Full wwPDB EM Validation Report (i)

Mar 9, 2024 – 09:14 AM EST

PDB ID	:	6OCE
EMDB ID	:	EMD-20017
Title	:	Structure of the rice hyperosmolality-gated ion channel OSCA1.2
Authors	:	Maity, K.; Heumann, J.M.; McGrath, A.P.; Chang, G.; Stowell, M.H.
Deposited on	:	2019-03-23
Resolution	:	4.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

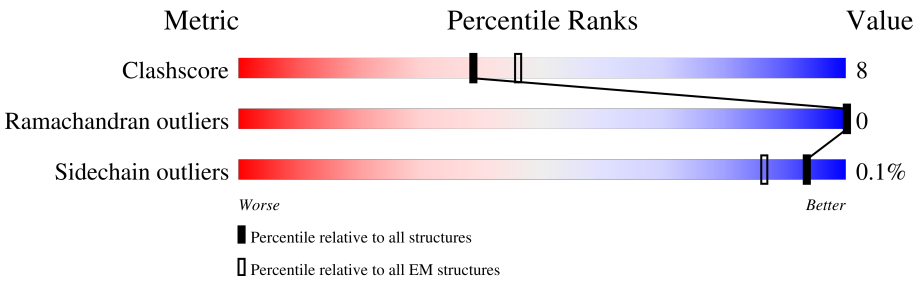
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.90 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 <=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	774	42% 77% 12% 11%
1	B	774	40% 76% 12% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11228 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 stress-gated cation channel 1.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	689	5614	3716	915	963	20	0	0
1	B	689	5614	3716	915	963	20	0	0

There are 16 discrepancies between the modelled and reference sequences:

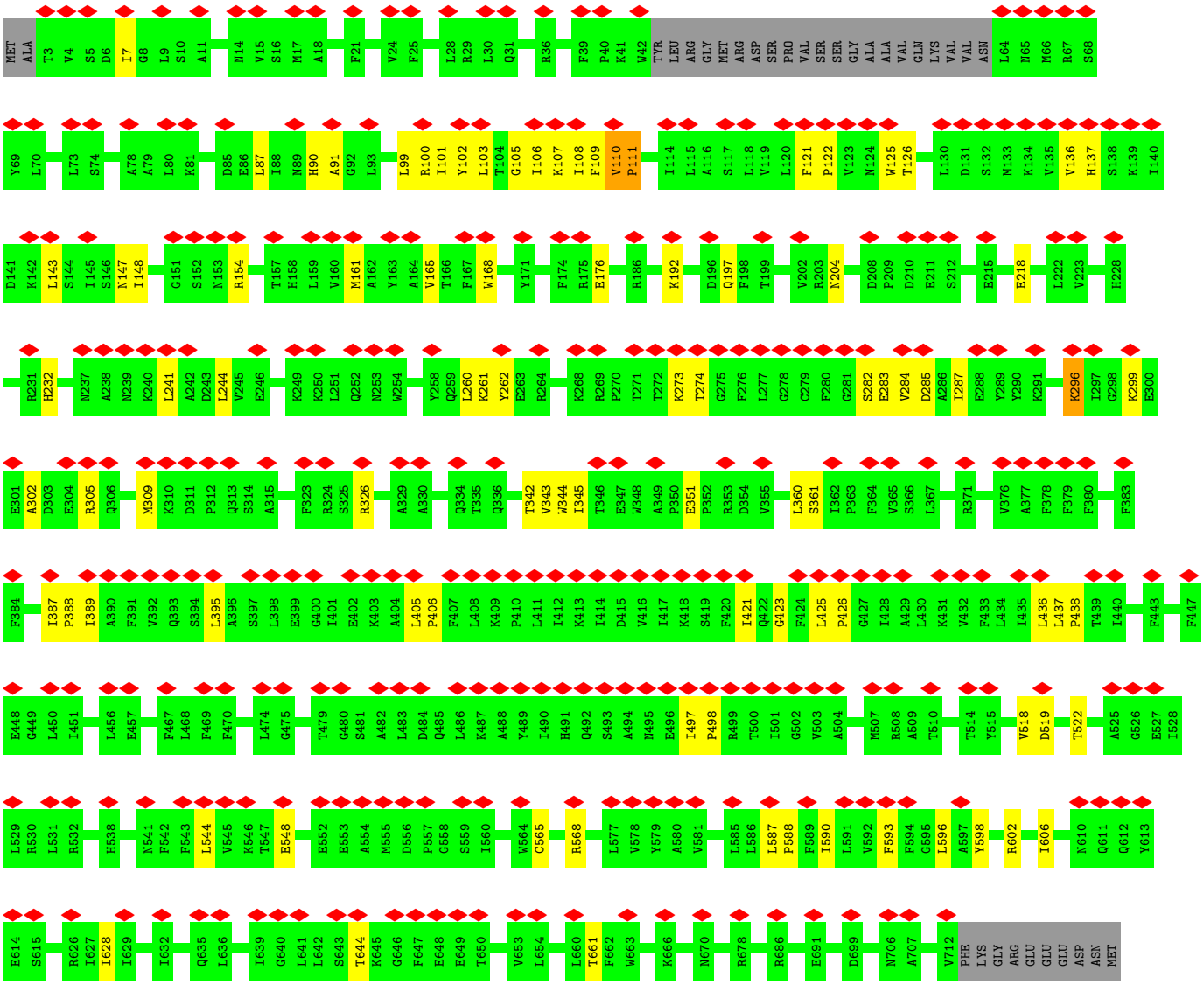
Chain	Residue	Modelled	Actual	Comment	Reference
A	767	ILE	-	expression tag	UNP Q5TKG1
A	768	LYS	-	expression tag	UNP Q5TKG1
A	769	PRO	-	expression tag	UNP Q5TKG1
A	770	GLN	-	expression tag	UNP Q5TKG1
A	771	LEU	-	expression tag	UNP Q5TKG1
A	772	GLU	-	expression tag	UNP Q5TKG1
A	773	GLY	-	expression tag	UNP Q5TKG1
A	774	SER	-	expression tag	UNP Q5TKG1
B	767	ILE	-	expression tag	UNP Q5TKG1
B	768	LYS	-	expression tag	UNP Q5TKG1
B	769	PRO	-	expression tag	UNP Q5TKG1
B	770	GLN	-	expression tag	UNP Q5TKG1
B	771	LEU	-	expression tag	UNP Q5TKG1
B	772	GLU	-	expression tag	UNP Q5TKG1
B	773	GLY	-	expression tag	UNP Q5TKG1
B	774	SER	-	expression tag	UNP Q5TKG1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: stress-gated cation channel 1.2

Chain A:



