



Full wwPDB EM Validation Report ⓘ

Jul 21, 2022 – 04:20 PM JST

PDB ID : 7YI0
EMDB ID : EMD-33845
Title : Cryo-EM structure of Rpd3S complex
Deposited on : 2022-07-14
Resolution : 3.20 Å (reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

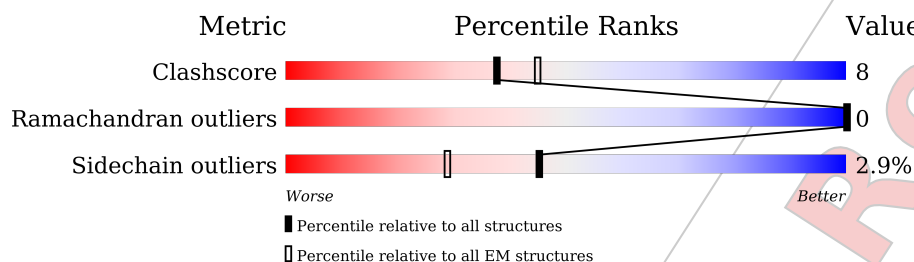
EMDB validation analysis : 0.0.1.dev8
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

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 3.20 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	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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1536	11% 25% 7% 67%
2	B	433	70% 14% 15%
3	C	401	38% 7% 55%
3	E	401	36% 27% 10% 62%
4	D	684	14% 35% 10% 55%
5	F	684	15% 13% 82%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13430 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	503	Total	C	N	O	S	0	0
			4233	2722	708	790	13		

- Molecule 2 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	368	Total	C	N	O	S	0	0
			2923	1858	495	545	25		

- Molecule 3 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	182	Total	C	N	O	S	0	0
			1473	944	237	283	9		
3	E	154	Total	C	N	O	S	0	0
			1259	815	201	235	8		

- Molecule 4 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	311	Total	C	N	O	S	0	0
			2553	1625	441	469	18		

- Molecule 5 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	120	Total	C	N	O	S	0	0
			982	635	166	171	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	567	ALA	PHE	engineered mutation	UNP Q04779

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

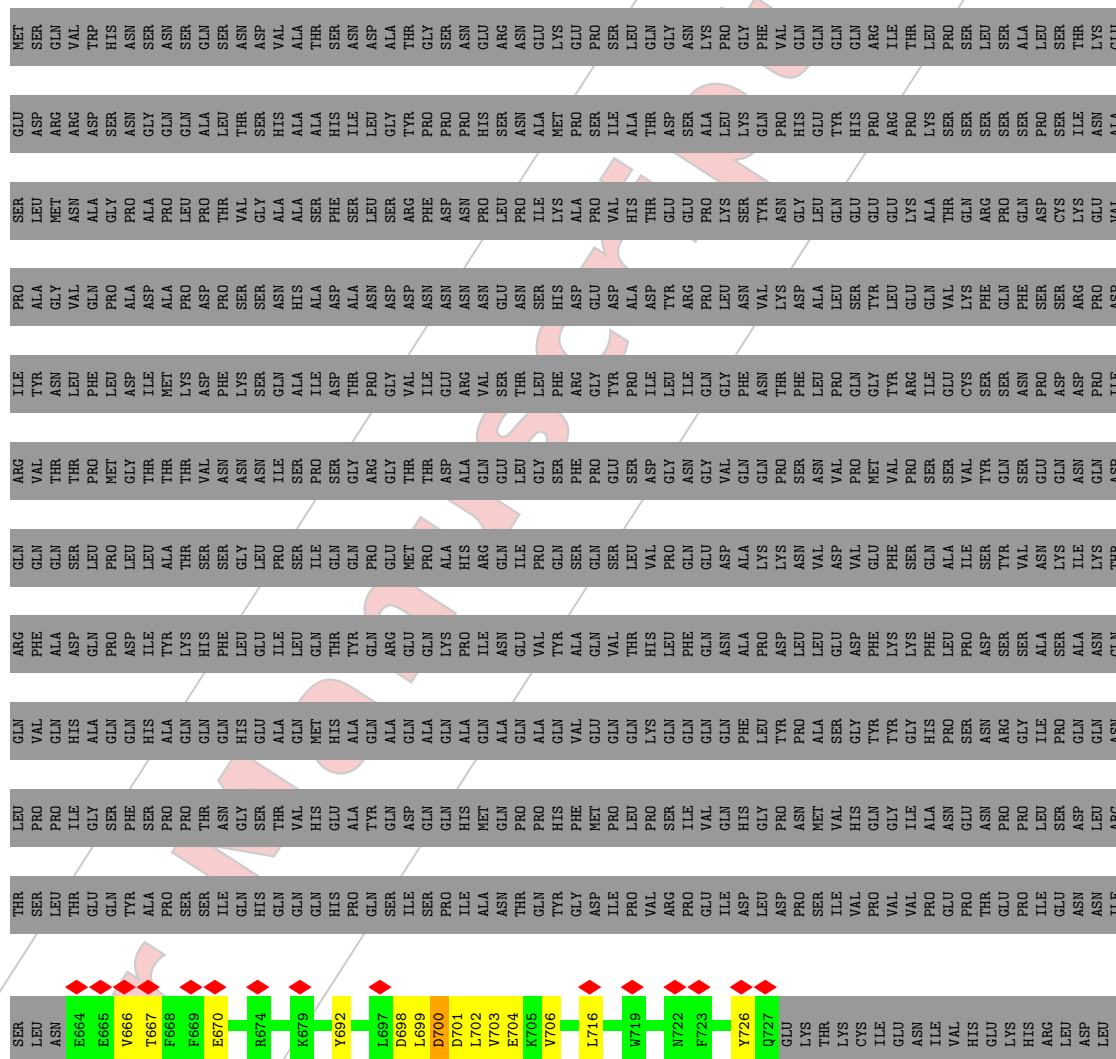
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total 1	Zn 1	0
6	D	4	Total 4	Zn 4	0
6	F	2	Total 2	Zn 2	0

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: Transcriptional regulatory protein SIN3

Chain A: 



