WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Nov 16, 2022 – 04:06 PM EST

PDB ID	:	7L2Z
EMDB ID	:	EMD-23146
Title	:	Bacterial cellulose synthase BcsB hexamer
Authors	:	Acheson, J.F.; Zimmer, J.
Deposited on	:	2020-12-17
Resolution	:	3.40 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.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.0%

Worse   *Better*

▌ Percentile relative to all structures

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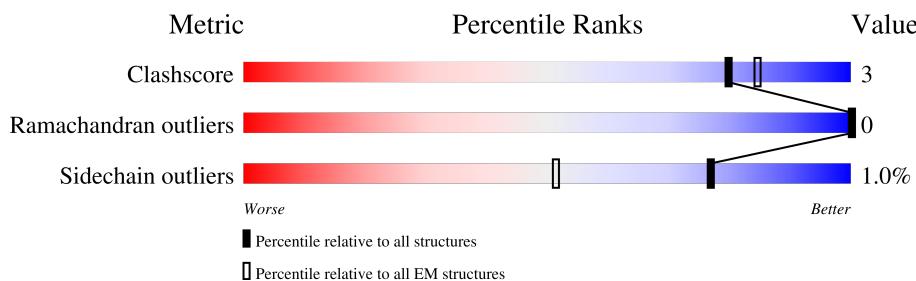
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	762	76% 5% 19%
1	B	762	78% 7% 15%
1	C	762	80% 5% 15%
1	D	762	78% 7% 15%
1	E	762	79% 6% 15%
1	F	762	18% 79% 8% 13%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 59631 atoms, of which 29676 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 Cyclic di-GMP-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	645	Total	C	H	N	O	S	0	0
			9952	3171	4953	851	953	24		
1	A	619	Total	C	H	N	O	S	0	0
			9550	3049	4752	814	912	23		
1	C	647	Total	C	H	N	O	S	0	0
			9971	3177	4960	853	957	24		
1	D	645	Total	C	H	N	O	S	0	0
			9938	3168	4942	850	954	24		
1	E	646	Total	C	H	N	O	S	0	0
			9957	3174	4953	851	955	24		
1	F	664	Total	C	H	N	O	S	0	0
			10263	3265	5116	879	979	24		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	TRP	-	expression tag	UNP P37652
B	19	SER	-	expression tag	UNP P37652
B	20	HIS	-	expression tag	UNP P37652
B	21	PRO	-	expression tag	UNP P37652
B	22	GLN	-	expression tag	UNP P37652
B	23	PHE	-	expression tag	UNP P37652
B	24	GLU	-	expression tag	UNP P37652
B	25	LYS	-	expression tag	UNP P37652
A	18	TRP	-	expression tag	UNP P37652
A	19	SER	-	expression tag	UNP P37652
A	20	HIS	-	expression tag	UNP P37652
A	21	PRO	-	expression tag	UNP P37652
A	22	GLN	-	expression tag	UNP P37652
A	23	PHE	-	expression tag	UNP P37652
A	24	GLU	-	expression tag	UNP P37652
A	25	LYS	-	expression tag	UNP P37652
C	18	TRP	-	expression tag	UNP P37652
C	19	SER	-	expression tag	UNP P37652

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W O R L D W I D E
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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	HIS	-	expression tag	UNP P37652
C	21	PRO	-	expression tag	UNP P37652
C	22	GLN	-	expression tag	UNP P37652
C	23	PHE	-	expression tag	UNP P37652
C	24	GLU	-	expression tag	UNP P37652
C	25	LYS	-	expression tag	UNP P37652
D	18	TRP	-	expression tag	UNP P37652
D	19	SER	-	expression tag	UNP P37652
D	20	HIS	-	expression tag	UNP P37652
D	21	PRO	-	expression tag	UNP P37652
D	22	GLN	-	expression tag	UNP P37652
D	23	PHE	-	expression tag	UNP P37652
D	24	GLU	-	expression tag	UNP P37652
D	25	LYS	-	expression tag	UNP P37652
E	18	TRP	-	expression tag	UNP P37652
E	19	SER	-	expression tag	UNP P37652
E	20	HIS	-	expression tag	UNP P37652
E	21	PRO	-	expression tag	UNP P37652
E	22	GLN	-	expression tag	UNP P37652
E	23	PHE	-	expression tag	UNP P37652
E	24	GLU	-	expression tag	UNP P37652
E	25	LYS	-	expression tag	UNP P37652
F	18	TRP	-	expression tag	UNP P37652
F	19	SER	-	expression tag	UNP P37652
F	20	HIS	-	expression tag	UNP P37652
F	21	PRO	-	expression tag	UNP P37652
F	22	GLN	-	expression tag	UNP P37652
F	23	PHE	-	expression tag	UNP P37652
F	24	GLU	-	expression tag	UNP P37652
F	25	LYS	-	expression tag	UNP P37652

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: Cyclic di-GMP-binding protein

