



Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 04:34 PM EDT

PDB ID : 7JG1 / pdb_00007jg1
EMDB ID : EMD-22309
Title : Dimeric Immunoglobulin A (dIgA)
Authors : Kumar Bharathkar, S.; Parker, B.P.; Malyutin, A.G.; Stadtmueller, B.M.
Deposited on : 2020-07-18
Resolution : 3.30 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 ⓘ 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

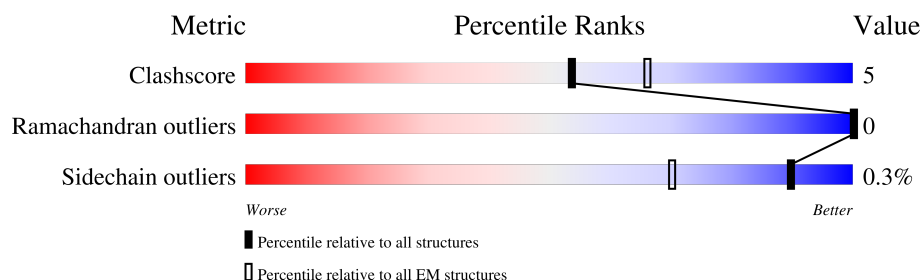
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	355	
1	B	355	
1	C	355	
1	D	355	
2	J	137	
3	E	2	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15850 atoms, of which 7847 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 Igh protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	231	Total	C	H	N	O	S	0	0
			3471	1100	1722	292	345	12		
1	B	224	Total	C	H	N	O	S	0	0
			3374	1069	1677	285	332	11		
1	C	231	Total	C	H	N	O	S	0	0
			3457	1094	1715	292	344	12		
1	D	228	Total	C	H	N	O	S	0	0
			3404	1079	1686	288	340	11		

- Molecule 2 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	J	131	Total	C	H	N	O	S	0	0
			2049	640	1008	180	209	12		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	2	Total	C	H	N	O		0	0
			47	16	19	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

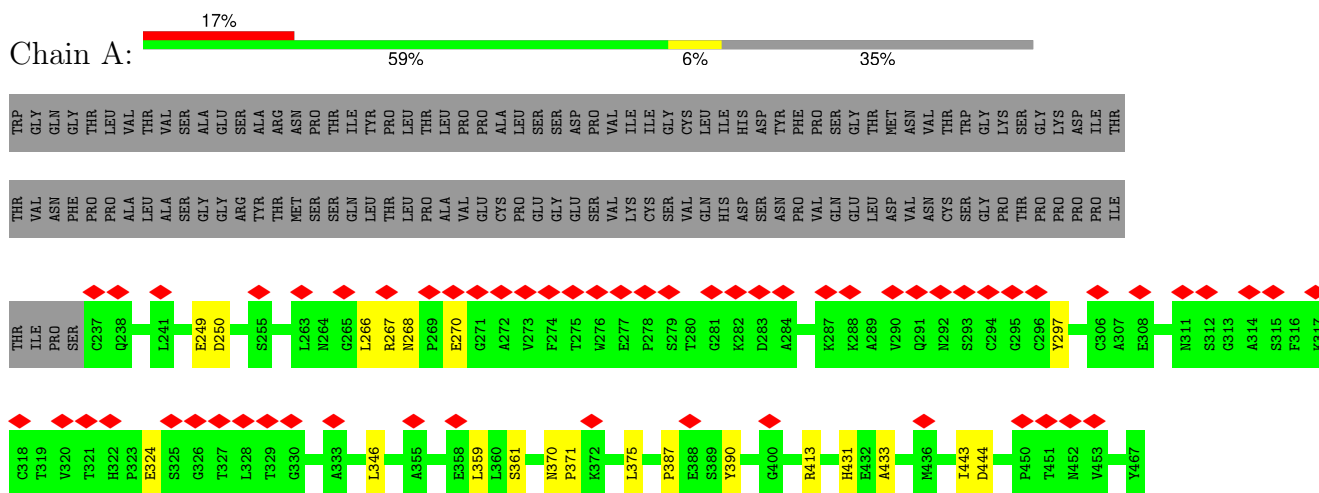


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	H	N	O	0
			24	8	10	1	5	
4	D	1	Total	C	H	N	O	0
			24	8	10	1	5	

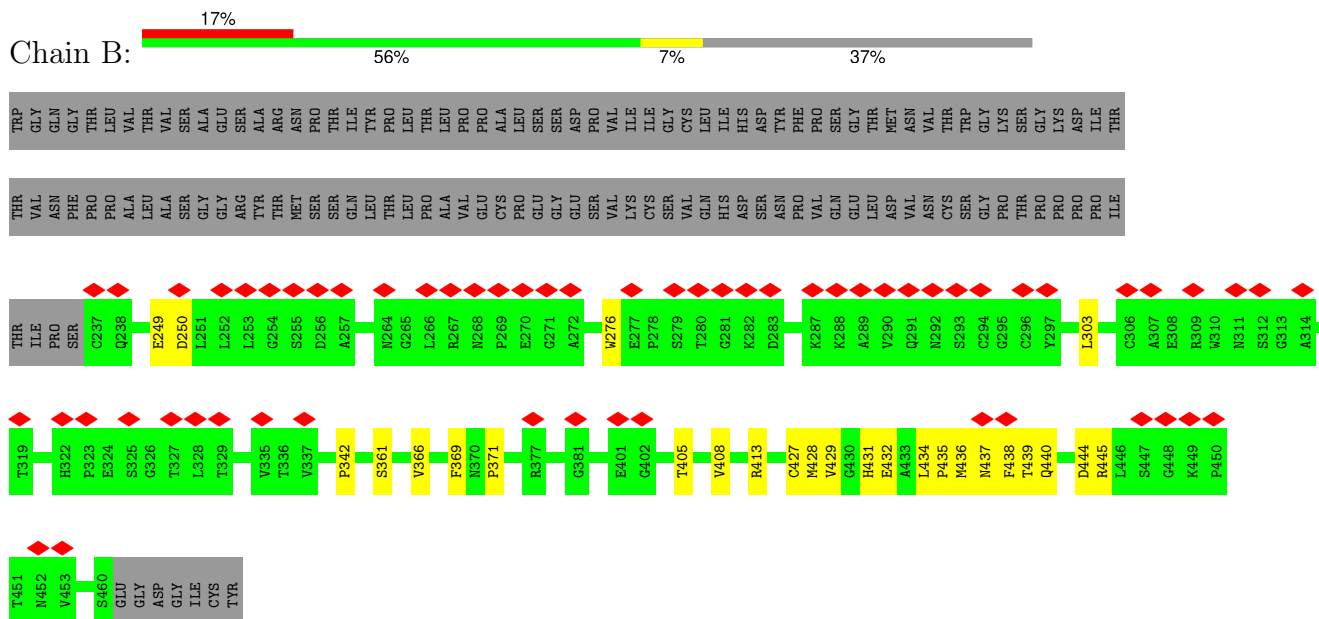
3 Residue-property plots [i](#)

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: Igh protein



- Molecule 1: Igh protein



- Molecule 1: Igh protein



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

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

THR ILE PRO C237 Q238 Q244 R245 L252 S255 I259 L263 N264 G265 L266 R267 E270 Q271 A272 T275 W276 T280 G281 K282 D283 Q286 K287 K288 A289 V290 Q291 N292 S293 C296 Y297 S298 E306 R309 W310 N311 S312 G313 A314 T319 V320 T321 H322 P323

E324 S325 G326 T327 G330 K334 V335 T336 V344 E353 E358 L359 V366 F369 N370 P371 K372 N382 L385 Y390 P395 A403 R413 V429 E430 H431 E432 A433 L434 F438 M452 S463 Y467

• Molecule 1: Igh protein



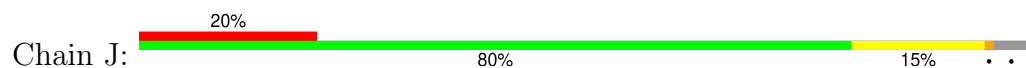
TRP GLY GLN GLY THR LEU VAL THR VAL VAL ALA ALA SER SER GLY SER ALA ARG ASN THR PRO THR ILE THR PRO THR LEU THR LEU VAL PRO PRO ALA ALA SER SER GLY GLY ARG TYR THR MET ASN SER SER GLN LEU THR PRO THR LEU VAL VAL PRO PRO GLU CYS ALA LEU SER SER GLY GLY SER VAL VAL ILE ILE CYS GLY LEU ILE HIS ASP ASP TYR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

