WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Nov 24, 2024 – 01:48 AM JST

PDB ID	:	8IB7
EMDB ID	:	EMD-35334
Title	:	Respiratory complex CIII2, focus-refined of type IA, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-09
Resolution	:	3.40 Å(reported)

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

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

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

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.40 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.
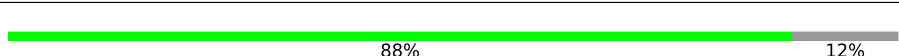
Metric	Percentile Ranks	Value
Ramachandran outliers		0
Sidechain outliers		0.0%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
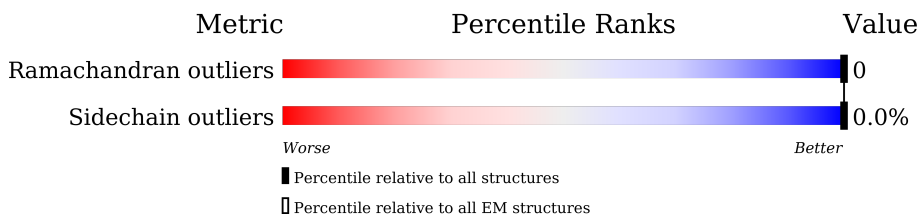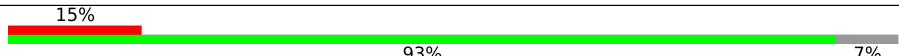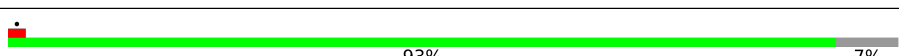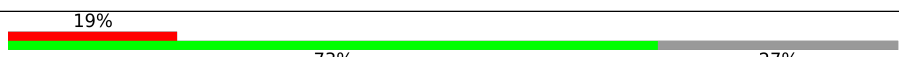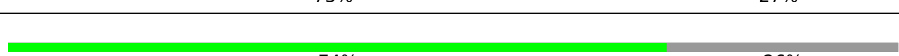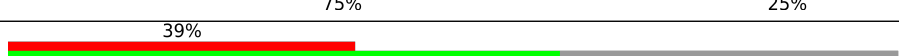
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	AA	480	83% 17%
1	Aa	480	86% 14%
2	AB	453	92% 8%
2	Ab	453	92% 8%
3	AC	381	98% ·
3	Ac	381	98% ·
4	AD	325	5% 73% 27%
4	Ad	325	73% 27%
5	AE	274	39% 67% 32%

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Mol	Chain	Length	Quality of chain
5	AI	274	18% · 81%
5	Ae	274	38% 67% 32%
6	AF	111	5% 88% 12%
6	Af	111	88% 12%
7	AG	82	15% 93% 7%
7	Ag	82	93% 7%
8	AH	89	19% 73% 27%
8	Ah	89	74% 26%
9	AJ	64	34% 64% 36%
9	Aj	64	8% 75% 25%
10	AK	56	39% 62% 38%
10	Ak	56	59% 79% 21%

2 Entry composition ⓘ

There are 17 unique types of molecules in this entry. The entry contains 31874 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	400	Total	C	N	O	S	0	0
			3128	1952	557	603	16		
1	Aa	412	Total	C	N	O	S	0	0
			3225	2016	569	624	16		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		
2	Ab	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		
3	Ac	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	238	Total	C	N	O	S	0	0
			1896	1211	326	345	14		
4	Ad	238	Total	C	N	O	S	0	0
			1895	1211	325	345	14		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	185	Total	C	N	O	S	0	0
			1427	902	250	268	7		
5	AI	51	Total	C	N	O		0	0
			345	221	64	60			
5	Ae	185	Total	C	N	O	S	0	0
			1432	905	250	270	7		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	98	Total	C	N	O	S	0	0
			864	552	154	155	3		
6	Af	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	76	Total	C	N	O	S	0	0
			643	418	116	108	1		
7	Ag	76	Total	C	N	O	S	0	0
			643	418	116	108	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	65	Total	C	N	O	S	0	0
			535	327	99	104	5		
8	Ah	66	Total	C	N	O	S	0	0
			544	333	101	105	5		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AJ	41	Total	C	N	O	0	0
			332	216	57	59		
9	Aj	48	Total	C	N	O	0	0
			392	257	67	68		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	35	Total	C	N	O	S	0	0
			281	184	52	44	1		
10	Ak	44	Total	C	N	O	S	0	0
			357	236	63	57	1		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					AltConf
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).

3PE

Mol	Chain	Residues	Atoms					AltConf
12	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	AF	1	Total	C	N	O	P	0
			42	32	1	8	1	
12	Ac	1	Total	C	N	O	P	0
			23	13	1	8	1	
12	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	Ag	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).
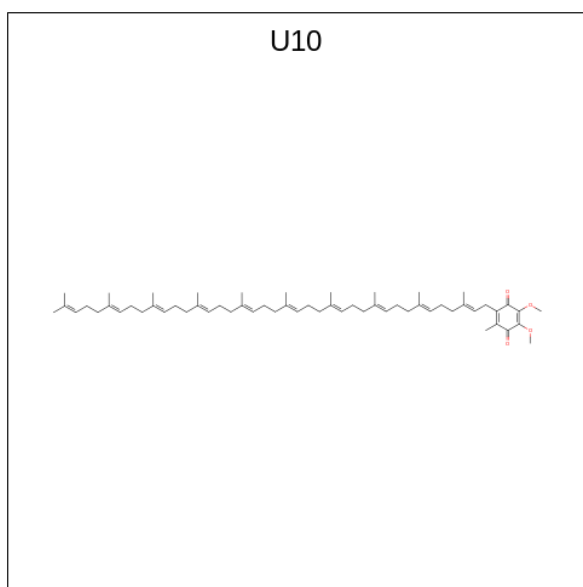
Mol	Chain	Residues	Atoms			AltConf
13	AC	1	Total 23	C 19	O 4	0
13	Ac	1	Total 38	C 34	O 4	0

- Molecule 14 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEX AENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms			AltConf
14	AC	1	Total 28	C 24	O 4	0

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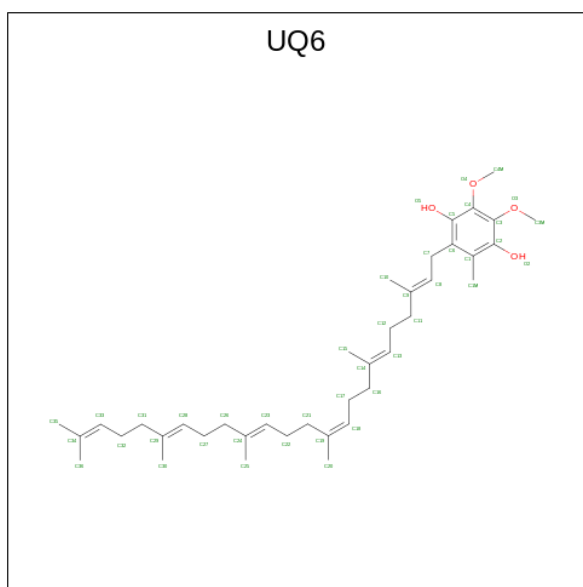
Mol	Chain	Residues	Atoms			AltConf
14	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

CDL

Mol	Chain	Residues	Atoms				AltConf
15	AC	1	Total	C	O	P	0
			56	37	17	2	
15	Aa	1	Total	C	O	P	0
			46	27	17	2	
15	Ac	1	Total	C	O	P	0
			42	23	17	2	
15	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

HEC

Mol	Chain	Residues	Atoms					AltConf
16	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).

