



## Full wwPDB EM Validation Report ⓘ

Feb 13, 2024 – 12:55 pm GMT

PDB ID : 8OQ3  
EMDB ID : EMD-17103  
Title : Structure of methylamine treated human complement C3  
Authors : Gadeberg, T.A.F.; Andersen, G.R.  
Deposited on : 2023-04-11  
Resolution : 2.90 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

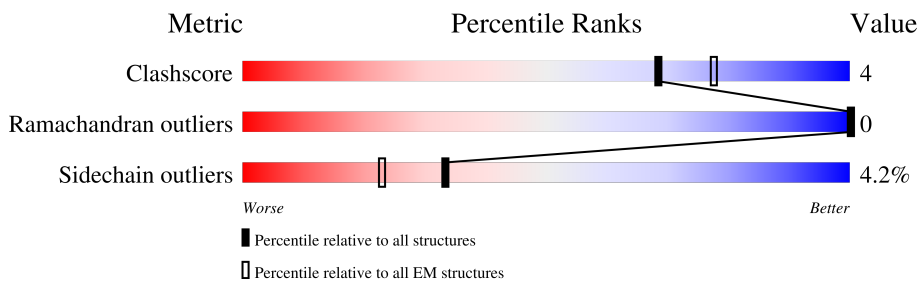
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1641	
1	D	1641	
2	C	129	
2	F	129	
3	G	3	
3	H	3	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 26596 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 C3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1556	12307	7811	2077	2366	53	0	0
1	D	1556	12307	7811	2077	2366	53	0	0

- Molecule 2 is a protein called nanobody hC3Nb1 with mutation.

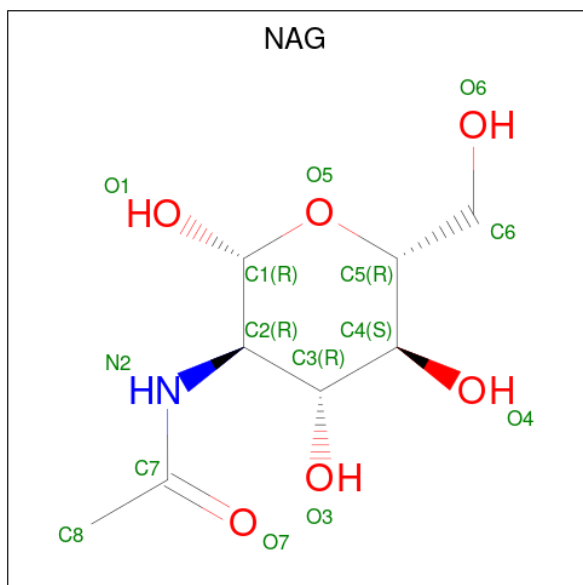
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	123	938	584	166	182	6	0	0
2	F	123	938	584	166	182	6	0	0

- Molecule 3 is an oligosaccharide called 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		
3	G	3	39	22	2	15	0	0
3	H	3	39	22	2	15	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

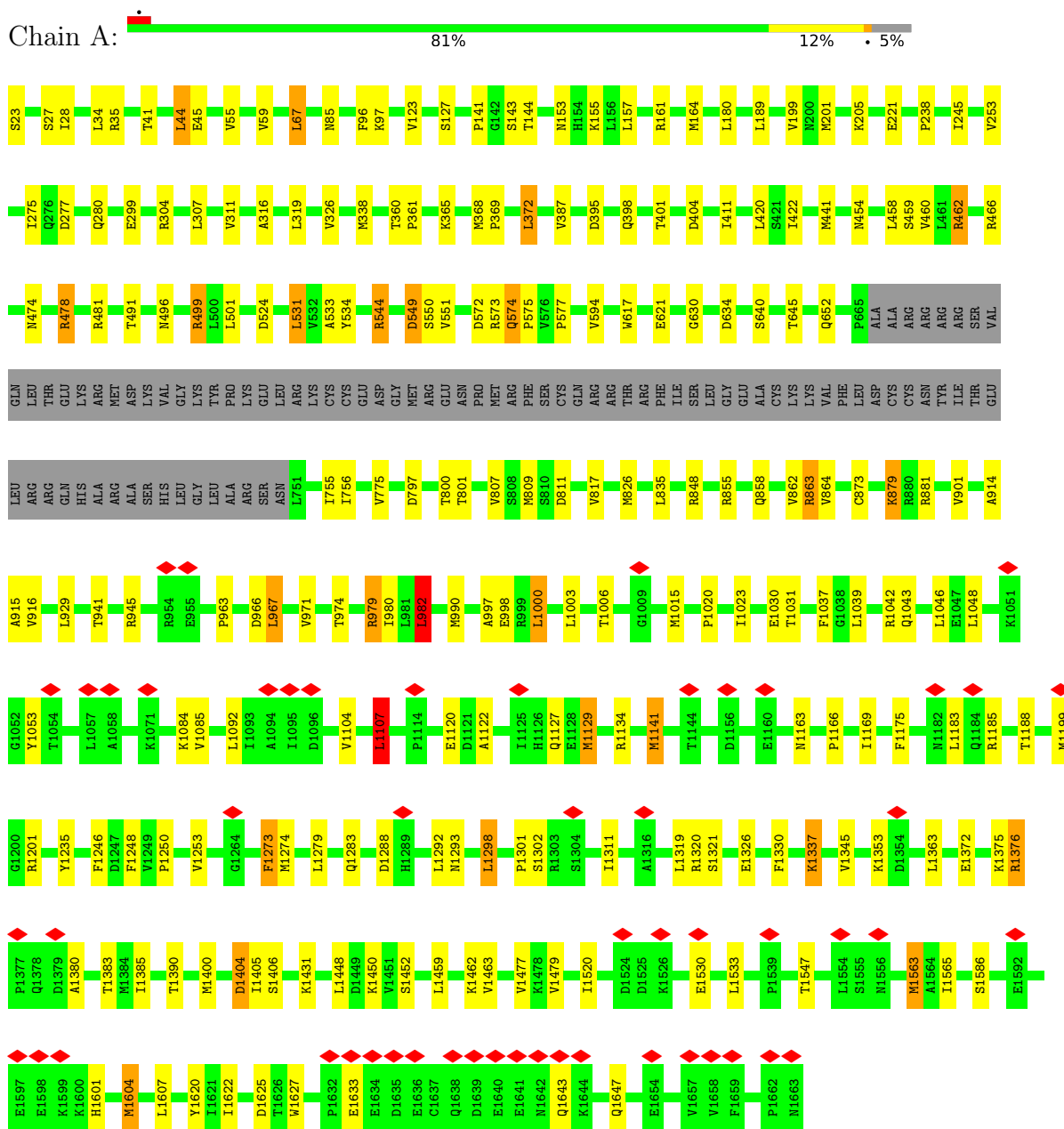


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	14	8	1	5	0
4	D	1	14	8	1	5	0