- Molecule 1: Cyclic di-GMP-binding protein
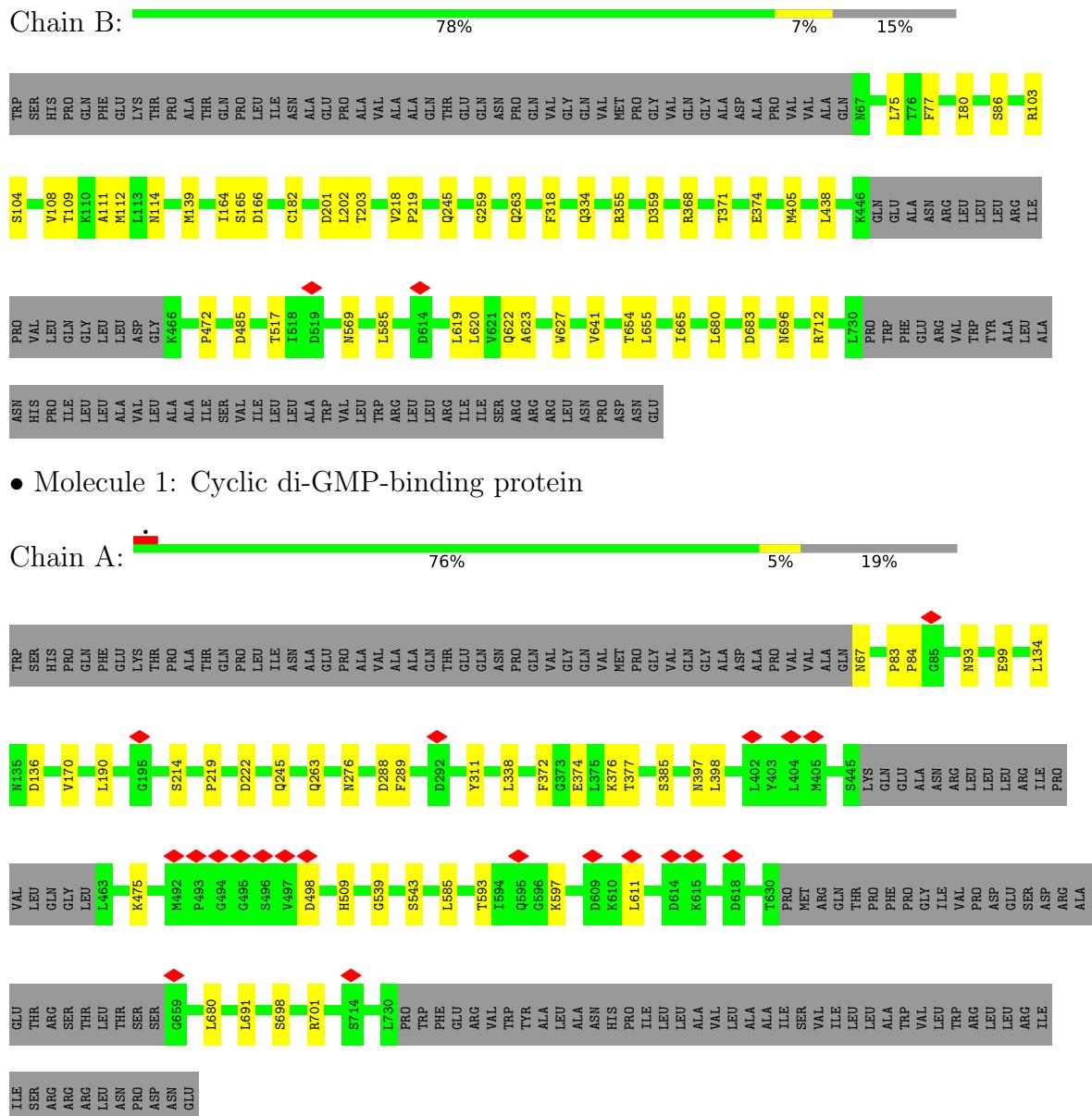
- Molecule 1: Cyclic di-GMP-binding protein
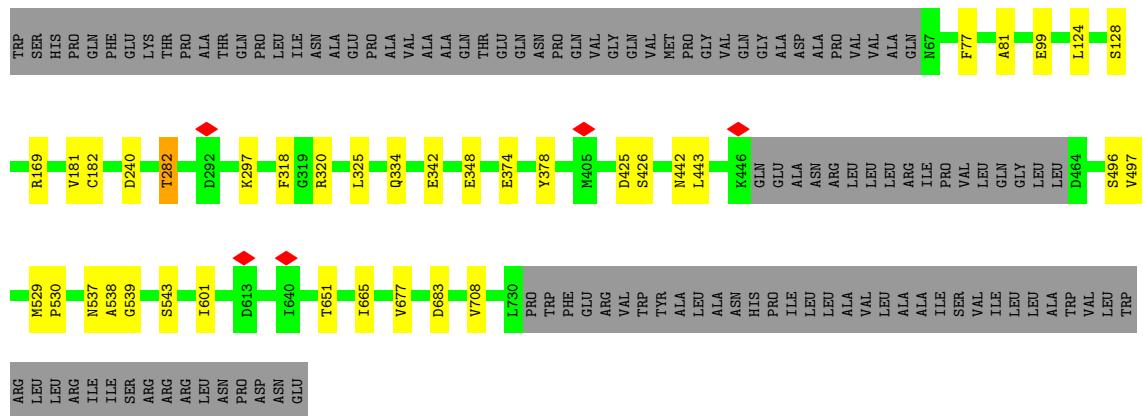
Chain C:

- Molecule 1: Cyclic di-GMP-binding protein

Chain D:
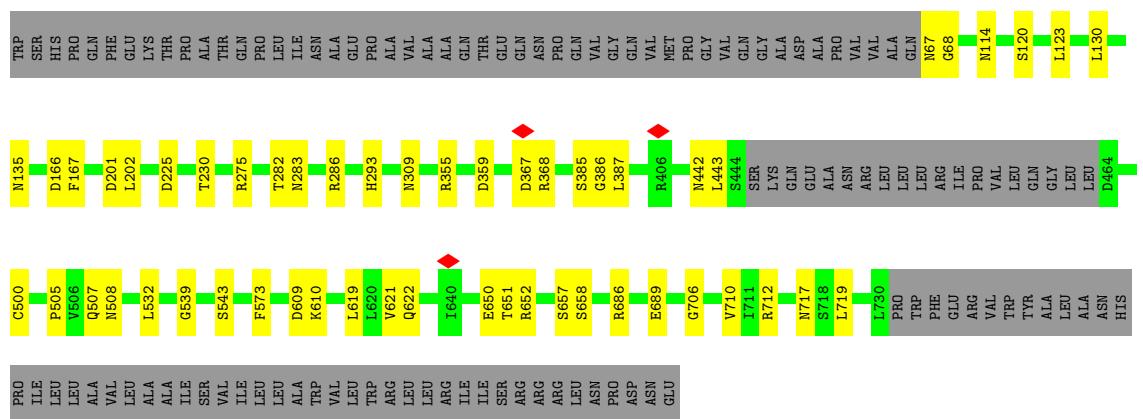
- Molecule 1: Cyclic di-GMP-binding protein

Chain E:

• Molecule 1: Cyclic di-GMP-binding protein

Chain F:

18%

79%   8%   13%

TRP SER HIS PRO GLN PHE GLU LYS THR PRO ALA THR GLN PRO LEU ILE ASN ALA GLU PRO ALA VAL ALA ALA GLN THR GLU GLN ASN PRO GLN VAL GLY GLN VAL MET PRO GLY VAL GLN GLY ALA ASP ALA PRO VAL VAL ALA GLN N67 G68 P69 S70 R71 D72 V73 K74 L75 T76 F77

A78 Q79 I80 P83 P84 I92 I98 E99 M102 E106 V107 K110 A111 M112 Y133 E137 L138 M139 G140 T145 K146 E147 Q156 N160 P161 L162 D166 V170 V181 S198 G199 L200 D201 L207 N208 V209 K210 N211 D212 L213 S214 V218 P219

S224 D225 N226 T230 L231 G237 A238 P239 D240 A246 G259 Q263 N270 Q271 L272 R275 D284 K285 R286 P287 D288 F289 L290 R291 D292 K297 V300 I304 N305 H306 P307 Q308 N309 R320 D321 D322 K323 Q327 A328 A329 G335 N336 I337 L338 F339

R340 G341 E342 V345 V346 N347 E348 V349 K350 P351 L352 L353 P354 R355 K356 D359 D367 E379 E380 Q383 D401 M405 R406 S407 T408 G409 I410 D411 P422 D425 R428 S444 S445 K446 Q447 E448 A449 N450 R451 L452 L453 L454 R455 I456 P457 V458 L459 Q460 G461

L462 L463 D464 D468 L474 E487 N490 G495 S496 V497 D498 N499 C500 F503 Q504 D515 I518 D519 H525 M529 P530 D531 D547 Q550 K557 L567 L568 G575 N584 G591 S592 T593 I594 Q595 D598 I601 G605 D609 K610

L611 K612 D613 D614 K615 D618 L619 L620 V621 Q622 A623 T624 E625 S626 W627 E644 S645 T651 R652 S653 T654 S657 D673 D683 S684 P685 D693 N696 D697 T703 M704 V710 I711 I716 D723 L730 PRO TRP PHE GLU ARG VAL TRP TYR ALA LEU ALA

ASN HIS PRO ILE LEU LEU ALA VAL LEU ALA ALA ILE SER VAL ILE LEU LEU LEU ALA TRP VAL LEU TRP ARG LEU LEU ARG ILE ILE SER ARG ARG ARG LEU ASN PRO ASP ASN GLU