3PH

Mol	Chain	Residues	Atoms				AltConf
17	AD	1	Total	C	O	P	0
			36	27	8	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	Ad	1	36	27	8	1	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.
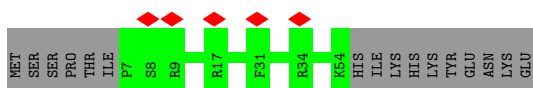
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AA:

• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Aa:

• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AB:

• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Ab:

• Molecule 3: Cytochrome b

Chain AC:

• Molecule 3: Cytochrome b

Chain Ac:

• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain AD:

• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Ad:

• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AE:

• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:

• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ae:

• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain AF:

• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain Af:

MET ALA GLY ARG SER ALA VAL SER ALA SER LYS TRP L14 K11

• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain AG:

15%

93%   7%

MET GLY ARG E4 A26 Y30 K33 G34 K71 R72 K73 A76 M77 Y78 E79 ASN ASP LYS

• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain Ag:

93%   7%

MET GLY ARG E4 L8 E79 ASN ASP LYS

• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AH:

19%

73%   27%

MET GLY LEU GLU ASP GLU ARG LYS MET LEU THR GLY SER GLY ASP PRO LYS GLU GLU GLU GLU GLU L24 V25 E33 K40 R47 L50 C51 D52 N53 R54 V55 S56 S57 R58 S59 Q60 T61 E62 E63 D64 L88 LYS

• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ah:

74%   26%

MET GLY LEU GLU ASP GLU ARG LYS MET LEU THR GLY SER GLY ASP PRO LYS GLU GLU GLU GLU GLU L24 K89

• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain AJ:

34%

64%   36%

MET SER SER PRO THR ILE PRO S8 R9 L10 Y11 S12 L13 L14 F15 R16 R17 A22 R34 A35 F36 D37 Q38 G39 A40 D41 A42 E45 H46 I47 N48 GLU GLY LYS LEU TRP LYS HIS ILE LYS HIS LYS TYR GLU ASN LYS GLU

• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain Aj:

8%

75%   25%

MET SER SER PRO THR ILE P7 S8 R9 R17 F31 R34 K54 HIS ILE LYS HIS LYS TYR GLU ASN LYS GLU

• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain AK:

39%

62%

38%

MET LEU SER ARG PHE LEU G7 P8 R9 Y10 R11 E12 L13 A14 R15 N16 W17 T20 M23 T26 A29 V30 G31 W34 D37 W38 R39 L40 I41 LEU ASP TRP VAL PRO TYR ILE ASN GLY LYS PHE LYS LYS ASP ASP

• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain Ak:

59%

79%

21%

MET LEU SER ARG PHE LEU G7 P8 R9 Y10 R11 E12 L13 A14 R15 N16 T20 M23 W24 G25 T26 V27 G28 A29 V30 G31 L32 V33 W34 A35 T36 D37 W38 R39 L40 I41 L42 D43 W44 V45 P46 Y47 I48 N49 G50 LYS PHE LYS LYS ASP ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.856	Depositor
Minimum map value	-1.742	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, 3PE, HEM, U10, CDL, HEC, UQ6

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	AA	0.41	0/3187	0.61	0/4320
1	Aa	0.42	0/3288	0.61	1/4462 (0.0%)
2	AB	0.35	0/3187	0.58	1/4308 (0.0%)
2	Ab	0.36	0/3187	0.56	0/4308
3	AC	0.35	0/3089	0.55	1/4221 (0.0%)
3	Ac	0.36	0/3089	0.56	1/4221 (0.0%)
4	AD	0.38	0/1955	0.53	0/2655
4	Ad	0.44	1/1954 (0.1%)	0.55	0/2655
5	AE	0.47	0/1459	0.63	1/1976 (0.1%)
5	AI	0.47	0/349	0.73	3/476 (0.6%)
5	Ae	0.47	0/1464	0.63	1/1983 (0.1%)
6	AF	0.32	0/884	0.50	0/1184
6	Af	0.32	0/884	0.50	0/1184
7	AG	0.37	0/662	0.55	0/895
7	Ag	0.42	0/662	0.53	0/895
8	AH	0.34	0/542	0.61	0/728
8	Ah	0.44	0/551	0.60	0/739
9	AJ	0.35	0/339	0.48	0/457
9	Aj	0.42	0/402	0.61	0/541
10	AK	0.31	0/291	0.49	0/399
10	Ak	0.41	0/371	0.55	0/511
All	All	0.39	1/31796 (0.0%)	0.57	9/43118 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Ad	180	PRO	N-CD	-8.24	1.36	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	261	ALA	N-CA-C	-5.85	95.20	111.00
5	AI	60	ALA	N-CA-CB	-5.83	101.94	110.10
3	Ac	17	SER	N-CA-CB	-5.66	102.01	110.50
3	AC	17	SER	N-CA-CB	-5.61	102.09	110.50
5	Ae	221	GLY	N-CA-C	5.51	126.87	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2　Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	AA	394/480 (82%)	381 (97%)	13 (3%)	0	100	100
1	Aa	408/480 (85%)	388 (95%)	20 (5%)	0	100	100
2	AB	416/453 (92%)	404 (97%)	12 (3%)	0	100	100
2	Ab	416/453 (92%)	405 (97%)	11 (3%)	0	100	100
3	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
3	Ac	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
4	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
4	Ad	236/325 (73%)	220 (93%)	16 (7%)	0	100	100
5	AE	181/274 (66%)	169 (93%)	12 (7%)	0	100	100
5	AI	43/274 (16%)	39 (91%)	4 (9%)	0	100	100
5	Ae	181/274 (66%)	166 (92%)	15 (8%)	0	100	100
6	AF	96/111 (86%)	96 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Af	96/111 (86%)	96 (100%)	0	0	100	100
7	AG	74/82 (90%)	74 (100%)	0	0	100	100
7	Ag	74/82 (90%)	73 (99%)	1 (1%)	0	100	100
8	AH	63/89 (71%)	62 (98%)	1 (2%)	0	100	100
8	Ah	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
9	AJ	39/64 (61%)	39 (100%)	0	0	100	100
9	Aj	46/64 (72%)	44 (96%)	2 (4%)	0	100	100
10	AK	33/56 (59%)	33 (100%)	0	0	100	100
10	Ak	42/56 (75%)	40 (95%)	2 (5%)	0	100	100
All	All	3880/4904 (79%)	3755 (97%)	125 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	338/398 (85%)	338 (100%)	0	100	100
1	Aa	349/398 (88%)	349 (100%)	0	100	100
2	AB	328/356 (92%)	328 (100%)	0	100	100
2	Ab	328/356 (92%)	328 (100%)	0	100	100
3	AC	325/333 (98%)	325 (100%)	0	100	100
3	Ac	325/333 (98%)	325 (100%)	0	100	100
4	AD	203/260 (78%)	203 (100%)	0	100	100
4	Ad	203/260 (78%)	203 (100%)	0	100	100
5	AE	155/224 (69%)	155 (100%)	0	100	100
5	AI	34/224 (15%)	33 (97%)	1 (3%)	37	61
5	Ae	156/224 (70%)	156 (100%)	0	100	100
6	AF	90/99 (91%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Af	90/99 (91%)	90 (100%)	0	100	100
7	AG	69/74 (93%)	69 (100%)	0	100	100
7	Ag	69/74 (93%)	69 (100%)	0	100	100
8	AH	62/83 (75%)	62 (100%)	0	100	100
8	Ah	63/83 (76%)	63 (100%)	0	100	100
9	AJ	33/55 (60%)	33 (100%)	0	100	100
9	Aj	39/55 (71%)	39 (100%)	0	100	100
10	AK	26/46 (56%)	26 (100%)	0	100	100
10	Ak	34/46 (74%)	34 (100%)	0	100	100
All	All	3319/4080 (81%)	3318 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
5	AI	78	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	Ab	304	ASN
4	Ad	190	ASN
2	Ab	415	GLN
3	Ac	341	GLN
5	Ae	135	GLN

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 (i)

