Full wwPDB EM Validation Report (i)

Oct 17, 2026 – 10:16 am BST

PDB ID	:	9TE8 / pdb_00009te8
EMDB ID	:	EMD-55823
Title	:	Cryo-EM structure of C5-CVFBb (state 1.1)
Authors	:	Joergensen, M.H.; Andersen, G.R.; Almeida, A.V.d.
Deposited on	:	2025-11-25
Resolution	:	3.48 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 (1)) were used in the production of this report:

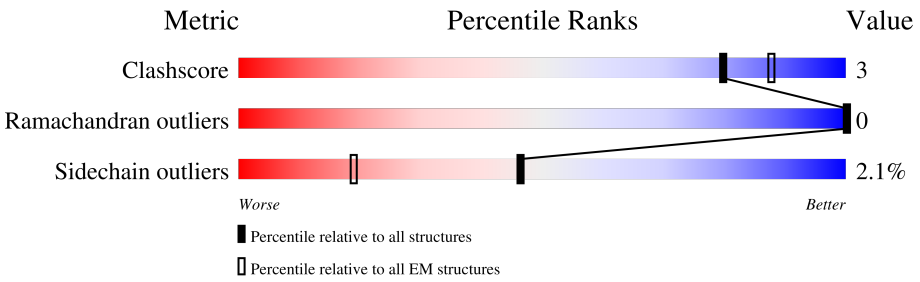
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

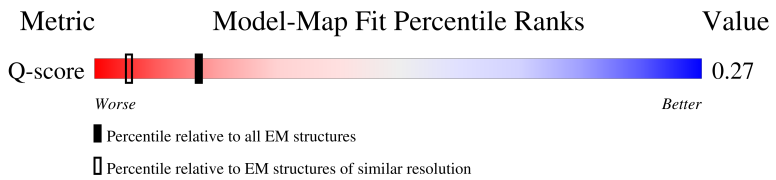
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.48 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13672 (2.98 - 3.98)

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	659	• 91% 9%
2	C	999	18% 89% 10%
3	B	627	• 93% 7%
4	D	252	10% 85% 7% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	379	19% 88% 10%
6	J	505	9% 87% 13%
7	F	5	80% 100%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 26956 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 Complement C5 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	658	5206	3336	842	1015	13	0	0

- Molecule 2 is a protein called Complement C5 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	999	7914	5055	1324	1494	41	0	0

- Molecule 3 is a protein called Cobra venom factor alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	626	4893	3125	824	928	16	0	0

- Molecule 4 is a protein called Cobra venom factor gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	234	1865	1199	312	349	5	0	0

- Molecule 5 is a protein called Cobra venom factor beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	373	3007	1895	507	585	20	0	0

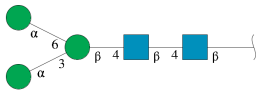
- Molecule 6 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	505	4007	2546	689	752	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	279	GLY	ASP	engineered mutation	UNP P00751
J	699	ALA	SER	engineered mutation	UNP P00751

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	F	5	61	34	2	25	0	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	J	1	1	1	0

- Molecule 9 is water.

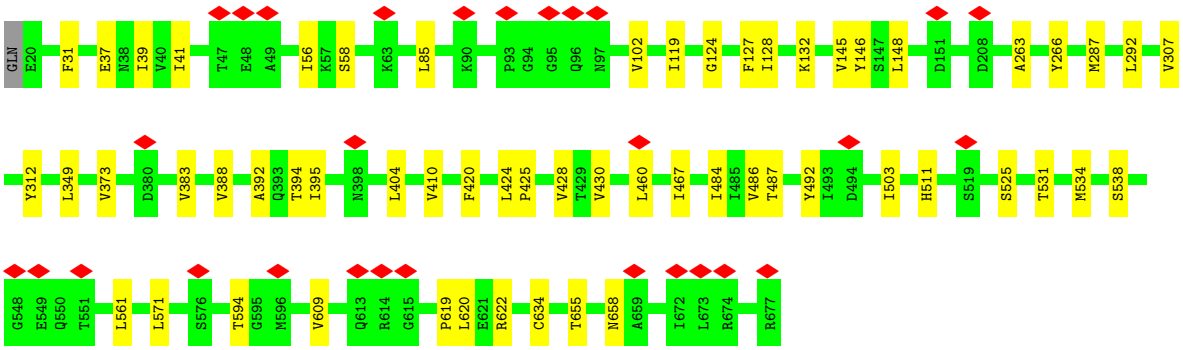
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
9	E	1	1	1	0
			Total	O	
9	J	1	1	1	0

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.

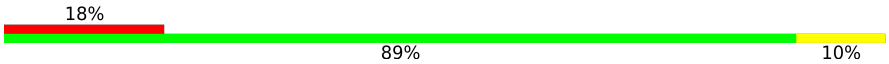
- Molecule 1: Complement C5 beta chain

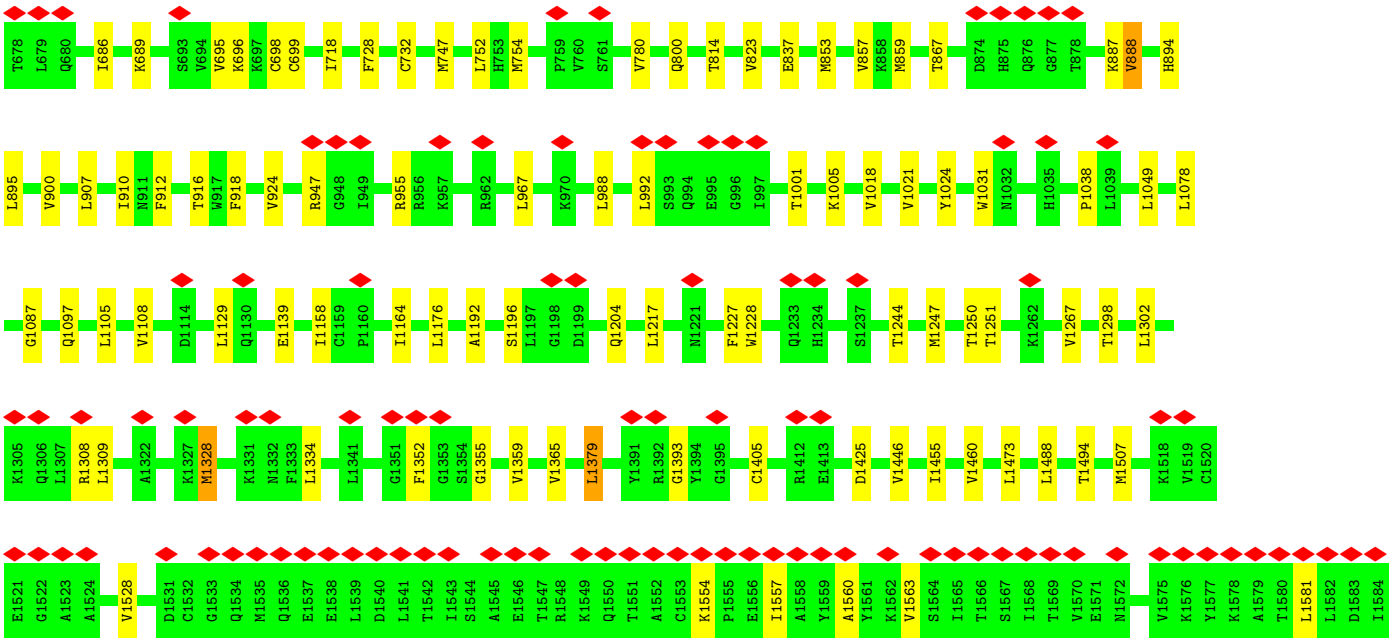
Chain A:

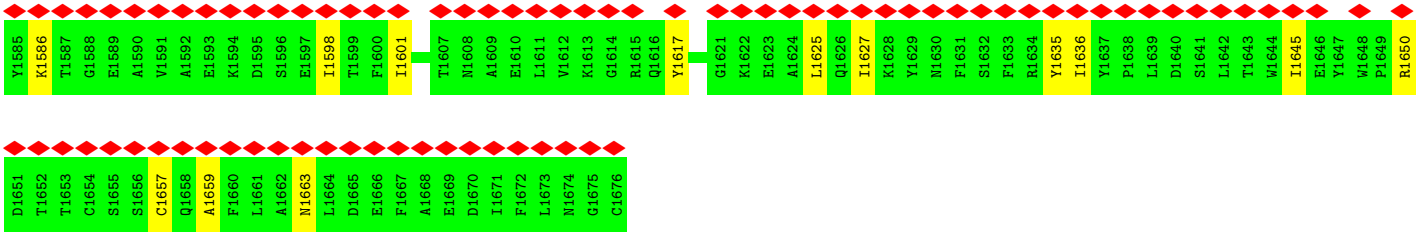


- Molecule 2: Complement C5 alpha chain

Chain C:

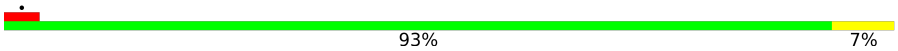


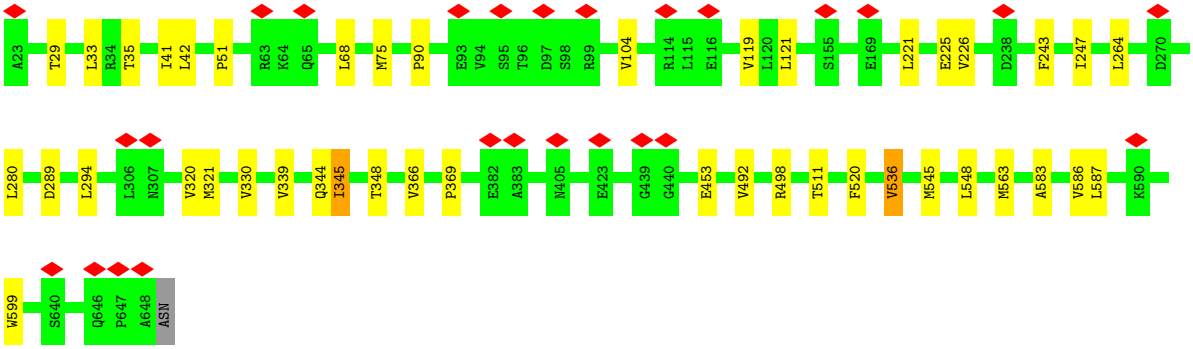




- Molecule 3: Cobra venom factor alpha chain

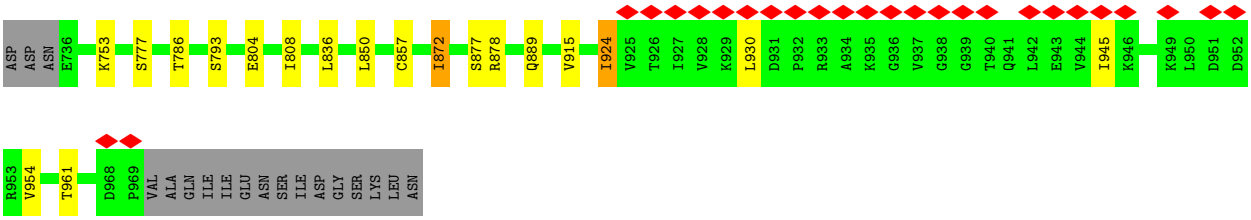
Chain B:





