4　Atom inclusion ⓘ
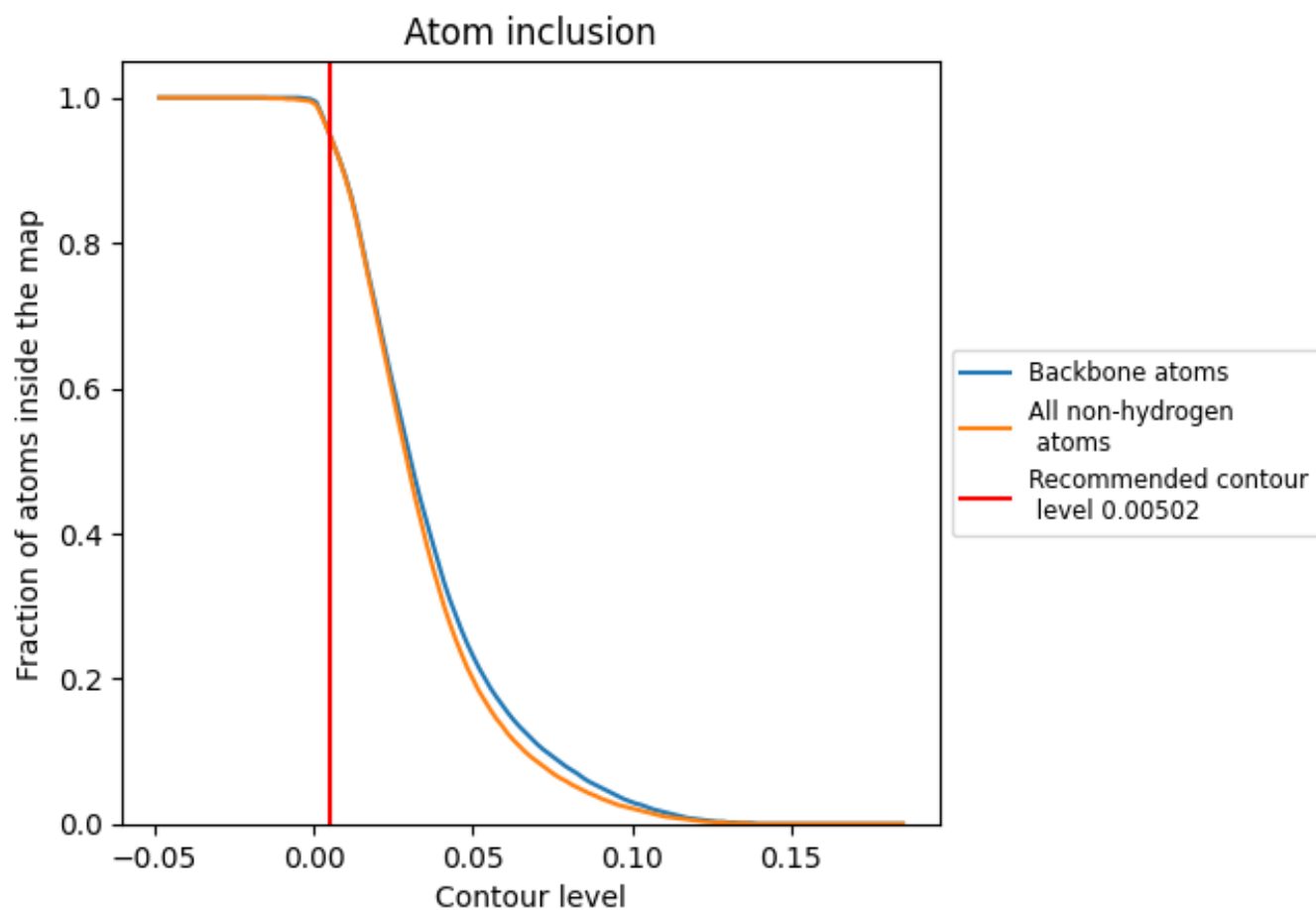
At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00502) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9490	0.0360
a	0.9690	0.0540
b	0.9790	0.0870
d	0.9900	0.0350
e	0.9700	0.0110
f	0.9870	0.0240
g	0.9670	0.0460
h	0.9630	0.0100
i	0.9840	0.0020
j	0.9860	0.0510
k	0.9990	0.0440
m	0.4430	0.0190
n	0.7180	0.0230
o	0.9890	0.0540
p	0.9760	0.0390
q	0.9660	-0.0370
r	0.9530	-0.0080

1.0

0.0
<0.0