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

THR ILE PRO C237 Q238 P239 Q240 L241 P246 L261 G264 S265 D266 A267 N264 G265 L266 R267 N268 P269 E270 G271 A272 V273 F274 T275 W276 E277 P278 S279 T280 G281 K282 D283 Q286 K287 K288 A289 V290 Q291 N292 S293 C294 G295 C296 Y297 L303 C306 A307 E308 W310

N311 S312 K317 T321 H322 P323 E324 S325 G326 T327 L328 T329 G330 T331 I332 N336 R367 A368 F369 N370 P371 E401 G402 L407 H431 E432 A433 L434 D444 R445 K449 P450 T451 N452 V453 S460 E461 G462 D463 G464 ILE CYS TYR

• Molecule 2: Immunoglobulin J chain



ASP ASP E3 I6 M13 C14 T15 R16 V17 T18 S19 R20 S24 T25 E26 D27 P28 N29 E30 D31 R46 E47 N48 I49 S54 P55 L56 R57 R58 D66 K69 V74 E75 V76 E77 L78 E79 V82 N92 E93 ASP ASP GLY V97 T100 C101 Y102 R106

N107 K108 Y118 H119 G120 E121 P131 D132 S133 C134 Y135 P136 ASP

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1 MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288823	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59808	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.347	Depositor
Minimum map value	-1.422	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.277	Depositor
Map size (Å)	300.96002, 300.96002, 300.96002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8360001, 0.8360001, 0.8360001	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: NAG

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	0.18	0/1788	0.43	0/2439
1	B	0.15	0/1735	0.45	0/2369
1	C	0.14	0/1780	0.41	0/2428
1	D	0.14	0/1756	0.41	0/2398
2	J	0.15	0/1058	0.42	0/1441
All	All	0.15	0/8117	0.42	0/11075

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 [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	1749	1722	1722	14	0
1	B	1697	1677	1679	28	0
1	C	1742	1715	1715	17	0
1	D	1718	1686	1686	9	0
2	J	1041	1008	1008	15	0
3	E	28	19	25	0	0
4	B	14	10	13	0	0
4	D	14	10	13	0	0
All	All	8003	7847	7861	80	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 5.

All (80) 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:434:LEU:CD1	1:B:435:PRO:HD2	1.67	1.24
1:B:434:LEU:HD12	1:B:435:PRO:CD	1.76	1.14
1:B:428:MET:HA	1:B:440:GLN:HG2	1.07	1.04
1:B:428:MET:HA	1:B:440:GLN:CG	1.86	1.03
1:B:434:LEU:HD12	1:B:435:PRO:HD2	1.06	1.03
1:B:428:MET:CA	1:B:440:GLN:HG2	1.90	1.00
1:B:429:VAL:O	1:B:439:THR:HG22	1.68	0.92
1:C:353:GLU:OE2	1:C:413:ARG:NH1	2.11	0.84
1:B:434:LEU:CD2	1:B:436:MET:O	2.31	0.78
1:B:434:LEU:HD23	1:B:436:MET:O	1.83	0.77
2:J:47:GLU:HB2	2:J:54:SER:OG	1.86	0.76
1:A:431:HIS:CE1	1:A:433:ALA:HB3	2.27	0.70
1:C:366:VAL:HG21	1:C:429:VAL:HG21	1.73	0.69
1:D:246:PRO:HG2	1:D:251:LEU:HD11	1.73	0.69
1:B:361:SER:OG	1:B:413:ARG:NH1	2.27	0.67
1:C:366:VAL:CG2	1:C:429:VAL:HG21	2.26	0.66
1:A:361:SER:OG	1:A:413:ARG:NH1	2.28	0.65
1:B:434:LEU:HG	1:B:436:MET:H	1.62	0.63
1:B:434:LEU:CG	1:B:435:PRO:HD2	2.29	0.62
1:D:276:TRP:CD2	1:D:303:LEU:HD12	2.34	0.62
1:B:276:TRP:CE3	1:B:303:LEU:HD22	2.36	0.61
1:D:278:PRO:HG3	1:D:303:LEU:HD11	1.86	0.57
1:D:278:PRO:HG3	1:D:303:LEU:CD1	2.35	0.56
1:B:249:GLU:O	1:B:250:ASP:HB2	2.04	0.56
1:B:444:ASP:OD1	1:B:445:ARG:N	2.37	0.56
1:B:342:PRO:HB3	1:B:369:PHE:CE1	2.41	0.56
1:D:278:PRO:O	1:D:279:SER:OG	2.12	0.55
2:J:13:MET:O	2:J:14:CYS:C	2.48	0.55
1:B:429:VAL:O	1:B:439:THR:CG2	2.49	0.55
1:C:244:GLN:O	1:C:259:ILE:HD12	2.06	0.55
1:C:371:PRO:HD2	1:C:431:HIS:NE2	2.21	0.55
1:A:267:ARG:N	1:A:324:GLU:OE1	2.40	0.54
1:B:434:LEU:HD12	1:B:435:PRO:HD3	1.81	0.53
1:C:344:VAL:HG22	1:C:366:VAL:HG22	1.89	0.53
1:D:370:ASN:HB3	1:D:371:PRO:HD3	1.90	0.53
1:A:444:ASP:OD2	2:J:46:ARG:NH2	2.43	0.52
1:B:437:ASN:O	1:B:438:PHE:CG	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:14:CYS:O	2:J:15:THR:HG23	2.12	0.50
2:J:6:ILE:HG12	2:J:18:THR:HG22	1.95	0.49
2:J:119:HIS:CG	2:J:119:HIS:O	2.65	0.49
1:A:370:ASN:HB3	1:A:371:PRO:HD3	1.96	0.48
1:B:439:THR:O	1:B:439:THR:HG23	2.13	0.48
1:C:252:LEU:HB3	1:C:438:PHE:CZ	2.48	0.48
1:B:369:PHE:O	1:B:405:THR:HA	2.15	0.47
1:D:276:TRP:CE3	1:D:303:LEU:HD12	2.49	0.47
1:C:370:ASN:N	1:C:371:PRO:CD	2.78	0.46
2:J:47:GLU:HA	2:J:57:ARG:HG3	1.97	0.46
2:J:76:VAL:O	2:J:82:VAL:HA	2.16	0.46
1:B:371:PRO:HG3	1:B:432:GLU:OE2	2.15	0.46
2:J:74:VAL:HG12	2:J:75:GLU:N	2.31	0.46
1:A:346:LEU:HB3	1:A:443:ILE:HD11	1.98	0.45
1:B:428:MET:CA	1:B:440:GLN:CG	2.71	0.45
1:A:250:ASP:OD1	2:J:118:TYR:OH	2.31	0.45
1:C:369:PHE:HZ	1:C:395:PRO:HB3	1.82	0.44
1:C:366:VAL:HG21	1:C:429:VAL:CG2	2.45	0.44
1:C:310:TRP:HB3	1:C:334:LYS:HD2	1.99	0.44
1:C:369:PHE:O	1:C:369:PHE:CD1	2.71	0.43
1:A:249:GLU:HB3	2:J:118:TYR:CE1	2.52	0.43
1:A:387:PRO:HA	1:A:390:TYR:CE2	2.53	0.43
2:J:15:THR:O	2:J:17:VAL:HG23	2.18	0.43
1:B:427:CYS:O	1:B:440:GLN:HG2	2.18	0.43
1:C:385:LEU:O	1:C:390:TYR:OH	2.27	0.43
2:J:47:GLU:N	2:J:55:PRO:O	2.49	0.43
1:B:429:VAL:HB	1:B:439:THR:HG23	2.01	0.43
1:C:369:PHE:CE1	1:C:372:LYS:HA	2.54	0.43
1:D:367:ARG:HG2	1:D:407:LEU:CD2	2.48	0.43
2:J:49:ILE:HG21	2:J:102:TYR:O	2.19	0.42
1:D:444:ASP:OD1	1:D:445:ARG:N	2.48	0.42
1:C:369:PHE:HE1	1:C:372:LYS:HA	1.84	0.42
1:A:266:LEU:HD12	1:A:297:TYR:HB2	2.02	0.42
1:A:359:LEU:HD23	1:A:413:ARG:HH21	1.85	0.42
1:A:249:GLU:HG2	1:A:375:LEU:HD22	2.01	0.42
1:C:353:GLU:HG2	1:C:359:LEU:O	2.21	0.41
1:A:266:LEU:HD12	1:A:266:LEU:C	2.46	0.41
1:B:369:PHE:CE1	1:B:431:HIS:HB2	2.56	0.41
1:C:432:GLU:O	1:C:434:LEU:N	2.52	0.41
1:B:366:VAL:HG23	1:B:408:VAL:HB	2.03	0.40
1:A:268:ASN:ND2	1:A:270:GLU:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:CD1	1:B:435:PRO:CD	2.56	0.40
2:J:66:ASP:O	2:J:69:LYS:HE2	2.21	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	229/355 (64%)	216 (94%)	13 (6%)	0	100	100
1	B	222/355 (62%)	205 (92%)	17 (8%)	0	100	100
1	C	229/355 (64%)	206 (90%)	23 (10%)	0	100	100
1	D	226/355 (64%)	215 (95%)	11 (5%)	0	100	100
2	J	127/137 (93%)	112 (88%)	15 (12%)	0	100	100
All	All	1033/1557 (66%)	954 (92%)	79 (8%)	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	201/309 (65%)	201 (100%)	0	100	100
1	B	196/309 (63%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	200/309 (65%)	200 (100%)	0	100	100
1	D	197/309 (64%)	195 (99%)	2 (1%)	73	84
2	J	125/130 (96%)	124 (99%)	1 (1%)	79	87
All	All	919/1366 (67%)	916 (100%)	3 (0%)	90	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	276	TRP
1	D	431	HIS
2	J	57	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
1	A	380	HIS
1	B	286	GLN
1	C	440	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	3,2	14,14,15	2.74	1 (7%)	17,19,21	4.00	3 (17%)
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	9.80	1.65	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	O5-C1-C2	-14.80	88.39	111.29
3	E	1	NAG	C4-C3-C2	5.42	118.97	111.02
3	E	1	NAG	C1-O5-C5	4.16	117.76	112.19