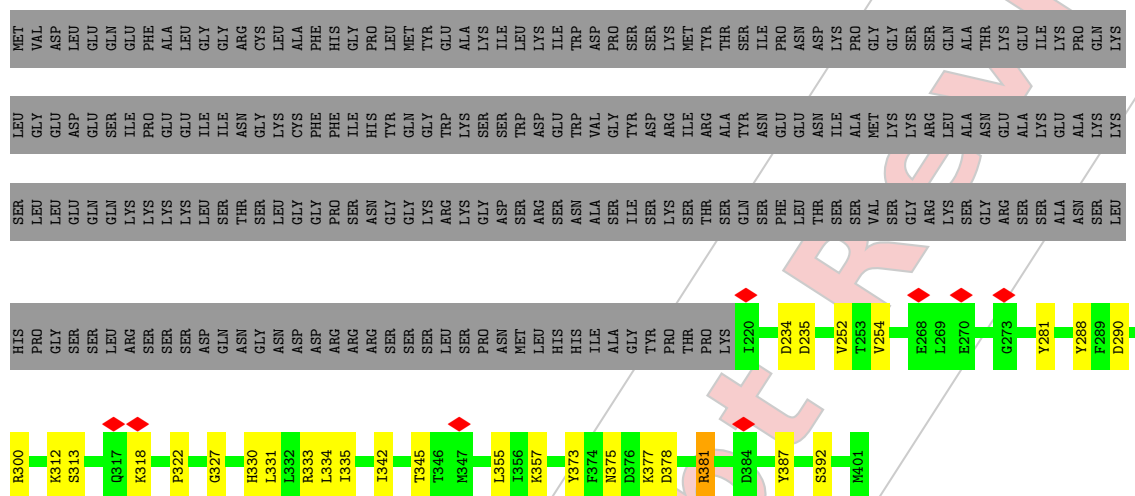


Frequency	Percentage
Often	70%
Sometimes	14%
Rarely	15%

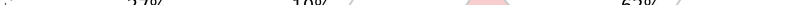


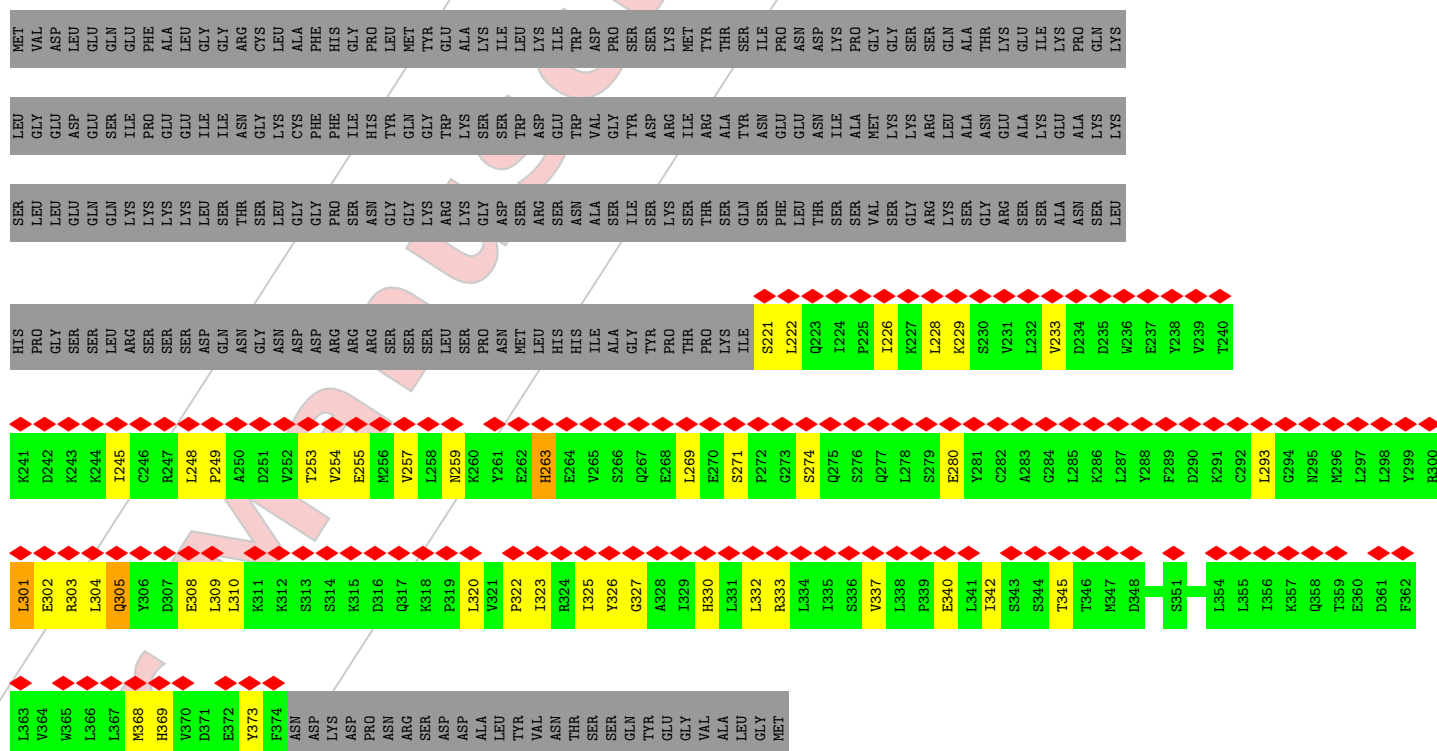
- Molecule 3: Chromatin modification-related protein EAF3

Chain C: 38% 7% 55%



- Molecule 3: Chromatin modification-related protein EAF3

Chain E: 



- Molecule 4: Transcriptional regulatory protein RCO1

Chain D:  35% 10% 55%

W301	H302	C303	N304	E305	C306	K307	F308	K309	I310	F311	I312	N313	N314	S315	M316	A317	T318	L319	K320	K321	I322	E323	Q329	N330	N331	N332	V333	K334	I335	F336	A337	K338	L339	L340	F341	N342	I343	D344	S345	H346	N347	F348	K349	Q350	F351	Q352	L353	P354	N355	Y356	I357	K358	GLU	THR	PHE	PRO	ALA	VAL
LYS	THR	GLY	SER	ARG	GLN	TYR	SER	GLU	ASN	ASP	LYS	PRO	LEU	THR	ASP	GLN	PHE	ASN	THR	THR	TYR	GLY	SER	ILE	LYS	LEU	ASP	SER	TYR	THR	THR	ASP	THR	ASN	SER	GLY	LYS	PHE	LEU	ILE	CYS	TYR	LYS	CYS	ASN	GLN	THR	ARG										
LEU	GLY	SER	TRP	HIS	PRO	GLU	ASN	ARG	LEU	ILE	MET	THR	CYS	ASP	TYR	GLN	THR	PRO	HIS	LEU	ASP	VAL	ARG	ALA	SER	PHE	LYS	ASN	LEU	GLY	LYS	TRP	THR	LYS	PRO	THR	LYS	VAL	ASN	TYR	LEU	ASP	LYS	ILE	HIS	CYS	GLN	GLU	ASP									
ASN	SER	VAL	ASN	TYR	LYS	VAL	TRP	GLN	LYS	LEU	ASN	LYS	ASN	GLN	LEU	TYR	GLU	PRO	LEU	GLN	ILE	GLY	TYR	GLN	ASN	GLY	ASN	ILE	GLN	ILE	PRO	THR	THR	ASN	TYR	ASP	PHE	ASN	GLN	PHE	LYS	THR	GLN	ILE	ASP	GLU												
N545	S546	I547	K548	Y549	D550	F551	F552	D553	K554	I555	Y556	K557	S558	K559	M560	V561	Q562	K563	R564	K565	L566	A567	GLN	PHE	GLN	GLU	SER	LEU	ILE	LYS	LEU	VAL	SER	ASN	GLY	ASN	SER	GLU	ASN	MET	VAL	LYS	ASP	ILE	ALA	SER	LEU	ILE	TYR	PHE	GLN	VAL	SER					
ASN	ASN	ASP	LYS	SER	ASN	LYS	ASN	ALA	SER	LYS	ASN	ASN	LEU	ARG	LYS	LEU	TRP	ASP	LYS	GLU	THR	VAL	VAL	VAL	VAL	PRO	ASN	GLU	LEU	LEU	ASP	SER	ASN	ASP	PHE	GLY	ASN	SER	SER	GLN	ASN	GLY	ILE	ASN	LYS	HIS	LEU	LEU	TYR	VAL	LYS	ASP	ILE	ILE	GLU	SER		
LYS	PRO	LYS	GLU	LEU	LEU	LYS	PHE	LEU	ASN	ILE	GLU	ASN	PRO	ASN	GLN	SER	GLU	ASN	GLY	ASN	GLN	SER	GLU																																			