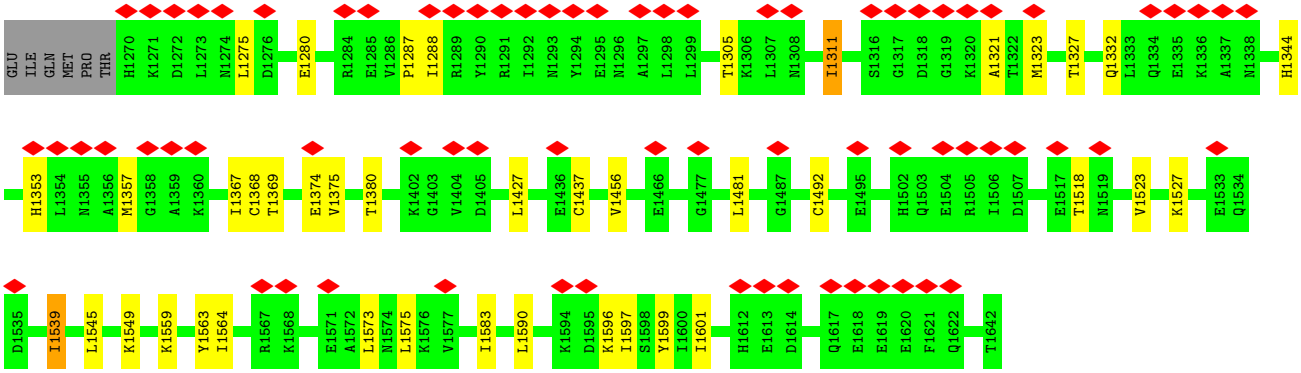
- Molecule 4: Cobra venom factor gamma chain

Chain D:



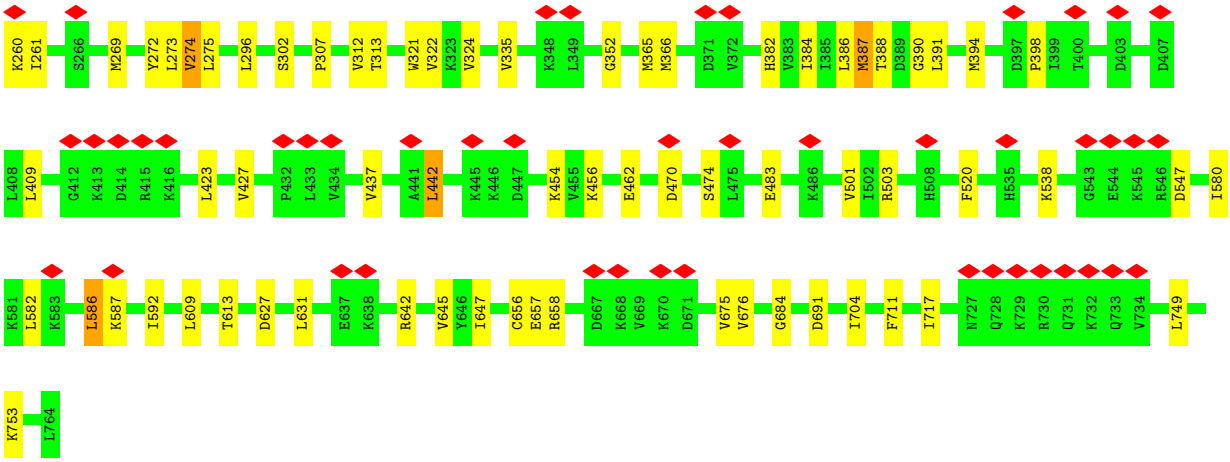
- Molecule 5: Cobra venom factor beta chain

Chain E:



- Molecule 6: Complement factor B

Chain J: 9% 87% 13%



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 80% 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	59.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.227	Depositor
Minimum map value	-0.489	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	387.0, 387.0, 387.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.29, 1.29, 1.29	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, BMA, MAN, MG

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	0.25	0/5327	0.55	0/7244
2	C	0.28	0/8078	0.62	3/10940 (0.0%)
3	B	0.23	0/5004	0.54	2/6809 (0.0%)
4	D	0.24	0/1903	0.52	0/2582
5	E	0.22	0/3061	0.53	0/4140
6	J	0.27	0/4095	0.68	6/5542 (0.1%)
All	All	0.25	0/27468	0.59	11/37257 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
5	E	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1657	CYS	CA-CB-SG	6.18	128.62	114.40
6	J	658	ARG	CB-CG-CD	6.00	125.10	111.30
6	J	366	MET	CA-CB-CG	5.61	125.33	114.10
2	C	1308	ARG	CB-CG-CD	5.60	124.18	111.30
6	J	387	MET	CA-CB-CG	5.56	125.22	114.10
6	J	366	MET	CB-CG-SD	5.39	128.88	112.70
6	J	587	LYS	CA-CB-CG	5.39	124.87	114.10
6	J	387	MET	CB-CG-SD	5.31	128.62	112.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1328	MET	CB-CG-SD	5.28	128.53	112.70
3	B	453	GLU	CB-CG-CD	5.07	121.22	112.60
3	B	453	GLU	N-CA-C	-5.03	104.73	111.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	910	ILE	Peptide
5	E	1353	HIS	Peptide