21 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	$\#|Z| > 2$
11	HEM	AC	402	3	41,50,50	1.47	8 (19%)	45,82,82	2.43	16 (35%)
17	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.13	3 (7%)
12	3PE	AF	201	-	41,41,50	1.00	2 (4%)	44,46,55	0.98	2 (4%)
13	U10	AC	404	-	23,23,63	1.78	2 (8%)	28,31,79	1.49	5 (17%)
12	3PE	Ac	401	-	22,22,50	0.38	0	25,27,55	0.48	0
12	3PE	Ac	404	-	34,34,50	1.09	2 (5%)	37,39,55	1.23	4 (10%)
14	UQ6	Ac	406	-	28,28,43	2.51	6 (21%)	33,37,55	1.59	9 (27%)
15	CDL	AC	406	-	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
11	HEM	AC	401	3	41,50,50	1.36	5 (12%)	45,82,82	1.88	10 (22%)
13	U10	Ac	405	-	38,38,63	1.37	2 (5%)	46,49,79	1.71	12 (26%)
15	CDL	Ac	407	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
15	CDL	Aa	501	-	45,45,99	0.36	0	51,57,111	0.42	0
14	UQ6	AC	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.80	10 (30%)
15	CDL	Ag	101	-	55,55,99	1.21	4 (7%)	61,67,111	1.26	6 (9%)
12	3PE	AC	403	-	34,34,50	1.10	2 (5%)	37,39,55	1.18	3 (8%)
11	HEM	Ac	402	3	41,50,50	1.42	6 (14%)	45,82,82	2.15	11 (24%)
12	3PE	Ag	102	-	38,38,50	1.04	2 (5%)	41,43,55	1.13	4 (9%)
16	HEC	AD	401	4	32,50,50	2.16	10 (31%)	24,82,82	2.57	6 (25%)
16	HEC	Ad	401	4	32,50,50	2.18	11 (34%)	24,82,82	2.45	6 (25%)
11	HEM	Ac	403	3	41,50,50	1.42	6 (14%)	45,82,82	1.84	11 (24%)
17	3PH	AD	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.21	3 (7%)

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
11	HEM	AC	402	3	-	4/12/54/54	-
17	3PH	Ad	402	-	-	8/37/37/49	-
12	3PE	AF	201	-	-	9/45/45/54	-
13	U10	AC	404	-	-	0/15/39/87	0/1/1/1
12	3PE	Ac	401	-	-	10/26/26/54	-
12	3PE	Ac	404	-	-	8/38/38/54	-
14	UQ6	Ac	406	-	-	7/21/21/39	0/1/1/1
15	CDL	AC	406	-	-	18/66/66/110	-
11	HEM	AC	401	3	-	6/12/54/54	-
13	U10	Ac	405	-	-	9/33/57/87	0/1/1/1
15	CDL	Ac	407	-	-	11/52/52/110	-
15	CDL	Aa	501	-	-	16/56/56/110	-
14	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
15	CDL	Ag	101	-	-	12/66/66/110	-
12	3PE	AC	403	-	-	12/38/38/54	-
11	HEM	Ac	402	3	-	3/12/54/54	-
12	3PE	Ag	102	-	-	5/42/42/54	-
16	HEC	AD	401	4	-	3/10/54/54	-
16	HEC	Ad	401	4	-	2/10/54/54	-
11	HEM	Ac	403	3	-	8/12/54/54	-
17	3PH	AD	402	-	-	8/37/37/49	-

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AC	404	U10	C6-C1	7.59	1.49	1.35
13	Ac	405	U10	C6-C1	7.42	1.48	1.35
16	Ad	401	HEC	C3C-C2C	6.23	1.47	1.40
14	AC	405	UQ6	C2-C3	5.95	1.49	1.39
14	Ac	406	UQ6	C2-C3	5.90	1.49	1.39

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AD	401	HEC	CMC-C2C-C3C	7.21	134.30	125.82
11	Ac	402	HEM	C4B-C3B-C2B	-6.98	101.57	107.11
16	Ad	401	HEC	C1D-C2D-C3D	-6.40	102.54	107.00
11	AC	402	HEM	CHC-C4B-NB	6.27	131.24	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	AD	401	HEC	C1D-C2D-C3D	-6.03	102.80	107.00

There are no chirality outliers.

5 of 162 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AC	402	HEM	C2B-C3B-CAB-CBB
11	AC	402	HEM	C4B-C3B-CAB-CBB
11	Ac	403	HEM	C2B-C3B-CAB-CBB
11	Ac	403	HEM	C4B-C3B-CAB-CBB
12	AC	403	3PE	C1-O11-P-O12

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 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 HEM AC 402	
Bond lengths	Bond angles
Torsions	Rings

Ligand 3PH Ad 402	
Bond lengths	Bond angles
Torsions	Rings

Ligand 3PE AF 201

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 AC 404

Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Ac 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Ac 404

Bond lengths

Bond angles

Torsions

Rings

Ligand UQ6 Ac 406

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL AC 406

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM AC 401	
Bond lengths	Bond angles
Torsions	Rings

Ligand U10 Ac 405	
Bond lengths	Bond angles
Torsions	Rings

Ligand CDL Ac 407

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL Aa 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UQ6 AC 405

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL Ag 101

Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE AC 403

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM Ac 402

Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Ag 102

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC AD 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC Ad 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM Ac 403

Bond lengths

Bond angles

Torsions

Rings

Ligand 3PH AD 402

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-35334. 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 ⓘ
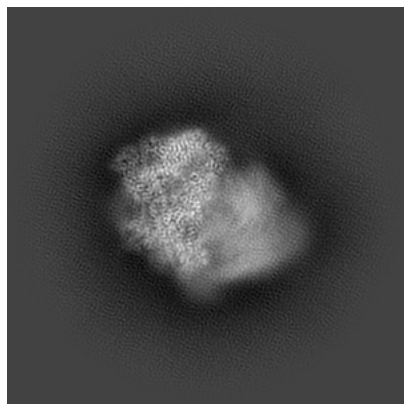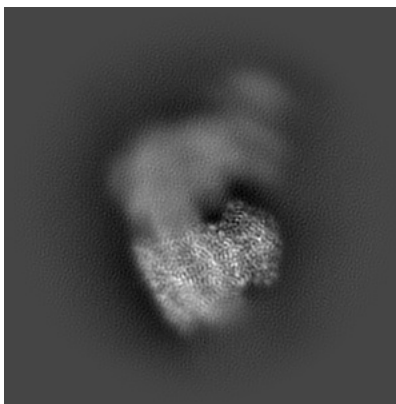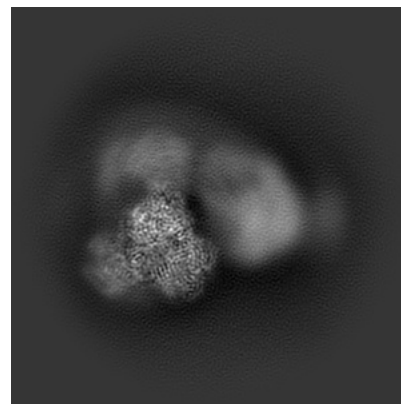
6.1.1 Primary map

X   Y   Z

6.1.2 Raw map

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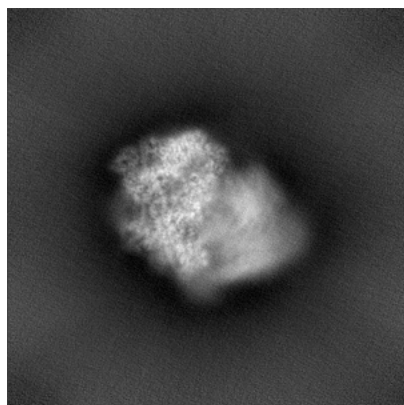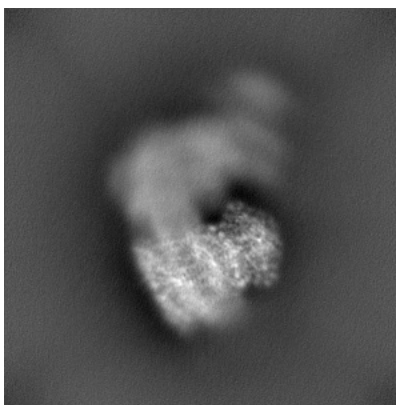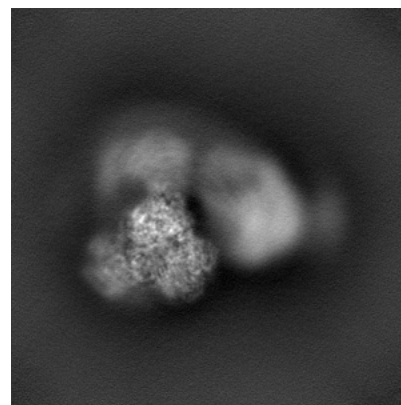
The images above show the map projected in three orthogonal directions.