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115289	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 $(e^-/\text{Å}^2)$	51	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.352	Depositor
Minimum map value	-0.962	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.24	0/4906	0.42	0/6675
1	B	0.25	0/5113	0.44	0/6959
1	C	0.25	0/5125	0.43	0/6975
1	D	0.25	0/5110	0.43	0/6956
1	E	0.25	0/5118	0.42	0/6967
1	F	0.25	0/5263	0.43	0/7164
All	All	0.25	0/30635	0.43	0/41696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4798	4752	4750	22	0
1	B	4999	4953	4951	34	0
1	C	5011	4960	4958	21	0
1	D	4996	4942	4940	29	0
1	E	5004	4953	4951	27	0
1	F	5147	5116	5114	39	0
All	All	29955	29676	29664	158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (158) 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:B:109:THR:OG1	1:B:203:THR:O	1.90	0.89
1:D:286:ARG:NH2	1:D:293:HIS:O	2.16	0.79
1:B:109:THR:OG1	1:B:203:THR:OG1	1.87	0.76
1:B:114:ASN:ND2	1:B:201:ASP:OD1	2.18	0.75
1:B:259:GLY:O	1:B:263:GLN:NE2	2.23	0.70
1:B:245:GLN:NE2	1:B:585:LEU:O	2.27	0.67
1:F:703:THR:OG1	1:F:716:ILE:HD11	1.96	0.65
1:A:219:PRO:O	1:A:276:ASN:ND2	2.29	0.65
1:D:135:ASN:O	1:E:196:ARG:NH1	2.31	0.64
1:F:448:GLU:OE1	1:F:449:ALA:N	2.31	0.64
1:E:348:GLU:OE2	1:F:652:ARG:NH2	2.32	0.63
1:C:342:GLU:N	1:C:342:GLU:OE1	2.32	0.63
1:F:77:PHE:N	1:F:198:SER:O	2.32	0.62
1:B:139:MET:SD	1:B:139:MET:N	2.72	0.62
1:C:348:GLU:OE1	1:D:652:ARG:NH2	2.32	0.62
1:A:680:LEU:HD13	1:A:691:LEU:HD21	1.81	0.61
1:D:387:LEU:HD11	1:D:505:PRO:HB2	1.82	0.61
1:B:438:LEU:HD11	1:B:472:PRO:HD2	1.83	0.61
1:D:114:ASN:ND2	1:D:201:ASP:OD1	2.34	0.59
1:F:428:ARG:NH2	1:F:487:GLU:OE1	2.35	0.59
1:F:230:THR:OG1	1:F:275:ARG:NH1	2.35	0.58
1:B:620:LEU:HD13	1:B:627:TRP:CZ2	2.38	0.58
1:F:619:LEU:HD23	1:F:620:LEU:N	2.19	0.57
1:D:712:ARG:NH1	1:D:717:ASN:OD1	2.37	0.56
1:D:230:THR:O	1:D:275:ARG:NH1	2.38	0.56
1:D:686:ARG:NH1	1:D:689:GLU:OE1	2.39	0.56
1:C:297:LYS:O	1:C:320:ARG:NH2	2.37	0.55
1:E:120:SER:OG	1:E:191:TRP:O	2.22	0.55
1:B:485:ASP:OD2	1:B:485:ASP:N	2.41	0.54
1:E:222:ASP:OD2	1:E:224:SER:OG	2.17	0.53
1:D:609:ASP:OD2	1:D:610:LYS:N	2.41	0.53
1:A:385:SER:HG	1:A:509:HIS:CG	2.26	0.53
1:A:374:GLU:N	1:A:374:GLU:OE2	2.40	0.53
1:D:532:LEU:N	1:D:706:GLY:O	2.41	0.53
1:C:124:LEU:O	1:C:128:SER:OG	2.18	0.52
1:A:288:ASP:OD1	1:A:289:PHE:N	2.42	0.52
1:D:67:ASN:OD1	1:D:68:GLY:N	2.43	0.52
1:F:102:MET:O	1:F:224:SER:OG	2.14	0.52
1:B:619:LEU:C	1:B:620:LEU:HD12	2.29	0.52
1:B:86:SER:OG	1:A:136:ASP:O	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:THR:OG1	1:F:146:LYS:N	2.43	0.52
1:B:108:VAL:HG21	1:B:164:ILE:HG21	1.91	0.51
1:B:112:MET:N	1:B:201:ASP:O	2.42	0.51
1:F:567:LEU:HD23	1:F:568:LEU:HD12	1.91	0.51
1:A:222:ASP:OD1	1:A:222:ASP:N	2.41	0.51
1:A:593:THR:O	1:A:597:LYS:NZ	2.37	0.51
1:B:622:GLN:O	1:B:623:ALA:HB3	2.11	0.51
1:D:619:LEU:HD21	1:D:710:VAL:HG22	1.92	0.51
1:C:665:ILE:HG22	1:C:708:VAL:HG23	1.93	0.50
1:F:422:PRO:O	1:F:447:GLN:NE2	2.45	0.50
1:E:306:HIS:HB2	1:E:312:VAL:HG13	1.92	0.50
1:B:619:LEU:HB3	1:B:665:ILE:HD11	1.94	0.49
1:A:190:LEU:H	1:A:190:LEU:HD23	1.76	0.49
1:E:213:LEU:N	1:E:341:GLY:O	2.43	0.49
1:B:355:ARG:NH2	1:B:359:ASP:OD2	2.40	0.49
1:A:397:ASN:OD1	1:A:397:ASN:N	2.45	0.49
1:E:590:ASP:OD1	1:E:592:SER:N	2.38	0.49
1:C:496:SER:OG	1:C:497:VAL:N	2.44	0.49
1:E:643:ASP:OD2	1:E:643:ASP:N	2.45	0.49
1:C:334:GLN:NE2	1:D:651:THR:HG21	2.28	0.49
1:E:351:PRO:HA	1:F:651:THR:HG22	1.94	0.49
1:C:683:ASP:OD1	1:C:683:ASP:N	2.46	0.49
1:B:218:VAL:N	1:B:219:PRO:CD	2.76	0.49
1:B:103:ARG:O	1:B:104:SER:OG	2.27	0.48
1:C:99:GLU:OE2	1:C:169:ARG:NH1	2.46	0.48
1:A:134:LEU:HD12	1:A:170:VAL:HG22	1.95	0.48
1:F:458:VAL:HG23	1:F:459:LEU:N	2.29	0.47
1:F:704:MET:HB3	1:F:716:ILE:HD12	1.96	0.47
1:B:112:MET:O	1:B:201:ASP:N	2.46	0.47