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	5206	0	5127	26	0
2	C	7914	0	7936	49	0
3	B	4893	0	4896	19	0
4	D	1865	0	1906	14	0
5	E	3007	0	2958	21	0
6	J	4007	0	3997	30	0
7	F	61	0	52	0	0
8	J	1	0	0	0	0
9	E	1	0	0	0	0
9	J	1	0	0	0	0
All	All	26956	0	26872	146	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 (146) 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)
3:B:563:MET:O	4:D:777:SER:HA	1.87	0.74
6:J:313:THR:HG22	6:J:321:TRP:HE1	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:SER:HB2	1:A:561:LEU:HB2	1.77	0.67
3:B:548:LEU:HD22	4:D:793:SER:HB3	1.80	0.62
6:J:388:THR:HG23	6:J:390:GLY:H	1.65	0.61
6:J:454:LYS:HD2	6:J:456:LYS:H	1.66	0.60
5:E:1539:ILE:HG23	5:E:1564:ILE:HG12	1.87	0.57
2:C:1625:LEU:HB2	2:C:1636:ILE:HG23	1.88	0.56
5:E:1344:HIS:O	5:E:1369:THR:HA	2.06	0.56
2:C:916:THR:HG23	2:C:918:PHE:H	1.71	0.55
1:A:467:ILE:HG22	1:A:486:VAL:HG22	1.87	0.55
6:J:324:VAL:H	6:J:365:MET:HE1	1.71	0.55
6:J:269:MET:HG3	6:J:307:PRO:HB3	1.88	0.54
1:A:594:THR:HG21	2:C:780:VAL:HG21	1.90	0.54
2:C:1108:VAL:HG11	2:C:1164:ILE:HG22	1.90	0.54
6:J:645:VAL:HG12	6:J:691:ASP:HB3	1.89	0.54
4:D:954:VAL:HG22	5:E:1332:GLN:HG3	1.90	0.54
6:J:586:LEU:HD12	6:J:592:ILE:HG21	1.90	0.53
6:J:631:LEU:HD11	6:J:642:ARG:HB3	1.89	0.53
1:A:128:ILE:HG22	1:A:145:VAL:HG22	1.89	0.53
3:B:344:GLN:HE22	3:B:369:PRO:HA	1.74	0.53
5:E:1368:CYS:HA	5:E:1437:CYS:HB2	1.90	0.52
4:D:786:THR:HA	4:D:808:ILE:O	2.09	0.52
4:D:924:ILE:HG13	5:E:1327:THR:HB	1.92	0.52
1:A:571:LEU:HD13	1:A:594:THR:HG22	1.92	0.52
6:J:274:VAL:HA	6:J:312:VAL:O	2.09	0.52
6:J:352:GLY:HA3	6:J:394:MET:HE1	1.91	0.52
2:C:837:GLU:HG2	2:C:1488:LEU:HA	1.93	0.51
6:J:386:LEU:HD12	6:J:427:VAL:HG13	1.92	0.51
2:C:1228:TRP:HE3	2:C:1251:THR:HG22	1.75	0.51
2:C:1087:GLY:HA2	2:C:1158:ILE:HD11	1.93	0.51
2:C:1405:CYS:HA	2:C:1473:LEU:O	2.10	0.51
2:C:1601:ILE:HB	2:C:1636:ILE:HD11	1.93	0.50
6:J:538:LYS:HB2	6:J:547:ASP:HB3	1.92	0.50
6:J:398:PRO:HB2	6:J:442:LEU:HD21	1.92	0.50
1:A:31:PHE:HZ	1:A:39:ILE:HD11	1.77	0.50
2:C:1563:VAL:HG12	2:C:1581:LEU:HA	1.94	0.50
4:D:872:ILE:HD12	4:D:878:ARG:HB2	1.94	0.49
6:J:684:GLY:HA2	6:J:691:ASP:HB2	1.94	0.49
1:A:424:LEU:HB3	1:A:428:VAL:HG21	1.95	0.49
2:C:853:MET:O	2:C:887:LYS:HA	2.13	0.49
2:C:1129:LEU:HD22	2:C:1139:GLU:HB3	1.93	0.49
2:C:1425:ASP:HB3	2:C:1494:THR:HG23	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1598:ILE:HD11	2:C:1635:TYR:HB2	1.95	0.49
2:C:800:GLN:HG3	2:C:814:THR:HG23	1.95	0.49
1:A:395:ILE:HB	1:A:430:VAL:HB	1.95	0.48
1:A:373:VAL:HG21	1:A:388:VAL:HG11	1.94	0.48
6:J:627:ASP:HA	6:J:647:ILE:O	2.13	0.48
2:C:1176:LEU:HD22	2:C:1204:GLN:HB3	1.95	0.48
5:E:1280:GLU:HG2	5:E:1287:PRO:HB3	1.95	0.48
6:J:275:LEU:HA	6:J:387:MET:HB2	1.95	0.48
6:J:501:VAL:HG12	6:J:503:ARG:HG3	1.95	0.48
2:C:1379:LEU:HD23	2:C:1507:MET:HG2	1.96	0.48
6:J:462:GLU:HG3	6:J:483:GLU:HB3	1.96	0.48
2:C:988:LEU:HD23	2:C:1021:VAL:HG22	1.96	0.47
1:A:619:PRO:HA	1:A:622:ARG:HH12	1.79	0.47
4:D:930:LEU:HG	5:E:1323:MET:HE2	1.96	0.47
5:E:1563:TYR:HB3	5:E:1601:ILE:HD11	1.96	0.47
2:C:1455:ILE:HG22	2:C:1460:VAL:HG22	1.96	0.47
2:C:1560:ALA:HB3	2:C:1586:LYS:H	1.79	0.47
1:A:56:ILE:HG12	1:A:85:LEU:HD22	1.97	0.47
1:A:531:THR:H	1:A:534:MET:HE2	1.79	0.47
2:C:1244:THR:HB	2:C:1247:MET:HG2	1.96	0.47
6:J:272:TYR:HB2	6:J:384:ILE:HG22	1.95	0.47
2:C:718:ILE:HG12	2:C:1446:VAL:HG22	1.96	0.47
4:D:945:ILE:HB	5:E:1311:ILE:HG23	1.97	0.47
3:B:264:LEU:HB2	3:B:280:LEU:HD13	1.98	0.46
2:C:689:LYS:HD3	2:C:696:LYS:HD2	1.97	0.46
2:C:1507:MET:HE3	2:C:1507:MET:HB2	1.83	0.46
3:B:29:THR:HG22	3:B:41:ILE:HD12	1.97	0.46
1:A:127:PHE:HB2	1:A:146:TYR:HD2	1.79	0.46
6:J:409:LEU:HD22	6:J:423:LEU:HD12	1.97	0.46
5:E:1374:GLU:HG2	5:E:1375:VAL:HG13	1.97	0.46
6:J:260:LYS:HD3	6:J:470:ASP:HB3	1.98	0.46
5:E:1380:THR:HB	5:E:1427:LEU:HB2	1.98	0.46
1:A:503:ILE:HB	1:A:511:HIS:HB2	1.98	0.45
5:E:1527:LYS:HB2	5:E:1545:LEU:HD11	1.99	0.45
6:J:322:VAL:HG11	6:J:335:VAL:HG23	1.97	0.45
6:J:520:PHE:HA	6:J:580:ILE:O	2.16	0.45
2:C:888:VAL:HB	2:C:894:HIS:HB2	1.98	0.45
3:B:243:PHE:HB3	3:B:294:LEU:HB3	1.99	0.45
2:C:1031:TRP:HB3	2:C:1038:PRO:HB3	1.99	0.45
2:C:823:VAL:HG11	2:C:853:MET:HG3	1.99	0.45
5:E:1559:LYS:HD3	5:E:1596:LYS:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1105:LEU:HA	2:C:1108:VAL:HG12	1.98	0.45
2:C:1617:TYR:HD2	2:C:1645:ILE:HD11	1.81	0.45
2:C:1554:LYS:HB2	2:C:1557:ILE:HG12	1.99	0.45
5:E:1590:LEU:HD12	5:E:1599:TYR:HE1	1.82	0.45
2:C:859:MET:HE2	2:C:912:PHE:HE1	1.80	0.45
2:C:1018:VAL:HG13	2:C:1049:LEU:HD22	1.98	0.45
3:B:247:ILE:O	3:B:289:ASP:HA	2.17	0.45
2:C:1247:MET:HA	2:C:1250:THR:HG22	1.98	0.45
3:B:33:LEU:HD23	3:B:119:VAL:HG11	1.98	0.45
2:C:1309:LEU:HB3	2:C:1328:MET:HE1	1.99	0.44
1:A:124:GLY:HA3	1:A:148:LEU:O	2.18	0.44
5:E:1573:LEU:HD22	5:E:1575:LEU:HD21	2.00	0.44
6:J:272:TYR:HE2	6:J:365:MET:HE3	1.82	0.44
2:C:1192:ALA:O	2:C:1196:SER:HB2	2.18	0.43
4:D:889:GLN:HA	4:D:915:VAL:HB	1.99	0.43
1:A:31:PHE:HB2	1:A:119:ILE:HG22	1.99	0.43
6:J:657:GLU:HG2	6:J:676:VAL:HG11	1.99	0.43
2:C:686:ILE:HG23	2:C:689:LYS:HE3	2.00	0.43
6:J:609:LEU:HD13	6:J:613:THR:HG21	2.00	0.43
3:B:520:PHE:HB3	3:B:536:VAL:HG13	2.00	0.43
2:C:1097:GLN:HG2	2:C:1158:ILE:HG22	2.00	0.43
4:D:961:THR:HB	5:E:1305:THR:HG23	1.99	0.43
5:E:1275:LEU:HD13	5:E:1321:ALA:HB2	2.01	0.43
2:C:955:ARG:HH22	2:C:1352:PHE:HA	1.84	0.43
1:A:263:ALA:HB3	1:A:292:LEU:HD23	2.00	0.42
3:B:68:LEU:HD12	3:B:90:PRO:HD2	2.00	0.42
2:C:747:MET:HG2	2:C:1393:GLY:HA3	2.01	0.42
5:E:1518:THR:HG21	6:J:391:LEU:HB3	2.00	0.42
2:C:728:PHE:O	2:C:732:CYS:HB2	2.19	0.42
2:C:1024:TYR:HB2	2:C:1298:THR:HG23	2.01	0.42
2:C:1024:TYR:HA	2:C:1302:LEU:HD11	2.01	0.42
5:E:1367:ILE:HD11	5:E:1456:VAL:HG11	2.01	0.42
3:B:221:LEU:HD11	4:D:753:LYS:HG2	2.02	0.42
3:B:583:ALA:O	3:B:587:LEU:HB2	2.19	0.42
3:B:545:MET:HE3	3:B:599:TRP:HH2	1.84	0.42
1:A:425:PRO:HG3	3:B:498:ARG:HD3	2.01	0.42
6:J:749:LEU:O	6:J:753:LYS:HB2	2.20	0.41
2:C:1217:LEU:HB2	2:C:1227:PHE:O	2.20	0.41
6:J:704:ILE:HD11	6:J:711:PHE:HB3	2.02	0.41
1:A:132:LYS:HG2	1:A:609:VAL:HG11	2.03	0.41
1:A:307:VAL:HB	1:A:312:TYR:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:947:ARG:HH12	2:C:1355:GLY:H	1.68	0.41
3:B:225:GLU:HG2	3:B:586:VAL:HG21	2.02	0.41
1:A:266:TYR:HB3	2:C:752:LEU:HD22	2.02	0.41
2:C:867:THR:HG22	2:C:900:VAL:HG12	2.02	0.41
2:C:967:LEU:HD13	2:C:1365:VAL:HG23	2.02	0.41
3:B:42:LEU:HD13	3:B:492:VAL:HG11	2.03	0.41
3:B:226:VAL:HG21	3:B:320:VAL:HG21	2.02	0.41
5:E:1523:VAL:HG23	5:E:1549:LYS:HE2	2.02	0.41
2:C:695:VAL:O	2:C:698:CYS:HB3	2.21	0.41
1:A:287:MET:HE2	1:A:287:MET:HB3	1.86	0.41
4:D:857:CYS:HB2	5:E:1492:CYS:HB2	1.86	0.41
6:J:382:HIS:O	6:J:423:LEU:HA	2.21	0.41
1:A:392:ALA:HB3	1:A:404:LEU:HB2	2.02	0.41
3:B:345:ILE:HG22	3:B:366:VAL:HG22	2.03	0.41
4:D:836:LEU:O	4:D:877:SER:HA	2.20	0.41
1:A:394:THR:HG23	1:A:428:VAL:HG13	2.03	0.40
1:A:484:ILE:O	1:A:525:SER:HA	2.21	0.40
2:C:1659:ALA:O	2:C:1663:ASN:HB2	2.20	0.40
3:B:51:PRO:HA	3:B:75:MET:O	2.20	0.40
1:A:655:THR:HG23	1:A:658:ASN:H	1.87	0.40
4:D:804:GLU:H	4:D:804:GLU:HG3	1.68	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	656/659 (100%)	634 (97%)	22 (3%)	0	100	100
2	C	997/999 (100%)	955 (96%)	42 (4%)	0	100	100
3	B	624/627 (100%)	606 (97%)	18 (3%)	0	100	100
4	D	232/252 (92%)	225 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	371/379 (98%)	361 (97%)	10 (3%)	0	100	100
6	J	503/505 (100%)	479 (95%)	24 (5%)	0	100	100
All	All	3383/3421 (99%)	3260 (96%)	123 (4%)	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	583/584 (100%)	570 (98%)	13 (2%)	45	65
2	C	886/886 (100%)	868 (98%)	18 (2%)	48	66
3	B	547/548 (100%)	537 (98%)	10 (2%)	51	69
4	D	211/227 (93%)	208 (99%)	3 (1%)	59	71
5	E	339/345 (98%)	332 (98%)	7 (2%)	47	66
6	J	444/444 (100%)	431 (97%)	13 (3%)	37	61
All	All	3010/3034 (99%)	2946 (98%)	64 (2%)	46	66