SER ILE SER GLU ASP VAL GLY MET GLU GLU GLU VAL ILE VAL PRO THR LYS ARG GLN SER ARG ARG ASN THR PRO ALA GLN SER LYS TYR GLU GLY SER ASP THR LEU SER LEU PRO GLU THR VAL HIS GLU ARG ILE LYS PRO GLN LEU GLU GLY SER
• Molecule 1: stress-gated cation channel 1.2
Chain B:
40%
76%
12%
11%
MET ALA T3 V4 S5 D6 I7 G8 L9 S10 A11 A12 I13 N14 V15 S16 M17 A18 F21 V24 F25 L28 R29 L30 Q31 D35 R36 F39 P40 K41 W42 TYR LEU ARG GLY MET ARG ASP SER PRO VAL SER SER GLY ALA ALA VAL GLN LYS VAL VAL ASN L64 N65 M66
R67 S68 Y69 L70 L73 S74 A78 A79 L80 K81 A91 G92 L93 I101 Y102 L103 T104 G105 I106 K107 I108 F109 V110 P111 I112 S113 I114 L115 A116 S117 L118 V119 L120 F121 P122 V123 N124 W125 T126 N127 D128 T129 L130 D131 S132 M133 K134 V135 V136 H137 S138 K139 I140 L143 S144
I145 S146 N147 I148 P149 Y150 G151 S152 N153 R154 T157 H158 L159 V160 M161 A162 Y163 A164 V165 T166 F167 W168 Y171 F174 R175 R186 K192 D196 Q197 N204 D208 P209 D210 E211 E215 L222 H228 R231 H232 Q233 N237 A238 N239 K240 L241 A242 D243
L244 V245 E246 K249 K250 L251 Q252 N253 W254 L255 D256 Y257 Y258 Q259 L260 K261 Y262 E263 R264 N265 P266 S267 K268 R269 P270 T271 T272 K273 T274 G275 F276 L277 G278 C279 F280 G281 S282 E283 V284 D285 A286 I287 E288 Y289 Y290 K291 I294 E295 K296 I297 G298 K299 E300 E301 E304 R305 Q306
M309 K310 D311 P312 Q313 S314 A315 R326 A329 A330 T342 V343 W344 I345 T346 E347 W348 A349 P350 E351 P352 R353 D354 V355 N358 I362 V365 S366 L367 R370 R371 V376 A377 F378 F379 F383 F384 I387 P388 I389 A390 F391 V392 Q393 S394 L395 A396 S397 L398
E399 G400 I401 E402 K403 A404 L405 P406 F407 L408 K409 P410 L411 I412 K413 I414 D415 V416 I417 K418 S419 F420 I421 F424 L425 P426 G427 I428 K431 V432 F433 L434 I435 L436 L437 P438 T439 I440 F443 F447 E448 G449 L450 I451 L456 E457 I466 F467 L468 F469 F470 F473 L474
G475 T479 G480 S481 A482 L483 D484 Q485 L486 K487 A488 Y489 I490 H491 Q492 S493 A494 N495 E496 I497 P498 R499 T500 I501 G502 V503 A504 M507 R508 A509 T510 Y515 V518 D519 T522 A525 G526 E527 I528 L529 R530 L531 R532 H538 N541 F542 F543 L544 V545 K546 T547 E548
E552 E553 A554 M555 D556 P557 G558 S559 I560 W564 R568 I569 Y572 L577 V578 Y579 A580 V581 L585 L586 L587 P588 F589 I590 L591 V592 F593 F594 Y598 R602 I605 Y609 N610 Q611 Q612 Y613 E614 S615 R626 I629 I632 Q635 L636 L637 L638 I639
G640 L641 L642 S643 T644 K645 G646 F647 E648 E649 T650 V653 L654 V655 V656 L657 P658 V659 L660 T661 F662 K666 N670 R678 E691 D699 L704 A707 Y708 V712 PHE LYS GLY ARG GLU GLU GLU ASP ASN MET SER ILE SER GLU ASP VAL GLY MET GLU GLU VAL
ILE VAL PRO THR LYS ARG GLN SER ARG ARG ASN THR PRO ALA GLN SER LYS TYR GLU GLY SER ASP THR LEU SER LEU PRO GLU THR VAL HIS GLU ARG ILE LYS PRO GLN LEU GLU GLY SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64096	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.30	1/5771 (0.0%)	0.44	4/7850 (0.1%)
1	B	0.30	1/5771 (0.0%)	0.44	2/7850 (0.0%)
All	All	0.30	2/11542 (0.0%)	0.44	6/15700 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	PRO	CB-CG	-6.80	1.16	1.50
1	B	111	PRO	CB-CG	-5.36	1.23	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	PRO	CA-N-CD	-9.79	97.80	111.50
1	B	111	PRO	CA-N-CD	-9.15	98.69	111.50
1	A	110	VAL	C-N-CD	5.72	140.41	128.40
1	A	285	ASP	N-CA-C	5.54	125.95	111.00
1	B	110	VAL	C-N-CD	5.47	139.88	128.40
1	A	296	LYS	N-CA-C	-5.20	96.97	111.00