There are no chirality outliers.

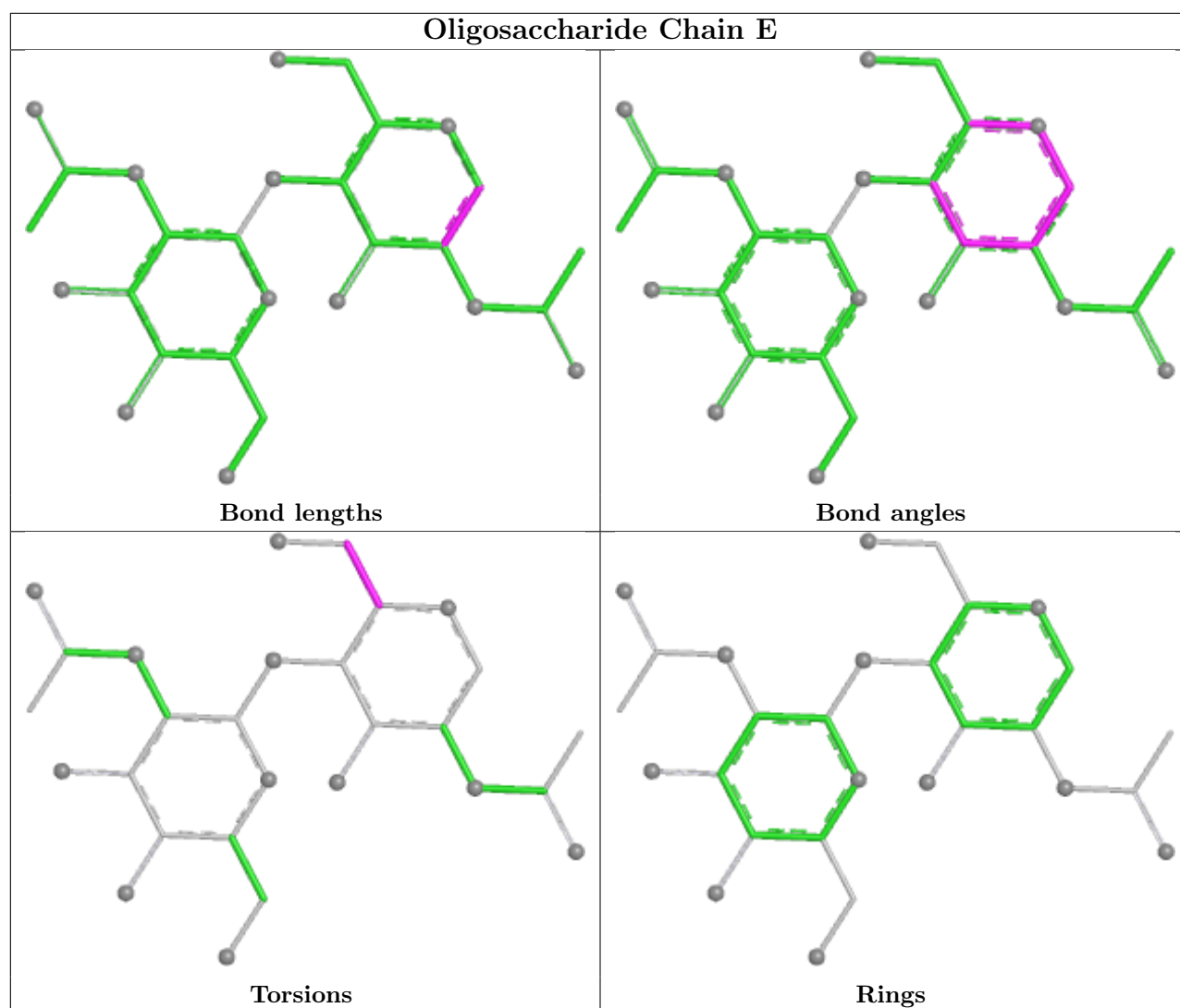
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	501	1	14,14,15	0.29	0	17,19,21	0.58	0
4	NAG	D	501	1	14,14,15	0.29	0	17,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	501	1	-	2/6/23/26	0/1/1/1
4	NAG	D	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	NAG	C1-C2-N2-C7
4	D	501	NAG	O5-C5-C6-O6
4	B	501	NAG	O5-C5-C6-O6
4	D	501	NAG	C4-C5-C6-O6

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.

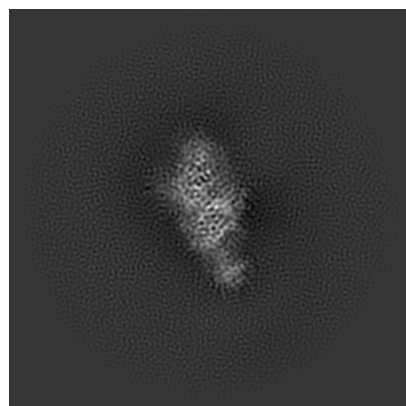
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22309. These allow visual inspection of the internal detail of the map and identification of artifacts.

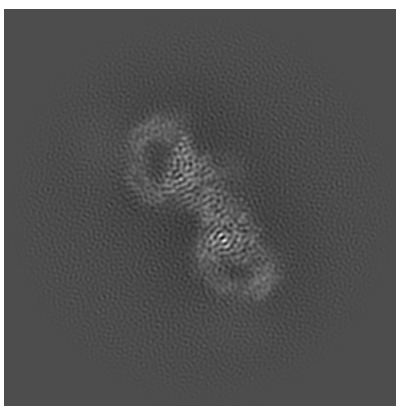
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