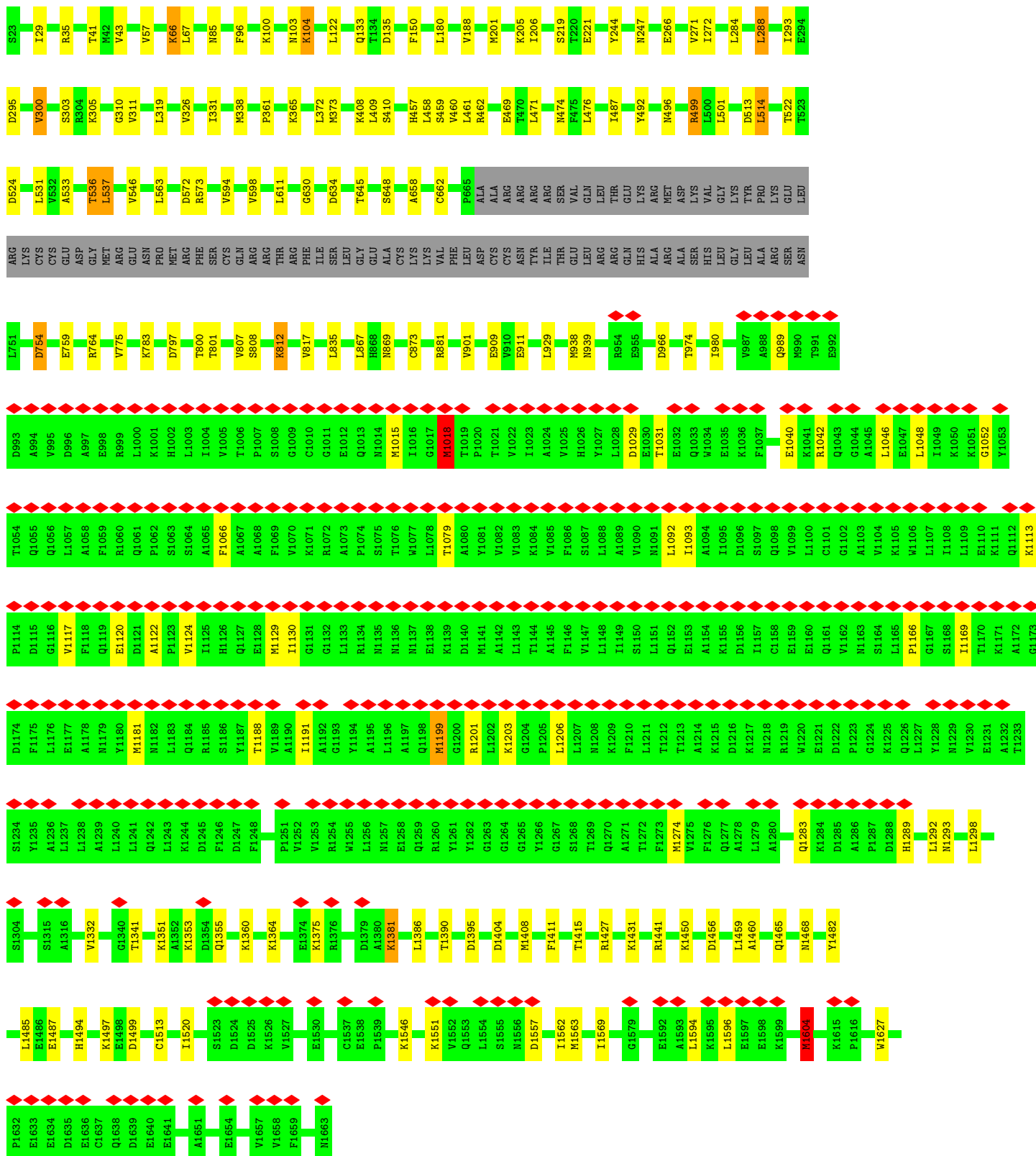
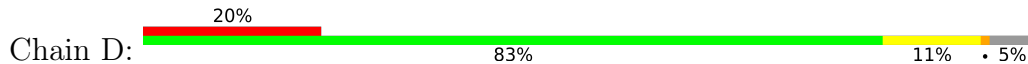
### 3 Residue-property plots i

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 C3

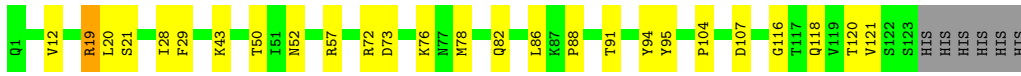


● Molecule 1: Complement C3




- Molecule 2: nanobody hC3Nb1 with mutation

Chain C:  75% 19% • 5%

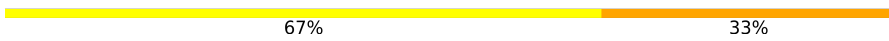


- Molecule 2: nanobody hC3Nb1 with mutation

Chain F:  78% 16% • 5%



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

Chain G:  67% 33%



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

Chain H:  33% 33% 33%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197438	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 ( $e^-/\text{\AA}^2$ )	59.5	Depositor
Minimum defocus (nm)	170	Depositor
Maximum defocus (nm)	2438	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.271	Depositor
Minimum map value	-0.146	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	310.56, 310.56, 310.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.647, 0.647, 0.647	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: BMA, 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	0.36	0/12555	0.70	20/17025 (0.1%)
1	D	0.35	0/12555	0.67	15/17025 (0.1%)
2	C	0.47	0/958	0.91	4/1295 (0.3%)
2	F	0.45	0/958	0.92	3/1295 (0.2%)
All	All	0.36	0/27026	0.70	42/36640 (0.1%)