6.2   Central slices   ⓘ
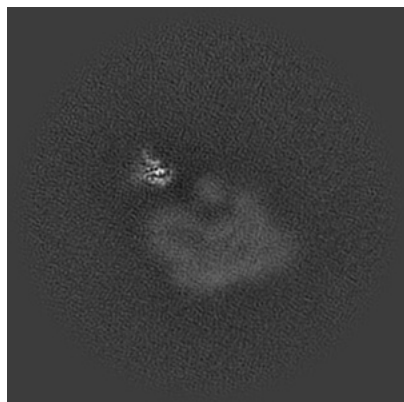
6.2.1   Primary map
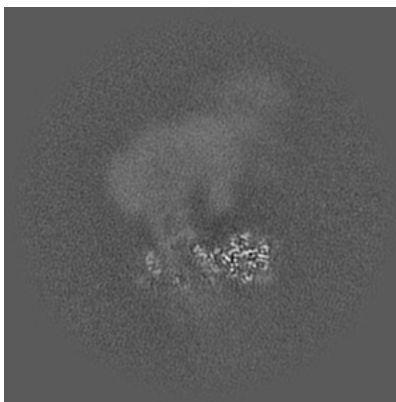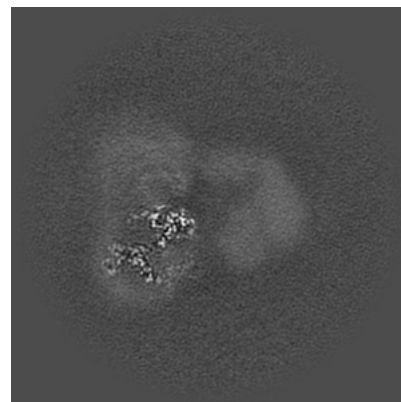
X Index: 192   Y Index: 192   Z Index: 192

6.2.2   Raw map
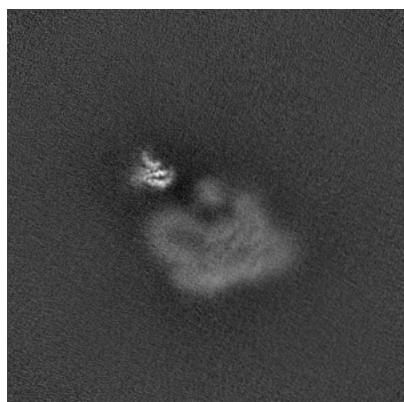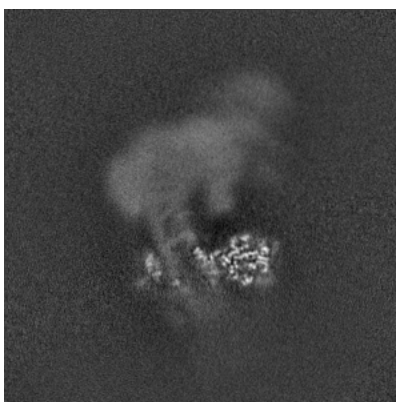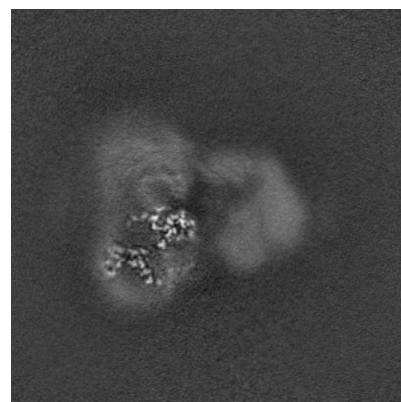
X Index: 192   Y Index: 192   Z Index: 192

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
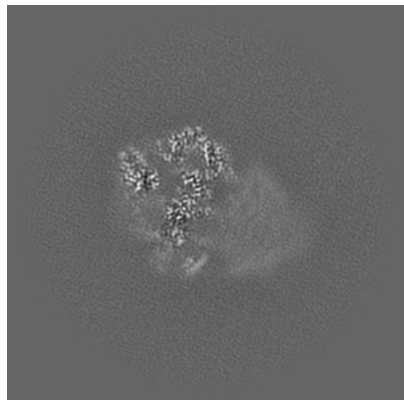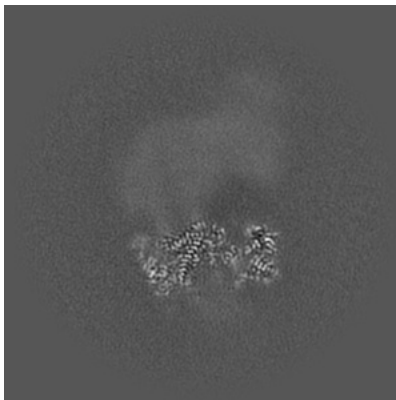
| X Index: 149 | Y Index: 168 | Z Index: 217 |
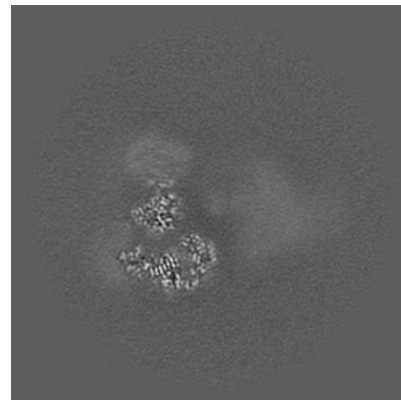
6.3.2 Raw map
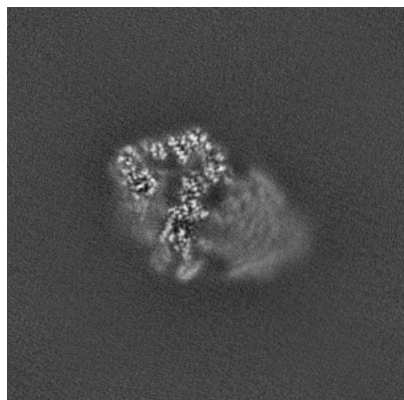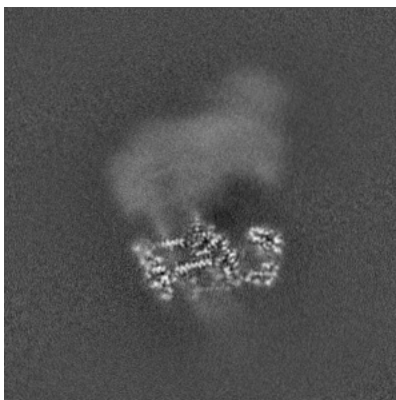
| X Index: 153 | Y Index: 175 | Z Index: 200 |
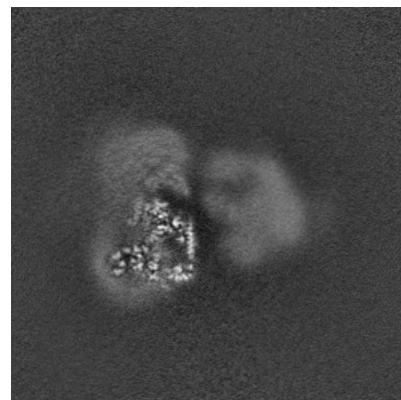
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