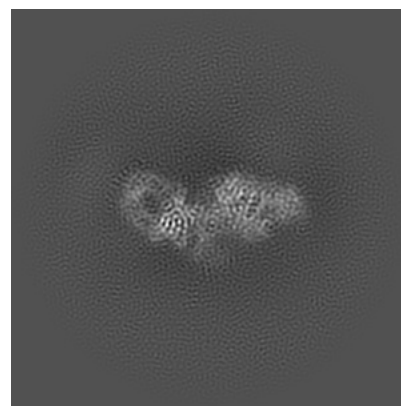
6.1.1 Primary map



X

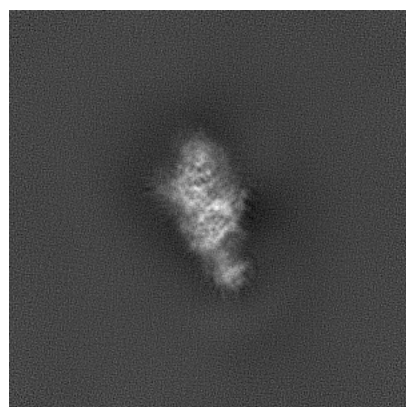


Y

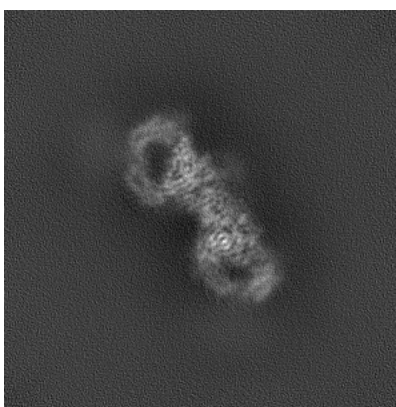


Z

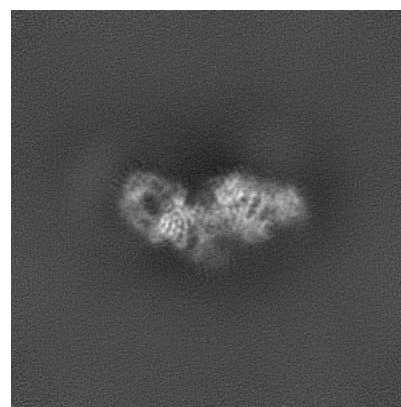
6.1.2 Raw map



X



Y

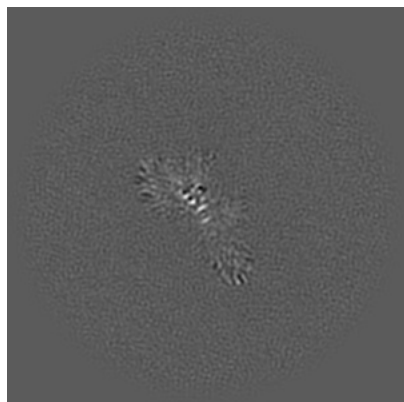


Z

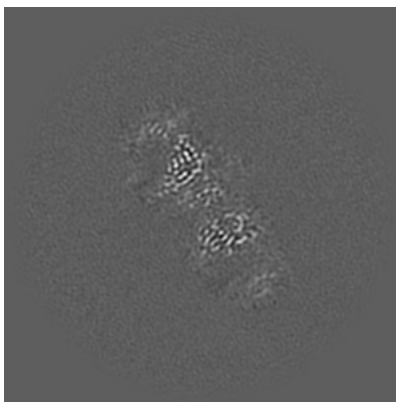
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

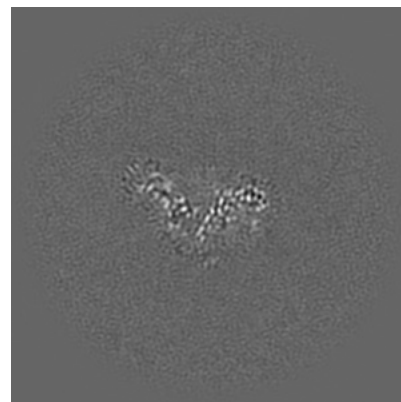
6.2.1 Primary map



X Index: 180

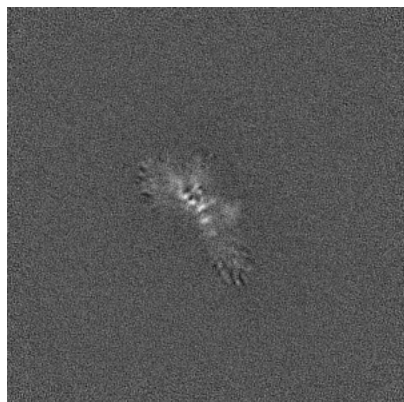


Y Index: 180

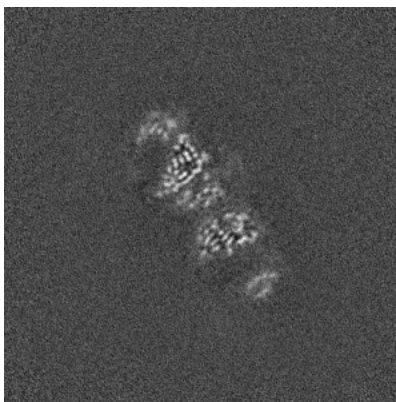


Z Index: 180

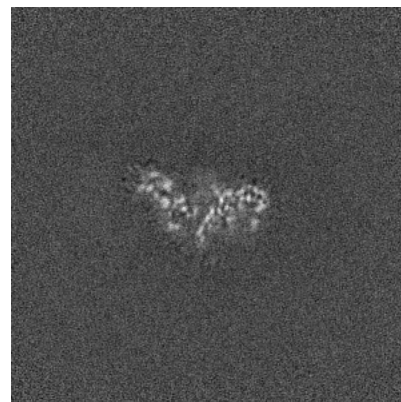
6.2.2 Raw map



X Index: 180



Y Index: 180

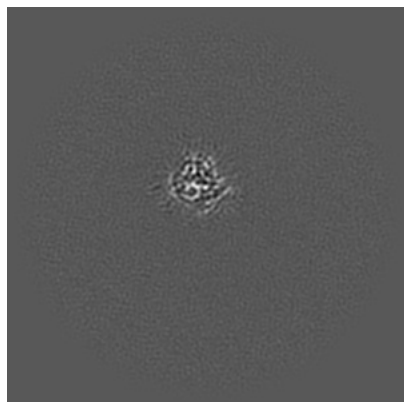


Z Index: 180

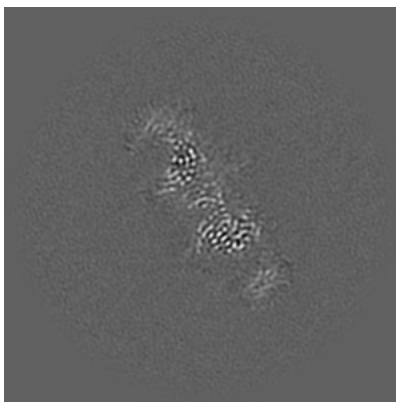
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

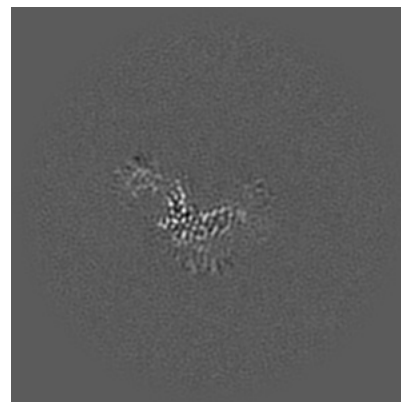
6.3.1 Primary map



X Index: 151

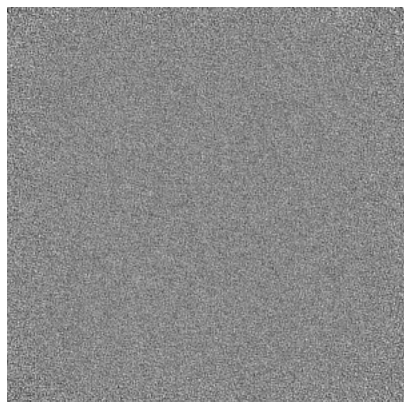


Y Index: 177

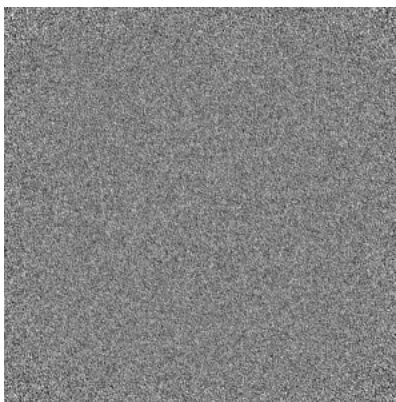


Z Index: 193

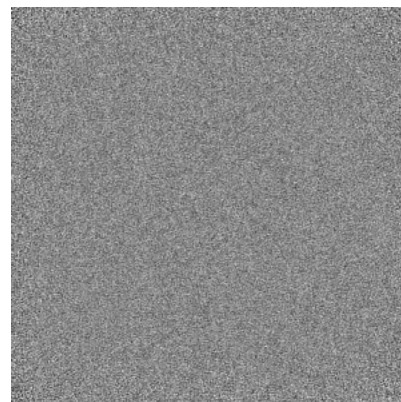
6.3.2 Raw map



X Index: 0



Y Index: 0

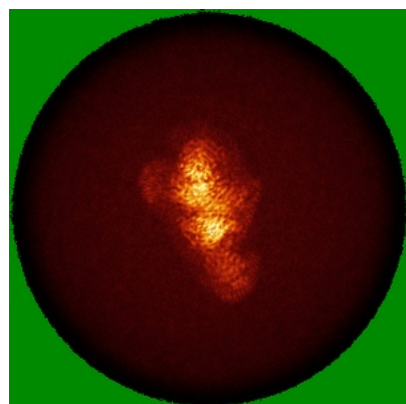


Z Index: 359

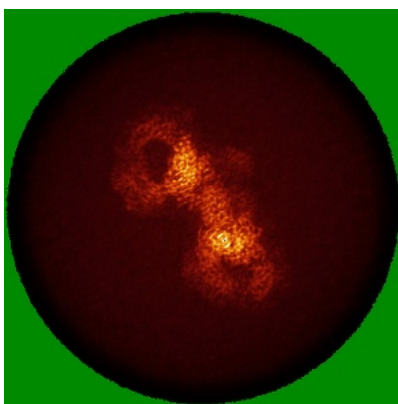
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