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
1	D	0	2

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	F	73	ASP	CB-CG-OD2	11.24	128.42	118.30
1	D	1499	ASP	CB-CG-OD2	11.03	128.22	118.30
2	C	73	ASP	CB-CG-OD1	9.27	126.64	118.30
1	A	1404	ASP	CB-CG-OD2	8.84	126.25	118.30
1	A	1000	LEU	CA-CB-CG	8.36	134.53	115.30
2	C	86	LEU	C-N-CA	8.06	141.85	121.70
1	D	122	LEU	CA-CB-CG	8.02	133.75	115.30
1	D	295	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	982	LEU	CA-CB-CG	7.50	132.56	115.30
1	D	1199	MET	CA-CB-CG	7.44	125.95	113.30
1	A	1107	LEU	CA-CB-CG	7.19	131.83	115.30
1	D	1018	MET	CA-CB-CG	7.05	125.28	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1279	LEU	CA-CB-CG	6.90	131.16	115.30
1	D	1092	LEU	CA-CB-CG	6.71	130.73	115.30
1	A	1298	LEU	CA-CB-CG	6.62	130.53	115.30
1	D	288	LEU	CA-CB-CG	6.54	130.34	115.30
1	A	1015	MET	CB-CG-SD	6.48	131.85	112.40
1	A	1292	LEU	CA-CB-CG	6.40	130.02	115.30
1	D	1274	MET	CG-SD-CE	-6.30	90.13	100.20
1	D	1604	MET	CA-CB-CG	6.28	123.98	113.30
1	A	1607	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	979	ARG	CB-CG-CD	6.02	127.25	111.60
1	D	1018	MET	CG-SD-CE	5.93	109.68	100.20
2	C	20	LEU	CA-CB-CG	5.91	128.90	115.30
1	D	1563	MET	CB-CG-SD	5.90	130.09	112.40
2	F	11	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	67	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	1563	MET	CB-CG-SD	5.73	129.58	112.40
2	F	73	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	A	1092	LEU	CA-CB-CG	5.64	128.28	115.30
1	D	537	LEU	CA-CB-CG	5.60	128.18	115.30
1	D	1499	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	A	44	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	1274	MET	CB-CG-SD	5.42	128.66	112.40
1	A	1353	LYS	CB-CG-CD	5.41	125.66	111.60
1	A	549	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	478	ARG	CA-CB-CG	5.31	125.09	113.40
1	A	1015	MET	CG-SD-CE	5.31	108.69	100.20
1	D	1485	LEU	CA-CB-CG	5.29	127.47	115.30
2	C	107	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	1337	LYS	CA-CB-CG	5.21	124.87	113.40
1	D	939	ASN	CB-CA-C	5.15	120.71	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1018	MET	Peptide
1	D	662	CYS	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	12307	0	12288	101	0
1	D	12307	0	12288	81	0
2	C	938	0	895	9	0
2	F	938	0	895	10	0
3	G	39	0	34	1	0
3	H	39	0	34	1	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0
All	All	26596	0	26460	200	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 4.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:ASN:HA	1:A:1311:ILE:O	1.77	0.85
1:A:1042:ARG:HH21	1:A:1046:LEU:HD21	1.58	0.69
2:C:12:VAL:O	2:C:121:VAL:HA	1.97	0.65
1:A:1039:LEU:O	1:A:1042:ARG:HB3	1.98	0.63
1:D:459:SER:HB2	1:D:474:ASN:HB2	1.82	0.62
2:C:94:TYR:O	2:C:116:GLY:HA2	1.99	0.62
1:A:756:ILE:HD11	1:A:863:ARG:HG2	1.82	0.61
2:F:94:TYR:O	2:F:116:GLY:HA2	2.01	0.60
1:A:1604:MET:HA	1:A:1627:TRP:O	2.02	0.59
1:A:1547:THR:HG22	1:A:1565:ILE:HA	1.85	0.57
1:D:1604:MET:HA	1:D:1627:TRP:O	2.04	0.57
1:D:873:CYS:HB3	1:D:901:VAL:HB	1.87	0.56
1:A:873:CYS:HB3	1:A:901:VAL:HB	1.89	0.55
1:D:85:ASN:N	1:D:85:ASN:OD1	2.39	0.55
1:A:459:SER:HB3	1:A:474:ASN:HB2	1.88	0.54
1:D:1120:GLU:HG3	1:D:1122:ALA:H	1.71	0.54
1:A:311:VAL:HG21	1:A:319:LEU:HD21	1.88	0.54
1:A:372:LEU:HD11	1:A:422:ILE:HD13	1.89	0.54
1:D:457:HIS:HB3	1:D:476:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:THR:HG21	3:G:1:NAG:H82	1.90	0.54
1:D:634:ASP:N	1:D:634:ASP:OD1	2.40	0.54
2:F:26:GLY:O	2:F:77:ASN:ND2	2.40	0.53
1:A:1003:LEU:HB3	1:A:1020:PRO:HB2	1.90	0.53
1:A:491:THR:O	1:A:533:ALA:HA	2.09	0.53
1:A:205:LYS:HG2	1:A:221:GLU:HG2	1.89	0.53
1:D:188:VAL:HG11	1:D:594:VAL:HG11	1.91	0.53
1:D:311:VAL:HG11	1:D:319:LEU:HD21	1.91	0.53
1:A:496:ASN:ND2	1:A:524:ASP:O	2.43	0.52
1:A:1043:GLN:HA	1:A:1046:LEU:HD12	1.92	0.52
1:A:1120:GLU:HG3	1:A:1122:ALA:H	1.75	0.52
2:C:19:ARG:HH21	2:C:82:GLN:HB2	1.74	0.52
1:A:41:THR:HG21	3:H:1:NAG:H82	1.92	0.52
1:D:272:ILE:HG13	1:D:288:LEU:HB2	1.91	0.52
2:F:67:ARG:NH2	2:F:90:ASP:OD2	2.43	0.52
1:A:634:ASP:OD2	1:A:634:ASP:N	2.43	0.52
1:A:800:THR:OG1	1:A:801:THR:N	2.43	0.51
1:D:372:LEU:HB2	1:D:409:LEU:HB2	1.93	0.51
1:A:1586:SER:HB2	1:A:1622:ILE:HD12	1.91	0.51
1:A:1031:THR:HG22	1:A:1283:GLN:HG3	1.93	0.51
1:A:1141:MET:HG3	1:A:1183:LEU:HD21	1.92	0.51
1:D:1124:VAL:HG11	1:D:1130:ILE:HD11	1.93	0.51
1:A:454:ASN:HA	1:A:478:ARG:O	2.11	0.51
1:D:1113:LYS:HD2	1:D:1117:VAL:HB	1.93	0.51
1:D:103:ASN:ND2	1:D:658:ALA:O	2.44	0.50
1:D:800:THR:OG1	1:D:801:THR:N	2.44	0.50
1:A:245:ILE:O	1:A:304:ARG:NH1	2.44	0.50
1:A:572:ASP:N	1:A:572:ASP:OD1	2.45	0.50
1:A:127:SER:O	1:A:161:ARG:NH1	2.44	0.50
2:F:50:THR:HG21	2:F:104:PRO:HB2	1.94	0.50
1:A:23:SER:O	1:A:544:ARG:NH2	2.45	0.50
1:D:754:ASP:OD2	1:D:754:ASP:N	2.42	0.50
1:D:759:GLU:OE2	2:F:57:ARG:NH1	2.45	0.50
1:A:997:ALA:HB1	1:A:1037:PHE:HB2	1.93	0.49
1:D:867:LEU:HB2	1:D:911:GLU:HB3	1.94	0.49
2:C:50:THR:HG21	2:C:104:PRO:HB2	1.95	0.49
1:D:1046:LEU:HG	1:D:1093:ILE:HD11	1.94	0.49
1:D:474:ASN:HD22	1:D:514:LEU:HD11	1.78	0.48
1:D:594:VAL:HG12	1:D:775:VAL:HG22	1.95	0.48
1:A:1301:PRO:HD2	1:A:1330:PHE:HD1	1.77	0.48
1:A:387:VAL:H	1:A:401:THR:HB	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD12	1:A:189:LEU:HD22	1.95	0.48
2:F:63:SER:O	2:F:67:ARG:NH1	2.47	0.48
1:A:862:VAL:HG22	1:A:916:VAL:HG22	1.94	0.48
1:D:1048:LEU:O	1:D:1052:GLY:N	2.46	0.48
1:D:205:LYS:HG2	1:D:221:GLU:HG2	1.95	0.48
1:D:1364:LYS:NZ	1:D:1456:ASP:OD2	2.45	0.48
1:A:945:ARG:HH22	1:A:963:PRO:HD3	1.79	0.47
1:A:1601:HIS:ND1	1:A:1633:GLU:OE2	2.48	0.47
1:D:1557:ASP:N	1:D:1557:ASP:OD1	2.46	0.47
1:A:143:SER:OG	1:A:144:THR:N	2.46	0.47
1:A:141:PRO:HB3	1:A:199:VAL:HG11	1.97	0.47
1:D:135:ASP:OD1	1:D:135:ASP:N	2.48	0.47
1:A:1385:ILE:HG12	1:A:1462:LYS:HG2	1.97	0.47
1:A:531:LEU:O	1:A:550:SER:HA	2.15	0.47
1:D:1408:MET:HB2	1:D:1411:PHE:HB2	1.97	0.47
1:D:764:ARG:HB3	1:D:797:ASP:HB3	1.97	0.46
1:D:835:LEU:HD13	1:D:929:LEU:HB3	1.97	0.46
1:D:1551:LYS:HB3	1:D:1562:ILE:HD13	1.97	0.46
1:D:96:PHE:O	1:D:104:LYS:NZ	2.47	0.46