1:D:619:LEU:O	1:D:621:VAL:HG23	2.15	0.47
1:F:380:GLU:OE2	1:F:383:GLN:NE2	2.47	0.47
1:E:112:MET:SD	1:E:156:GLN:NE2	2.88	0.47
1:A:99:GLU:N	1:A:99:GLU:OE1	2.48	0.46
1:A:67:ASN:N	1:A:311:TYR:HH	2.14	0.46
1:E:438:LEU:HD13	1:E:471:ILE:HG23	1.96	0.46
1:F:259:GLY:O	1:F:263:GLN:NE2	2.49	0.46
1:B:569:ASN:ND2	1:B:696:ASN:OD1	2.49	0.46
1:A:376:LYS:O	1:A:377:THR:OG1	2.26	0.46
1:E:365:ARG:NH2	1:E:367:ASP:OD2	2.48	0.46
1:D:507:GLN:O	1:E:428:ARG:NH2	2.49	0.46
1:E:340:ARG:NE	1:F:657:SER:OG	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:529:MET:O	1:F:531:ASP:N	2.48	0.46
1:F:683:ASP:OD1	1:F:683:ASP:N	2.46	0.46
1:B:75:LEU:HD12	1:B:80:ILE:HD13	1.98	0.46
1:D:120:SER:HB3	1:D:123:LEU:HD13	1.97	0.46
1:B:368:ARG:NH2	1:B:374:GLU:OE2	2.50	0.45
1:F:218:VAL:N	1:F:219:PRO:CD	2.79	0.45
1:F:231:LEU:H	1:F:231:LEU:HD23	1.80	0.45
1:B:334:GLN:NE2	1:C:651:THR:HG21	2.31	0.45
1:A:698:SER:OG	1:A:701:ARG:NH1	2.50	0.45
1:C:537:ASN:O	1:C:538:ALA:HB3	2.15	0.45
1:B:683:ASP:N	1:B:683:ASP:OD1	2.50	0.45
1:C:529:MET:N	1:C:530:PRO:CD	2.79	0.45
1:D:282:THR:HG22	1:D:282:THR:O	2.16	0.45
1:F:458:VAL:HG23	1:F:459:LEU:H	1.80	0.45
1:F:468:ASP:OD1	1:F:468:ASP:N	2.48	0.45
1:B:712:ARG:NH2	1:A:214:SER:OG	2.50	0.45
1:E:330:LYS:NZ	1:E:583:ILE:O	2.50	0.45
1:C:601:ILE:HB	1:C:677:VAL:HG13	1.99	0.45
1:B:202:LEU:H	1:B:202:LEU:HD23	1.82	0.45
1:F:547:ASP:OD2	1:F:584:ASN:ND2	2.50	0.45
1:D:367:ASP:OD1	1:D:368:ARG:N	2.50	0.44
1:E:83:PRO:N	1:E:84:PRO:HD2	2.32	0.44
1:B:111:ALA:HA	1:B:202:LEU:HA	1.99	0.44
1:E:268:LEU:H	1:E:268:LEU:HD23	1.82	0.44
1:F:83:PRO:N	1:F:84:PRO:HD2	2.32	0.44
1:D:166:ASP:OD1	1:D:167:PHE:N	2.49	0.44
1:A:263:GLN:N	1:A:263:GLN:OE1	2.51	0.44
1:C:181:VAL:HG13	1:C:182:CYS:N	2.32	0.44
1:F:133:TYR:O	1:F:170:VAL:HA	2.17	0.44
1:C:539:GLY:O	1:C:543:SER:OG	2.32	0.43
1:D:385:SER:OG	1:D:386:GLY:N	2.51	0.43
1:E:80:ILE:HD12	1:E:98:ILE:HD12	2.00	0.43
1:E:99:GLU:N	1:E:99:GLU:OE1	2.51	0.43
1:C:282:THR:HG22	1:C:325:LEU:HD11	2.00	0.43
1:B:108:VAL:HG11	1:B:164:ILE:CD1	2.49	0.43
1:F:218:VAL:HG12	1:F:219:PRO:HD3	2.00	0.43
1:B:654:THR:C	1:B:655:LEU:HD12	2.38	0.43
1:A:498:ASP:OD1	1:A:498:ASP:N	2.52	0.43
1:C:425:ASP:O	1:C:426:SER:OG	2.32	0.43
1:E:609:ASP:N	1:E:609:ASP:OD1	2.52	0.43
1:F:619:LEU:CD1	1:F:710:VAL:HG12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:PHE:O	1:C:81:ALA:HB3	2.19	0.42
1:F:622:GLN:O	1:F:623:ALA:HB3	2.19	0.42
1:C:334:GLN:HE22	1:D:651:THR:HG21	1.84	0.42
1:F:405:MET:SD	1:F:405:MET:N	2.84	0.42
1:A:245:GLN:NE2	1:A:585:LEU:O	2.50	0.42
1:D:657:SER:OG	1:D:658:SER:N	2.51	0.42
1:D:309:ASN:OD1	1:D:309:ASN:N	2.53	0.42
1:F:75:LEU:O	1:F:200:LEU:N	2.48	0.42
1:A:83:PRO:N	1:A:84:PRO:HD2	2.35	0.42
1:C:374:GLU:N	1:C:374:GLU:OE2	2.53	0.42
1:B:165:SER:OG	1:B:166:ASP:N	2.53	0.41
1:E:312:VAL:HG13	1:E:312:VAL:O	2.19	0.41
1:E:498:ASP:OD1	1:E:499:ASN:N	2.53	0.41
1:F:356:LYS:NZ	1:F:367:ASP:OD1	2.53	0.41
1:F:711:ILE:HD12	1:F:716:ILE:HG22	2.03	0.41
1:B:108:VAL:HG11	1:B:164:ILE:HD13	2.02	0.41
1:A:680:LEU:HD13	1:A:691:LEU:CD2	2.49	0.41
1:E:348:GLU:O	1:F:654:THR:OG1	2.37	0.41
1:D:622:GLN:OE1	1:D:622:GLN:N	2.53	0.41
1:E:234:VAL:HG13	1:E:234:VAL:O	2.20	0.41
1:B:371:THR:HG22	1:B:517:THR:HG22	2.02	0.41
1:C:442:ASN:OD1	1:C:443:LEU:N	2.54	0.41
1:D:539:GLY:O	1:D:543:SER:OG	2.34	0.41
1:E:347:ASN:ND2	1:F:625:GLU:OE1	2.48	0.41
1:F:410:ILE:HD12	1:F:518:ILE:HD11	2.03	0.41
1:D:355:ARG:NH2	1:D:359:ASP:OD1	2.53	0.40
1:D:442:ASN:OD1	1:D:443:LEU:N	2.53	0.40
1:E:76:THR:OG1	1:E:77:PHE:N	2.55	0.40
1:B:405:MET:SD	1:B:641:VAL:HG22	2.60	0.40
1:F:401:ASP:OD2	1:F:401:ASP:N	2.54	0.40
1:A:539:GLY:O	1:A:543:SER:OG	2.24	0.40
1:D:650:GLU:HG2	1:D:651:THR:HG23	2.03	0.40
1:F:80:ILE:HD12	1:F:98:ILE:CG2	2.52	0.40
1:E:500:CYS:O	1:F:495:GLY:N	2.42	0.40
1:B:218:VAL:HG22	1:B:219:PRO:HD3	2.03	0.40
1:D:508:ASN:OD1	1:D:508:ASN:N	2.53	0.40