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	5614	0	5718	78	0
1	B	5614	0	5718	101	0
All	All	11228	0	11436	179	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 (179) 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:107:LYS:O	1:A:110:VAL:HG22	1.06	1.23
1:B:107:LYS:O	1:B:110:VAL:CG2	1.87	1.21
1:A:107:LYS:O	1:A:110:VAL:CG2	1.93	1.17
1:B:107:LYS:O	1:B:110:VAL:HG22	0.94	1.11
1:B:395:LEU:HD11	1:B:426:PRO:HB3	1.42	0.97
1:A:110:VAL:HG23	1:A:111:PRO:HD3	1.49	0.94
1:B:106:ILE:O	1:B:110:VAL:HG13	1.71	0.91
1:A:110:VAL:HG23	1:A:111:PRO:CD	2.02	0.90
1:B:108:ILE:O	1:B:111:PRO:HD2	1.73	0.88
1:B:395:LEU:HD11	1:B:426:PRO:CB	2.06	0.85
1:B:110:VAL:HG23	1:B:111:PRO:HD3	1.59	0.84
1:B:110:VAL:HG23	1:B:111:PRO:CD	2.08	0.84
1:B:101:ILE:HG21	1:B:569:ILE:HD13	1.61	0.81
1:B:275:GLY:HA2	1:B:283:GLU:HA	1.63	0.79
1:B:108:ILE:O	1:B:111:PRO:CG	2.30	0.79
1:A:108:ILE:O	1:A:111:PRO:HD2	1.84	0.78
1:A:106:ILE:O	1:A:110:VAL:HG13	1.82	0.77
1:B:638:LEU:HD21	1:B:642:LEU:HD21	1.65	0.77
1:B:108:ILE:O	1:B:111:PRO:CD	2.33	0.76
1:A:108:ILE:O	1:A:111:PRO:CG	2.32	0.76
1:A:110:VAL:CG2	1:A:111:PRO:CD	2.63	0.76
1:B:275:GLY:CA	1:B:283:GLU:HA	2.17	0.73
1:A:262:TYR:HB2	1:A:287:ILE:HD13	1.68	0.73
1:B:110:VAL:CG2	1:B:111:PRO:CD	2.66	0.72
1:A:108:ILE:O	1:A:111:PRO:CD	2.40	0.69
1:B:241:LEU:HD22	1:B:309:MET:HG3	1.75	0.69
1:A:108:ILE:O	1:A:111:PRO:HG2	1.92	0.69
1:B:143:LEU:O	1:B:147:ASN:ND2	2.26	0.69
1:A:519:ASP:O	1:A:568:ARG:NH1	2.27	0.67
1:A:110:VAL:CG2	1:A:111:PRO:HD3	2.20	0.67
1:B:519:ASP:O	1:B:568:ARG:NH1	2.28	0.67
1:B:101:ILE:CG2	1:B:569:ILE:HD13	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:C	1:A:111:PRO:HD2	2.16	0.66
1:B:244:LEU:HD23	1:B:305:ARG:HD2	1.78	0.66
1:B:262:TYR:HB2	1:B:287:ILE:HD13	1.78	0.64
1:B:192:LYS:O	1:B:326:ARG:NH1	2.30	0.64
1:A:143:LEU:O	1:A:147:ASN:ND2	2.31	0.64
1:B:108:ILE:C	1:B:111:PRO:HD2	2.17	0.64
1:A:548:GLU:N	1:A:548:GLU:OE1	2.31	0.63
1:B:436:LEU:HD12	1:B:437:LEU:N	2.14	0.62
1:B:395:LEU:HD11	1:B:426:PRO:CG	2.29	0.62
1:A:296:LYS:O	1:A:299:LYS:N	2.33	0.62
1:B:102:TYR:HB3	1:B:598:TYR:HB2	1.82	0.62
1:A:192:LYS:O	1:A:326:ARG:NH1	2.33	0.61
1:A:241:LEU:HD22	1:A:309:MET:HG3	1.82	0.61
1:A:436:LEU:HD12	1:A:437:LEU:N	2.15	0.61
1:A:107:LYS:C	1:A:110:VAL:HG22	2.12	0.59
1:B:548:GLU:OE1	1:B:548:GLU:N	2.34	0.59
1:B:351:GLU:OE1	1:B:351:GLU:N	2.36	0.59
1:A:87:LEU:CD2	1:A:606:ILE:HD11	2.33	0.59
1:B:110:VAL:CG2	1:B:111:PRO:HD3	2.27	0.58
1:A:351:GLU:N	1:A:351:GLU:OE1	2.36	0.58
1:B:395:LEU:CD1	1:B:426:PRO:HB3	2.27	0.57
1:B:108:ILE:O	1:B:111:PRO:HG2	2.05	0.56
1:B:110:VAL:HG23	1:B:111:PRO:N	2.21	0.56
1:B:122:PRO:O	1:B:126:THR:OG1	2.24	0.55
1:A:260:LEU:HD12	1:A:261:LYS:N	2.21	0.55
1:B:497:ILE:HG23	1:B:498:PRO:CD	2.37	0.55
1:B:497:ILE:HG23	1:B:498:PRO:HD3	1.89	0.55
1:B:497:ILE:CG2	1:B:498:PRO:HD3	2.37	0.55
1:B:103:LEU:HD12	1:B:602:ARG:NH2	2.22	0.55
1:A:136:VAL:HG23	1:A:137:HIS:H	1.72	0.54
1:B:136:VAL:HG23	1:B:137:HIS:H	1.72	0.54
1:A:395:LEU:HD11	1:A:426:PRO:HB3	1.89	0.54
1:A:110:VAL:HG23	1:A:111:PRO:N	2.23	0.54
1:A:218:GLU:OE1	1:A:218:GLU:N	2.41	0.53
1:B:638:LEU:CD2	1:B:642:LEU:HD21	2.38	0.53
1:A:161:MET:O	1:A:165:VAL:HG23	2.09	0.53
1:B:265:ASN:HB3	1:B:266:PRO:HD3	1.89	0.53
1:B:393:GLN:NE2	1:B:479:THR:OG1	2.38	0.53
1:A:497:ILE:HB	1:A:498:PRO:HD3	1.91	0.53
1:A:122:PRO:O	1:A:126:THR:OG1	2.27	0.52
1:A:148:ILE:HD12	1:A:154:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ILE:HA	1:B:593:PHE:CE2	2.45	0.51
1:B:409:LYS:HE3	1:B:412:ILE:HD11	1.93	0.51
1:A:590:ILE:HA	1:A:593:PHE:CE2	2.45	0.51
1:A:241:LEU:HD12	1:A:244:LEU:HD21	1.93	0.50
1:A:244:LEU:CD2	1:A:305:ARG:HB2	2.42	0.50
1:B:260:LEU:HD22	1:B:543:PHE:CE2	2.47	0.50
1:A:100:ARG:HG3	1:A:176:GLU:OE2	2.12	0.50
1:B:161:MET:O	1:B:165:VAL:HG23	2.11	0.50
1:A:282:SER:OG	1:A:283:GLU:OE1	2.18	0.49
1:B:251:LEU:HD13	1:B:294:ILE:HG23	1.94	0.49
1:B:273:LYS:HD2	1:B:284:VAL:HG23	1.93	0.49
1:A:395:LEU:HD11	1:A:426:PRO:CG	2.43	0.49
1:A:218:GLU:OE2	1:A:232:HIS:ND1	2.46	0.48
1:B:294:ILE:HG22	1:B:294:ILE:O	2.13	0.48
1:B:342:THR:HG23	1:B:343:VAL:HG23	1.95	0.48
1:B:273:LYS:CD	1:B:284:VAL:HG23	2.44	0.48
1:B:425:LEU:N	1:B:426:PRO:HD2	2.29	0.48
1:B:262:TYR:HB2	1:B:287:ILE:HG21	1.95	0.48