X   Y   Z

6.4.2 Raw map

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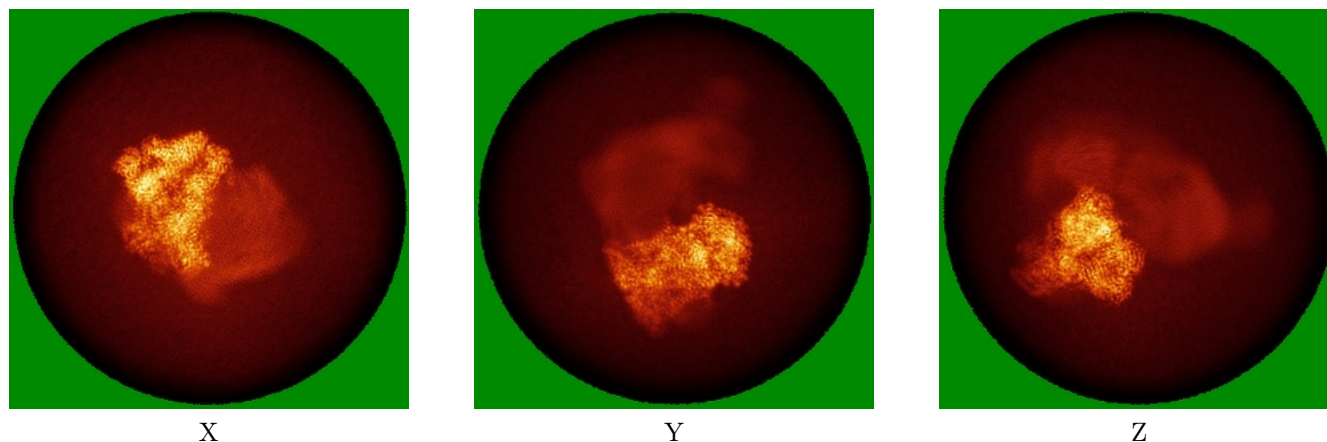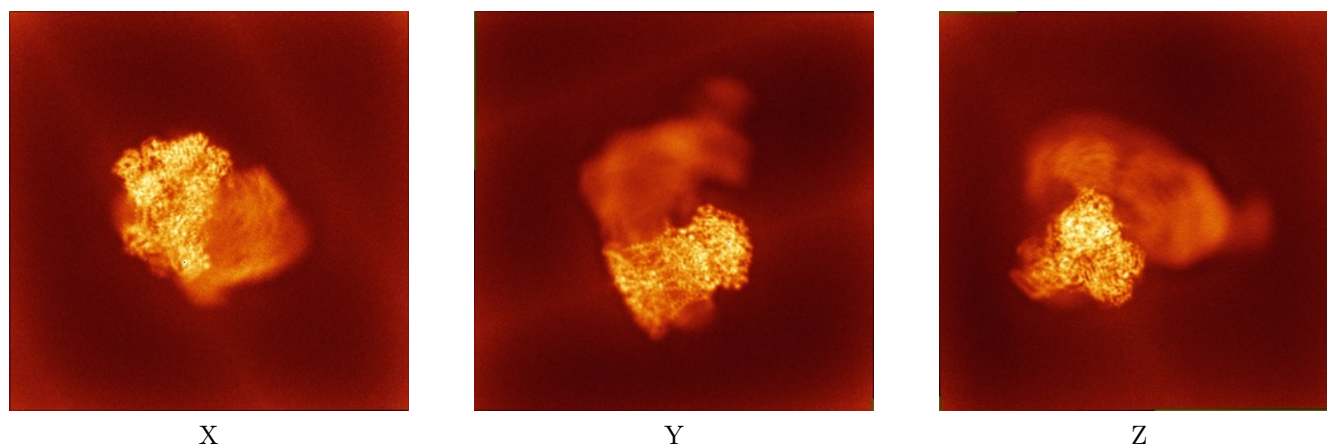
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
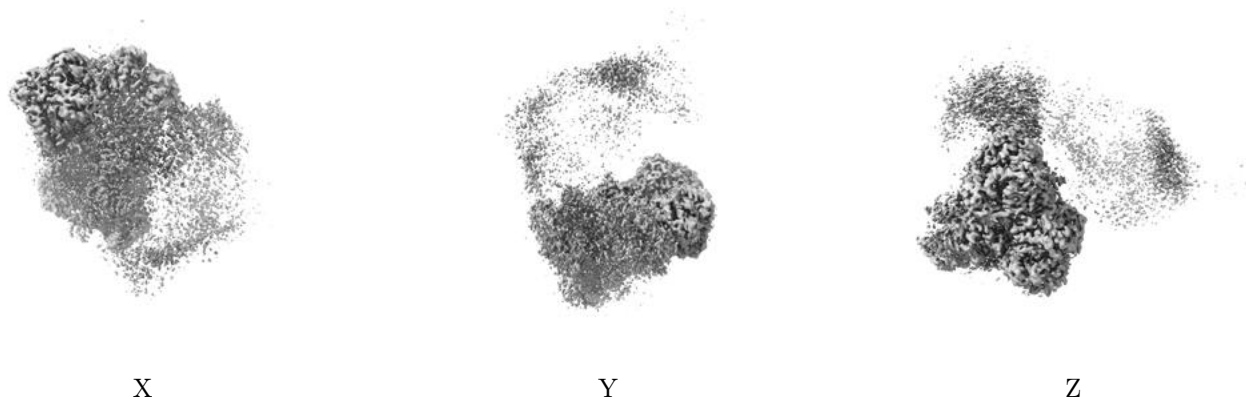
The images above show the 3D surface view of the map at the recommended contour level 0.35.
These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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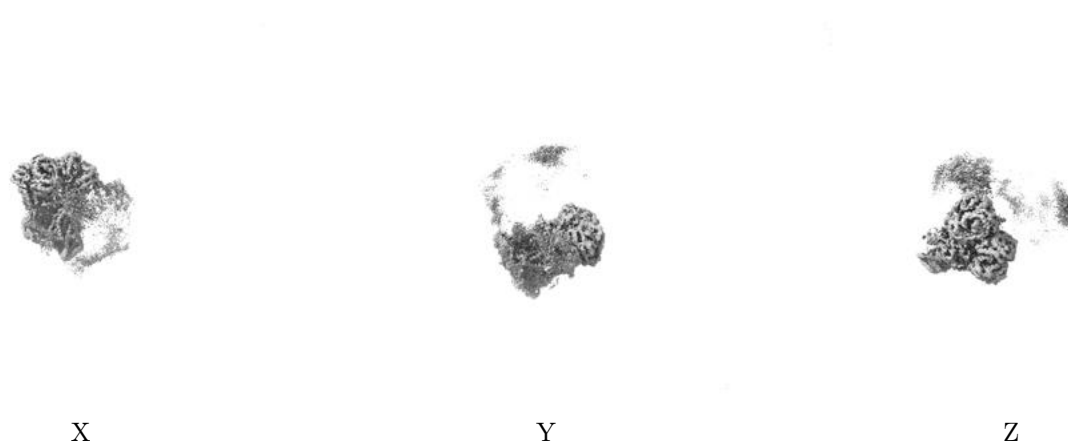
These images show the 3D surface of the raw map. The raw map's contour level was selected so
that its surface encloses the same volume as the primary map does at its recommended contour
level.

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_35334_msk_1.map ⓘ
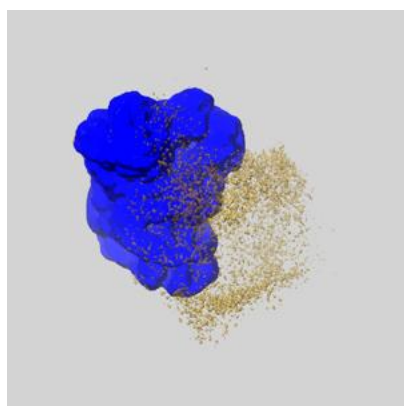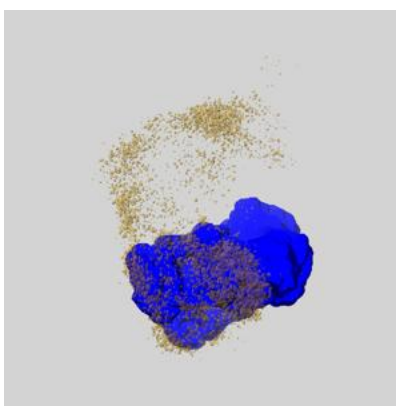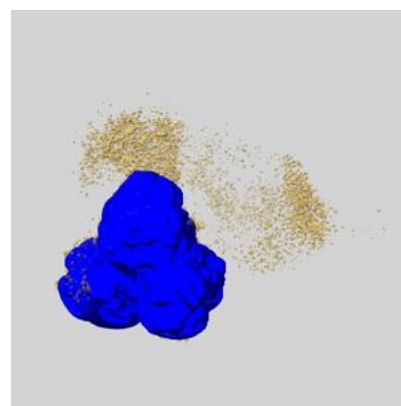
X   Y   Z