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	41	ILE
1	A	58	SER
1	A	102	VAL
1	A	349	LEU
1	A	383	VAL
1	A	410	VAL
1	A	420	PHE
1	A	460	LEU
1	A	487	THR
1	A	492	TYR
1	A	620	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	634	CYS
2	C	699	CYS
2	C	754	MET
2	C	857	VAL
2	C	888	VAL
2	C	895	LEU
2	C	907	LEU
2	C	924	VAL
2	C	992	LEU
2	C	1001	THR
2	C	1005	LYS
2	C	1078	LEU
2	C	1267	VAL
2	C	1334	LEU
2	C	1359	VAL
2	C	1379	LEU
2	C	1528	VAL
2	C	1627	ILE
2	C	1650	ARG
3	B	35	THR
3	B	104	VAL
3	B	121	LEU
3	B	321	MET
3	B	330	VAL
3	B	339	VAL
3	B	345	ILE
3	B	348	THR
3	B	511	THR
3	B	536	VAL
4	D	850	LEU
4	D	872	ILE
4	D	924	ILE
5	E	1288	ILE
5	E	1311	ILE
5	E	1357	MET
5	E	1481	LEU
5	E	1539	ILE
5	E	1583	ILE
5	E	1597	ILE
6	J	261	ILE
6	J	273	LEU
6	J	274	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	J	296	LEU
6	J	302	SER
6	J	437	VAL
6	J	442	LEU
6	J	474	SER
6	J	582	LEU
6	J	586	LEU
6	J	656	CYS
6	J	675	VAL
6	J	717	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	179	HIS
1	A	320	ASN
1	A	423	ASN
1	A	483	ASN
1	A	533	ASN
1	A	562	ASN
1	A	570	GLN
1	A	574	HIS
1	A	586	GLN
1	A	591	ASN
1	A	642	ASN
1	A	658	ASN
2	C	692	HIS
2	C	1029	ASN
2	C	1043	GLN
2	C	1098	ASN
2	C	1125	GLN
2	C	1178	ASN
2	C	1204	GLN
2	C	1231	ASN
2	C	1233	GLN
2	C	1278	GLN
2	C	1324	HIS
2	C	1550	GLN
2	C	1616	GLN
2	C	1630	ASN
3	B	65	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	102	GLN
3	B	124	GLN
3	B	244	HIS
3	B	344	GLN
3	B	368	ASN
3	B	475	GLN
3	B	495	GLN
3	B	525	GLN
3	B	528	ASN
3	B	615	GLN
3	B	635	ASN
3	B	638	GLN
4	D	868	GLN
4	D	869	GLN
4	D	892	HIS
4	D	921	GLN
5	E	1293	ASN
5	E	1419	GLN
5	E	1537	ASN
5	E	1570	GLN
6	J	340	ASN
6	J	467	GLN
6	J	562	ASN
6	J	706	HIS
6	J	737	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

5 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	$\#\|Z\| > 2$
7	NAG	F	1	7,2	14,14,15	0.87	1 (7%)	17,19,21	1.81	7 (41%)
7	NAG	F	2	7	14,14,15	0.75	0	17,19,21	1.62	3 (17%)
7	BMA	F	3	7	11,11,12	1.09	1 (9%)	15,15,17	3.21	5 (33%)
7	MAN	F	4	7	11,11,12	0.80	0	15,15,17	1.37	2 (13%)
7	MAN	F	5	7	11,11,12	0.84	0	15,15,17	1.96	3 (20%)

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
7	NAG	F	1	7,2	-	4/6/23/26	0/1/1/1
7	NAG	F	2	7	-	1/6/23/26	0/1/1/1
7	BMA	F	3	7	-	1/2/19/22	0/1/1/1
7	MAN	F	4	7	-	2/2/19/22	0/1/1/1
7	MAN	F	5	7	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	3	BMA	C2-C3	2.95	1.56	1.52
7	F	1	NAG	C4-C5	2.06	1.57	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	3	BMA	C1-O5-C5	10.14	125.93	112.19
7	F	5	MAN	C1-O5-C5	5.65	119.85	112.19
7	F	2	NAG	O5-C1-C2	-4.89	103.57	111.29
7	F	3	BMA	C2-C3-C4	4.12	118.02	110.89
7	F	4	MAN	C1-O5-C5	3.46	116.89	112.19
7	F	1	NAG	O3-C3-C4	3.27	117.90	110.35
7	F	3	BMA	C1-C2-C3	3.04	113.40	109.67
7	F	1	NAG	O3-C3-C2	-2.84	103.60	109.47
7	F	2	NAG	C1-O5-C5	2.76	115.93	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	1	NAG	O5-C1-C2	-2.72	106.99	111.29
7	F	5	MAN	C2-C3-C4	2.55	115.31	110.89
7	F	1	NAG	C2-N2-C7	2.55	126.53	122.90
7	F	5	MAN	C1-C2-C3	2.49	112.72	109.67
7	F	1	NAG	C1-C2-N2	2.45	114.67	110.49
7	F	1	NAG	O5-C5-C6	2.36	110.91	107.20
7	F	4	MAN	C2-C3-C4	2.27	114.82	110.89
7	F	1	NAG	O4-C4-C5	2.14	114.61	109.30
7	F	3	BMA	O5-C1-C2	2.09	114.00	110.77
7	F	3	BMA	O2-C2-C1	-2.02	105.02	109.15
7	F	2	NAG	C4-C3-C2	2.02	113.98	111.02

There are no chirality outliers.

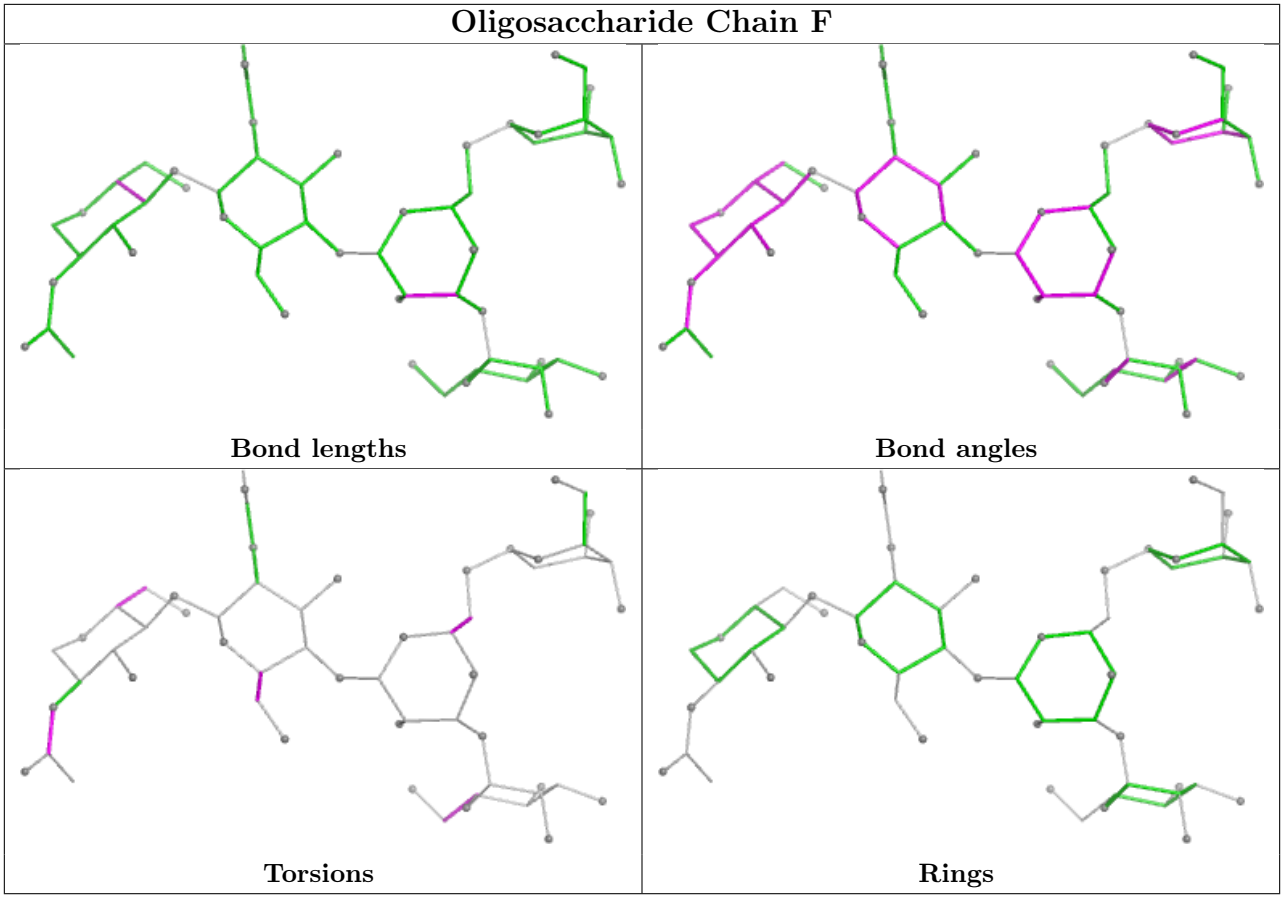
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	4	MAN	C4-C5-C6-O6
7	F	4	MAN	O5-C5-C6-O6
7	F	1	NAG	C8-C7-N2-C2
7	F	1	NAG	O7-C7-N2-C2
7	F	1	NAG	O5-C5-C6-O6
7	F	1	NAG	C4-C5-C6-O6
7	F	2	NAG	O5-C5-C6-O6
7	F	3	BMA	C4-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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

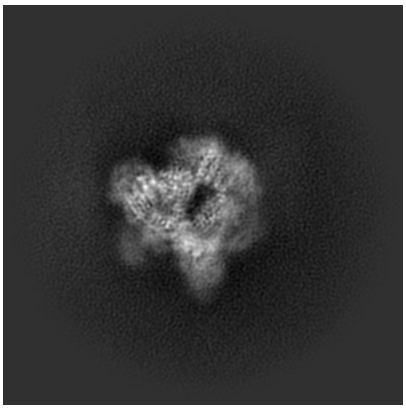
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55823. These allow visual inspection of the internal detail of the map and identification of artifacts.