4 Experimental information [i](#)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	670000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.26	0/4321	0.48	0/5814
2	B	0.27	0/2997	0.48	0/4051
3	C	0.25	0/1499	0.43	0/2028
3	E	0.26	0/1282	0.50	1/1733 (0.1%)
4	D	0.26	0/2614	0.47	0/3517
5	F	0.26	0/1007	0.44	0/1351
All	All	0.26	0/13720	0.47	1/18494 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	301	LEU	CA-CB-CG	5.51	127.98	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4233	0	4188	72	0
2	B	2923	0	2805	40	0
3	C	1473	0	1497	19	0
3	E	1259	0	1300	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2553	0	2507	57	0
5	F	982	0	976	23	0
6	B	1	0	0	0	0
6	D	4	0	0	0	0
6	F	2	0	0	0	0
All	All	13430	0	13273	217	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 8.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:GLN:HE21	1:A:1188:SER:HB2	1.26	0.96
4:D:259:ASN:N	4:D:259:ASN:HD22	1.70	0.89
2:B:140:ASP:OD1	2:B:140:ASP:N	2.19	0.76
1:A:985:PHE:HB3	1:A:1018:ILE:HD11	1.68	0.75
2:B:187:VAL:HG22	2:B:274:ASP:HB3	1.71	0.72
4:D:113:LEU:HD11	4:D:120:SER:HB2	1.71	0.72
4:D:510:GLN:NE2	4:D:513:GLY:O	2.22	0.72
3:E:248:LEU:HB3	3:E:249:PRO:HD2	1.72	0.71
2:B:123:SER:OG	2:B:165:ASP:OD1	2.11	0.69
3:C:313:SER:OG	3:C:318:LYS:O	2.11	0.69
2:B:213:GLU:HG2	4:D:460:LEU:HD12	1.73	0.69
3:C:234:ASP:OD1	4:D:496:ARG:NH1	2.26	0.68
5:F:357:ILE:HG23	3:E:229:LYS:HG2	1.76	0.68
1:A:921:GLN:NE2	1:A:1188:SER:HB2	2.07	0.65
2:B:84:ASP:OD2	2:B:88:ARG:NH1	2.30	0.65
1:A:982:LYS:HD2	1:A:1024:ILE:HG23	1.80	0.64
3:C:300:ARG:NH1	4:D:268:GLN:OE1	2.30	0.64
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.80	0.63
3:E:249:PRO:HB3	3:E:325:ILE:HA	1.79	0.63
1:A:701:ASP:HA	1:A:704:GLU:HG2	1.80	0.62
2:B:256:LYS:O	2:B:260:GLU:HG2	1.99	0.62
4:D:114:PRO:HD2	4:D:117:LYS:HG2	1.81	0.61
3:E:253:THR:HA	3:E:327:GLY:HA3	1.81	0.61
3:E:342:ILE:O	3:E:345:THR:OG1	2.17	0.61
3:C:252:VAL:HG11	3:C:373:TYR:HE1	1.65	0.61
2:B:128:MET:HB3	4:D:182:ARG:HD2	1.83	0.61
1:A:863:TYR:O	1:A:867:ILE:HG12	2.00	0.60
4:D:543:ASP:OD1	4:D:544:GLU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:GLU:N	2:B:342:GLU:OE1	2.33	0.59
4:D:259:ASN:N	4:D:259:ASN:ND2	2.44	0.59
5:F:290:PRO:HD2	3:E:310:LEU:HD12	1.84	0.59
5:F:319:LEU:HD22	5:F:320:LYS:H	1.68	0.59
3:C:235:ASP:OD2	3:C:333:ARG:NH2	2.35	0.58
2:B:189:HIS:H	2:B:216:PRO:HG2	1.67	0.58
3:C:375:ASN:HD22	3:C:377:LYS:HE2	1.69	0.58
4:D:437:ILE:HD11	4:D:446:PRO:HB2	1.86	0.58
2:B:118:GLU:CD	2:B:118:GLU:H	2.07	0.58
2:B:88:ARG:HH21	2:B:97:PHE:HE1	1.50	0.58
1:A:919:LEU:HB2	4:D:127:SER:HB3	1.86	0.57
2:B:365:THR:OG1	4:D:450:ASP:OD2	2.21	0.57
1:A:698:ASP:OD1	1:A:698:ASP:N	2.33	0.57
4:D:509:LEU:HD11	5:F:338:LYS:HE3	1.87	0.57
4:D:309:LYS:HA	4:D:313:ASN:HB2	1.86	0.57
1:A:786:PRO:HB3	2:B:216:PRO:O	2.05	0.56
3:C:375:ASN:ND2	3:C:377:LYS:HE2	2.20	0.56
1:A:975:LEU:HB2	1:A:1314:ILE:HB	1.86	0.56
2:B:244:ASP:OD2	2:B:287:SER:OG	2.22	0.56
3:C:342:ILE:HD11	3:C:355:LEU:HD23	1.89	0.55
4:D:542:ILE:O	4:D:546:SER:OG	2.19	0.55
2:B:50:SER:OG	2:B:342:GLU:OE1	2.25	0.55
4:D:372:TYR:OH	4:D:496:ARG:NH2	2.40	0.55
2:B:243:ASP:OD1	2:B:362:ASN:ND2	2.41	0.53
1:A:1300:MET:HG2	1:A:1301:PHE:N	2.23	0.53
5:F:282:PHE:HE1	5:F:347:ASN:HB3	1.74	0.53
4:D:511:LYS:HD3	5:F:334:LYS:HD3	1.91	0.53
2:B:90:THR:HG22	2:B:92:ASP:H	1.73	0.53
5:F:275:CYS:SG	5:F:276:ASP:N	2.82	0.53
1:A:945:THR:HG22	1:A:1146:ILE:HG13	1.92	0.52
5:F:273:LEU:N	5:F:282:PHE:O	2.42	0.52
1:A:826:ARG:HG3	1:A:826:ARG:HH11	1.74	0.52
1:A:1169:THR:O	1:A:1173:ASN:ND2	2.43	0.52
4:D:318:THR:O	4:D:322:ILE:HG13	2.10	0.52
1:A:1007:LYS:O	1:A:1011:LYS:HG3	2.10	0.52
3:E:228:LEU:HD13	3:E:332:LEU:HD11	1.91	0.52
1:A:876:GLY:O	1:A:880:ILE:HG13	2.10	0.51
1:A:1264:GLU:OE1	1:A:1293:HIS:ND1	2.43	0.51
2:B:177:HIS:HB3	2:B:265:SER:HB2	1.91	0.51
5:F:322:ILE:HD12	5:F:322:ILE:H	1.76	0.51
3:E:226:ILE:HA	3:E:229:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:283:HIS:HB2	4:D:286:CYS:HB2	1.92	0.51
4:D:296:LEU:HD12	4:D:297:PRO:HD2	1.93	0.51
1:A:785:HIS:CE1	3:C:392:SER:HB3	2.46	0.51
3:E:245:ILE:HD11	3:E:301:LEU:HD13	1.92	0.51
2:B:243:ASP:OD1	2:B:243:ASP:N	2.44	0.51
3:C:378:ASP:HB3	3:C:381:ARG:HG3	1.93	0.51
5:F:280:LYS:NZ	5:F:347:ASN:OD1	2.44	0.51
3:C:281:TYR:HA	4:D:335:ILE:HD11	1.93	0.51
1:A:768:SER:OG	2:B:80:ASP:OD2	2.25	0.50
1:A:896:LYS:HD2	1:A:897:ARG:N	2.26	0.50
2:B:133:ARG:HG2	4:D:181:ILE:HD11	1.93	0.50
3:E:305:GLN:O	3:E:308:GLU:HG3	2.12	0.50
3:C:342:ILE:O	3:C:345:THR:OG1	2.29	0.49
5:F:357:ILE:HD12	3:E:229:LYS:HG2	1.94	0.49
3:E:221:SER:OG	3:E:222:LEU:N	2.45	0.49
5:F:300:ASP:OD2	5:F:302:HIS:NE2	2.45	0.49
1:A:983:ASN:HA	1:A:986:TYR:CD1	2.47	0.49
1:A:893:VAL:HA	1:A:896:LYS:HE3	1.95	0.49
4:D:125:ARG:NH1	4:D:130:ASN:O	2.42	0.49
1:A:826:ARG:HG3	1:A:826:ARG:NH1	2.27	0.49
3:E:255:GLU:HG2	3:E:259:ASN:HD21	1.78	0.49
1:A:1305:PHE:CE2	1:A:1307:LYS:HG2	2.48	0.48
2:B:186:ASP:OD1	2:B:187:VAL:N	2.47	0.48
2:B:295:VAL:HG21	2:B:325:GLU:HG2	1.95	0.48
1:A:1278:THR:HB	1:A:1282:ASP:HB2	1.95	0.48
3:C:331:LEU:HD12	3:C:334:LEU:HD23	1.95	0.48
4:D:120:SER:O	4:D:123:ILE:N	2.47	0.48
4:D:351:PHE:O	4:D:352:GLN:NE2	2.41	0.48
4:D:278:CYS:SG	4:D:280:LYS:NZ	2.87	0.48
5:F:296:LEU:O	5:F:298:LYS:HD2	2.14	0.48
3:C:254:VAL:HG23	3:C:327:GLY:HA2	1.95	0.48
4:D:476:LYS:HG3	4:D:490:LYS:HB2	1.94	0.48
4:D:560:MET:HE2	4:D:560:MET:HB2	1.58	0.47
5:F:276:ASP:N	5:F:276:ASP:OD1	2.43	0.47
1:A:1206:GLN:OE1	1:A:1209:ARG:NH2	2.38	0.47
5:F:264:SER:O	5:F:264:SER:OG	2.20	0.47
4:D:542:ILE:HG13	4:D:546:SER:OG	2.14	0.47
2:B:32:TYR:CD1	2:B:115:GLY:HA3	2.50	0.47
1:A:700:ASP:OD1	1:A:700:ASP:N	2.48	0.47