There are no symmetry-related clashes.

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	A	613/762 (80%)	590 (96%)	23 (4%)	0	100	100
1	B	641/762 (84%)	611 (95%)	30 (5%)	0	100	100
1	C	643/762 (84%)	622 (97%)	21 (3%)	0	100	100
1	D	641/762 (84%)	620 (97%)	21 (3%)	0	100	100
1	E	642/762 (84%)	625 (97%)	17 (3%)	0	100	100
1	F	662/762 (87%)	636 (96%)	26 (4%)	0	100	100
All	All	3842/4572 (84%)	3704 (96%)	138 (4%)	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	533/657 (81%)	527 (99%)	6 (1%)	73	86
1	B	557/657 (85%)	553 (99%)	4 (1%)	84	92
1	C	558/657 (85%)	554 (99%)	4 (1%)	84	92
1	D	556/657 (85%)	549 (99%)	7 (1%)	69	84
1	E	557/657 (85%)	550 (99%)	7 (1%)	69	84
1	F	573/657 (87%)	568 (99%)	5 (1%)	78	90
All	All	3334/3942 (85%)	3301 (99%)	33 (1%)	77	88

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	PHE
1	B	182	CYS
1	B	318	PHE
1	B	680	LEU
1	A	93	ASN
1	A	338	LEU
1	A	372	PHE
1	A	398	LEU
1	A	475	LYS
1	A	611	LEU
1	C	240	ASP
1	C	282	THR
1	C	318	PHE
1	C	378	TYR
1	D	130	LEU
1	D	202	LEU
1	D	225	ASP
1	D	283	ASN
1	D	500	CYS
1	D	573	PHE
1	D	719	LEU
1	E	77	PHE
1	E	118	THR
1	E	153	THR
1	E	168	ASN
1	E	504	GLN
1	E	532	LEU
1	E	573	PHE
1	F	77	PHE
1	F	349	VAL
1	F	462	LEU
1	F	618	ASP
1	F	627	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	577	GLN
1	A	211	ASN
1	A	569	ASN
1	C	179	GLN

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Mol	Chain	Res	Type
1	C	293	HIS
1	C	490	ASN
1	D	393	ASN
1	E	480	ASN
1	F	508	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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-23146. 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 ⓘ

6.1.1 Primary map

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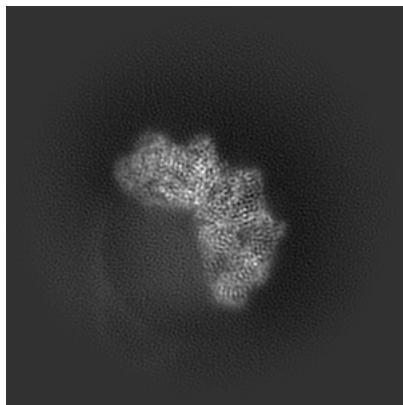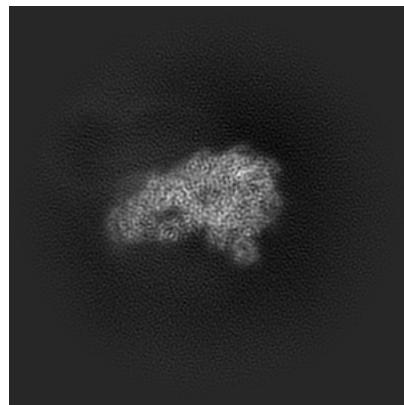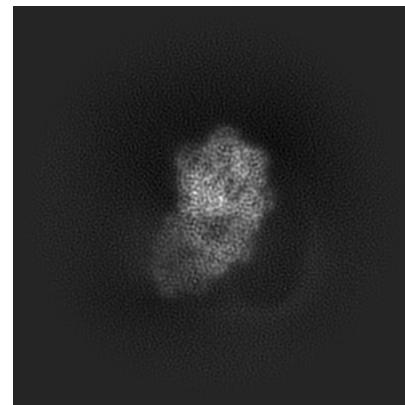
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
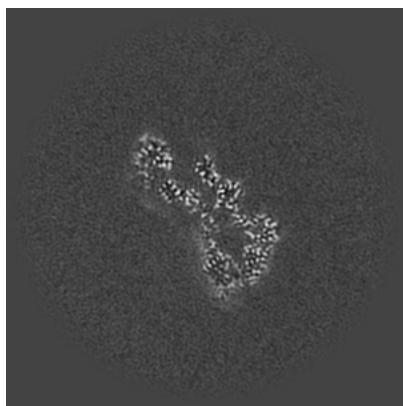
6.2.1 Primary map
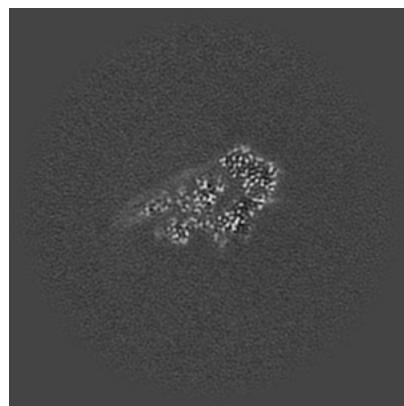
| X Index: 180 | Y Index: 180 | Z Index: 180 |
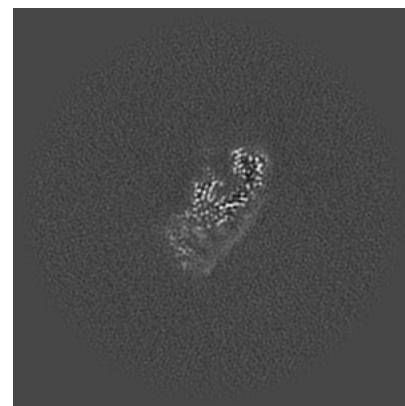
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
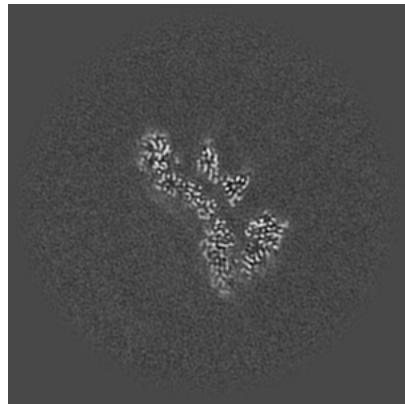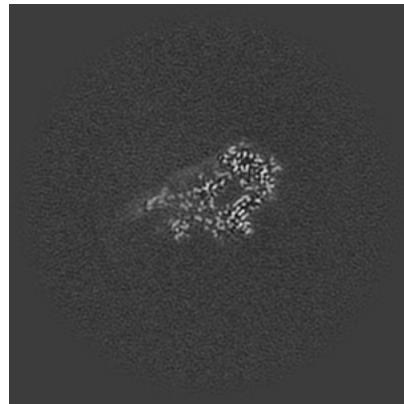
| X Index: 186 | Y Index: 178 | Z Index: 204 |
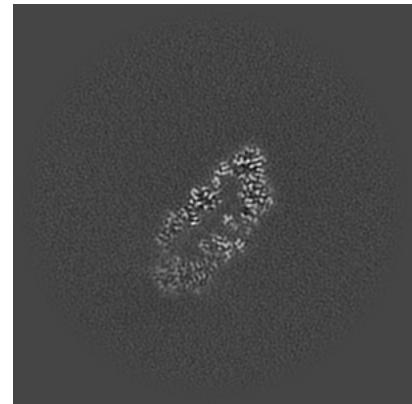
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

| X | Y | Z |
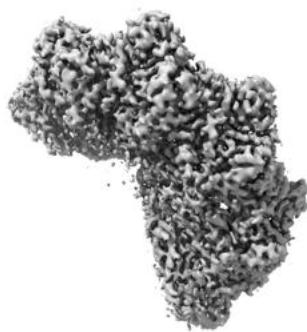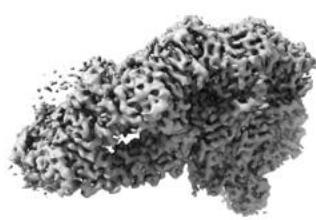
The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5　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