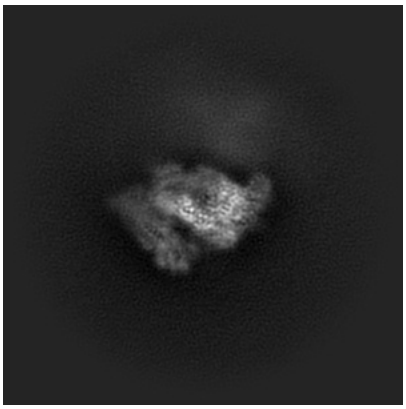
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

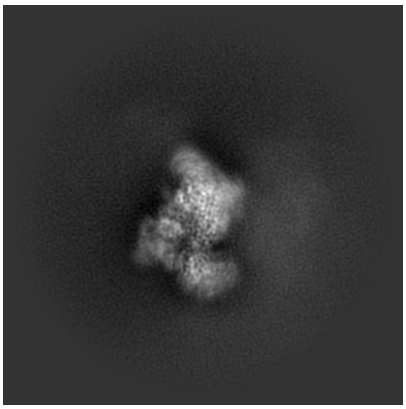
6.1.1 Primary map



X

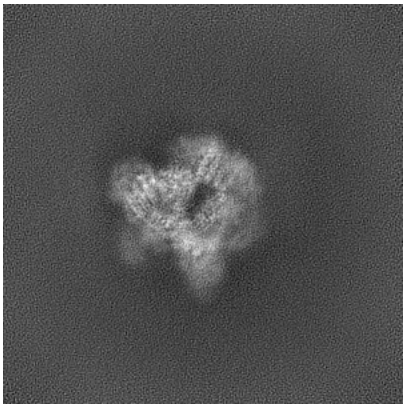


Y

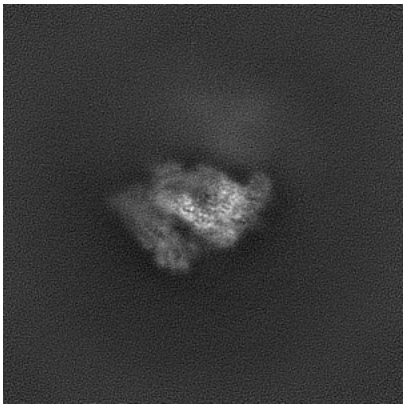


Z

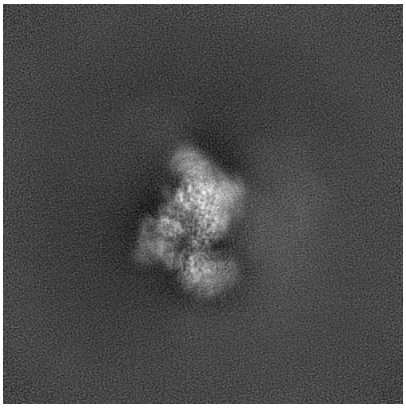
6.1.2 Raw map



X



Y

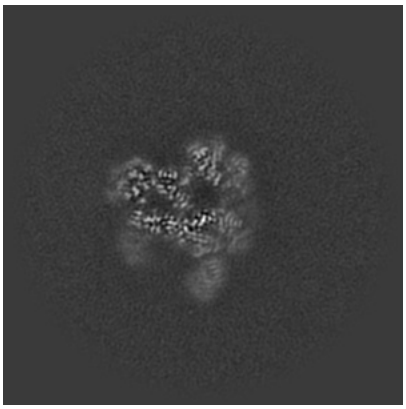


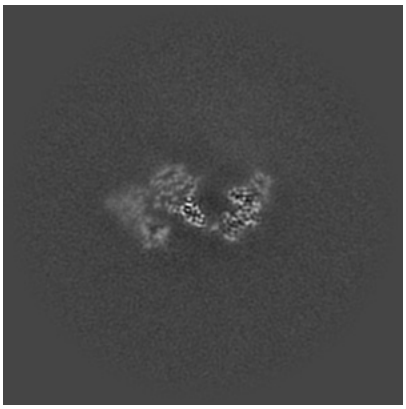
Z

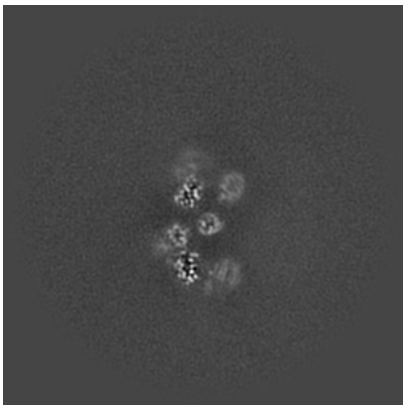
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

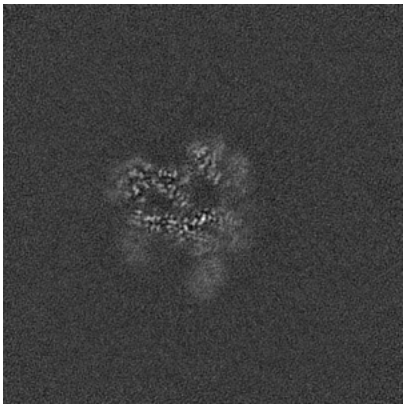
6.2.1 Primary map

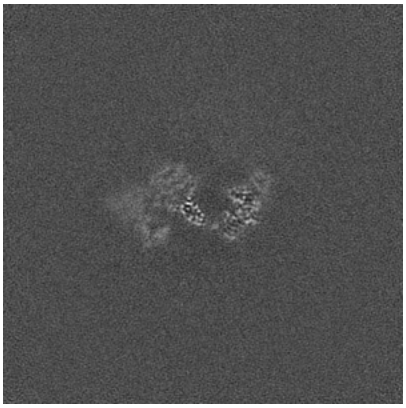

X Index: 150

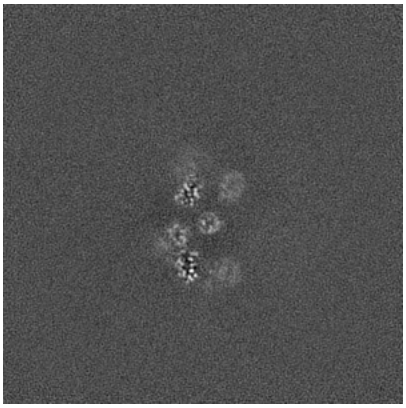

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

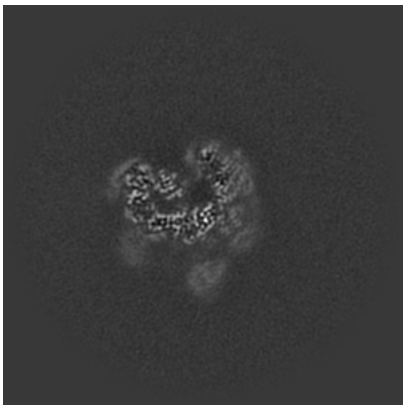

Y Index: 150

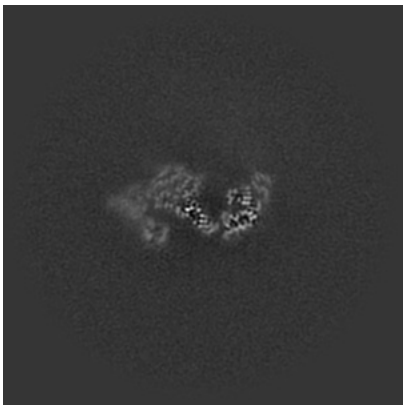

Z Index: 150

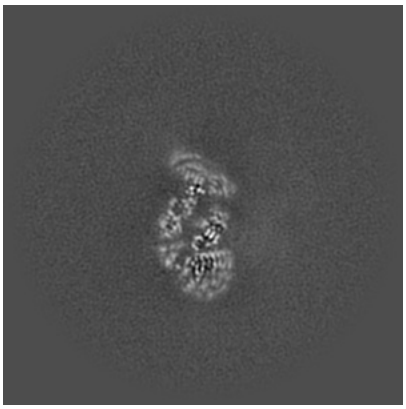
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