1:A:395:LEU:HD12	1:A:395:LEU:C	2.35	0.48
1:B:395:LEU:C	1:B:395:LEU:HD12	2.34	0.48
1:B:121:PHE:O	1:B:125:TRP:N	2.47	0.48
1:B:109:PHE:HE2	1:B:590:ILE:HD12	1.79	0.47
1:B:256:ASP:O	1:B:260:LEU:HB3	2.14	0.47
1:A:7:ILE:HD13	1:A:421:ILE:HB	1.97	0.47
1:A:273:LYS:HB3	1:A:284:VAL:CG2	2.45	0.47
1:B:395:LEU:HD11	1:B:426:PRO:CD	2.44	0.47
1:A:204:ASN:O	1:A:343:VAL:HG13	2.15	0.47
1:B:659:VAL:HA	1:B:662:PHE:CE2	2.50	0.47
1:B:244:LEU:HD12	1:B:245:VAL:N	2.29	0.47
1:A:197:GLN:OE1	1:A:197:GLN:N	2.48	0.46
1:A:102:TYR:HB3	1:A:598:TYR:HB2	1.97	0.46
1:A:342:THR:HG23	1:A:343:VAL:HG23	1.97	0.45
1:B:103:LEU:HD12	1:B:602:ARG:HH22	1.81	0.45
1:A:598:TYR:OH	1:A:602:ARG:NH2	2.49	0.45
1:A:244:LEU:HD22	1:A:302:ALA:HA	1.99	0.45
1:B:204:ASN:O	1:B:343:VAL:HG13	2.17	0.45
1:B:260:LEU:C	1:B:260:LEU:HD12	2.36	0.45
1:B:251:LEU:O	1:B:255:LEU:N	2.46	0.45
1:B:387:ILE:N	1:B:388:PRO:CD	2.80	0.45
1:B:109:PHE:O	1:B:112:ILE:HB	2.17	0.45
1:B:166:THR:HG21	1:B:657:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:HD11	1:A:426:PRO:CB	2.46	0.45
1:B:239:ASN:ND2	1:B:358:ASN:O	2.48	0.44
1:B:244:LEU:HD21	1:B:305:ARG:HB2	1.99	0.44
1:B:393:GLN:HE22	1:B:479:THR:CB	2.29	0.44
1:A:102:TYR:OH	1:A:565:CYS:SG	2.74	0.44
1:A:387:ILE:N	1:A:388:PRO:CD	2.80	0.44
1:A:360:LEU:O	1:A:361:SER:OG	2.32	0.44
1:A:109:PHE:HE2	1:A:590:ILE:HD12	1.81	0.44
1:B:103:LEU:HB2	1:B:598:TYR:CE1	2.52	0.43
1:B:110:VAL:HG22	1:B:111:PRO:CD	2.47	0.43
1:B:233:GLN:NE2	1:B:708:TYR:O	2.49	0.43
1:A:103:LEU:O	1:A:107:LYS:HG2	2.18	0.43
1:B:251:LEU:HD22	1:B:294:ILE:CD1	2.48	0.43
1:A:343:VAL:HG12	1:A:344:TRP:CD1	2.54	0.43
1:B:655:VAL:O	1:B:659:VAL:HG23	2.18	0.43
1:A:148:ILE:HD12	1:A:154:ARG:HH12	1.83	0.43
1:B:197:GLN:OE1	1:B:197:GLN:N	2.48	0.43
1:B:265:ASN:N	1:B:266:PRO:CD	2.82	0.43
1:A:518:VAL:O	1:A:522:THR:OG1	2.36	0.43
1:A:405:LEU:HB3	1:A:406:PRO:HD3	2.02	0.42
1:B:107:LYS:O	1:B:111:PRO:HD2	2.19	0.42
1:B:593:PHE:CD1	1:B:594:PHE:N	2.87	0.42
1:A:274:THR:O	1:A:283:GLU:HB2	2.19	0.42
1:B:251:LEU:HD22	1:B:294:ILE:HD12	2.01	0.42
1:B:102:TYR:CB	1:B:598:TYR:HB2	2.49	0.42
1:B:275:GLY:HA2	1:B:283:GLU:CA	2.41	0.42
1:A:110:VAL:HG22	1:A:111:PRO:CD	2.47	0.42
1:B:437:LEU:N	1:B:438:PRO:CD	2.82	0.42
1:B:587:LEU:N	1:B:588:PRO:CD	2.83	0.42
1:A:437:LEU:N	1:A:438:PRO:CD	2.82	0.42
1:B:343:VAL:HG12	1:B:344:TRP:CD1	2.54	0.42
1:A:593:PHE:O	1:A:596:LEU:HG	2.20	0.42
1:A:395:LEU:HD11	1:A:426:PRO:CD	2.49	0.42
1:A:587:LEU:N	1:A:588:PRO:CD	2.83	0.42
1:B:121:PHE:HB2	1:B:122:PRO:HD3	2.02	0.42
1:B:402:GLU:OE1	1:B:414:ILE:HD13	2.20	0.42
1:A:105:GLY:O	1:A:108:ILE:HG12	2.20	0.41
1:A:204:ASN:ND2	1:A:345:ILE:HD12	2.35	0.41
1:A:389:ILE:HD12	1:A:389:ILE:N	2.35	0.41
1:B:297:ILE:O	1:B:297:ILE:HG22	2.19	0.41
1:A:425:LEU:N	1:A:426:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PRO:HB3	1:A:168:TRP:CD1	2.55	0.41
1:A:136:VAL:HG23	1:A:137:HIS:N	2.36	0.41
1:B:644:THR:HG22	1:B:644:THR:O	2.20	0.41
1:B:7:ILE:HD13	1:B:421:ILE:HB	2.02	0.41
1:A:628:ILE:HD11	1:A:661:THR:CG2	2.50	0.41
1:A:644:THR:O	1:A:644:THR:HG22	2.20	0.41
1:B:204:ASN:ND2	1:B:345:ILE:HD12	2.35	0.41
1:B:605:ILE:HD13	1:B:609:TYR:CD2	2.56	0.41
1:A:99:LEU:C	1:A:101:ILE:H	2.24	0.41
1:B:389:ILE:HD12	1:B:389:ILE:N	2.35	0.41
1:B:425:LEU:N	1:B:426:PRO:CD	2.84	0.41
1:A:121:PHE:O	1:A:125:TRP:N	2.53	0.41
1:A:423:GLY:O	1:A:426:PRO:HD2	2.21	0.41
1:B:105:GLY:O	1:B:108:ILE:HG12	2.21	0.41
1:B:244:LEU:HD12	1:B:244:LEU:C	2.41	0.41
1:A:90:HIS:CG	1:A:91:ALA:H	2.39	0.40
1:B:103:LEU:C	1:B:103:LEU:HD23	2.41	0.40
1:B:421:ILE:HD12	1:B:421:ILE:C	2.42	0.40
1:B:581:VAL:HG11	1:B:638:LEU:HD11	2.03	0.40
1:A:425:LEU:N	1:A:426:PRO:HD2	2.36	0.40
1:A:544:LEU:N	1:A:544:LEU:HD12	2.36	0.40
1:B:106:ILE:HG12	1:B:591:LEU:HD11	2.02	0.40
1:B:518:VAL:O	1:B:522:THR:OG1	2.38	0.40
1:B:545:VAL:HG13	1:B:548:GLU:HB2	2.04	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	685/774 (88%)	620 (90%)	65 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	685/774 (88%)	615 (90%)	70 (10%)	0	100	100
All	All	1370/1548 (88%)	1235 (90%)	135 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	612/688 (89%)	612 (100%)	0	100	100
1	B	612/688 (89%)	611 (100%)	1 (0%)	93	96
All	All	1224/1376 (89%)	1223 (100%)	1 (0%)	93	96