1:A:702:LEU:O	1:A:706:VAL:HG23	2.15	0.47
1:A:831:LEU:O	1:A:835:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:SER:HB2	2:B:218:THR:HG22	1.97	0.46
4:D:553:ASP:OD1	3:E:271:SER:HB3	2.15	0.46
3:E:303:ARG:HE	3:E:303:ARG:HB3	1.59	0.46
3:C:357:LYS:HE3	3:C:357:LYS:HB3	1.67	0.46
4:D:378:LYS:HB3	4:D:463:LYS:HG3	1.97	0.46
5:F:305:GLU:H	5:F:347:ASN:HD21	1.63	0.46
4:D:121:GLU:HA	4:D:124:LYS:HG3	1.97	0.46
2:B:70:THR:O	2:B:74:MET:HG3	2.16	0.46
2:B:350:ASP:HB2	2:B:352:LYS:HD3	1.98	0.46
1:A:1000:THR:O	1:A:1000:THR:HG23	2.16	0.46
1:A:1202:ASP:HB3	1:A:1205:LYS:HE2	1.96	0.46
2:B:38:HIS:CE1	2:B:40:MET:HB3	2.51	0.45
3:E:255:GLU:O	3:E:259:ASN:ND2	2.49	0.45
3:E:263:HIS:ND1	3:E:263:HIS:C	2.69	0.45
1:A:1142:THR:O	1:A:1146:ILE:HG12	2.16	0.45
1:A:703:VAL:HG21	1:A:726:TYR:CD1	2.52	0.45
4:D:124:LYS:O	4:D:128:LEU:HB2	2.17	0.45
3:E:253:THR:O	3:E:257:VAL:HG23	2.17	0.45
3:E:254:VAL:HG23	3:E:327:GLY:HA2	1.98	0.45
4:D:511:LYS:NZ	3:E:280:GLU:OE1	2.50	0.45
1:A:900:GLN:O	1:A:904:GLU:HG2	2.17	0.45
4:D:335:ILE:HG13	4:D:336:PHE:CD1	2.51	0.45
3:E:326:TYR:HD2	3:E:330:HIS:CD2	2.35	0.45
1:A:868:ARG:HG3	1:A:868:ARG:HH11	1.81	0.45
1:A:1014:LEU:O	1:A:1018:ILE:HG22	2.16	0.45
1:A:1178:VAL:HB	1:A:1182:LYS:HB3	1.98	0.45
2:B:148:GLY:HA2	2:B:166:ILE:HD11	1.98	0.45
3:E:337:VAL:HG22	3:E:340:GLU:HB3	1.97	0.45
1:A:906:ARG:HG2	1:A:906:ARG:HH11	1.82	0.45
2:B:275:SER:HB2	2:B:286:LEU:HD12	1.99	0.45
5:F:322:ILE:HD12	5:F:322:ILE:N	2.32	0.45
4:D:264:SER:HB2	4:D:282:PHE:CE1	2.52	0.45
5:F:272:PHE:CD1	5:F:283:HIS:CE1	3.05	0.45
1:A:1015:LYS:HD3	1:A:1030:GLU:HG2	1.99	0.44
4:D:564:ARG:HA	4:D:564:ARG:HD3	1.77	0.44
1:A:936:LYS:O	1:A:937:GLN:HG3	2.17	0.44
1:A:1013:LEU:HD12	1:A:1257:MET:HG3	1.99	0.44
4:D:499:ASN:OD1	4:D:499:ASN:N	2.50	0.44
2:B:50:SER:O	2:B:54:ASN:ND2	2.47	0.44
3:E:229:LYS:O	3:E:233:VAL:HG23	2.18	0.44
3:C:290:ASP:HA	3:C:322:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:439:THR:HG23	4:D:439:THR:O	2.18	0.44
1:A:756:LYS:O	1:A:782:TRP:HA	2.18	0.44
1:A:1294:MET:HG2	1:A:1298:GLU:OE2	2.18	0.44
3:E:257:VAL:HG22	3:E:373:TYR:CE1	2.53	0.44
3:E:320:LEU:HD12	3:E:322:PRO:HD3	1.99	0.44
2:B:67:LYS:HD3	4:D:185:ILE:HD11	2.00	0.43
3:E:293:LEU:HD21	3:E:326:TYR:CD1	2.53	0.43
1:A:1156:GLU:HG3	1:A:1157:ARG:N	2.34	0.43
1:A:1243:ASP:OD1	1:A:1243:ASP:N	2.50	0.43
3:E:309:LEU:HD12	3:E:309:LEU:HA	1.85	0.43
2:B:340:TYR:HA	2:B:344:TYR:CD1	2.54	0.43
2:B:63:ILE:HG22	4:D:176:THR:HG22	2.00	0.43
3:C:330:HIS:HA	3:C:333:ARG:HG2	1.99	0.43
3:C:331:LEU:O	3:C:335:ILE:HG12	2.18	0.43
4:D:306:CYS:HA	4:D:309:LYS:HG2	2.00	0.43
1:A:1295:SER:OG	1:A:1296:ASN:N	2.50	0.43
4:D:168:LYS:HB2	4:D:170:PHE:CE1	2.54	0.43
1:A:666:VAL:HG23	1:A:667:THR:HG23	1.99	0.43
1:A:915:VAL:HA	4:D:128:LEU:HD11	2.01	0.42
1:A:1148:PHE:CZ	1:A:1312:VAL:HG11	2.54	0.42
4:D:338:LYS:HE2	4:D:338:LYS:HB2	1.88	0.42
4:D:369:ARG:NH1	4:D:369:ARG:HB2	2.35	0.42
1:A:1226:GLU:OE2	1:A:1230:GLN:NE2	2.36	0.42
2:B:216:PRO:C	2:B:218:THR:H	2.22	0.42
2:B:267:VAL:O	2:B:305:MET:HA	2.18	0.42
4:D:374:ASP:N	4:D:374:ASP:OD1	2.52	0.42
1:A:1150:HIS:O	1:A:1154:ILE:HG13	2.19	0.42
3:C:235:ASP:OD1	3:C:387:TYR:OH	2.30	0.42
1:A:699:LEU:O	1:A:703:VAL:HG23	2.19	0.42
2:B:244:ASP:OD1	2:B:244:ASP:N	2.53	0.42
5:F:285:LEU:HD23	5:F:285:LEU:H	1.83	0.42
5:F:349:LYS:HE3	5:F:349:LYS:HB2	1.78	0.42
4:D:320:LYS:HD3	4:D:320:LYS:HA	1.84	0.41
5:F:340:LEU:O	5:F:343:ILE:HG22	2.20	0.41
1:A:1268:LEU:HD11	1:A:1293:HIS:CD2	2.55	0.41
1:A:1169:THR:HG22	1:A:1173:ASN:ND2	2.36	0.41
1:A:763:THR:HG23	1:A:780:ASP:HB3	2.03	0.41
1:A:785:HIS:HA	1:A:786:PRO:HD2	1.86	0.41
1:A:716:LEU:HD23	1:A:716:LEU:HA	1.91	0.41
1:A:796:ILE:H	2:B:213:GLU:HB3	1.85	0.41
3:E:255:GLU:CG	3:E:259:ASN:HD21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:PHE:HD2	1:A:1250:VAL:HG21	1.86	0.41
4:D:322:ILE:HG12	4:D:341:PHE:CE1	2.56	0.41
1:A:912:TRP:HB3	1:A:916:TRP:CH2	2.56	0.41
2:B:141:VAL:HG22	2:B:305:MET:HG2	2.03	0.41
4:D:335:ILE:HG13	4:D:336:PHE:HD1	1.86	0.41
5:F:551:PHE:HE1	5:F:555:ILE:HD11	1.86	0.41
1:A:1196:LEU:HB3	1:A:1227:SER:HB3	2.03	0.41
1:A:952:ILE:HG12	1:A:1316:TYR:HB2	2.03	0.40
1:A:831:LEU:HD23	1:A:831:LEU:HA	1.90	0.40
1:A:907:ARG:O	1:A:911:GLU:HG2	2.21	0.40
1:A:912:TRP:HH2	4:D:123:ILE:HD12	1.86	0.40
5:F:308:PHE:HA	5:F:311:PHE:HB3	2.02	0.40
1:A:692:TYR:O	4:D:554:LYS:NZ	2.52	0.40
1:A:813:GLU:OE1	1:A:916:TRP:NE1	2.55	0.40
1:A:867:ILE:HD12	1:A:880:ILE:HG12	2.03	0.40
3:E:245:ILE:HG12	3:E:302:GLU:HG2	2.02	0.40
3:E:269:LEU:HD13	3:E:274:SER:HB2	2.03	0.40
1:A:880:ILE:HG22	1:A:884:HIS:CE1	2.57	0.40
2:B:211:TYR:CB	2:B:237:PRO:HB3	2.52	0.40
4:D:287:LEU:HD12	4:D:287:LEU:HA	1.98	0.40
4:D:304:ASN:OD1	4:D:304:ASN:N	2.53	0.40
4:D:416:ILE:O	4:D:446:PRO:HG2	2.21	0.40
1:A:1291:ARG:HD3	1:A:1321:ASP:OD2	2.21	0.40
4:D:130:ASN:OD1	4:D:130:ASN:N	2.54	0.40
3:E:255:GLU:N	3:E:323:ILE:HG22	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	491/1536 (32%)	472 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	366/433 (84%)	350 (96%)	16 (4%)	0	100	100
3	C	180/401 (45%)	171 (95%)	9 (5%)	0	100	100
3	E	152/401 (38%)	141 (93%)	11 (7%)	0	100	100
4	D	299/684 (44%)	272 (91%)	27 (9%)	0	100	100
5	F	116/684 (17%)	106 (91%)	10 (9%)	0	100	100
All	All	1604/4139 (39%)	1512 (94%)	92 (6%)	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	A	469/1391 (34%)	459 (98%)	10 (2%)	53	79
2	B	311/367 (85%)	299 (96%)	12 (4%)	32	67
3	C	171/359 (48%)	168 (98%)	3 (2%)	59	82
3	E	147/359 (41%)	141 (96%)	6 (4%)	30	66
4	D	294/653 (45%)	284 (97%)	10 (3%)	37	70
5	F	114/652 (18%)	111 (97%)	3 (3%)	46	76
All	All	1506/3781 (40%)	1462 (97%)	44 (3%)	45	74