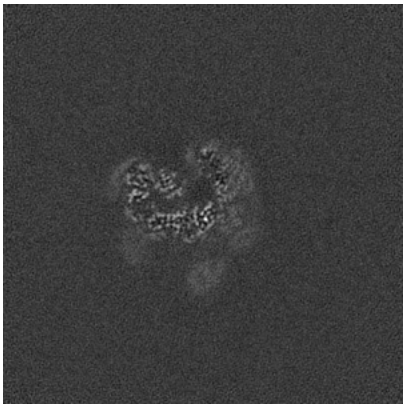
6.3.1 Primary map

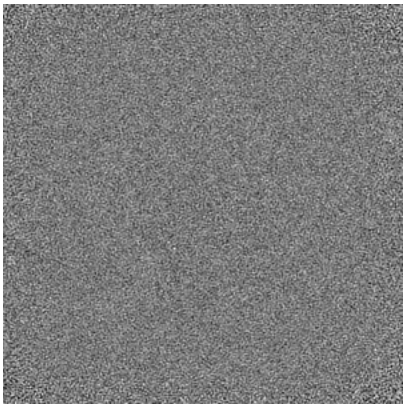

X Index: 146

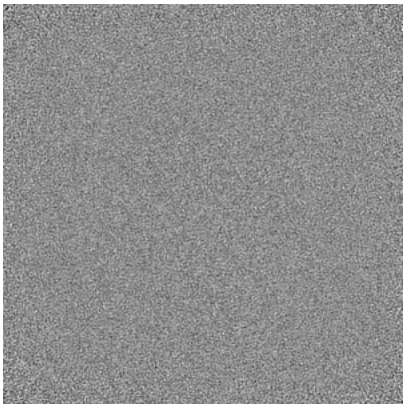

Y Index: 152


Z Index: 166

6.3.2 Raw map


X Index: 146

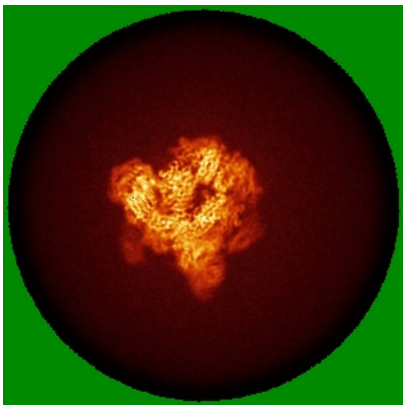

Y Index: 0

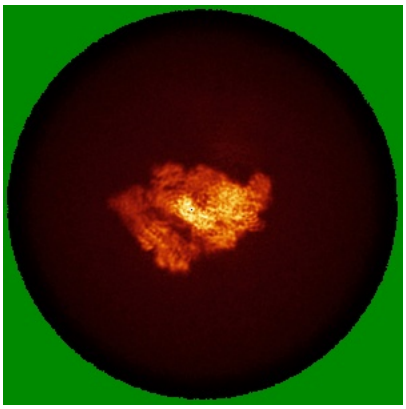

Z Index: 299

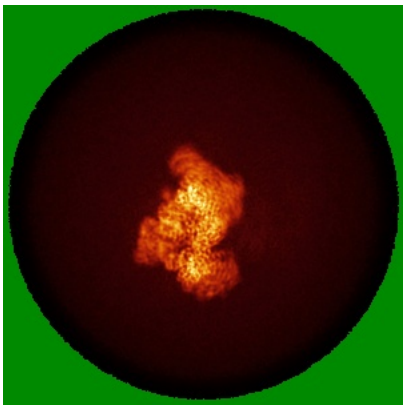
The images above show the largest variance slices of the map in three orthogonal directions.

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

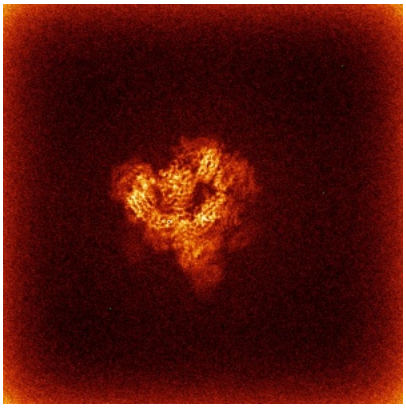
6.4.1 Primary map

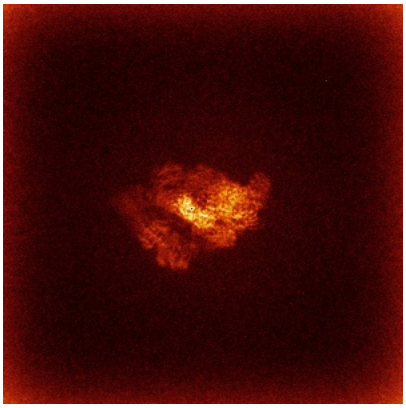

X

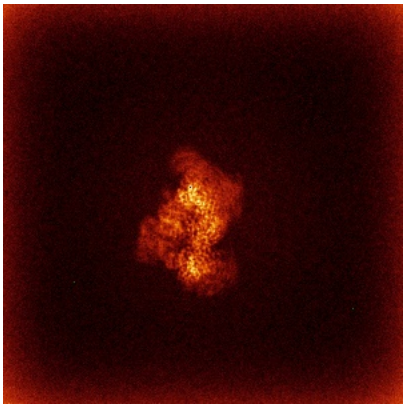

Y


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.

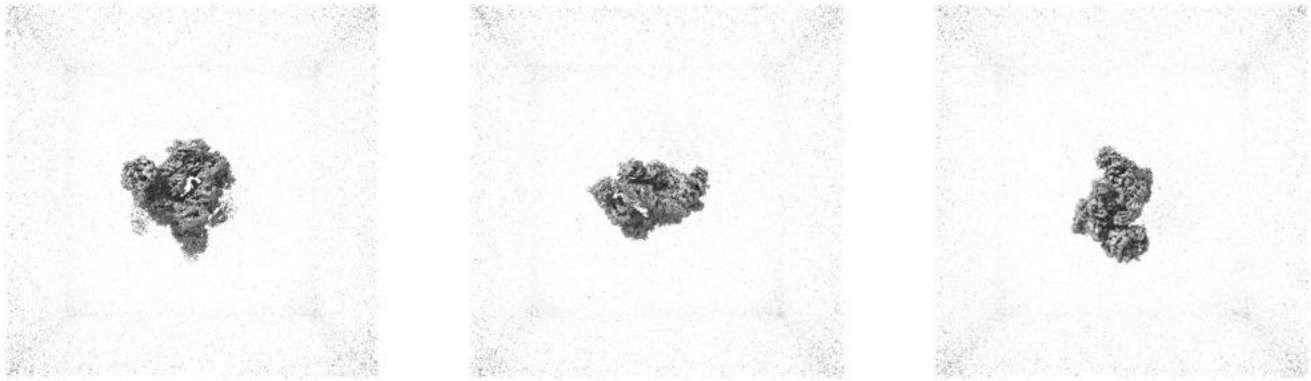
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

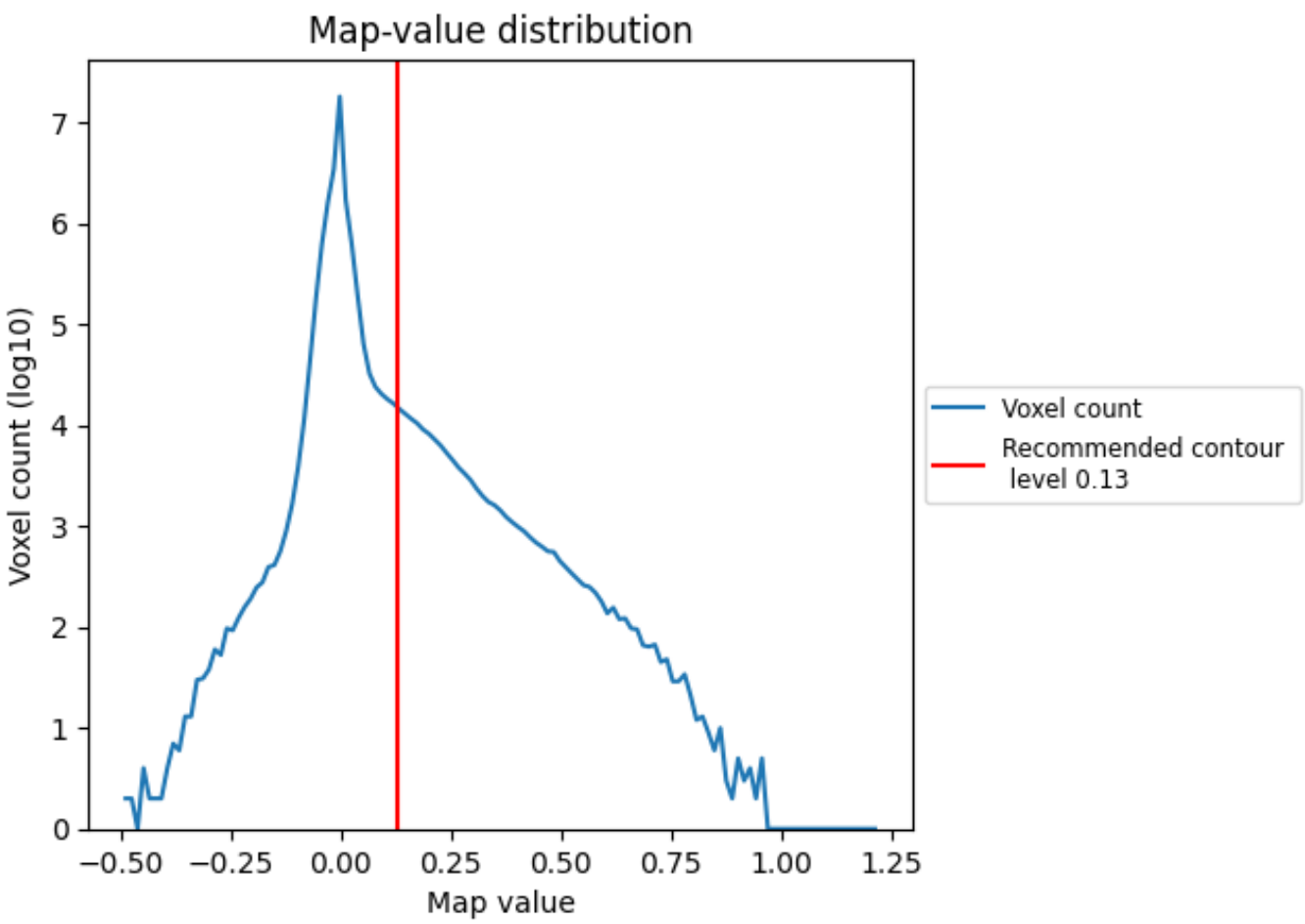
6.6 Mask visualisation (i)