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

Mol	Chain	Res	Type
1	B	662	PHE

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

Mol	Chain	Res	Type
1	B	336	GLN

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)

There are no ligands in this entry.

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.

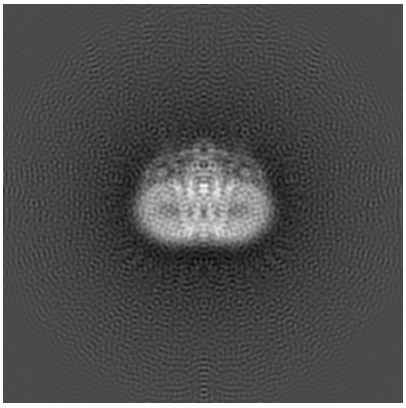
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20017. These allow visual inspection of the internal detail of the map and identification of artifacts.

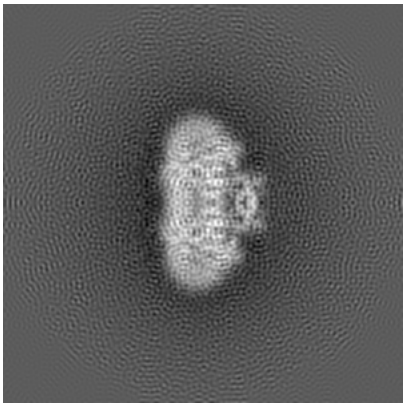
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

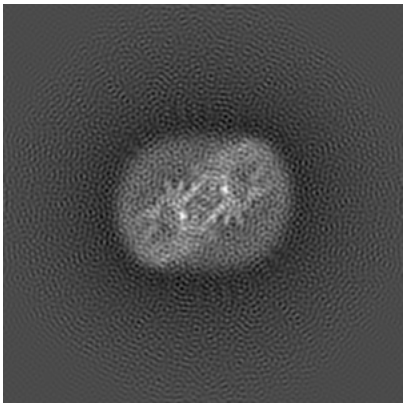
6.1.1 Primary map



X



Y

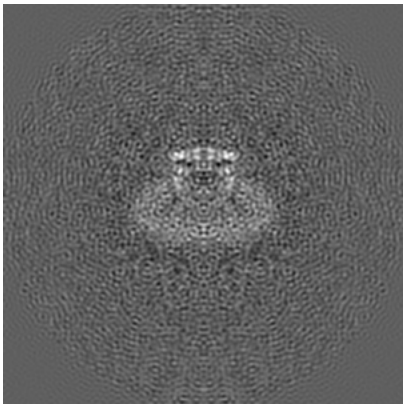


Z

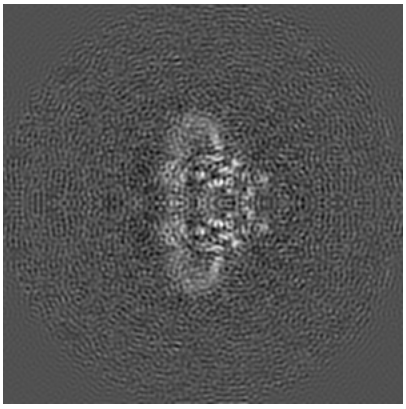
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

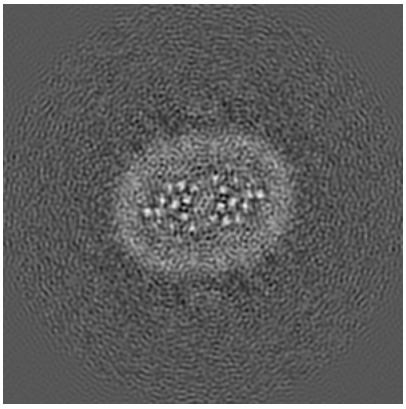
6.2.1 Primary map



X Index: 120



Y Index: 120

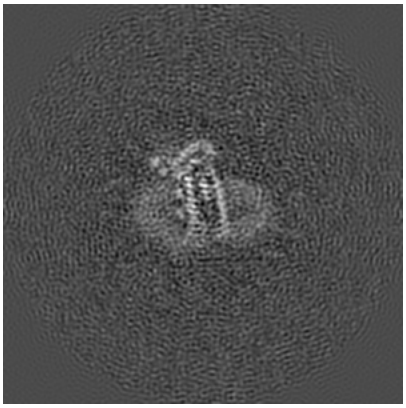


Z Index: 120

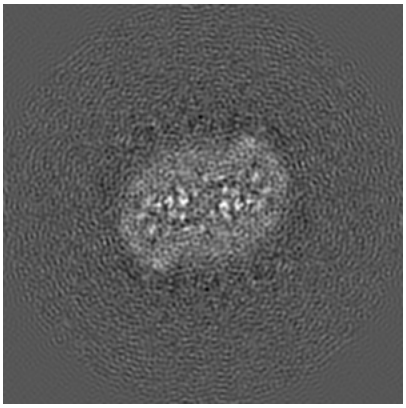
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 107

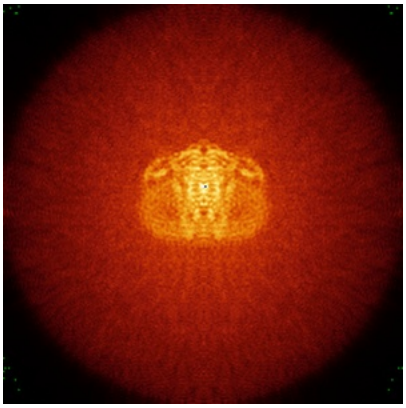
Y Index: 127

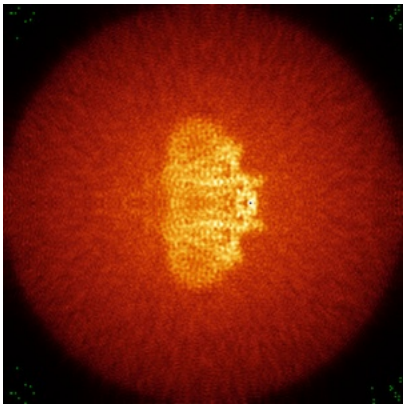

Z Index: 130

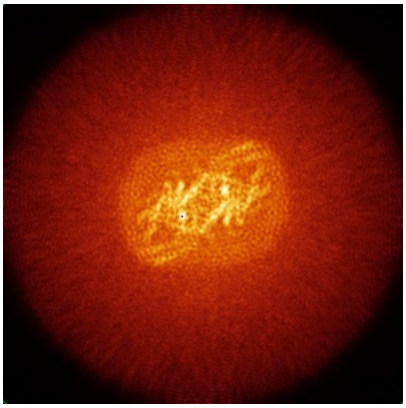
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