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	670	GLU
1	A	700	ASP
1	A	764	PHE
1	A	770	ARG
1	A	818	ASP
1	A	885	GLU
1	A	896	LYS
1	A	902	ASP

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Mol	Chain	Res	Type
1	A	1186	LEU
1	A	1187	LEU
2	B	20	ARG
2	B	81	GLU
2	B	114	ASP
2	B	128	MET
2	B	140	ASP
2	B	153	LYS
2	B	156	GLU
2	B	214	PHE
2	B	257	LYS
2	B	270	GLN
2	B	350	ASP
2	B	373	MET
3	C	288	TYR
3	C	312	LYS
3	C	381	ARG
4	D	259	ASN
4	D	303	CYS
4	D	304	ASN
4	D	334	LYS
4	D	378	LYS
4	D	419	LYS
4	D	440	CYS
4	D	500	LYS
4	D	553	ASP
4	D	557	LYS
5	F	264	SER
5	F	316	MET
5	F	548	LYS
3	E	263	HIS
3	E	304	LEU
3	E	305	GLN
3	E	333	ARG
3	E	368	MET
3	E	369	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	921	GLN
4	D	510	GLN

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Mol	Chain	Res	Type
5	F	283	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33845. These allow visual inspection of the internal detail of the map and identification of artifacts.

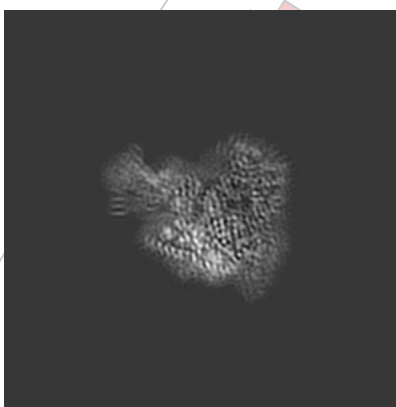
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

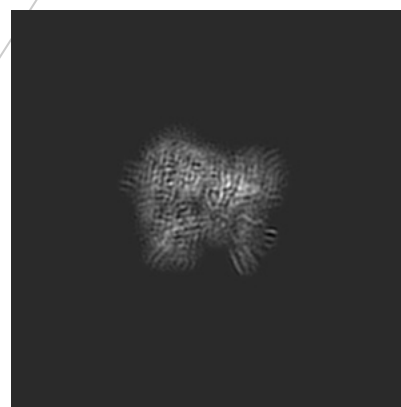
6.1.1 Primary map



X

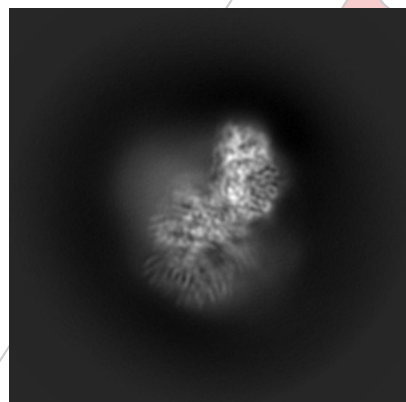


Y

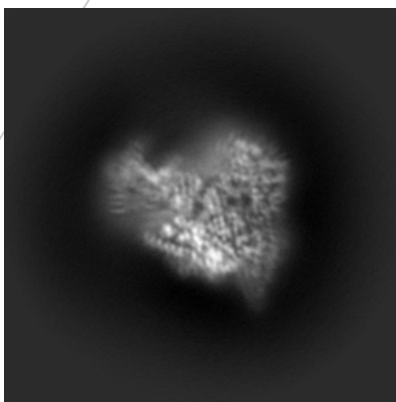


Z

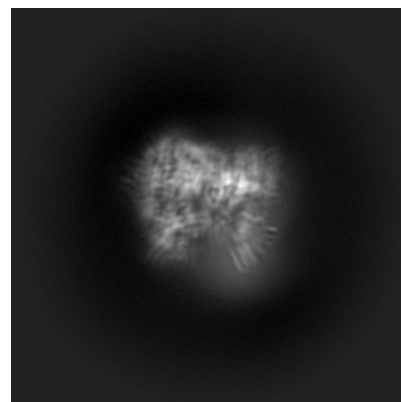
6.1.2 Raw map



X



Y

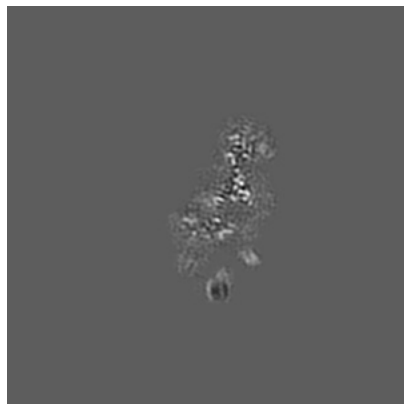


Z

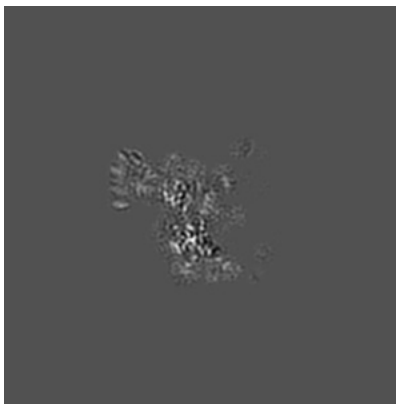
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

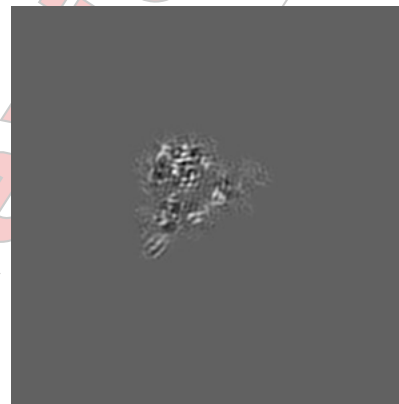
6.2.1 Primary map



X Index: 128

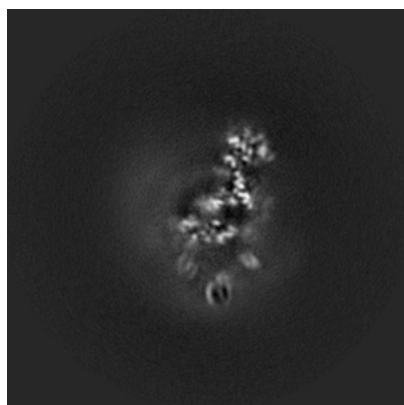


Y Index: 128

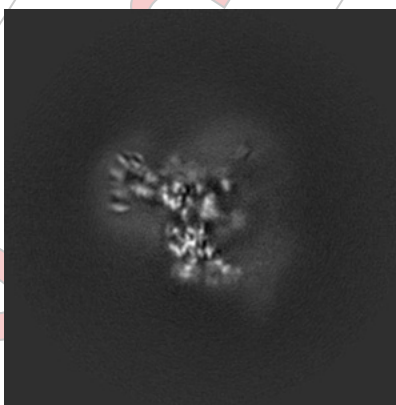


Z Index: 128

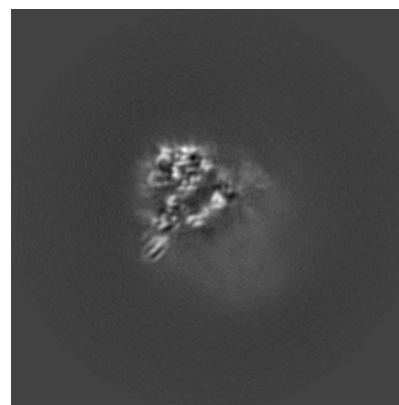
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