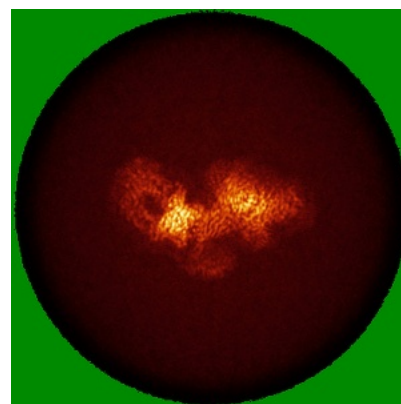
6.4.1 Primary map



X

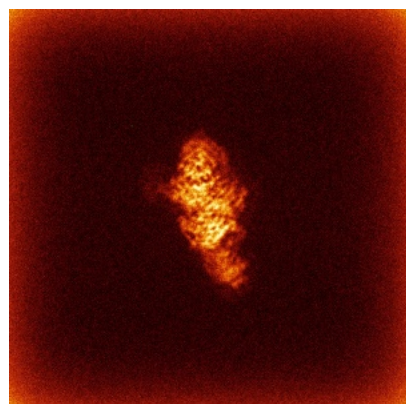


Y

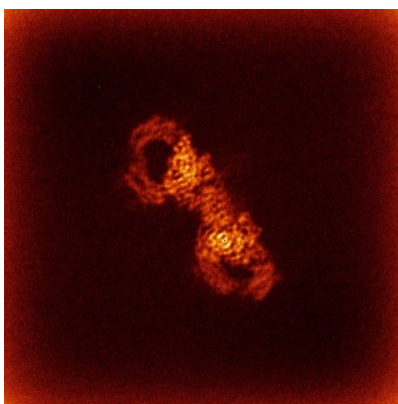


Z

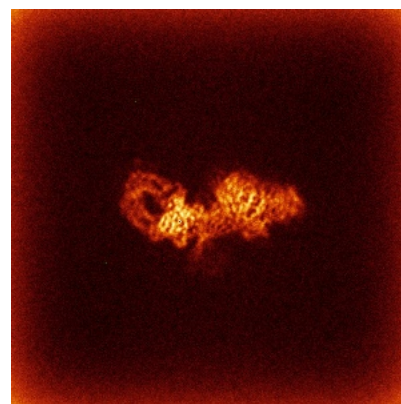
6.4.2 Raw map



X



Y

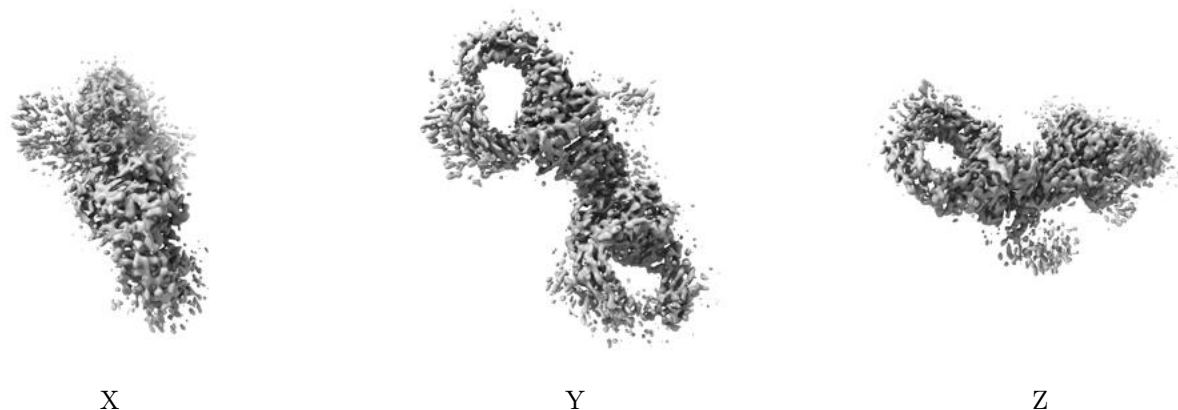


Z

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

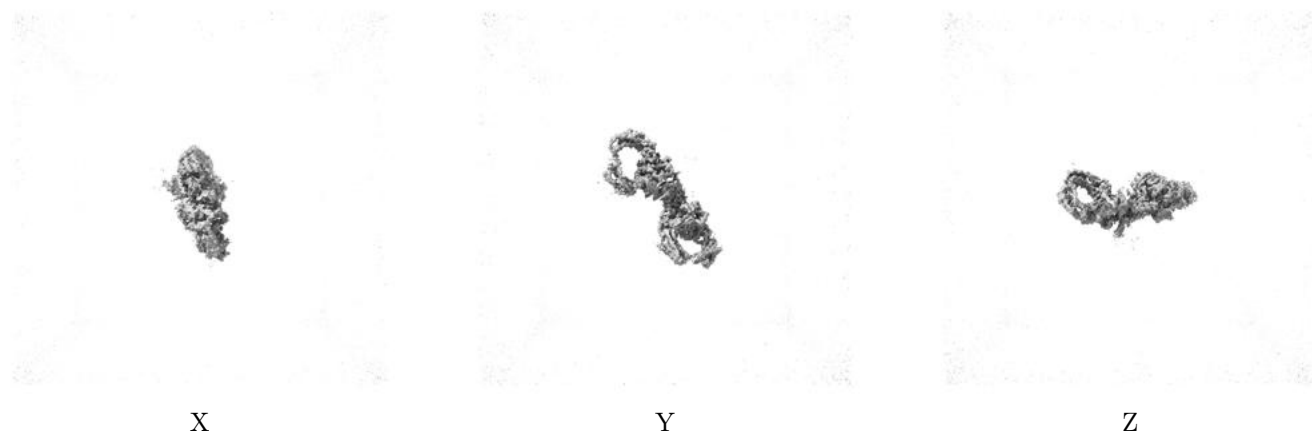
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.277. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

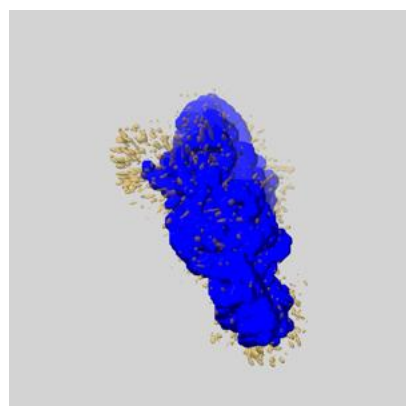
6.6 Mask visualisation [i](#)

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

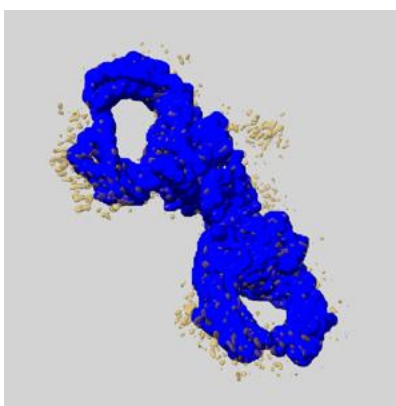
A mask typically either:

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

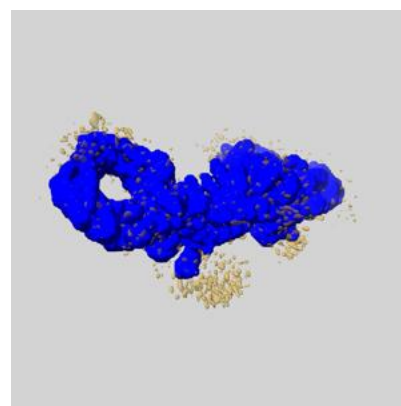
6.6.1 emd_22309_msk_1.map [i](#)