7 Map analysis (i)

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

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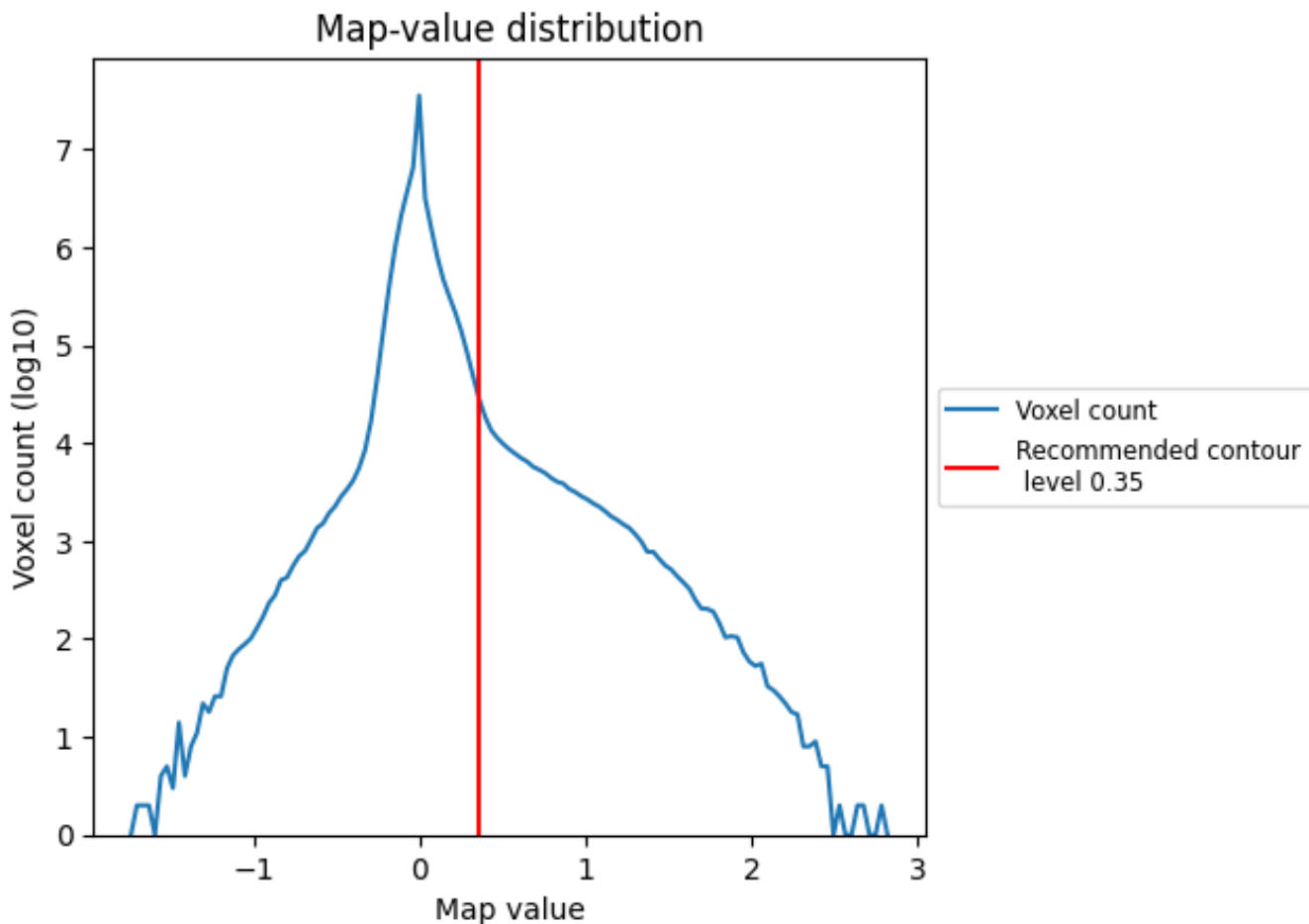
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
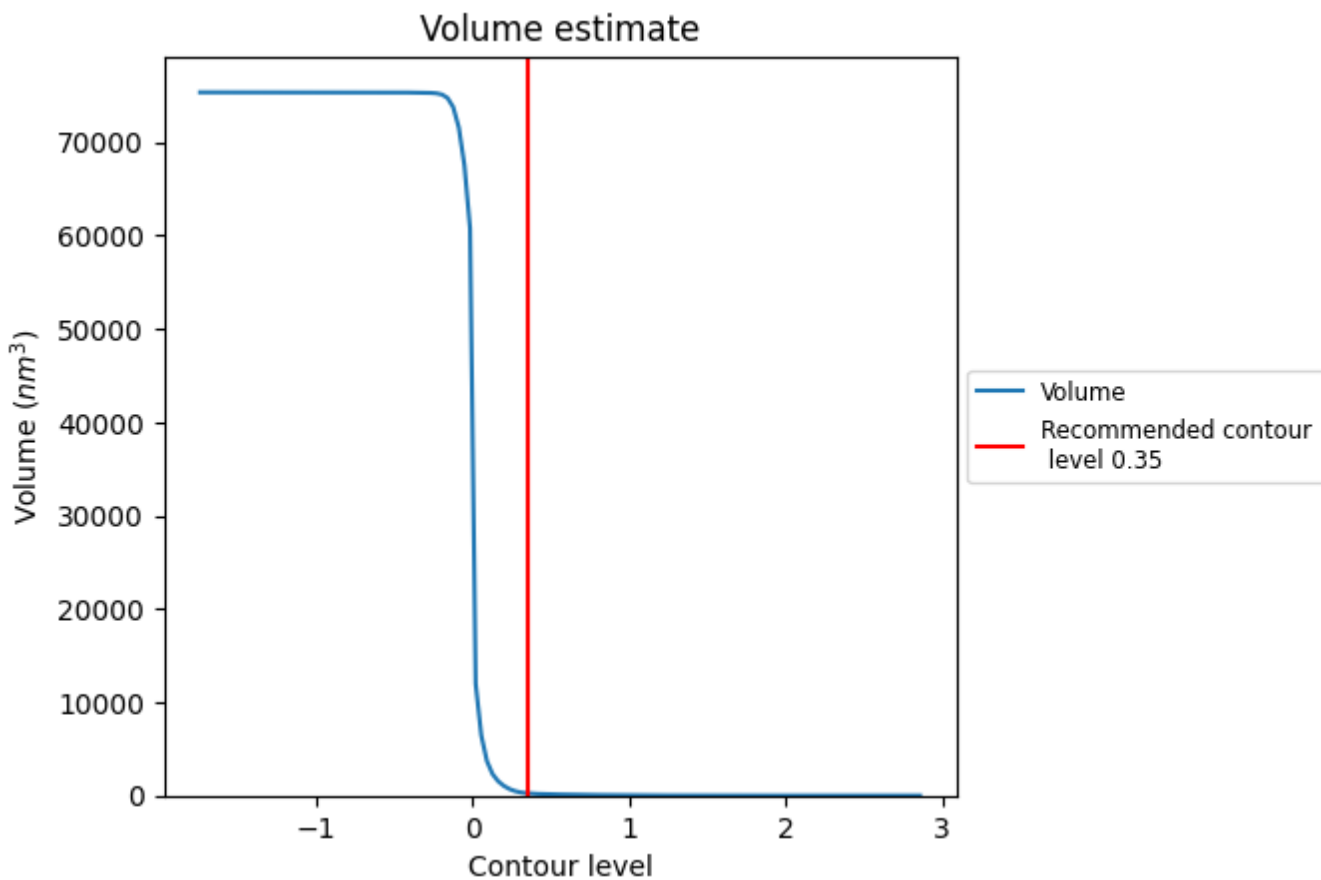
The volume at the recommended contour level is 244 nm^3; this corresponds to an approximate mass of 220 kDa.