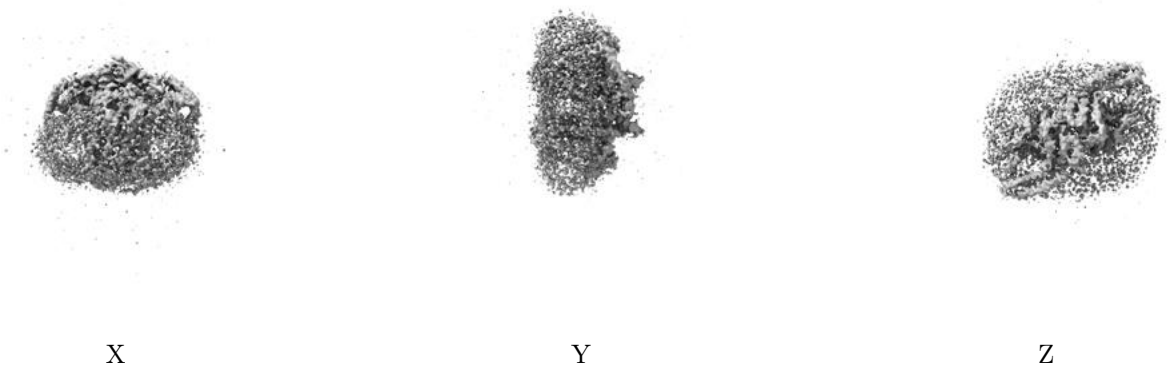

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

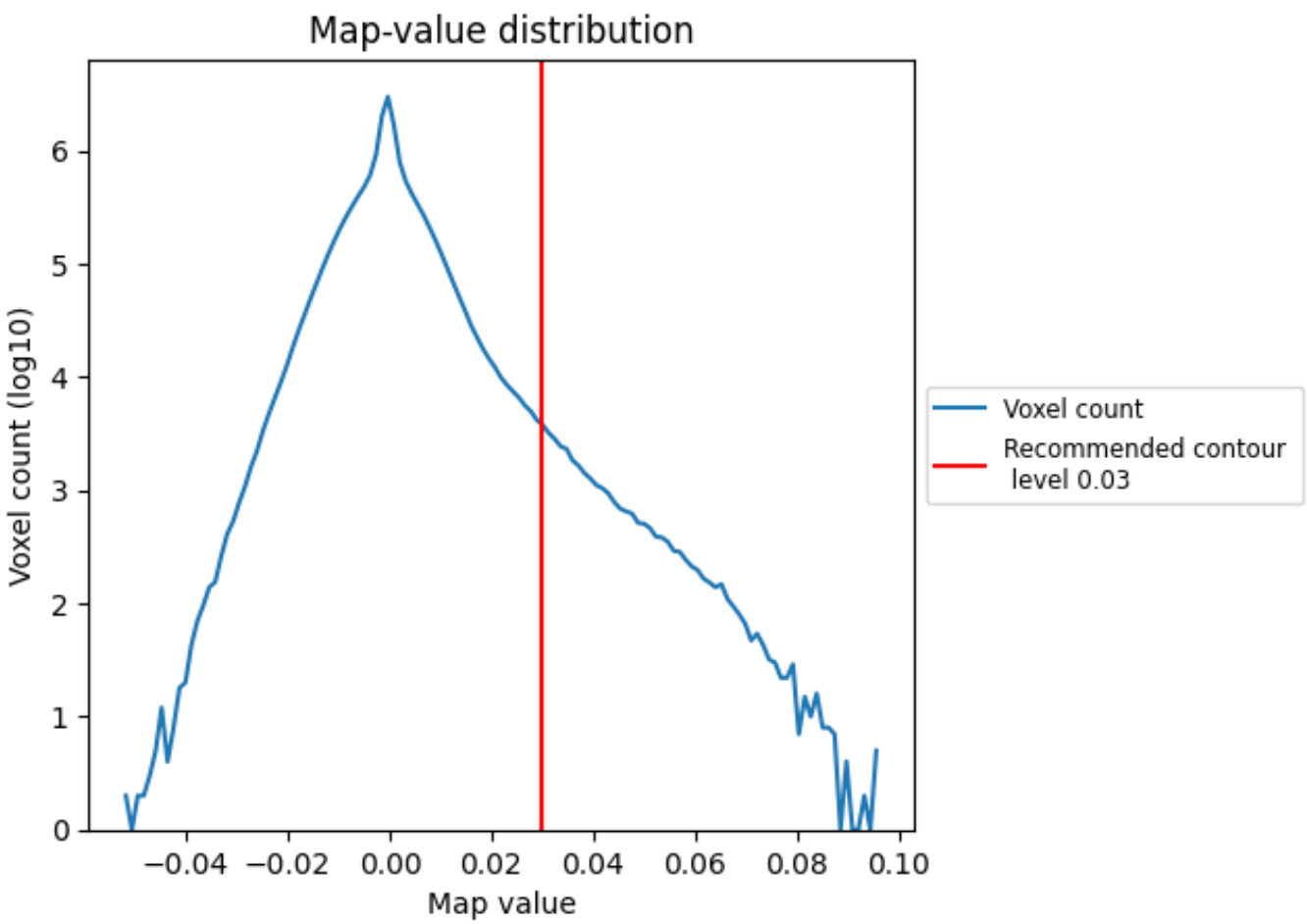
6.6 Mask visualisation (i)

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

7 Map analysis (i)

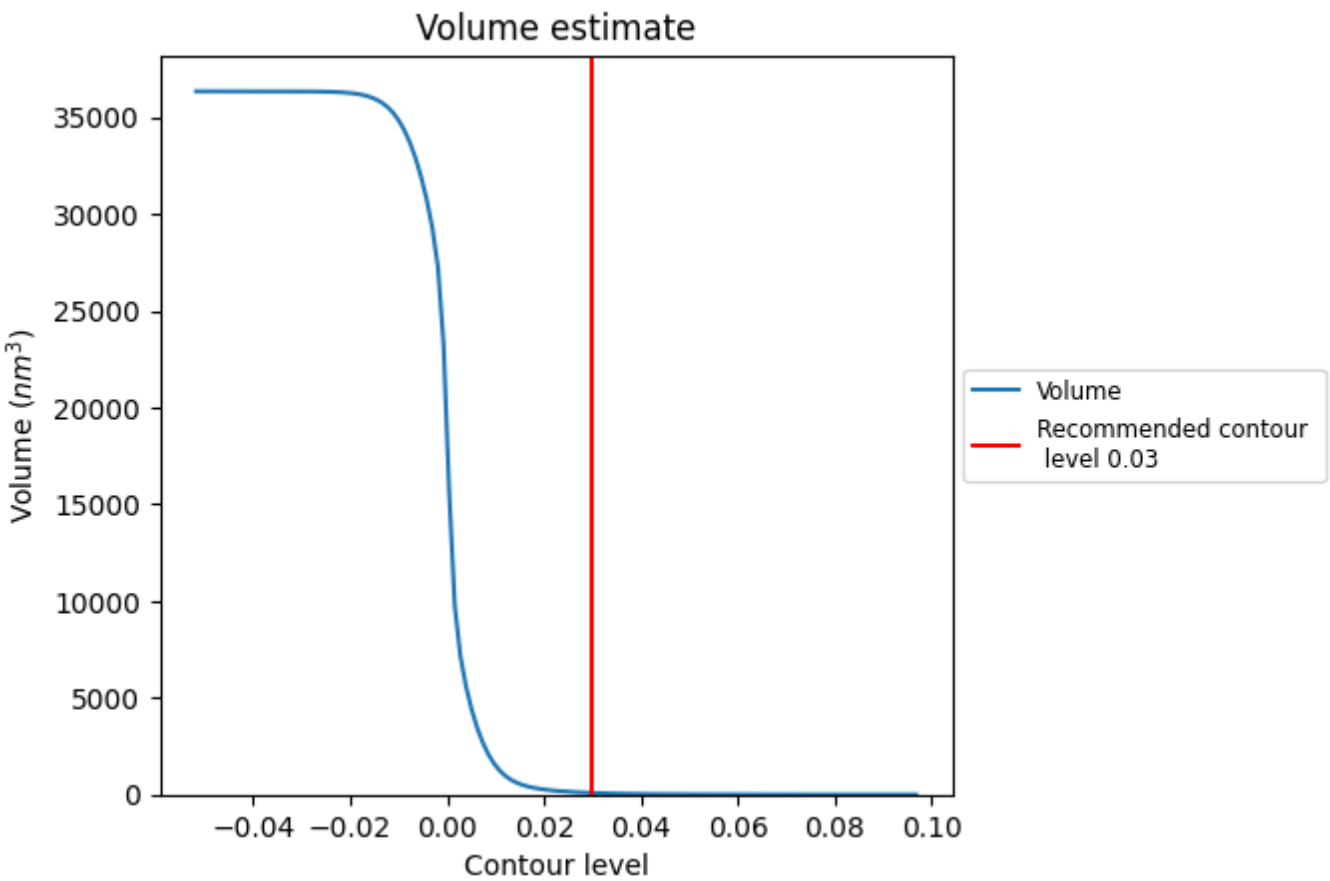
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