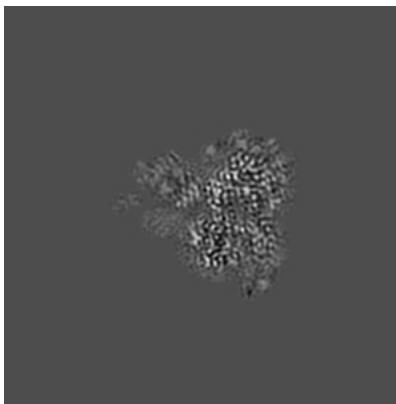
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map



X Index: 108

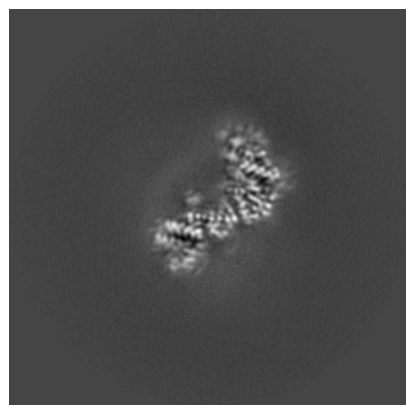


Y Index: 143

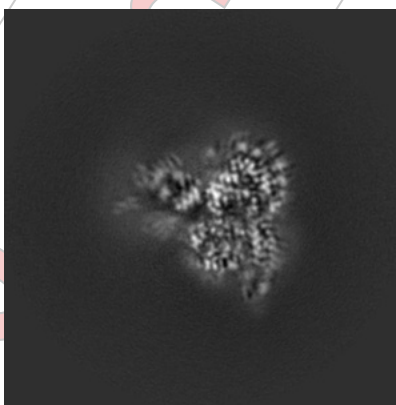


Z Index: 136

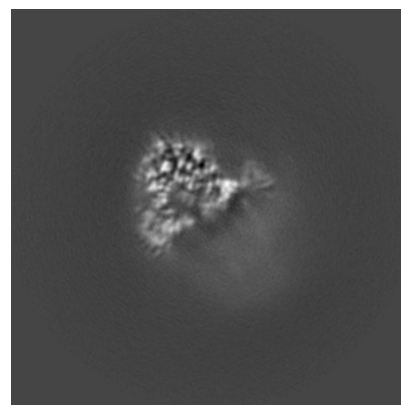
6.3.2 Raw map



X Index: 108



Y Index: 143



Z Index: 134

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

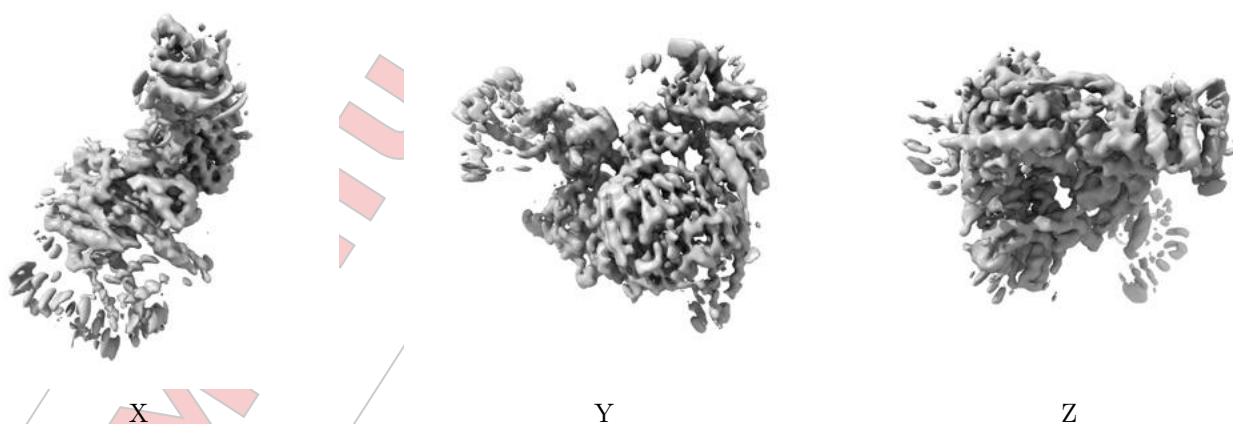
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

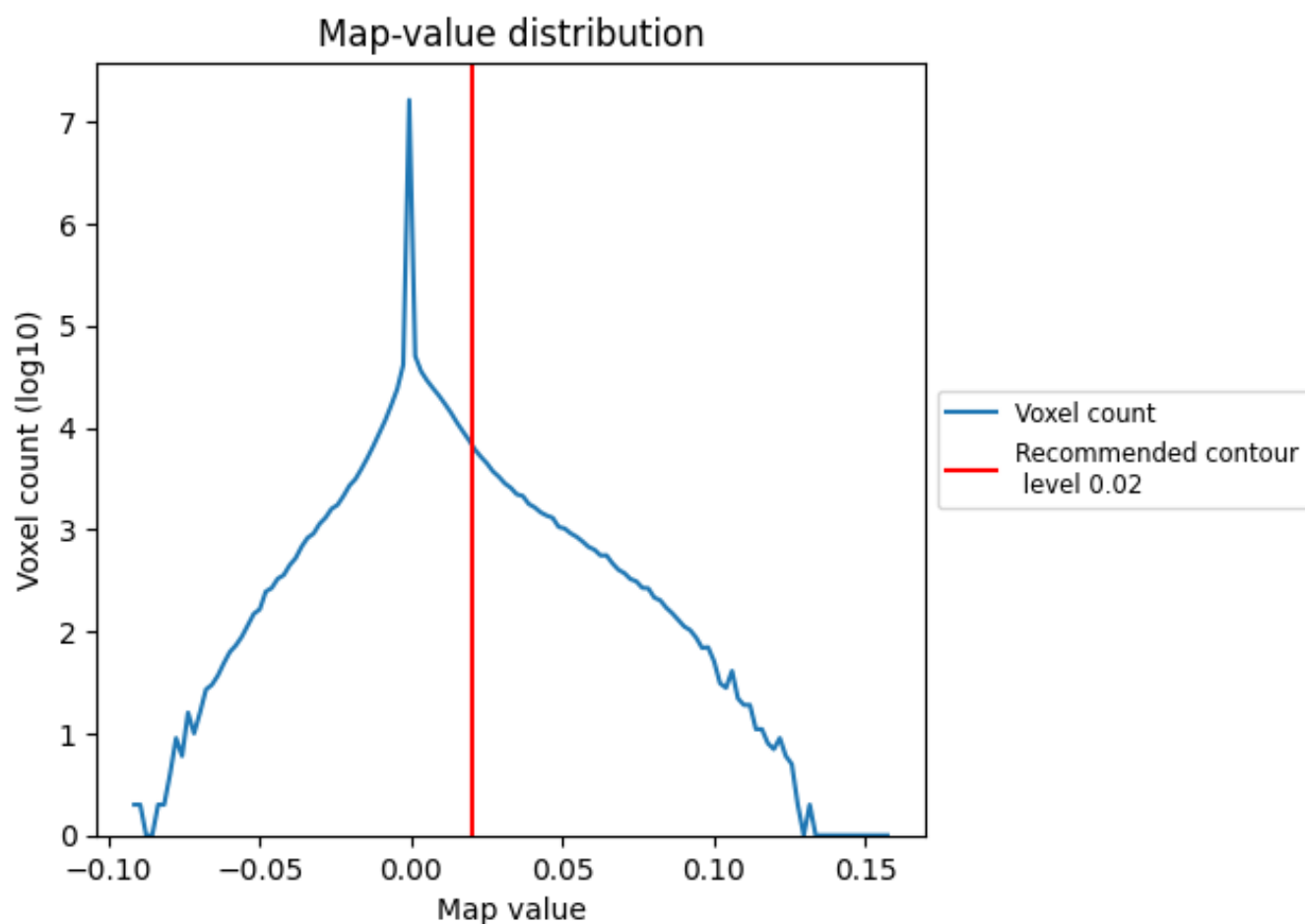
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