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 ⓘ
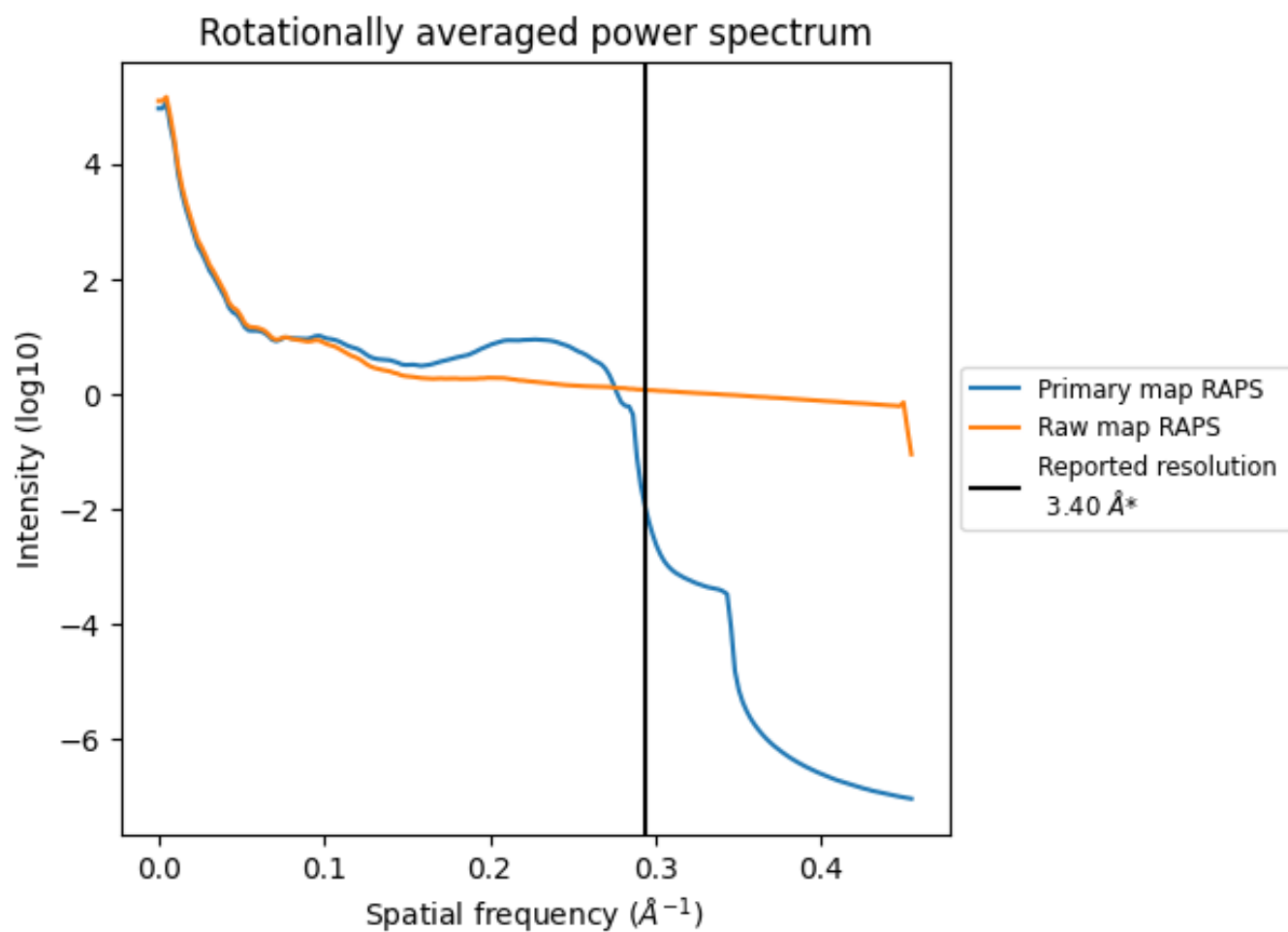
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)
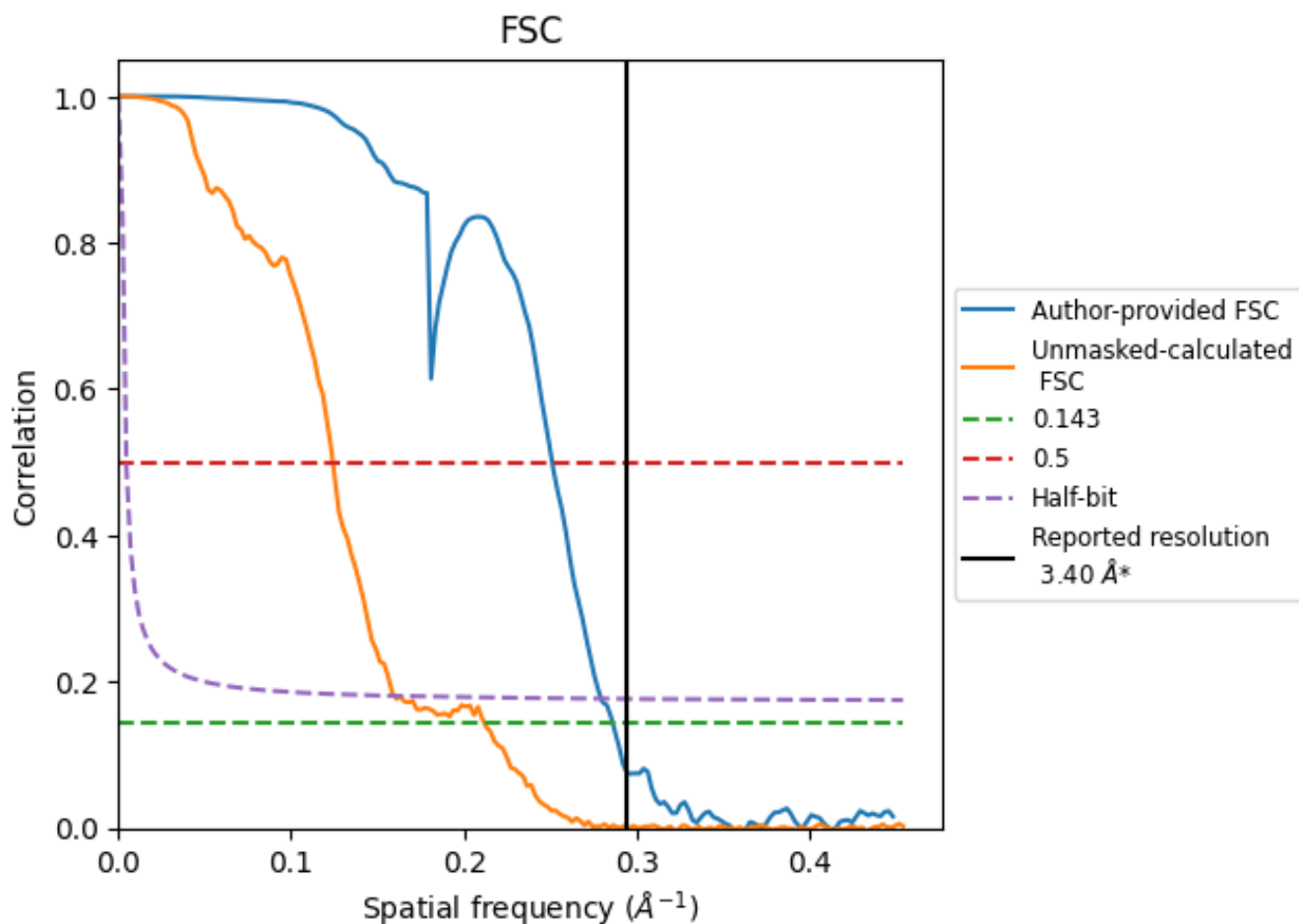
*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.49	3.98	3.58
Unmasked-calculated*	4.72	8.05	6.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.72 differs from the reported value 3.4 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-35334 and PDB model 8IB7. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay ⓘ

X   Y   Z
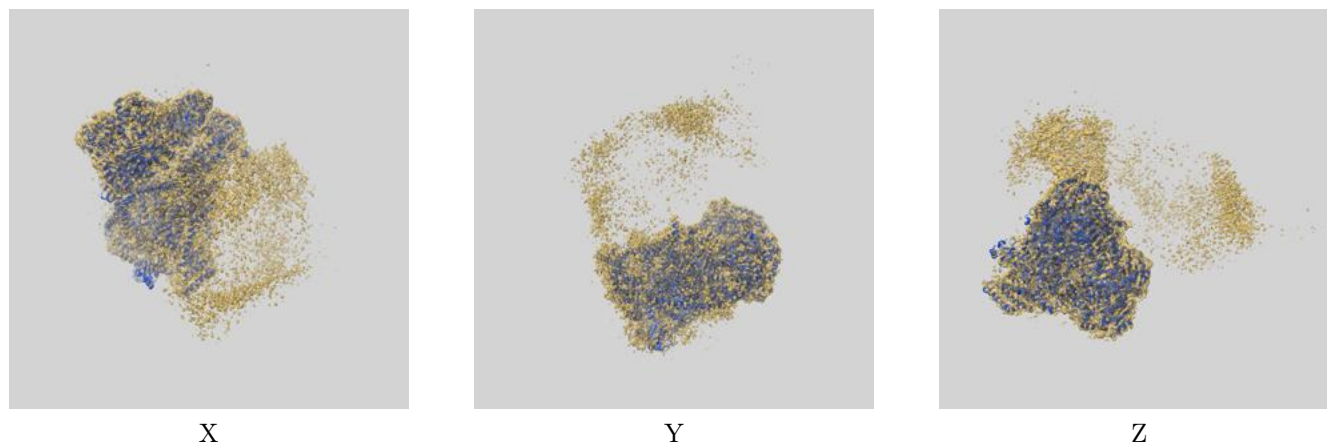
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model　ⓘ