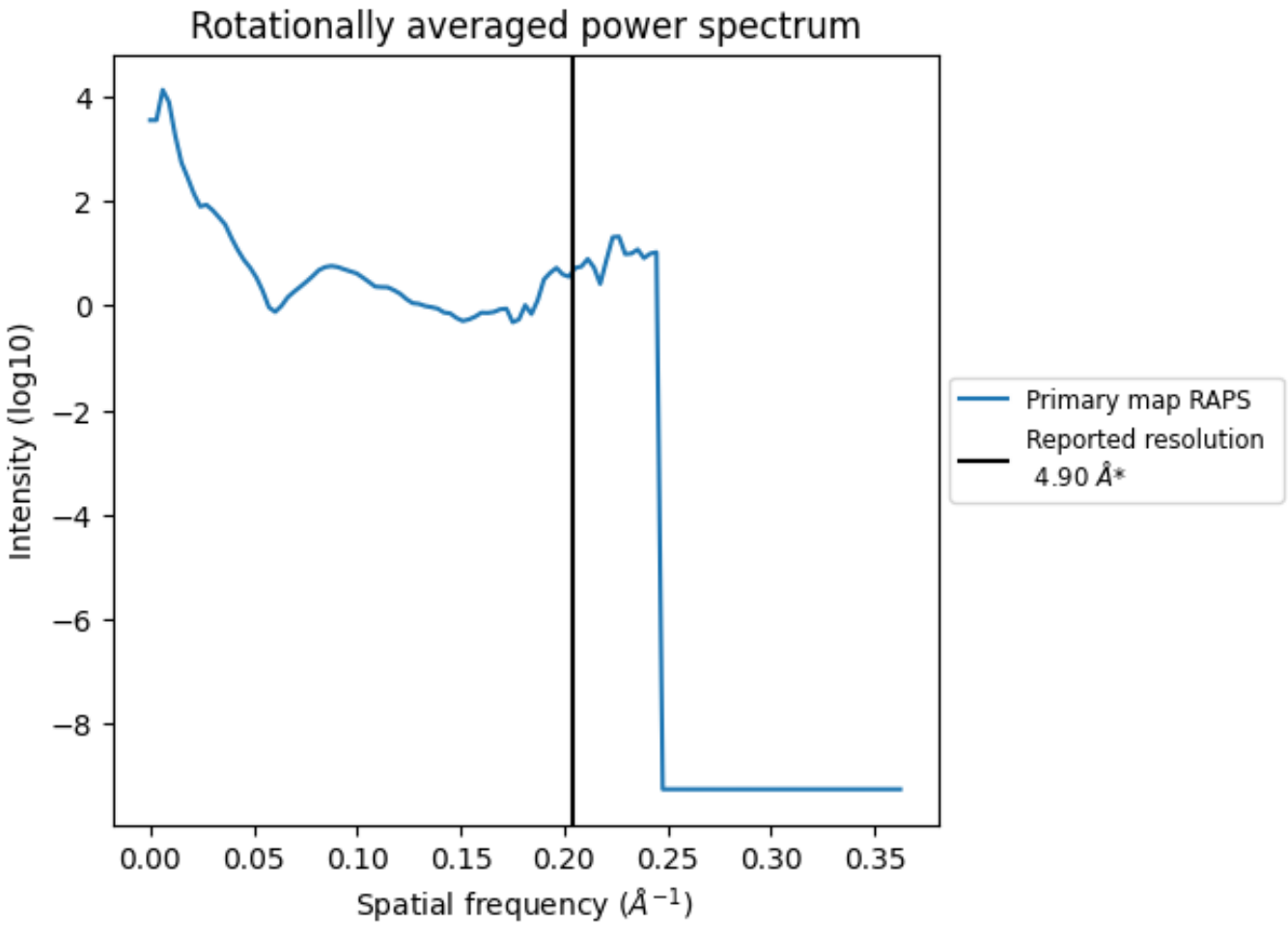
7.2 Volume estimate (i)



The volume at the recommended contour level is 84 nm^3; this corresponds to an approximate mass of 76 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.204 Å^{-1}

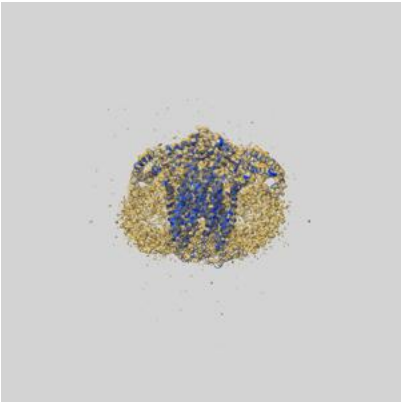
8 Fourier-Shell correlation (i)

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

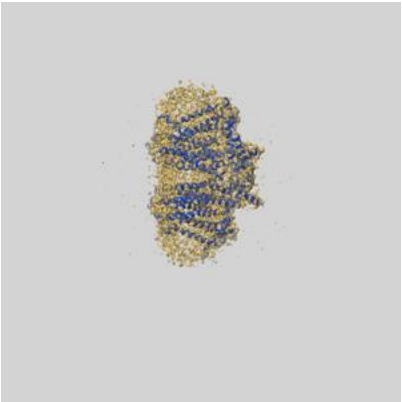
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20017 and PDB model 6OCE. Per-residue inclusion information can be found in section 3 on page 4.