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

7 Map analysis (i)

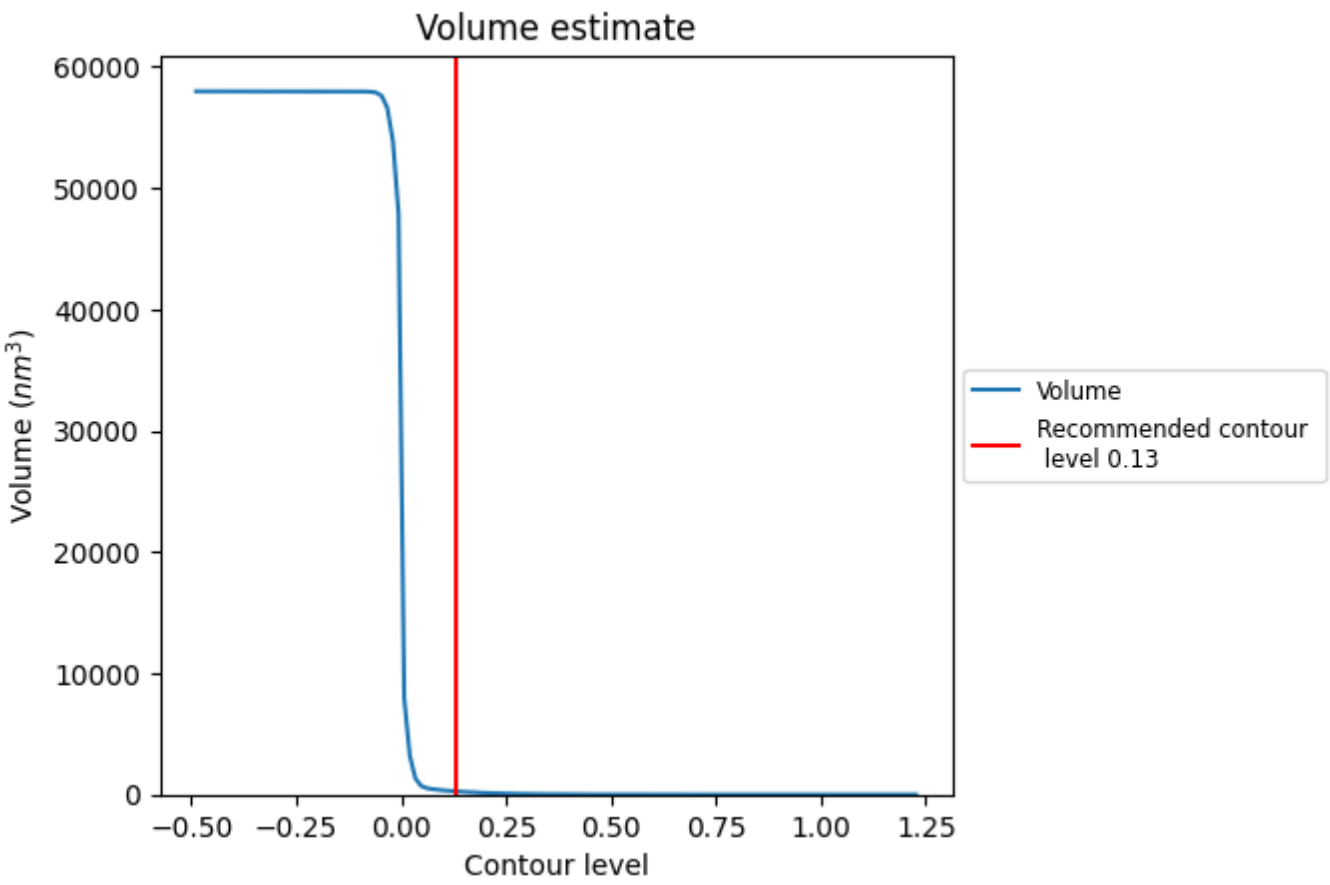
This section contains the results of statistical analysis of the map.

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.

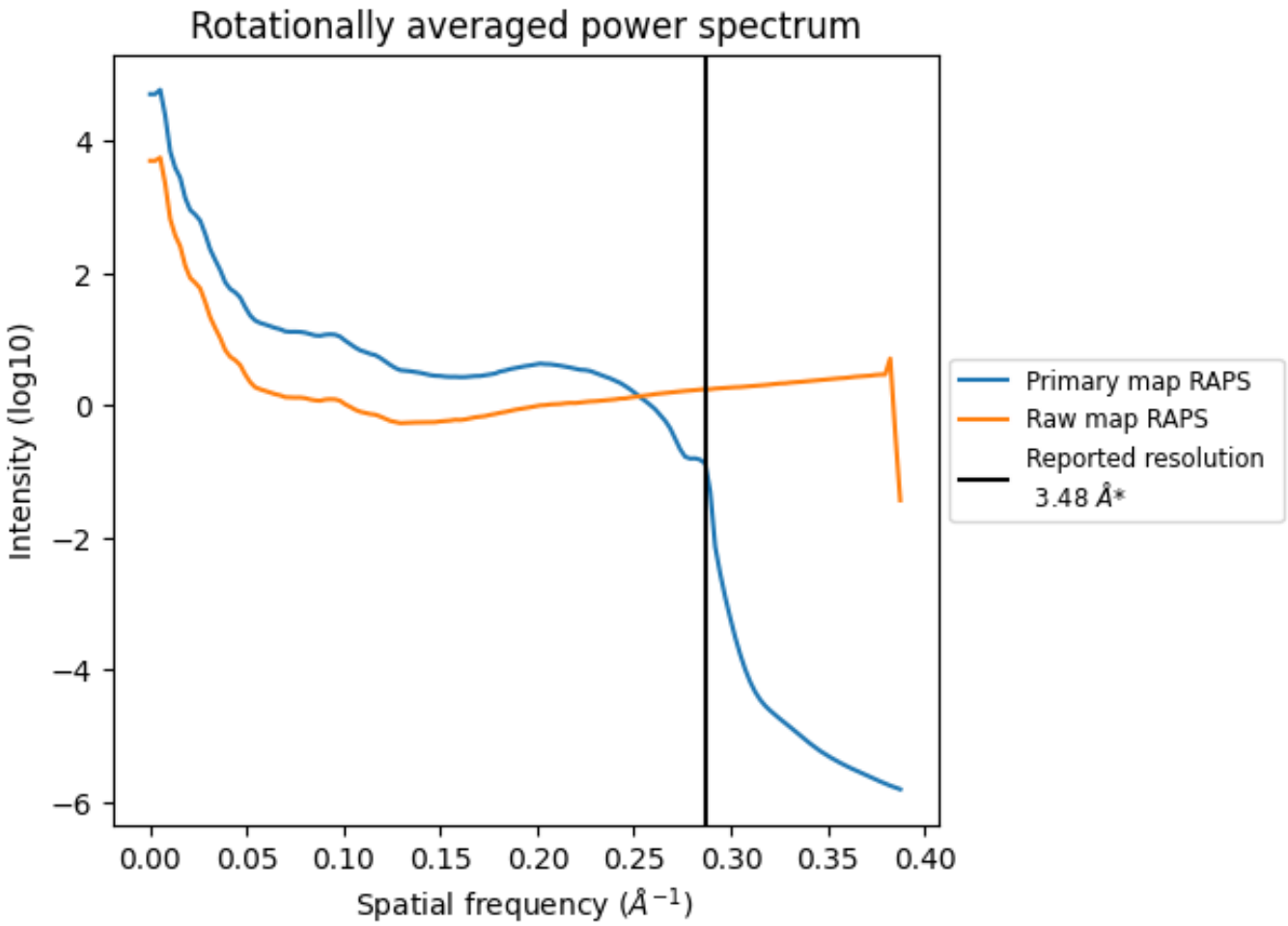
7.2 Volume estimate (i)



The volume at the recommended contour level is 265 nm^3; this corresponds to an approximate mass of 240 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)

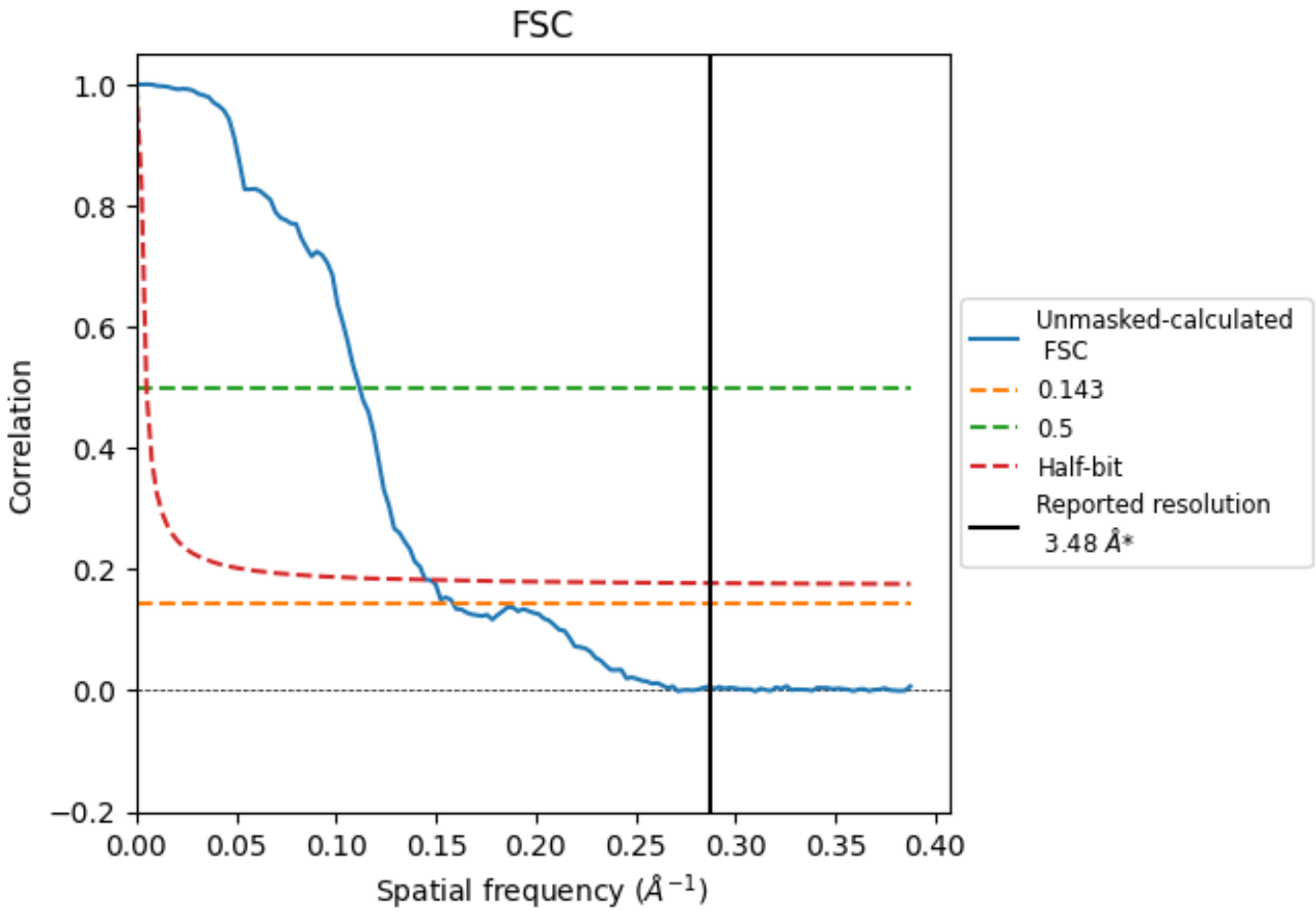


*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

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 0.287 Å^{-1}

8.2 Resolution estimates (i)

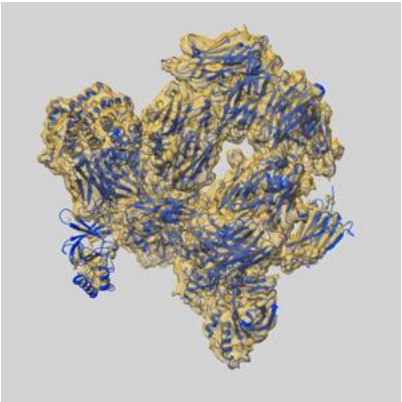
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.30	8.94	6.79