6.5.1　emd_23146_msk_1.map ⓘ

X　　　　　　　　　　　Y　　　　　　　　　　　Z
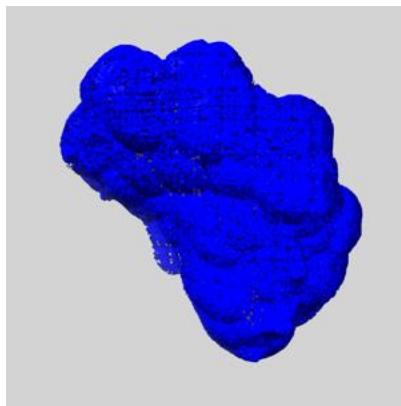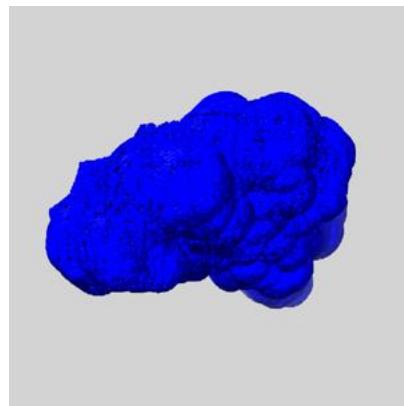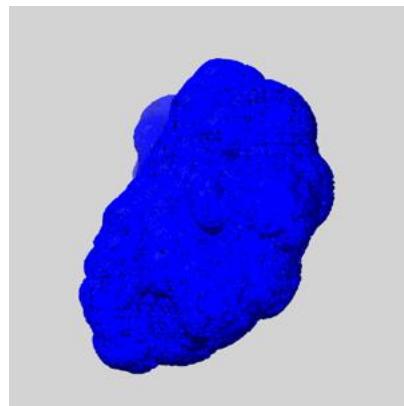
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

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

7.2 Volume estimate (i)
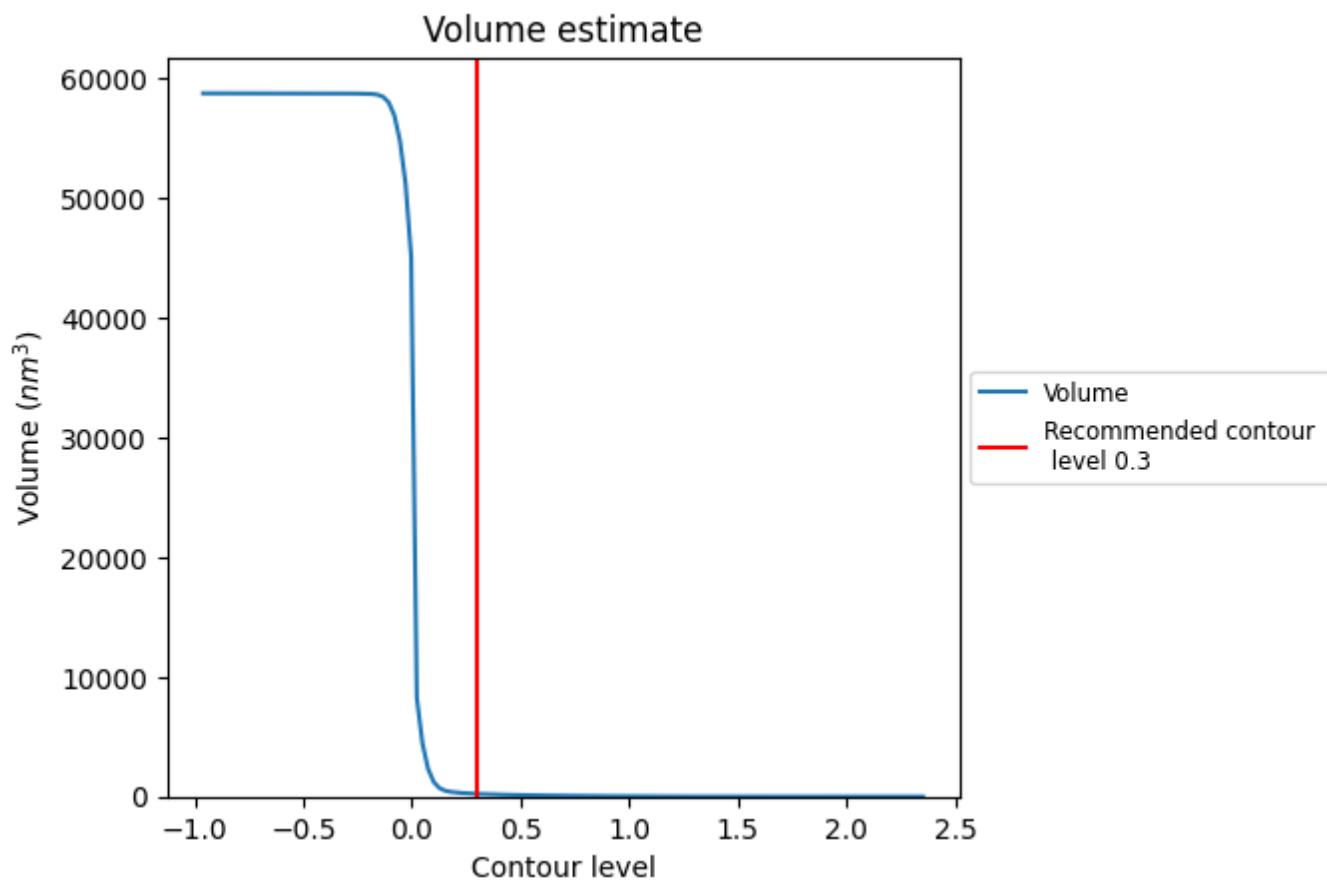
The volume at the recommended contour level is 226 nm^3; this corresponds to an approximate mass of 204 kDa.