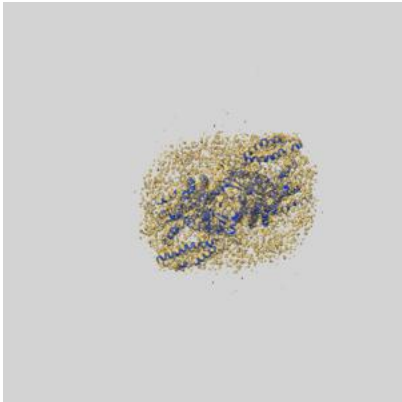
9.1 Map-model overlay (i)



X



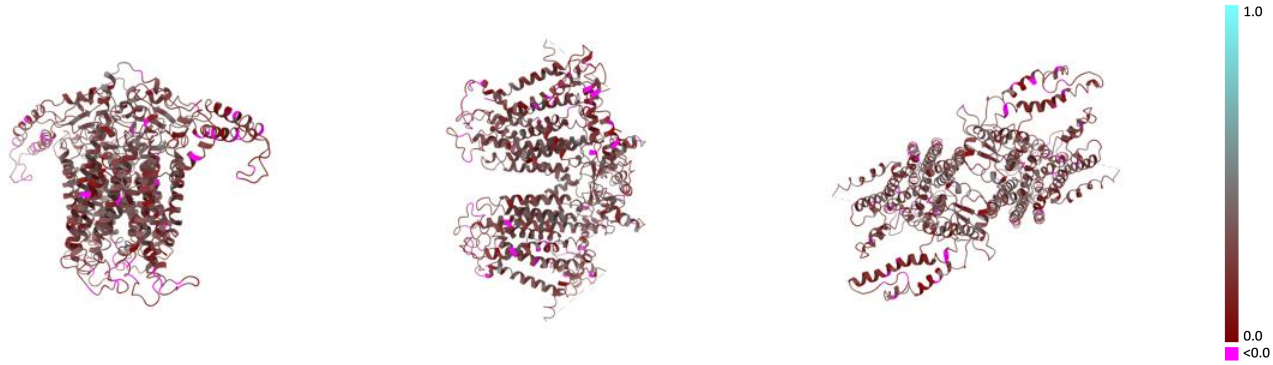
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

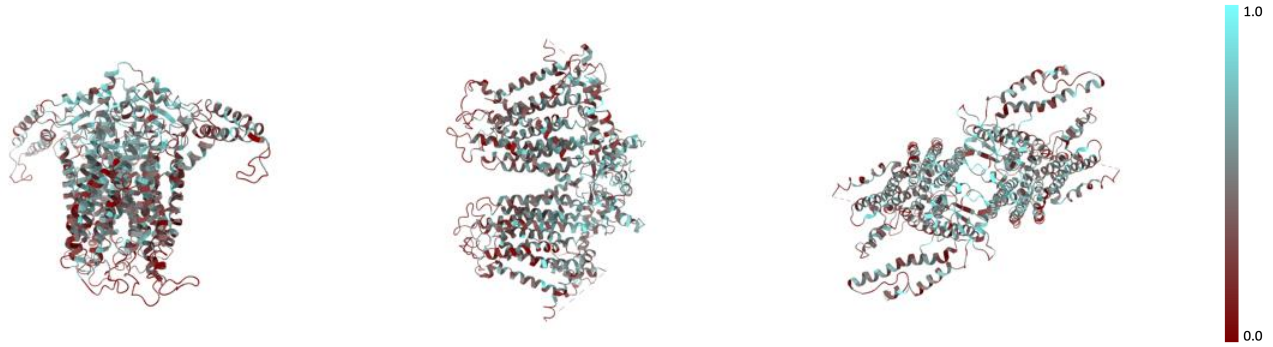
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

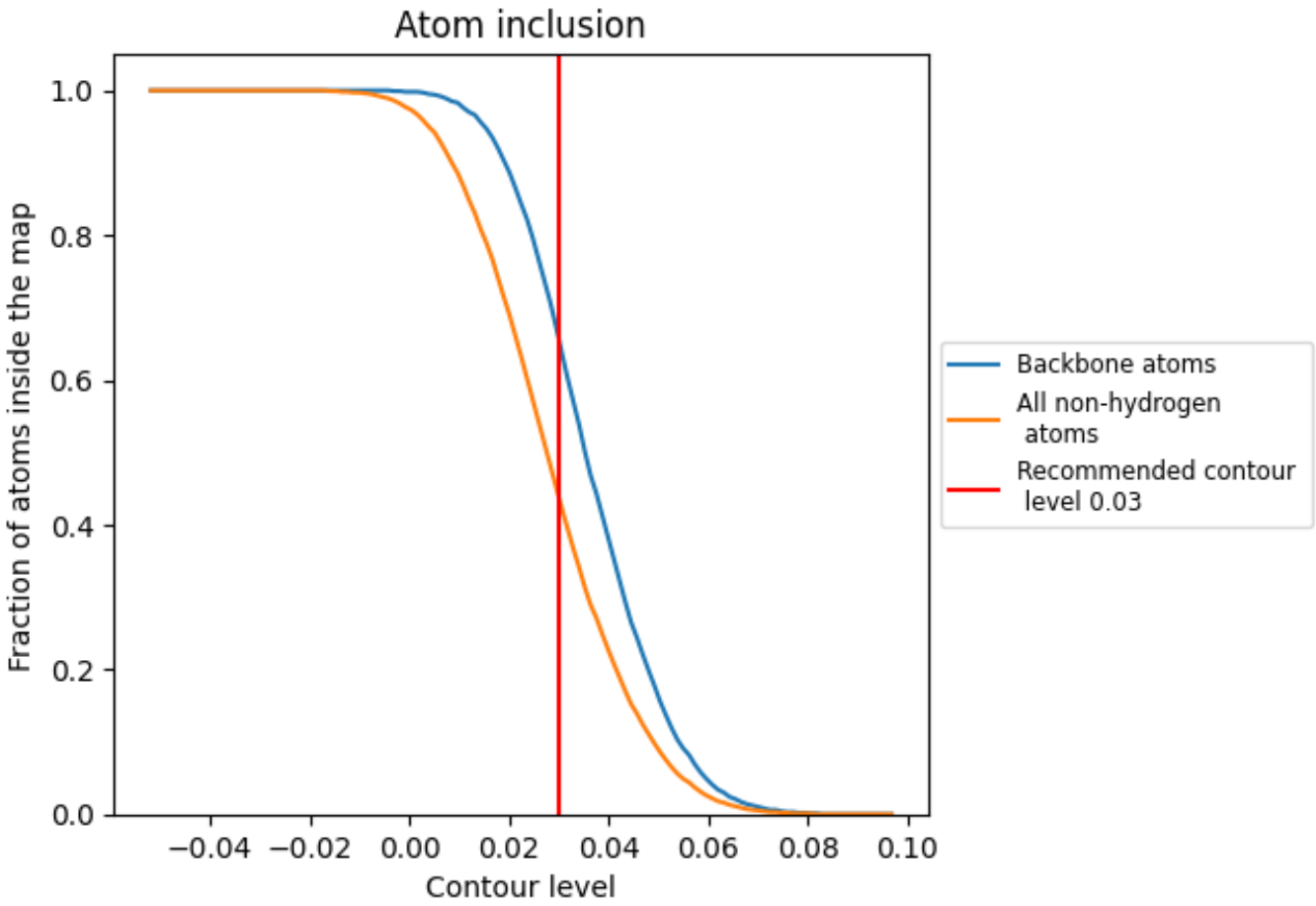
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 44% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4390	0.2400
A	0.4380	0.2400
B	0.4400	0.2400