1:A:34:LEU:HB2	1:A:123:VAL:HG12	1.95	0.46
1:D:206:ILE:O	1:D:219:SER:HA	2.16	0.46
1:D:980:ILE:HG21	1:D:1298:LEU:HD21	1.96	0.46
1:D:1029:ASP:OD2	1:D:1042:ARG:NH2	2.45	0.46
1:A:404:ASP:OD1	1:A:404:ASP:N	2.45	0.46
1:A:941:THR:HA	1:A:1345:VAL:HG22	1.97	0.46
1:D:1298:LEU:HG	1:D:1332:VAL:HG22	1.96	0.46
1:D:1415:THR:HG22	1:D:1441:ARG:HH22	1.80	0.46
1:D:1494:HIS:HB3	1:D:1497:LYS:HB2	1.97	0.46
1:A:360:THR:HG21	1:A:441:MET:HE1	1.98	0.46
1:A:1084:LYS:NZ	1:A:1235:TYR:OH	2.49	0.46
1:D:812:LYS:HE3	1:D:812:LYS:HB3	1.82	0.46
1:D:1188:THR:HA	1:D:1191:ILE:HG22	1.97	0.46
1:A:496:ASN:O	1:A:499:ARG:NH1	2.49	0.46
1:A:980:ILE:O	1:A:1321:SER:HA	2.16	0.46
1:D:284:LEU:HD22	1:D:310:GLY:HA3	1.98	0.46
1:D:460:VAL:HG13	1:D:471:LEU:HD11	1.97	0.46
1:A:1127:GLN:HB3	1:A:1134:ARG:HD2	1.97	0.46
1:D:1381:LYS:HE3	1:D:1381:LYS:HB3	1.81	0.46
1:D:29:ILE:HB	1:D:43:VAL:HB	1.99	0.45
1:A:28:ILE:HG22	1:A:44:LEU:HD13	1.97	0.45
1:D:1546:LYS:HB2	1:D:1569:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:GLN:HG2	1:D:150:PHE:HE2	1.81	0.45
1:A:275:ILE:HD11	1:A:307:LEU:HD11	1.99	0.45
1:A:369:PRO:HA	1:A:411:ILE:O	2.16	0.45
1:A:848:ARG:NH2	1:A:1406:SER:OG	2.47	0.45
1:A:1530:GLU:HA	1:A:1533:LEU:HD12	1.98	0.45
1:A:1250:PRO:HA	1:A:1253:VAL:HB	1.99	0.45
1:D:361:PRO:HG3	1:D:630:GLY:HA3	1.99	0.45
1:A:460:VAL:HG12	1:A:462:ARG:HB3	1.99	0.45
1:A:755:ILE:HG23	1:A:915:ALA:HB3	1.99	0.45
1:A:544:ARG:O	1:A:652:GLN:NE2	2.50	0.45
1:A:1643:GLN:HE21	1:A:1647:GLN:HE22	1.65	0.45
1:D:462:ARG:NH2	1:D:469:GLU:OE1	2.50	0.45
1:D:492:TYR:HB2	1:D:531:LEU:HD11	1.99	0.45
1:D:1203:LYS:HB2	1:D:1206:LEU:HG	1.98	0.45
1:A:45:GLU:OE1	1:A:534:TYR:OH	2.31	0.44
1:D:408:LYS:HE2	1:D:461:LEU:HD22	1.99	0.44
1:D:522:THR:OG1	1:D:524:ASP:OD1	2.32	0.44
1:D:244:TYR:HB3	1:D:247:ASN:HB2	1.99	0.44
1:D:1465:GLN:HE21	1:D:1468:ASN:HA	1.81	0.44
1:A:1376:ARG:NH2	1:A:1380:ALA:O	2.50	0.44
1:D:496:ASN:O	1:D:499:ARG:NH1	2.51	0.44
1:A:153:ASN:HD21	1:A:157:LEU:HB2	1.83	0.44
1:D:271:VAL:HG21	1:D:300:VAL:HG11	2.00	0.44
1:D:572:ASP:N	1:D:572:ASP:OD1	2.46	0.44
1:D:1066:PHE:HD2	1:D:1079:THR:HG23	1.81	0.44
1:D:1427:ARG:HH21	1:D:1459:LEU:HB3	1.83	0.44
1:A:971:VAL:O	1:A:974:THR:OG1	2.35	0.43
1:A:998:GLU:N	1:A:998:GLU:OE2	2.51	0.43
1:A:1185:ARG:O	1:A:1188:THR:OG1	2.34	0.43
1:D:1520:ILE:HD12	1:D:1627:TRP:HB2	2.00	0.43
1:A:1006:THR:HG22	1:A:1048:LEU:HD11	2.01	0.43
1:D:1360:LYS:HG3	1:D:1487:GLU:HG3	2.00	0.43
1:A:245:ILE:HG13	1:A:316:ALA:HB1	2.01	0.43
1:A:855:ARG:HA	1:A:855:ARG:HD2	1.91	0.43
1:A:1383:THR:HA	1:A:1463:VAL:O	2.18	0.43
2:C:88:PRO:HA	2:C:121:VAL:HG13	2.01	0.43
1:D:1386:LEU:O	1:D:1460:ALA:HA	2.19	0.43
2:C:28:ILE:O	2:C:72:ARG:NH2	2.51	0.43
1:D:365:LYS:HE2	1:D:365:LYS:HB2	1.81	0.43
1:D:1031:THR:HG22	1:D:1283:GLN:HG3	2.00	0.43
1:D:133:GLN:HB3	1:D:611:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1166:PRO:HA	1:D:1169:ILE:HB	2.01	0.43
1:A:1085:VAL:HG22	1:A:1273:PHE:HE1	1.84	0.42
1:D:100:LYS:HB2	1:D:1289:HIS:HE1	1.83	0.42
1:D:1594:LEU:HB3	1:D:1596:LEU:HG	2.01	0.42
1:A:879:LYS:H	1:A:879:LYS:HG2	1.55	0.42
1:A:967:LEU:H	1:A:967:LEU:HG	1.53	0.42
1:A:549:ASP:OD2	1:A:550:SER:N	2.53	0.42
2:C:91:THR:HG22	2:C:120:THR:HA	2.02	0.42
1:A:277:ASP:HB3	1:A:280:GLN:HE21	1.84	0.42
2:F:36:TRP:HD1	2:F:70:ILE:HD12	1.84	0.42
1:A:398:GLN:HE21	1:A:398:GLN:HB2	1.61	0.42
1:A:864:VAL:HG23	1:A:914:ALA:HB2	2.02	0.42
1:D:869:ASN:ND2	1:D:909:GLU:O	2.41	0.42
1:D:1015:MET:HA	1:D:1018:MET:HG2	2.01	0.42
1:D:1404:ASP:N	1:D:1404:ASP:OD1	2.52	0.42
1:A:1023:ILE:HD12	1:A:1023:ILE:HA	1.86	0.42
2:C:21:SER:OG	2:C:78:MET:SD	2.77	0.42
1:A:155:LYS:HE2	1:A:155:LYS:HB2	1.88	0.42
1:A:361:PRO:HG3	1:A:630:GLY:HA3	2.02	0.42
1:A:499:ARG:HH12	1:A:501:LEU:HB2	1.84	0.42
1:A:577:PRO:HB3	1:A:797:ASP:HA	2.00	0.42
1:A:848:ARG:NH2	1:A:1404:ASP:OD2	2.53	0.42
2:C:52:ASN:HD22	2:C:57:ARG:HB2	1.85	0.42
1:D:458:LEU:HD21	1:D:533:ALA:HB3	2.01	0.42
1:A:1104:VAL:HA	1:A:1107:LEU:HD12	2.01	0.42
1:A:1363:LEU:HD22	1:A:1479:VAL:HG12	2.02	0.42
1:A:617:TRP:O	1:A:621:GLU:HB2	2.20	0.41
1:A:858:GLN:H	1:A:858:GLN:HG2	1.67	0.41
1:D:1351:LYS:HD2	1:D:1351:LYS:HA	1.77	0.41
1:A:420:LEU:HD23	1:A:422:ILE:HD11	2.03	0.41
1:A:1129:MET:SD	1:A:1129:MET:N	2.91	0.41
1:A:574:GLN:HE21	1:A:575:PRO:HD2	1.85	0.41
1:A:807:VAL:HG22	1:A:817:VAL:HG22	2.02	0.41
1:D:266:GLU:HA	1:D:293:ILE:O	2.19	0.41
1:A:365:LYS:HE2	1:A:365:LYS:HB2	1.89	0.41
1:A:395:ASP:OD1	1:A:395:ASP:N	2.54	0.41
2:F:12:VAL:O	2:F:121:VAL:HA	2.20	0.41
1:A:594:VAL:HG12	1:A:775:VAL:HG22	2.01	0.41
1:A:1405:ILE:HG12	1:A:1477:VAL:HG22	2.03	0.41
2:F:29:PHE:O	2:F:53:ARG:NH1	2.45	0.41
1:A:1302:SER:OG	1:A:1326:GLU:OE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:GLU:HG3	1:A:1375:LYS:HD3	2.02	0.41
1:A:1400:MET:HA	1:A:1448:LEU:O	2.20	0.41
1:A:1520:ILE:HD12	1:A:1627:TRP:HB2	2.01	0.41
2:F:72:ARG:HA	2:F:79:VAL:HG23	2.03	0.41
1:A:238:PRO:HA	1:A:253:VAL:HA	2.02	0.41
1:D:563:LEU:HD22	1:D:808:SER:HB3	2.03	0.41
1:D:873:CYS:HB2	1:D:1513:CYS:HB2	1.95	0.41
1:A:1020:PRO:HA	1:A:1023:ILE:HG22	2.03	0.40
1:A:1166:PRO:HA	1:A:1169:ILE:HB	2.02	0.40
1:D:536:THR:HG23	1:D:546:VAL:HG22	2.03	0.40
1:A:835:LEU:HD13	1:A:929:LEU:HB3	2.03	0.40
1:A:982:LEU:O	1:A:1319:LEU:HA	2.21	0.40
1:D:807:VAL:HG22	1:D:817:VAL:HG22	2.03	0.40
1:A:1431:LYS:HA	1:A:1431:LYS:HD2	1.81	0.40
1:D:1353:LYS:HB2	1:D:1355:GLN:HG2	2.03	0.40
1:D:66:LYS:HE2	1:D:66:LYS:HB3	1.92	0.40
1:D:499:ARG:HH12	1:D:501:LEU:HB2	1.86	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	1552/1641 (95%)	1500 (97%)	52 (3%)	0	100	100
1	D	1552/1641 (95%)	1503 (97%)	49 (3%)	0	100	100
2	C	121/129 (94%)	115 (95%)	6 (5%)	0	100	100
2	F	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
All	All	3346/3540 (94%)	3234 (97%)	112 (3%)	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	1375/1450 (95%)	1311 (95%)	64 (5%)	26	59
1	D	1375/1450 (95%)	1326 (96%)	49 (4%)	35	69
2	C	97/103 (94%)	91 (94%)	6 (6%)	18	47
2	F	97/103 (94%)	92 (95%)	5 (5%)	23	55
All	All	2944/3106 (95%)	2820 (96%)	124 (4%)	33	63