X



Y

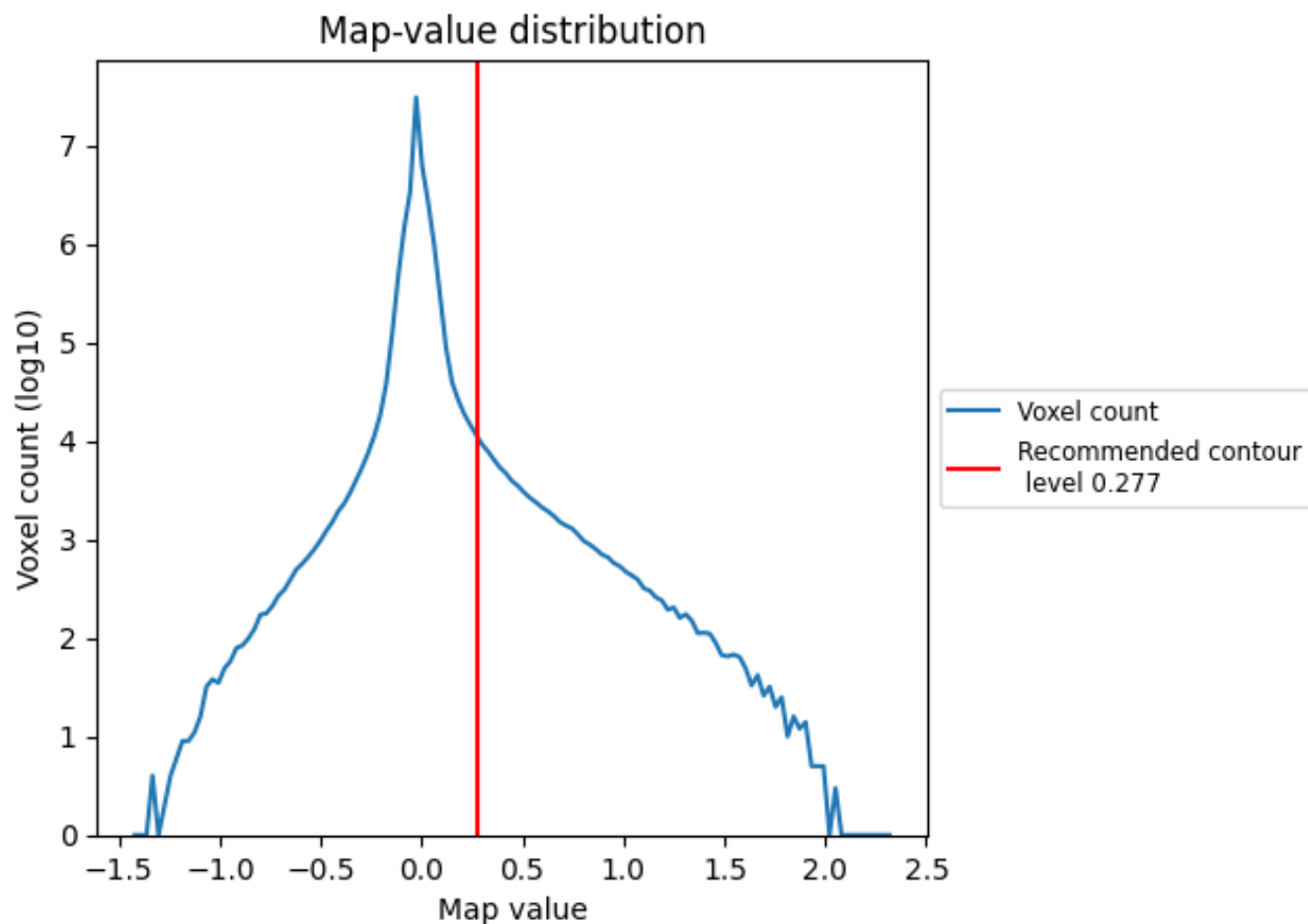


Z

7 Map analysis [i](#)

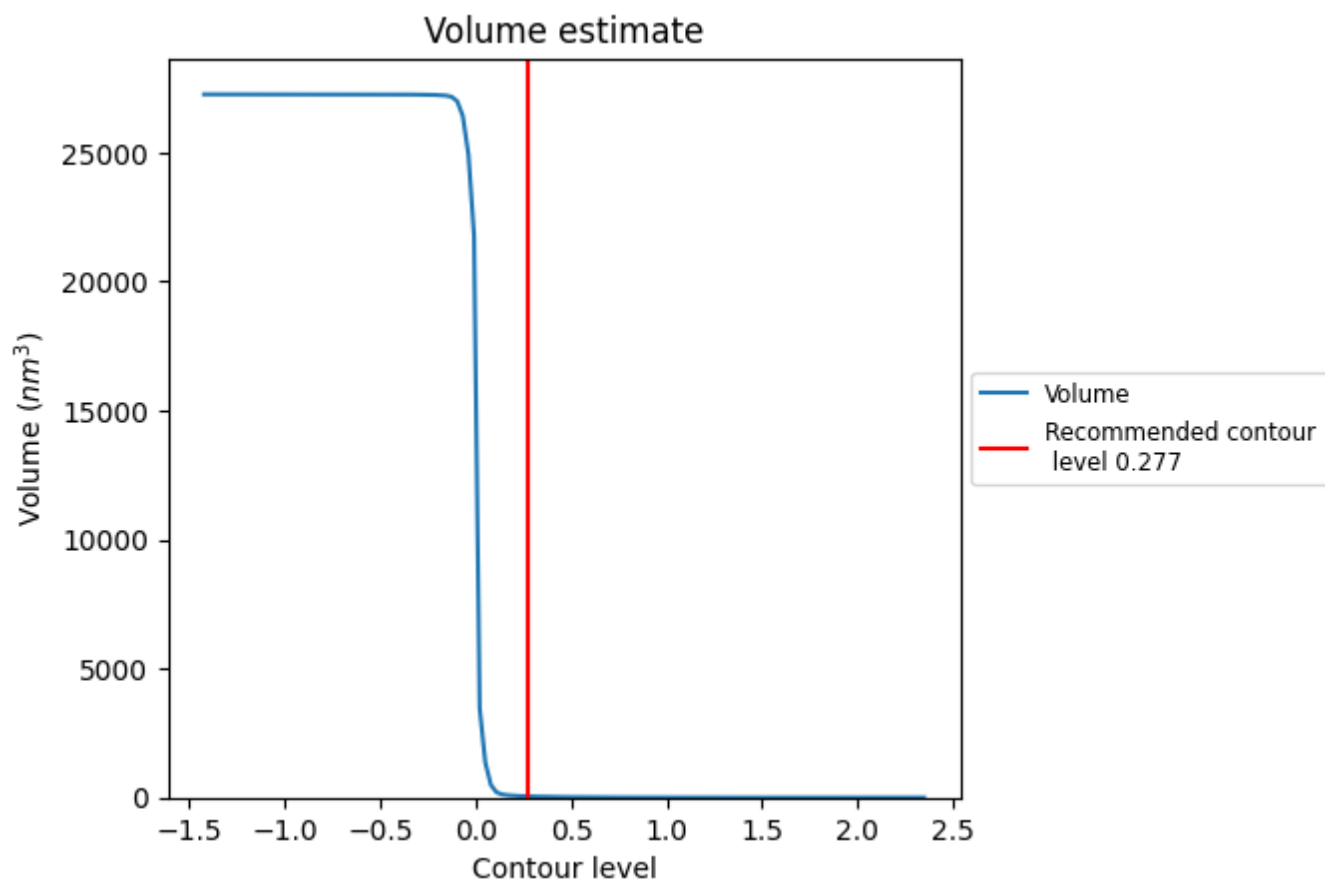
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