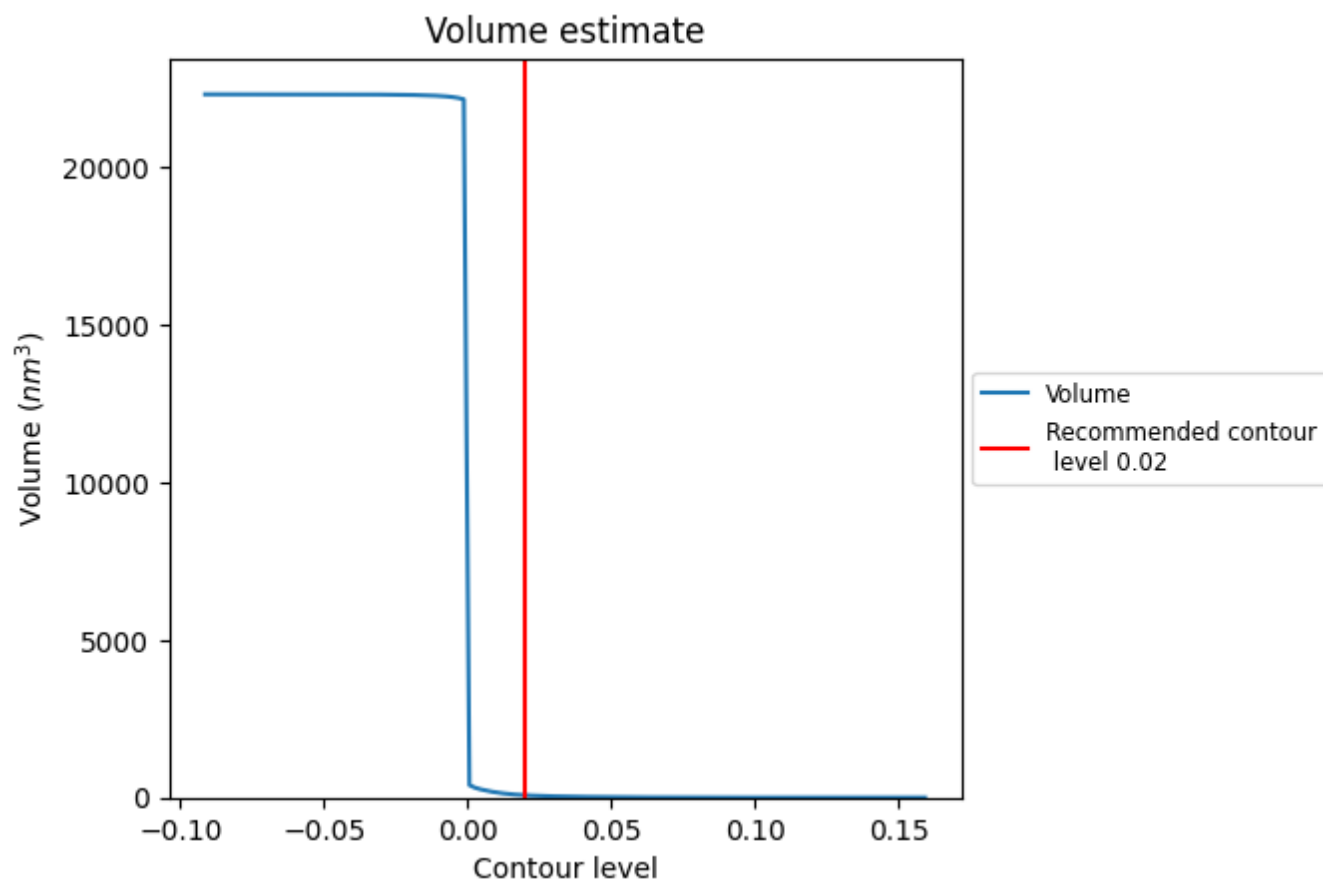
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

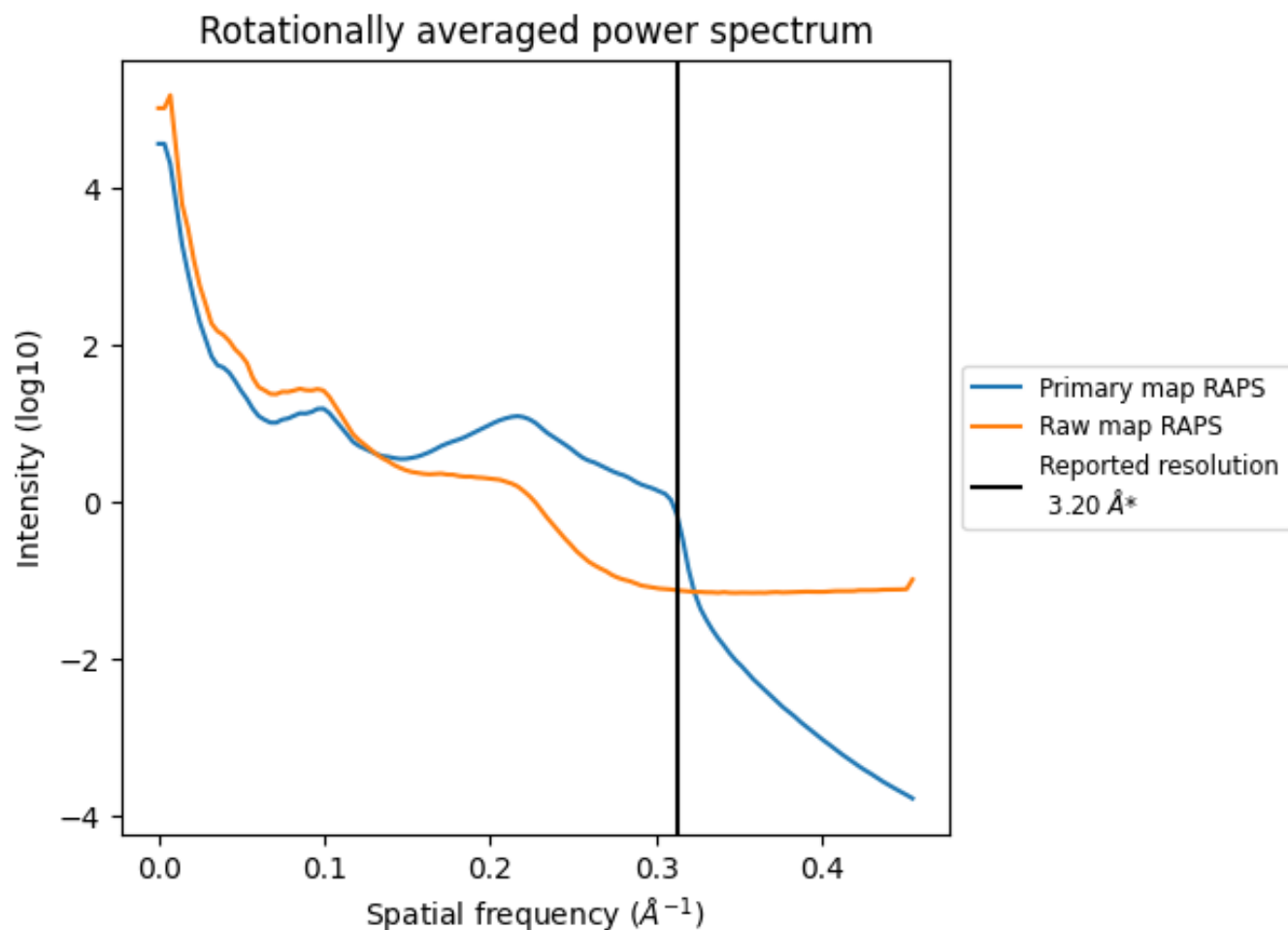
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm^3 ; this corresponds to an approximate mass of 66 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 ⓘ