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	35	ARG
1	A	55	VAL
1	A	59	VAL
1	A	67	LEU
1	A	85	ASN
1	A	96	PHE
1	A	97	LYS
1	A	164	MET
1	A	201	MET
1	A	299	GLU
1	A	326	VAL
1	A	338	MET
1	A	368	MET
1	A	372	LEU
1	A	458	LEU
1	A	462	ARG
1	A	466	ARG
1	A	481	ARG
1	A	499	ARG
1	A	531	LEU
1	A	544	ARG
1	A	551	VAL
1	A	573	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	574	GLN
1	A	640	SER
1	A	645	THR
1	A	809	MET
1	A	811	ASP
1	A	826	MET
1	A	863	ARG
1	A	879	LYS
1	A	881	ARG
1	A	966	ASP
1	A	967	LEU
1	A	979	ARG
1	A	982	LEU
1	A	990	MET
1	A	1000	LEU
1	A	1030	GLU
1	A	1053	TYR
1	A	1107	LEU
1	A	1129	MET
1	A	1141	MET
1	A	1163	ASN
1	A	1175	PHE
1	A	1199	MET
1	A	1201	ARG
1	A	1246	PHE
1	A	1248	PHE
1	A	1273	PHE
1	A	1288	ASP
1	A	1298	LEU
1	A	1320	ARG
1	A	1337	LYS
1	A	1376	ARG
1	A	1390	THR
1	A	1450	LYS
1	A	1452	SER
1	A	1459	LEU
1	A	1563	MET
1	A	1604	MET
1	A	1620	TYR
1	A	1625	ASP
2	C	19	ARG
2	C	29	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	43	LYS
2	C	76	LYS
2	C	95	TYR
2	C	118	GLN
1	D	35	ARG
1	D	57	VAL
1	D	66	LYS
1	D	67	LEU
1	D	104	LYS
1	D	180	LEU
1	D	201	MET
1	D	300	VAL
1	D	303	SER
1	D	305	LYS
1	D	326	VAL
1	D	331	ILE
1	D	338	MET
1	D	373	MET
1	D	410	SER
1	D	487	ILE
1	D	499	ARG
1	D	513	ASP
1	D	514	LEU
1	D	536	THR
1	D	537	LEU
1	D	573	ARG
1	D	598	VAL
1	D	645	THR
1	D	648	SER
1	D	754	ASP
1	D	783	LYS
1	D	812	LYS
1	D	881	ARG
1	D	938	MET
1	D	966	ASP
1	D	974	THR
1	D	989	GLN
1	D	1040	GLU
1	D	1129	MET
1	D	1181	MET
1	D	1199	MET
1	D	1201	ARG