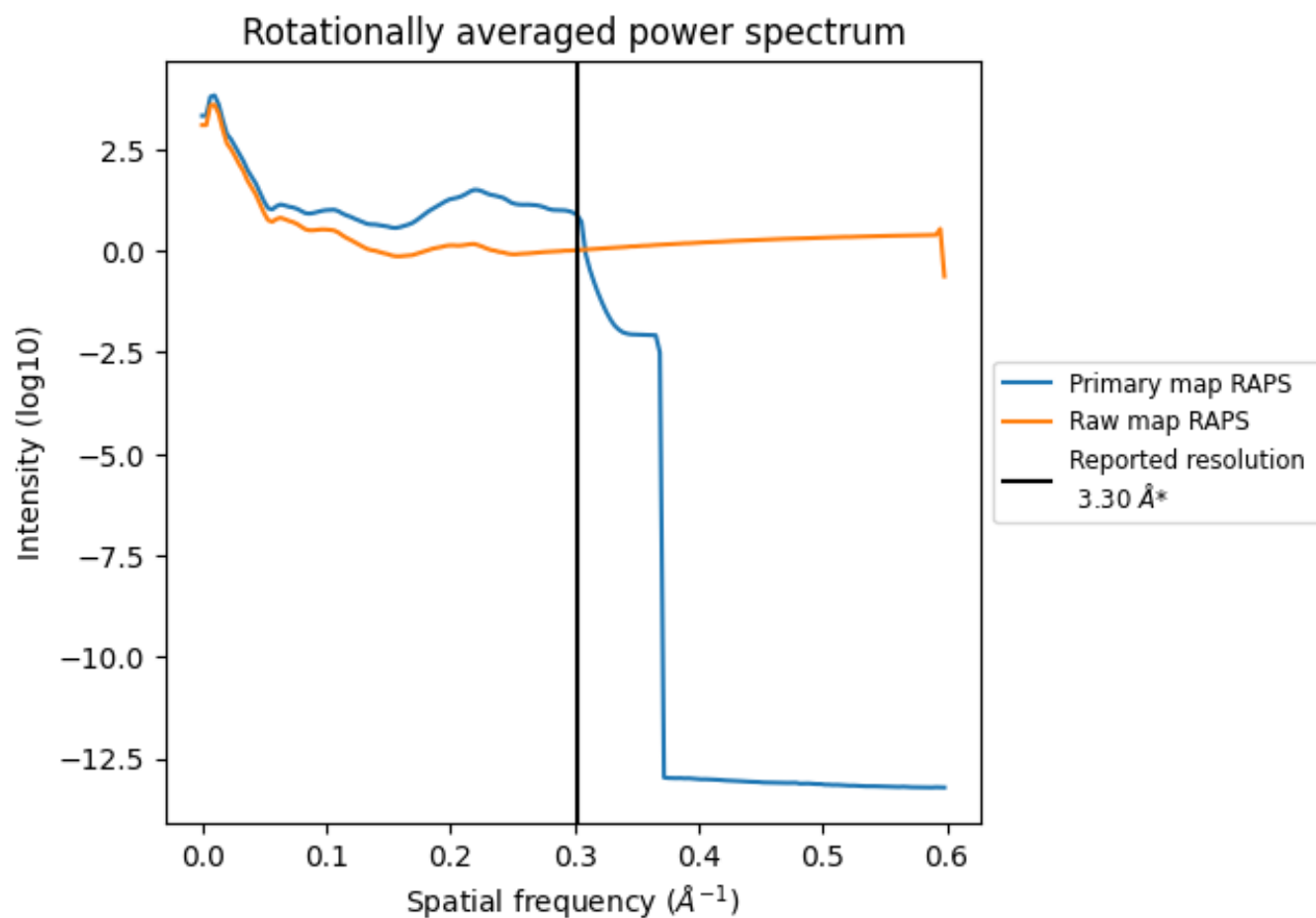
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm³; this corresponds to an approximate mass of 41 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 ⓘ

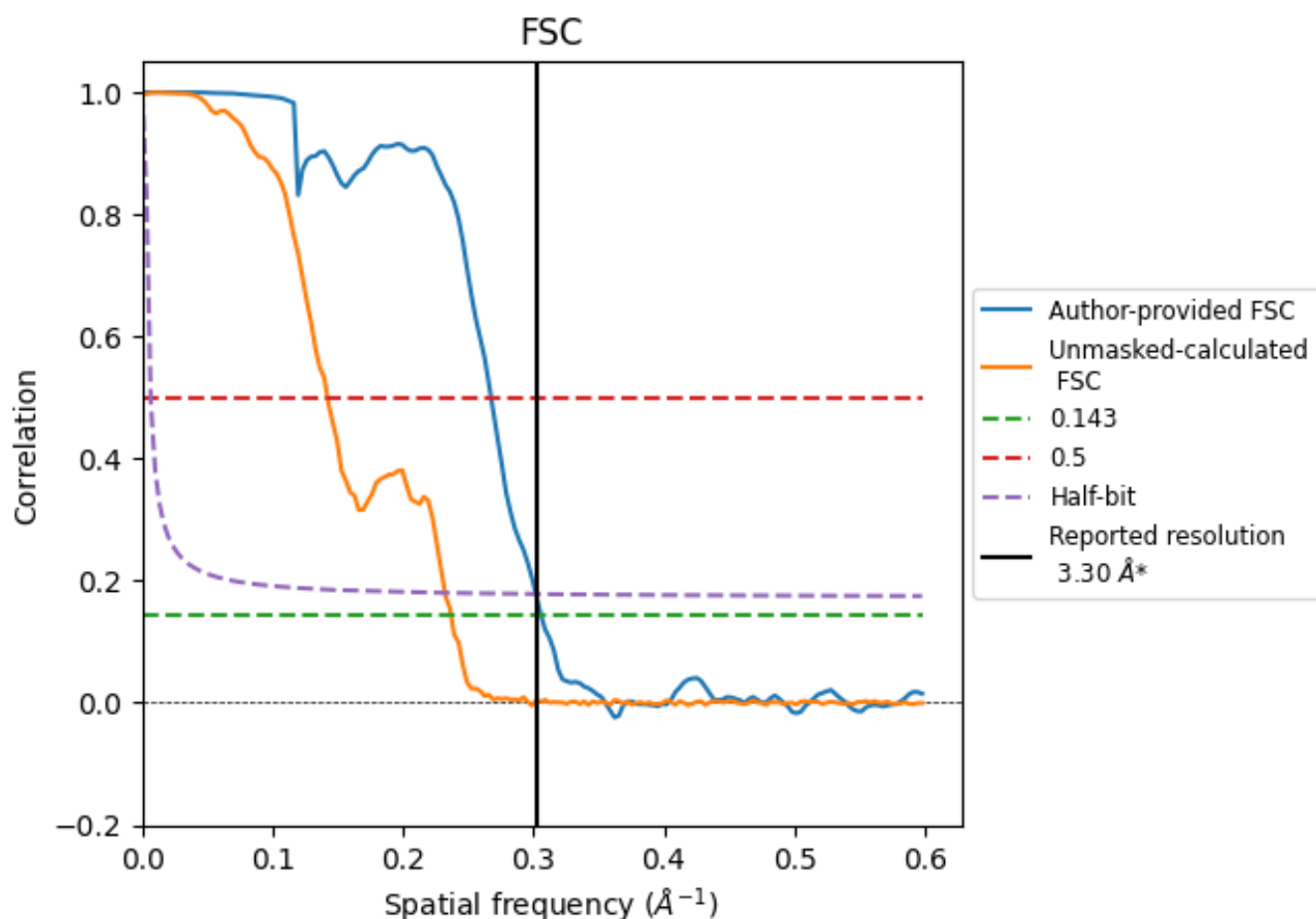


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

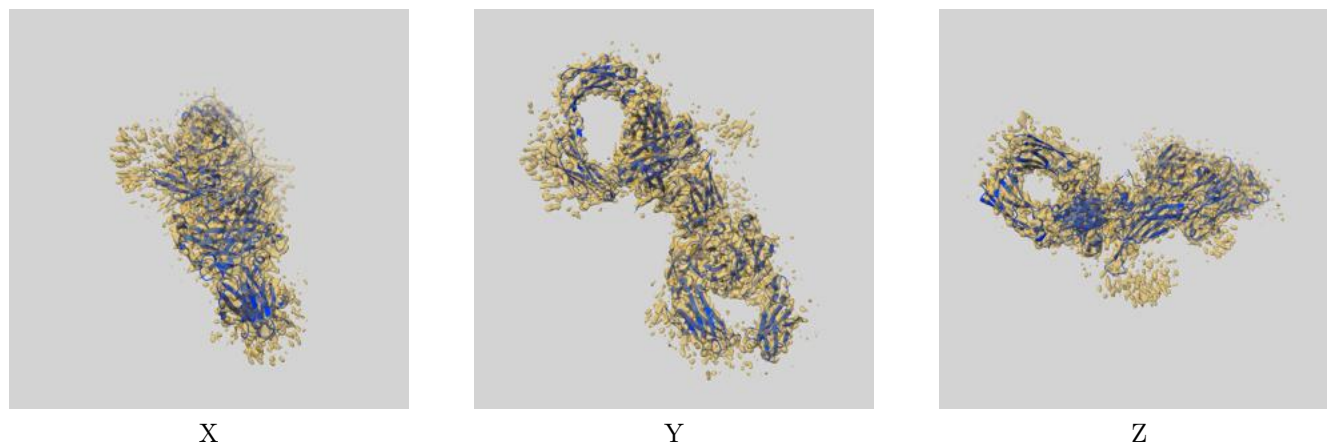
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.74	3.31
Unmasked-calculated*	4.22	7.04	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