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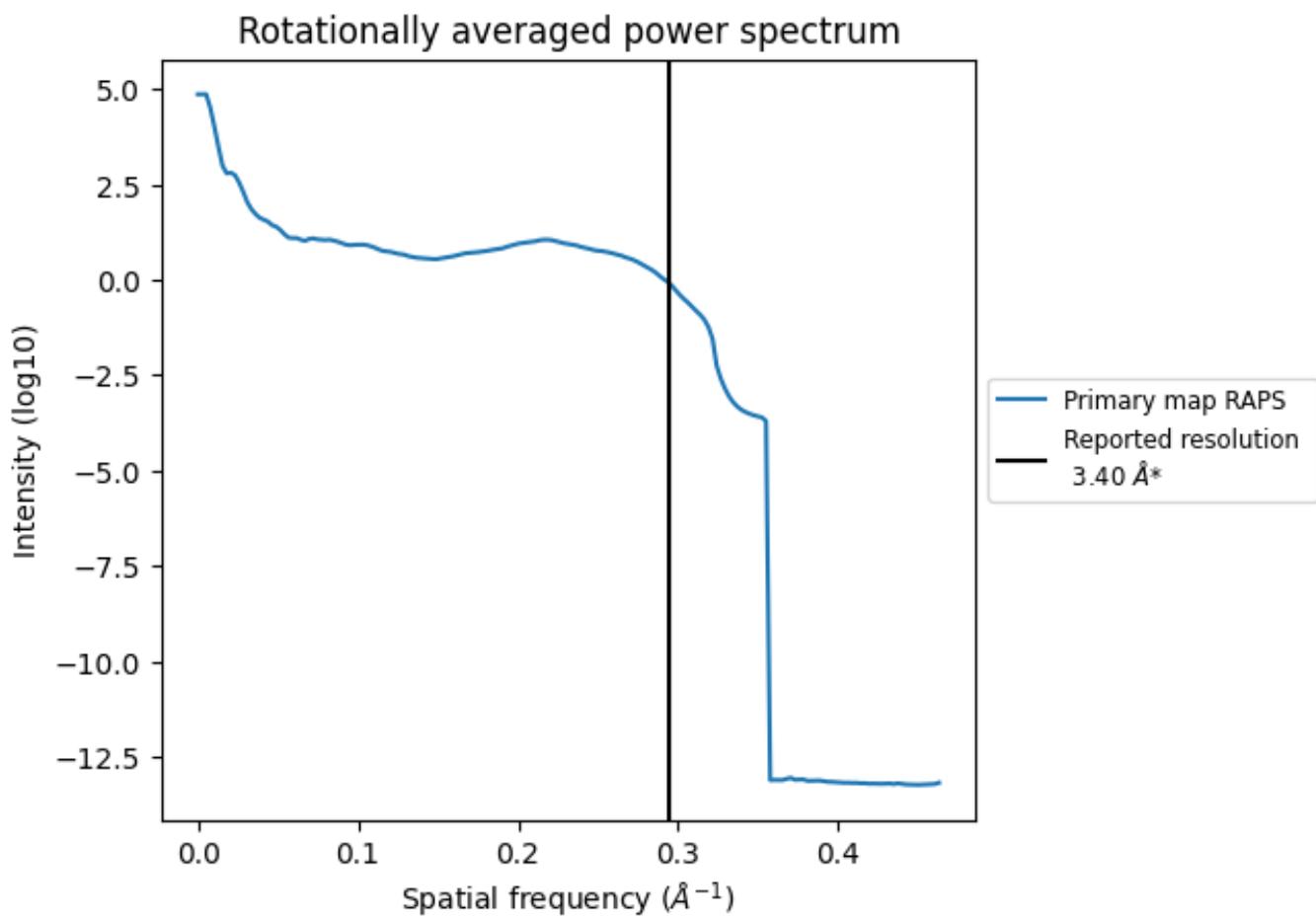
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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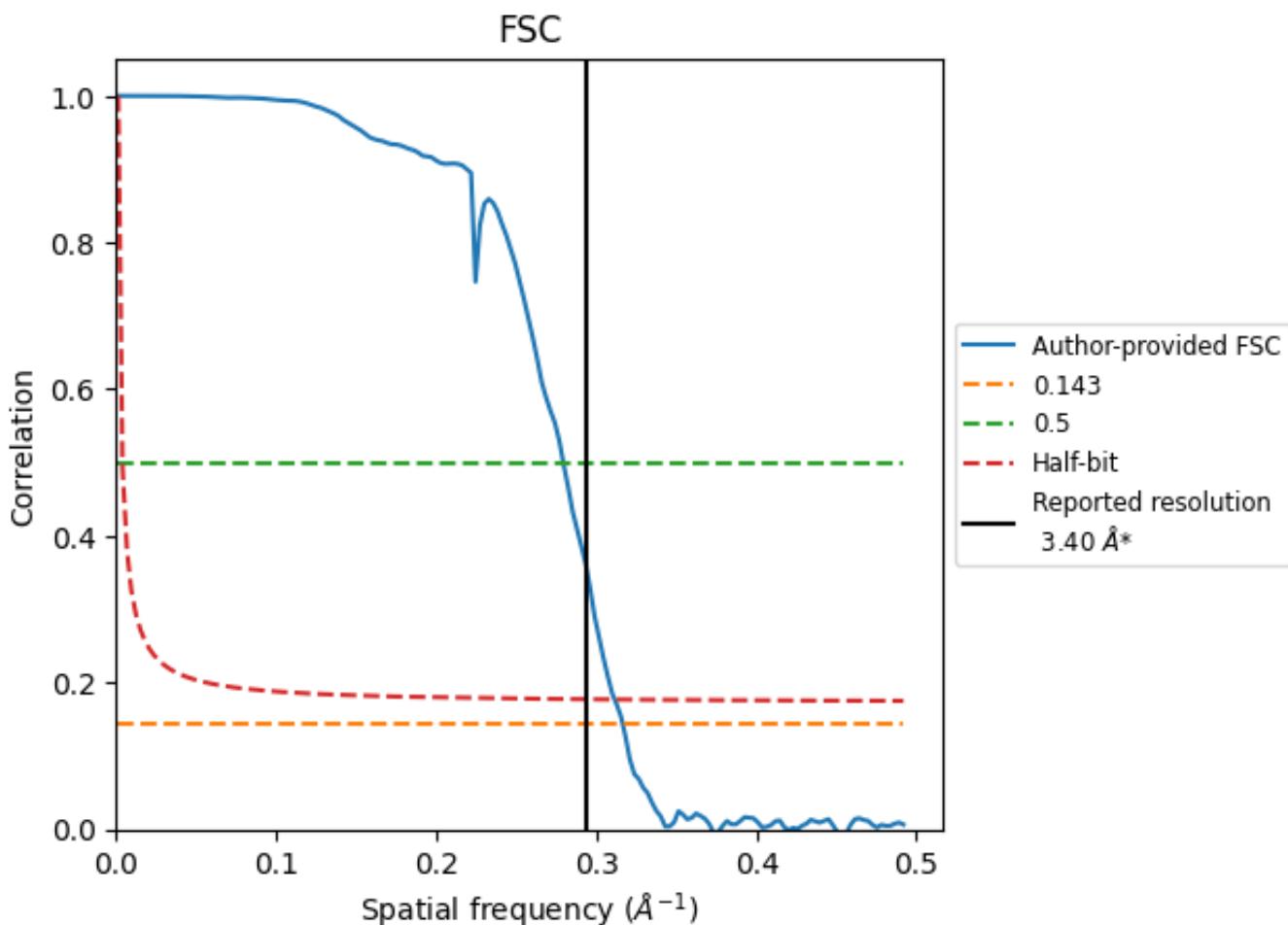
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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	3.16	3.58	3.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-23146 and PDB model 7L2Z. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ