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Mol	Chain	Res	Type
1	D	1292	LEU
1	D	1293	ASN
1	D	1341	THR
1	D	1375	LYS
1	D	1381	LYS
1	D	1390	THR
1	D	1395	ASP
1	D	1431	LYS
1	D	1450	LYS
1	D	1482	TYR
1	D	1604	MET
2	F	21	SER
2	F	22	CYS
2	F	29	PHE
2	F	67	ARG
2	F	122	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	103	ASN
1	A	154	HIS
1	A	313	ASN
1	A	333	HIS
1	A	398	GLN
1	A	496	ASN
1	A	1043	GLN
1	A	1112	GLN
1	A	1136	ASN
1	A	1152	GLN
1	A	1182	ASN
1	A	1309	HIS
1	A	1643	GLN
1	D	474	ASN
1	D	1056	GLN
1	D	1136	ASN
1	D	1198	GLN
1	D	1289	HIS
1	D	1293	ASN
1	D	1473	GLN
2	F	1	GLN

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Mol	Chain	Res	Type
2	F	3	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

6 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	G	1	3,1	14,14,15	0.42	0	17,19,21	0.82	1 (5%)
3	NAG	G	2	3	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
3	BMA	G	3	3	11,11,12	1.16	1 (9%)	15,15,17	0.99	1 (6%)
3	NAG	H	1	3,1	14,14,15	0.40	0	17,19,21	0.87	1 (5%)
3	NAG	H	2	3	14,14,15	0.62	0	17,19,21	0.61	0
3	BMA	H	3	3	11,11,12	1.12	2 (18%)	15,15,17	1.22	1 (6%)

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. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	BMA	C2-C3	2.36	1.56	1.52
3	H	3	BMA	C2-C3	2.17	1.55	1.52
3	H	3	BMA	C1-C2	2.00	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-O5-C5	3.40	116.80	112.19
3	G	2	NAG	C1-O5-C5	2.61	115.72	112.19
3	G	3	BMA	C1-O5-C5	2.47	115.54	112.19
3	G	1	NAG	C1-O5-C5	2.24	115.23	112.19
3	H	1	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