*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 6.30 differs from the reported value 3.48 by more than 10 %

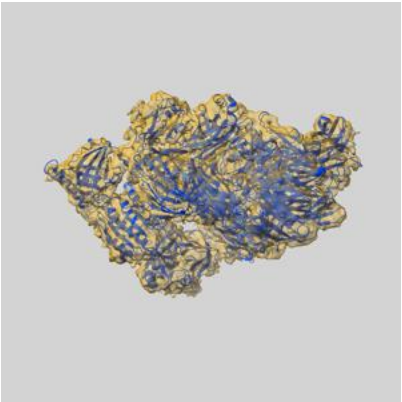
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55823 and PDB model 9TE8. Per-residue inclusion information can be found in section 3 on page 6.

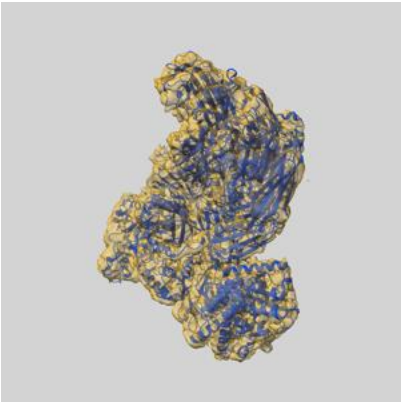
9.1 Map-model overlay (i)



X



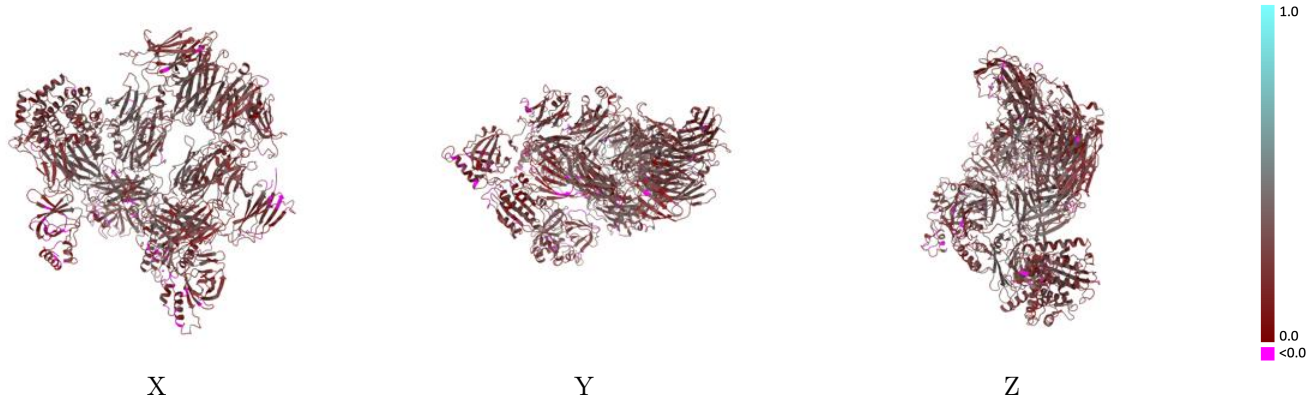
Y



Z

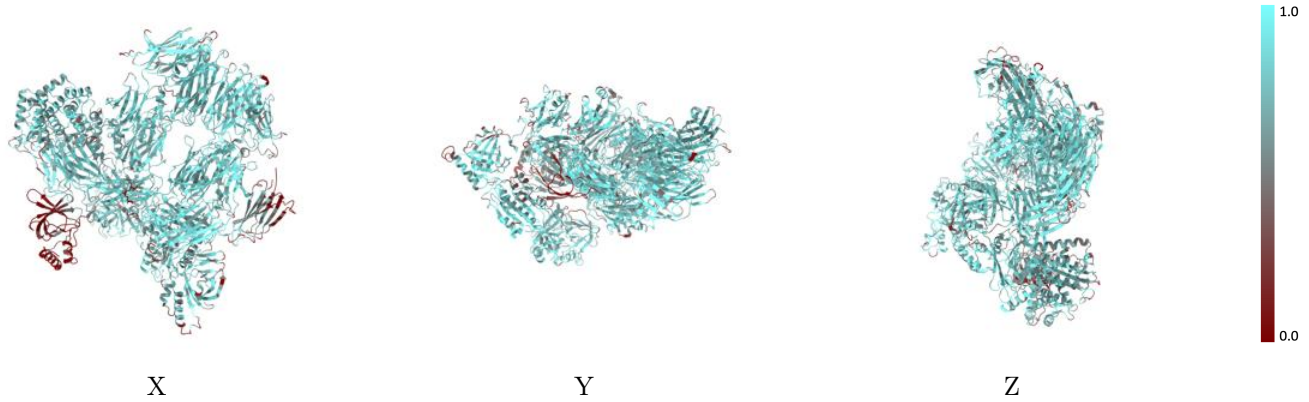
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



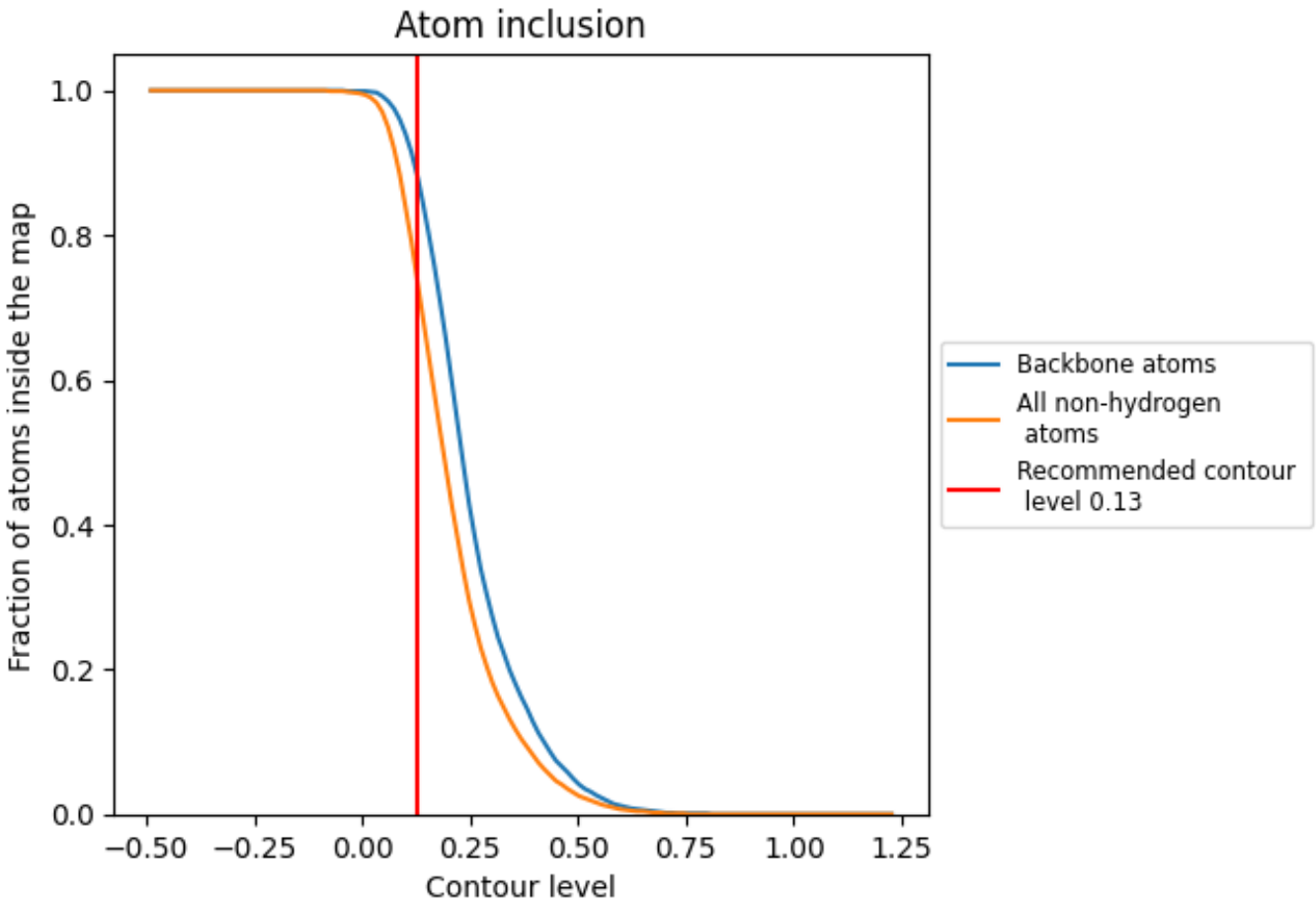
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 73% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7300	0.2700
A	0.7970	0.3080
B	0.7970	0.2770
C	0.6620	0.2770
D	0.7370	0.3000
E	0.6600	0.2220
F	0.2790	0.1520
J	0.7600	0.2250