| X | Y | Z |
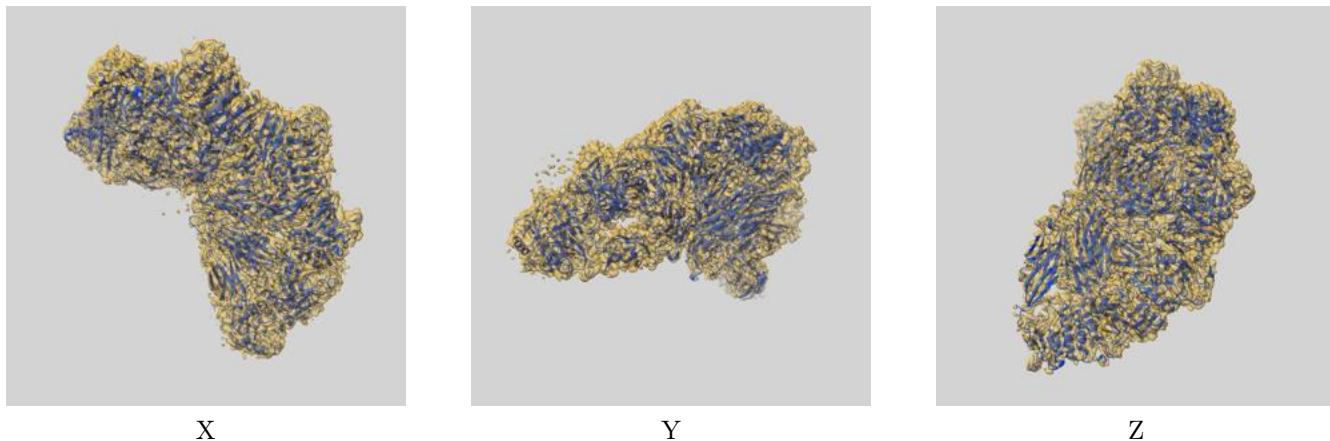
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X Y Z
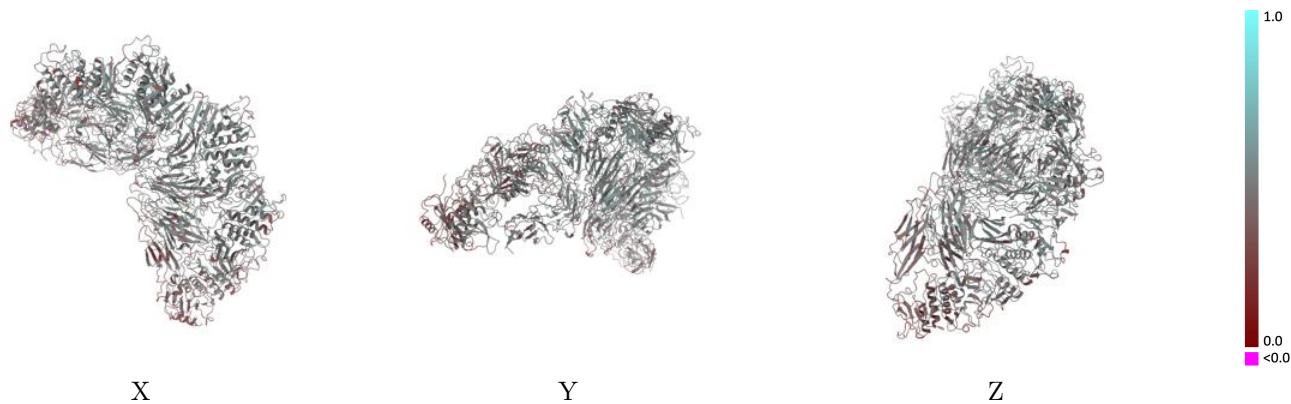
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
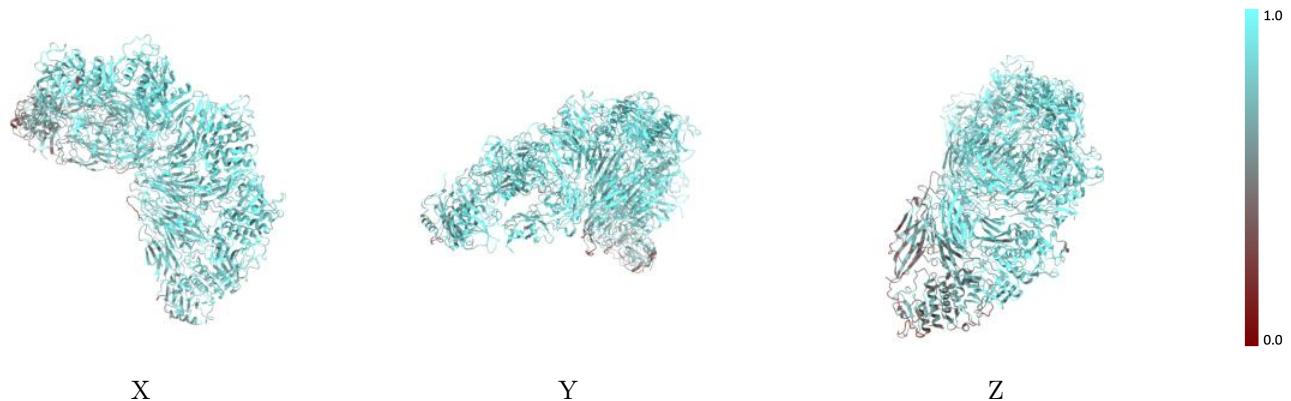
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4   Atom inclusion ⓘ
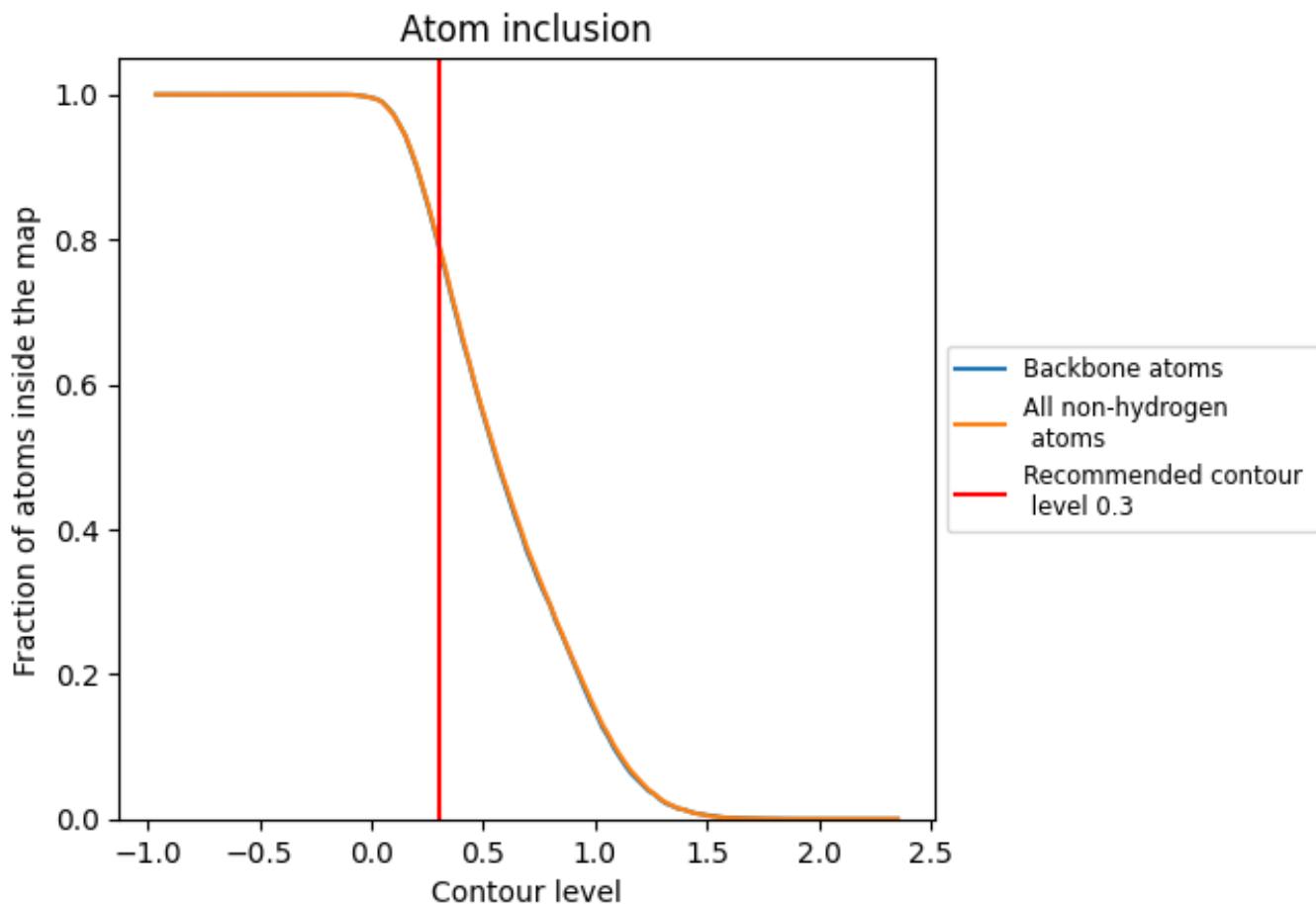
At the recommended contour level, 79% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7941	0.4490
A	0.7860	0.4000
B	0.8555	0.4640
C	0.8636	0.4820
D	0.8638	0.4820
E	0.8544	0.4690
F	0.5820	0.3960

1.0

0.0
<0.0