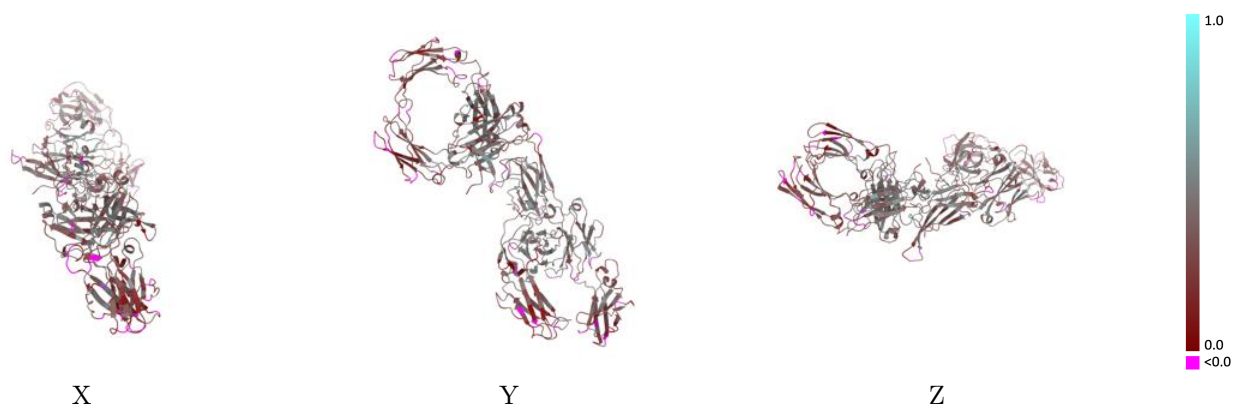
This section contains information regarding the fit between EMDB map EMD-22309 and PDB model 7JG1. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



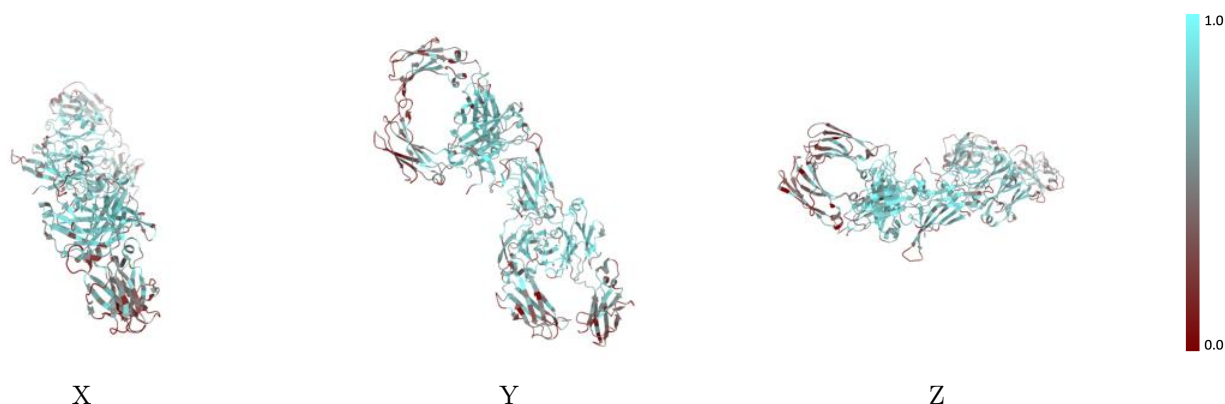
The images above show the 3D surface view of the map at the recommended contour level 0.277 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



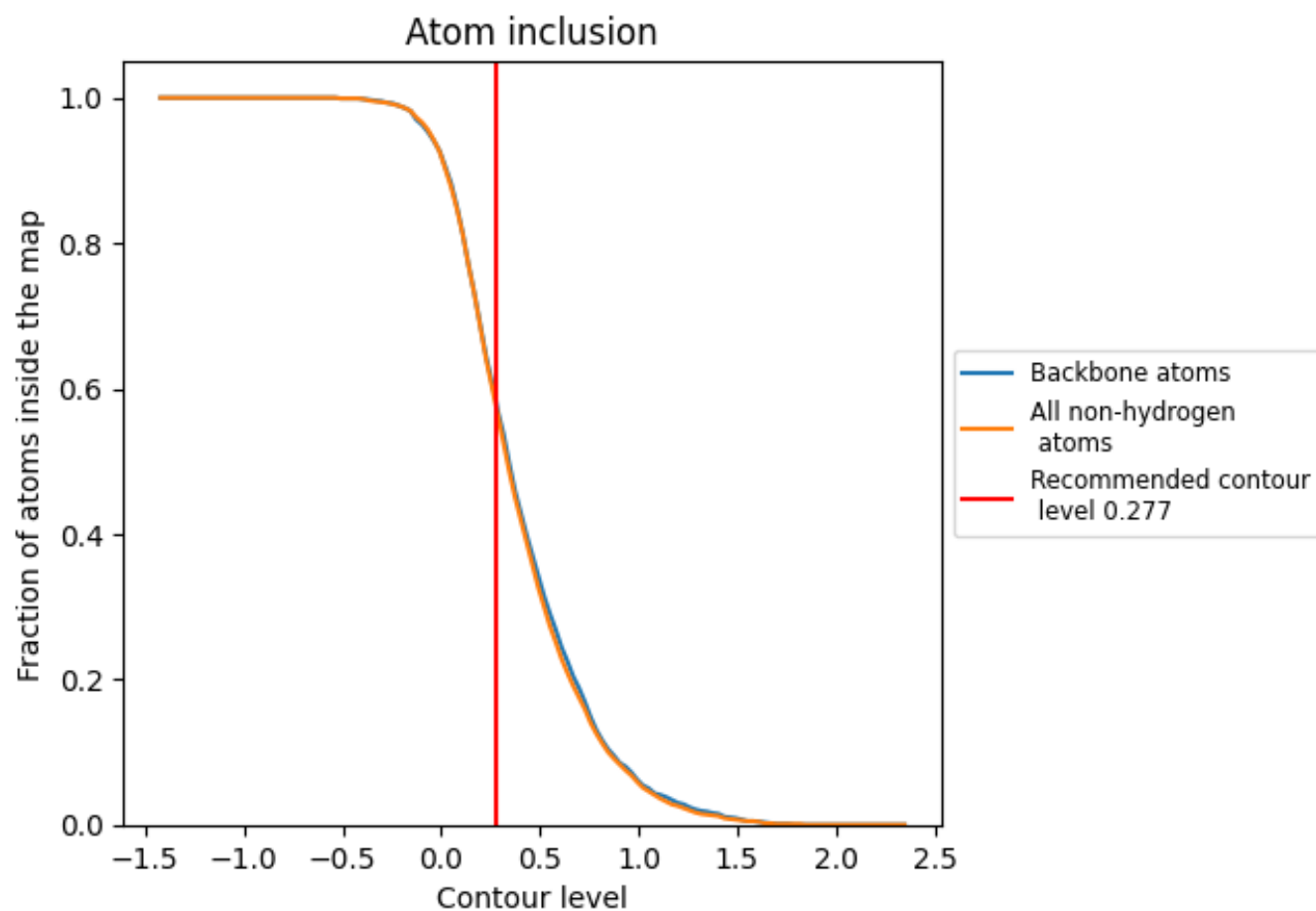
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.277).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.277) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.5780</div>	<div><div></div>0.3280</div>
A	<div><div></div>0.5740</div>	<div><div></div>0.3160</div>
B	<div><div></div>0.5400</div>	<div><div></div>0.3040</div>
C	<div><div></div>0.6240</div>	<div><div></div>0.3480</div>
D	<div><div></div>0.5550</div>	<div><div></div>0.3210</div>
E	<div><div></div>0.4640</div>	<div><div></div>0.3780</div>
J	<div><div></div>0.6200</div>	<div><div></div>0.3660</div>

1.0

0.0

<0.0