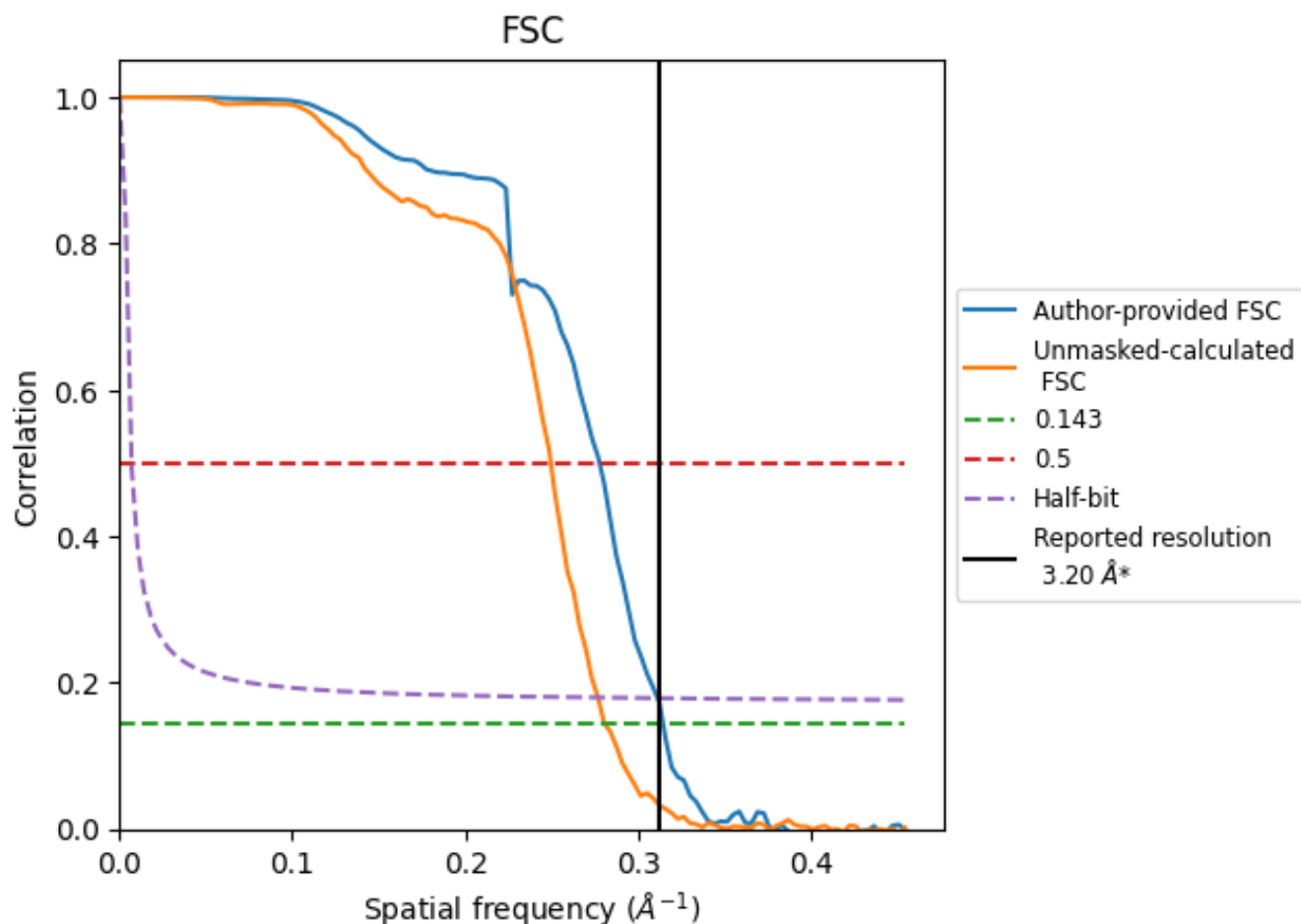


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 Å⁻¹

8.2 Resolution estimates ⓘ

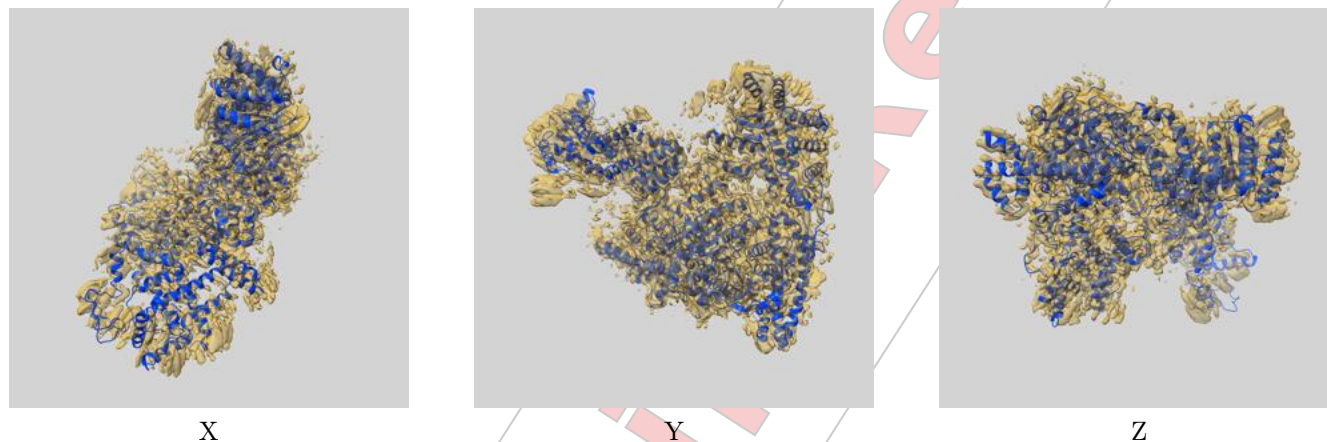
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.60	3.21
Unmasked-calculated*	3.56	4.00	3.61

*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 3.56 differs from the reported value 3.2 by more than 10 %

9 Map-model fit ⓘ

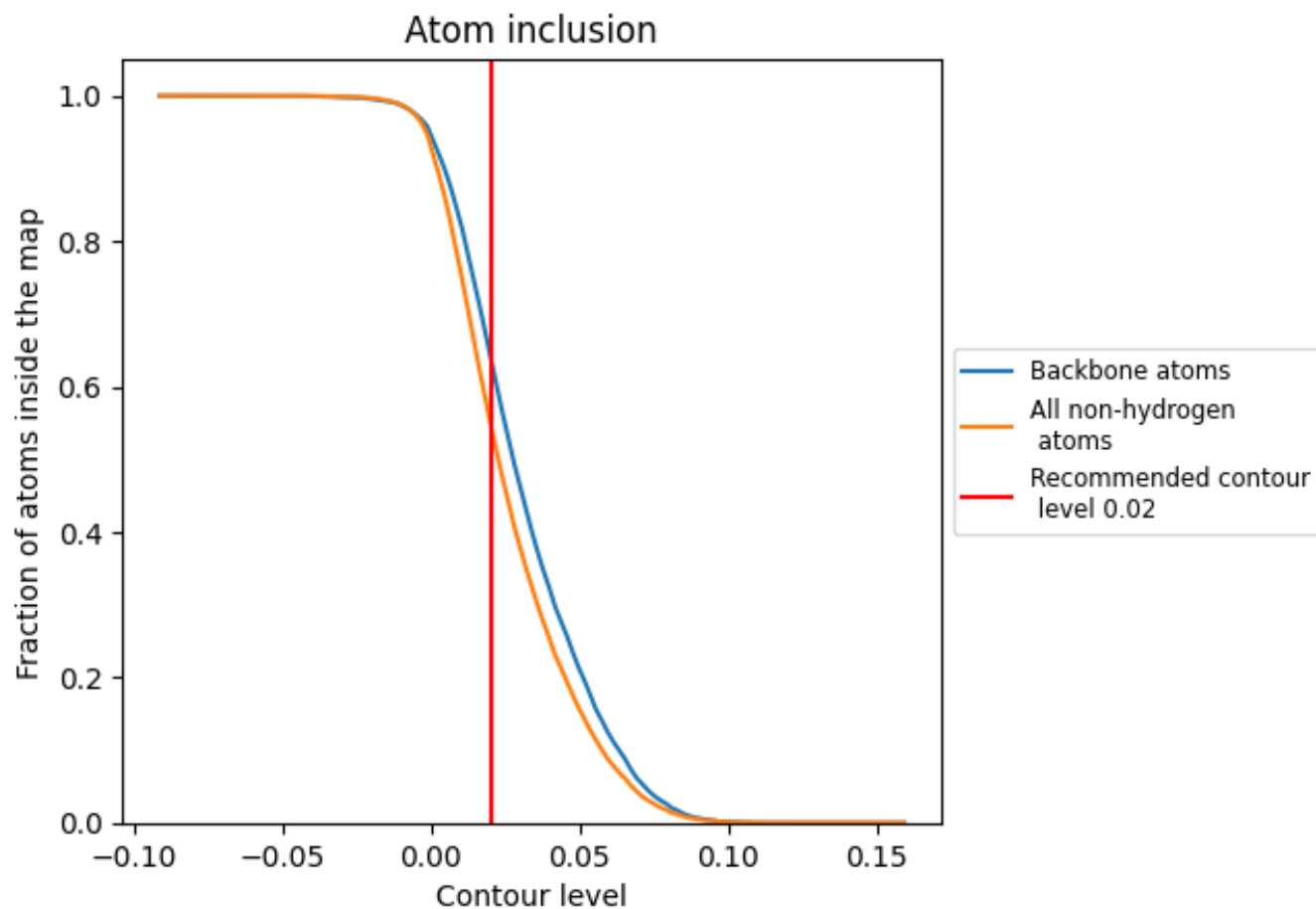
This section contains information regarding the fit between EMDB map EMD-33845 and PDB model 7YI0. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ



The images above show the 3D surface view of the map at the recommended contour level 0.02 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 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.