| X | Y | Z |
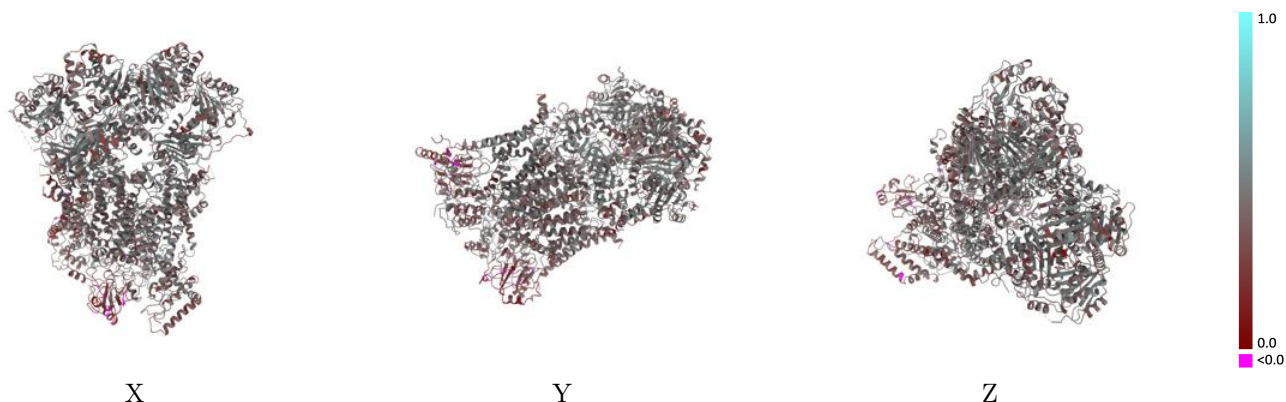
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 |
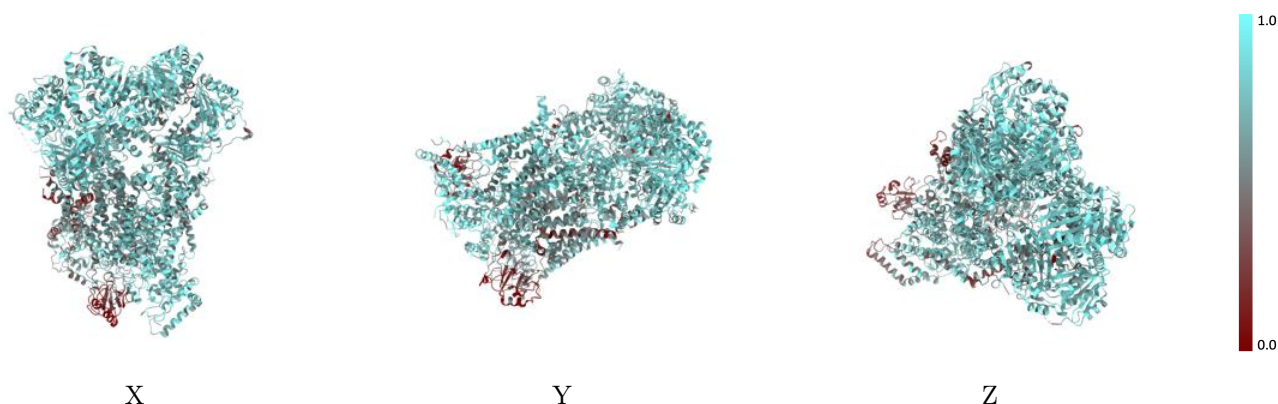
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4　Atom inclusion ⓘ
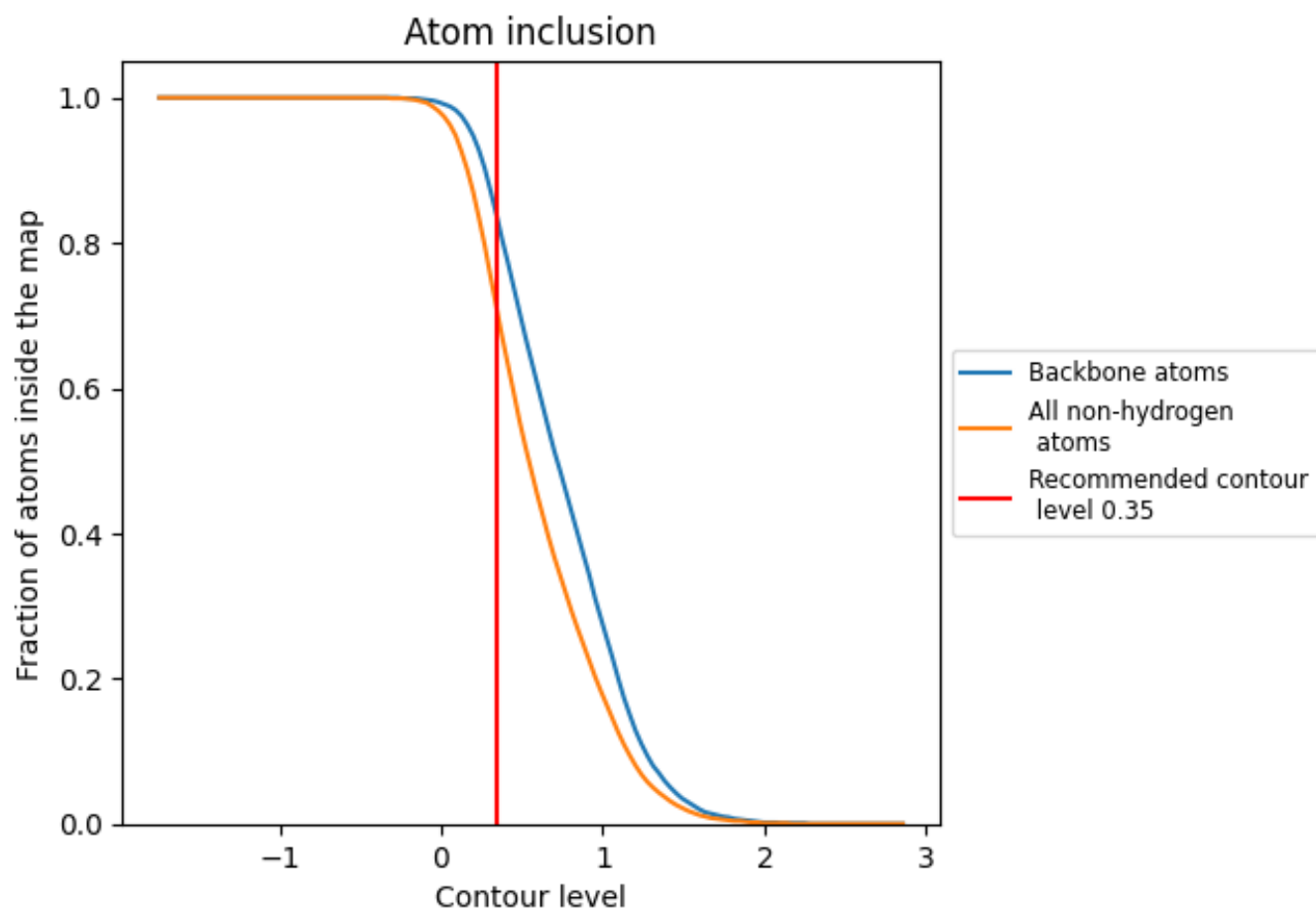
At the recommended contour level, 83% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.4070
AA	0.7960	0.4360
AB	0.7840	0.4260
AC	0.7000	0.4210
AD	0.7040	0.3820
AE	0.3450	0.2790
AF	0.7160	0.4100
AG	0.6480	0.3710
AH	0.5430	0.2770
AI	0.5790	0.4280
AJ	0.3540	0.2930
AK	0.3360	0.3550
Aa	0.7780	0.4360
Ab	0.7910	0.4330
Ac	0.7620	0.4450
Ad	0.7940	0.4150
Ae	0.3540	0.2940
Af	0.7660	0.4520
Ag	0.7480	0.4470
Ah	0.7740	0.3640
Aj	0.6120	0.3990
Ak	0.2570	0.3700

1.0

0.0
<0.0