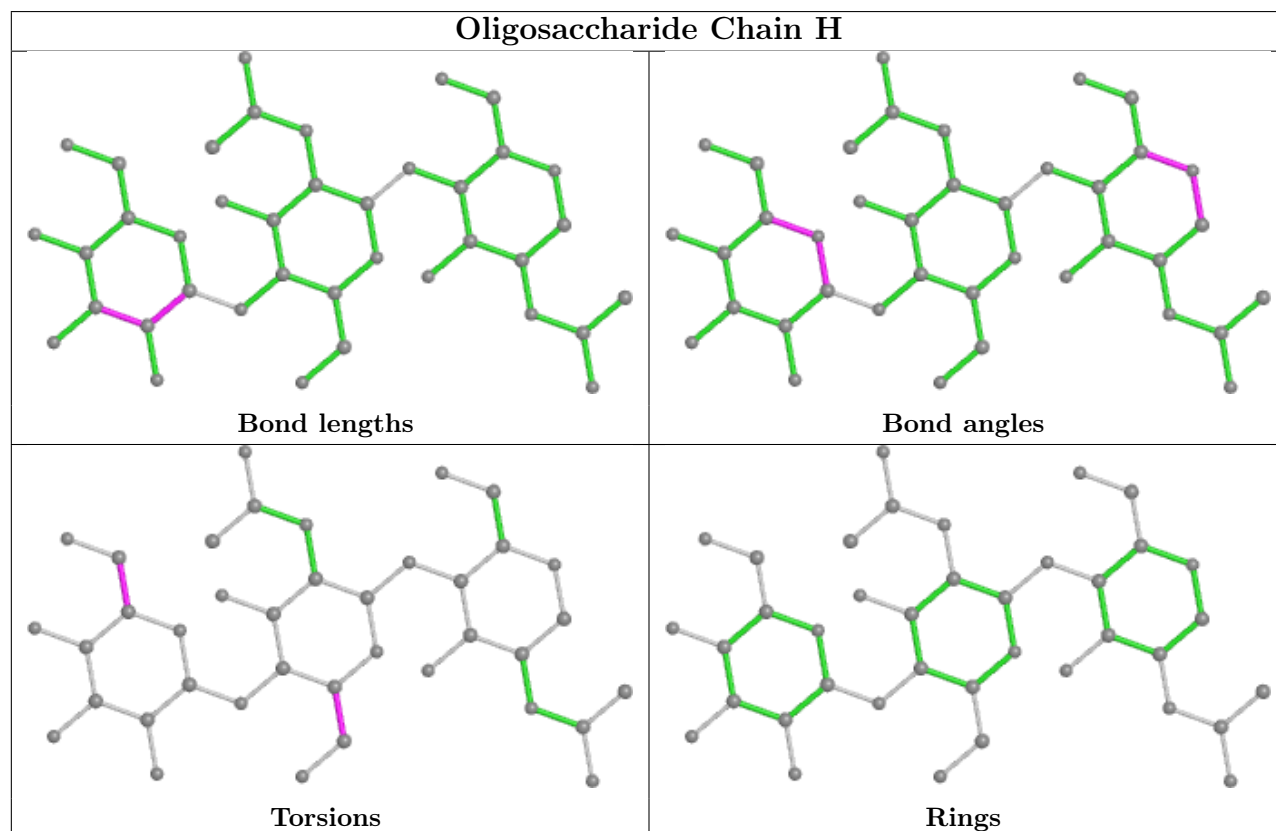
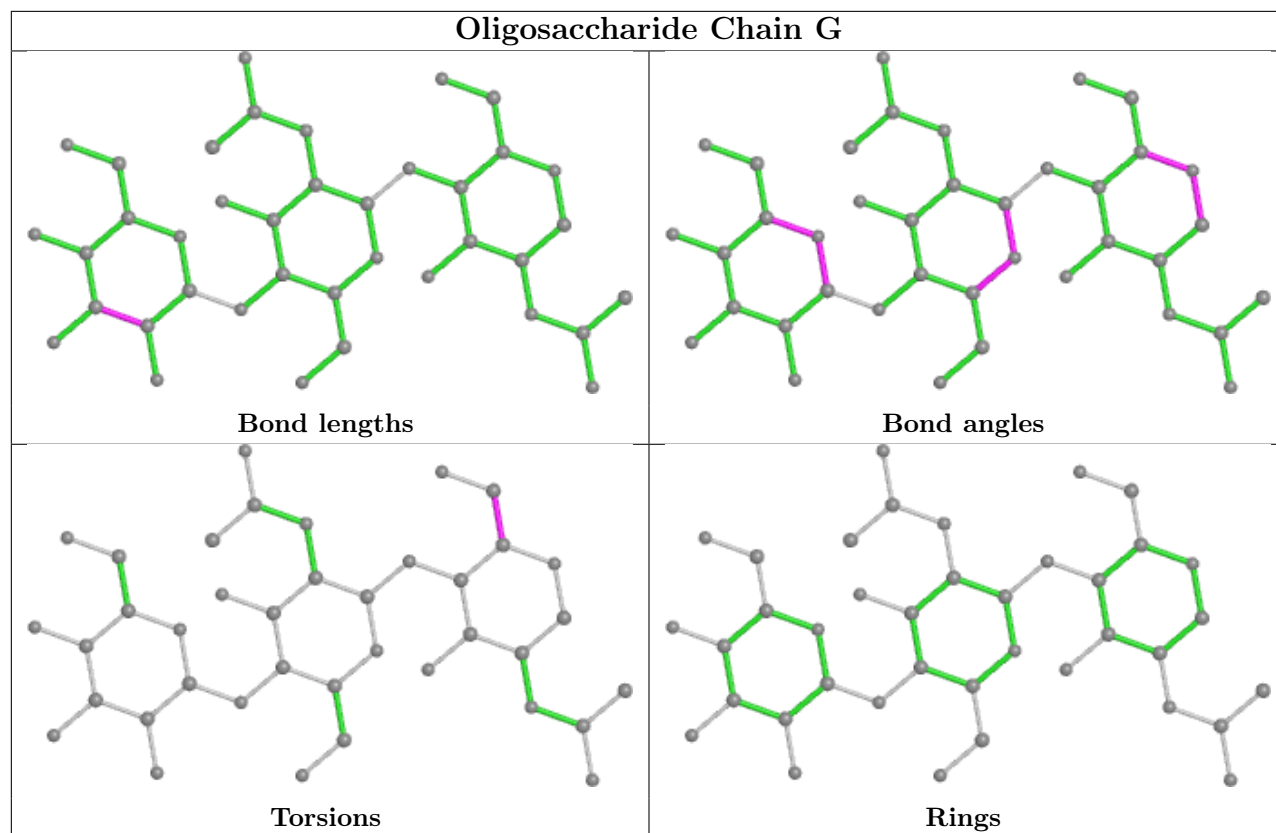
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	H	1	NAG	1	0

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

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	A	1701	1	14,14,15	1.11	2 (14%)	17,19,21	0.54	0
4	NAG	D	1701	1	14,14,15	0.62	0	17,19,21	0.75	1 (5%)

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	A	1701	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1701	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1701	NAG	O5-C1	3.42	1.49	1.43
4	A	1701	NAG	C1-C2	2.14	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1701	NAG	C1-O5-C5	2.31	115.33	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1701	NAG	O5-C5-C6-O6
4	A	1701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	1701	NAG	C4-C5-C6-O6
4	A	1701	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.

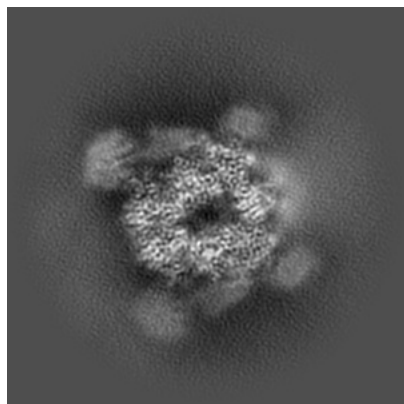
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17103. These allow visual inspection of the internal detail of the map and identification of artifacts.

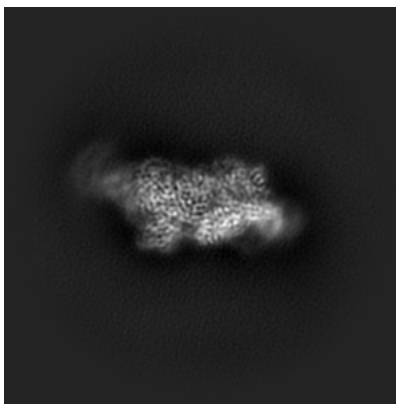
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

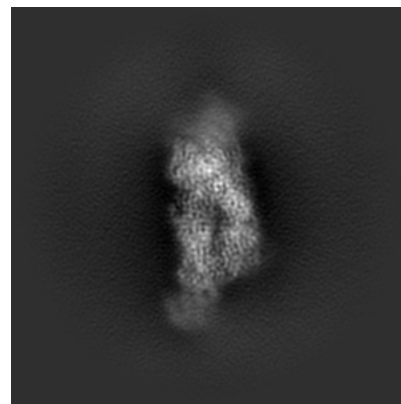
#### 6.1.1 Primary map



X

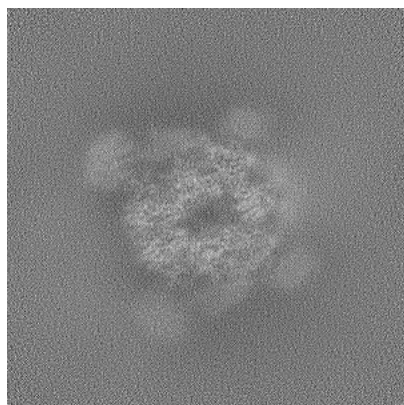


Y

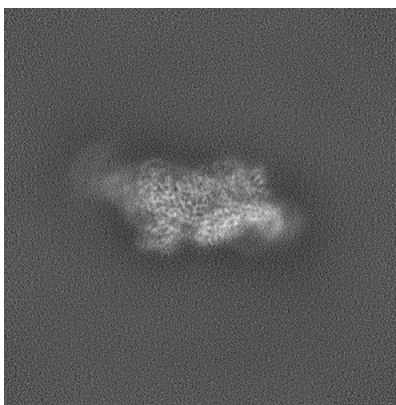


Z

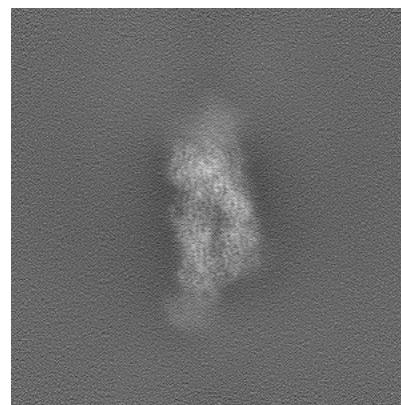
#### 6.1.2 Raw map



X



Y

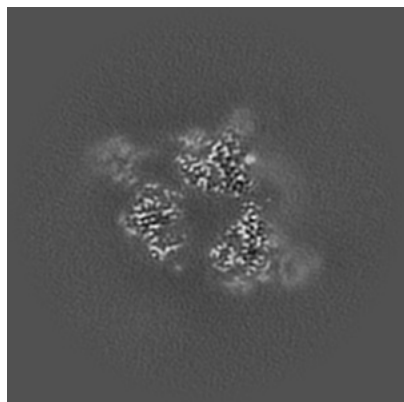


Z

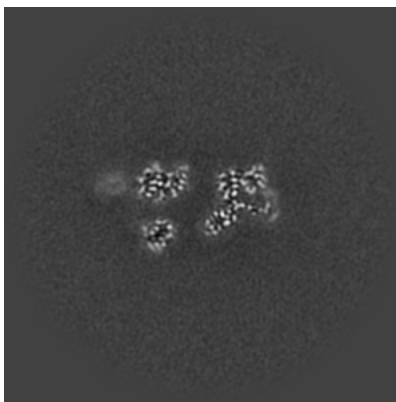
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

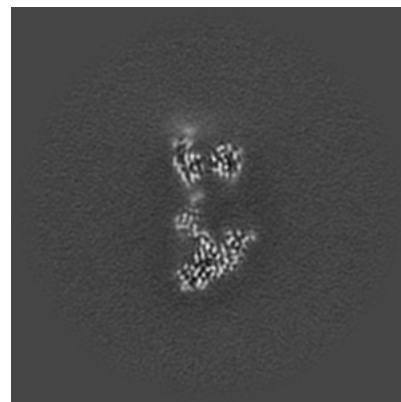
### 6.2.1 Primary map



X Index: 240

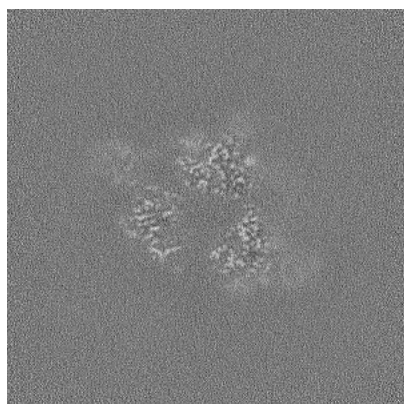


Y Index: 240

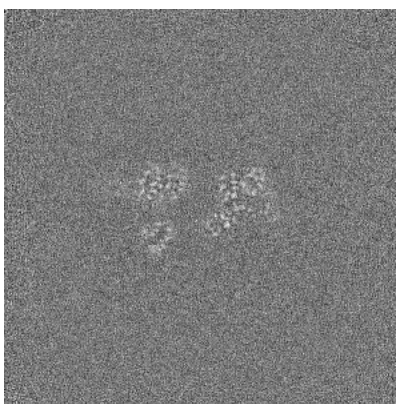


Z Index: 240

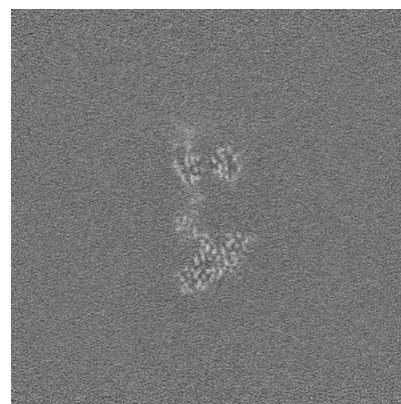
### 6.2.2 Raw map



X Index: 240



Y Index: 240

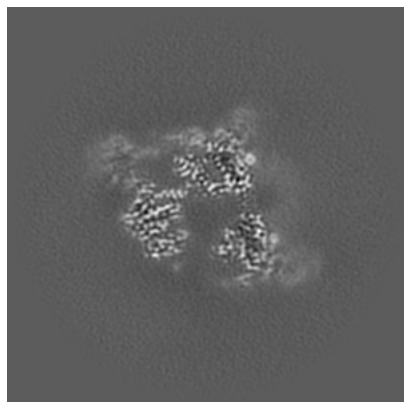


Z Index: 240

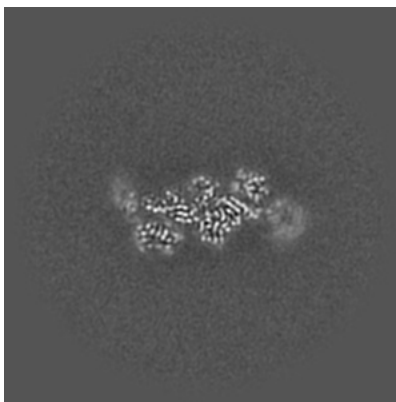
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

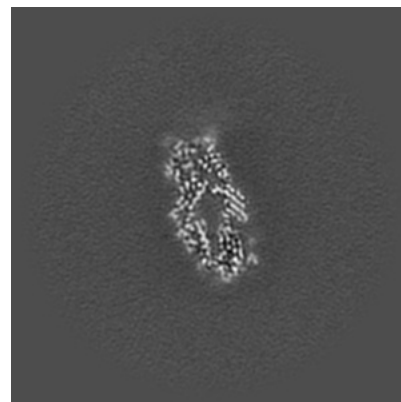
### 6.3.1 Primary map



X Index: 236

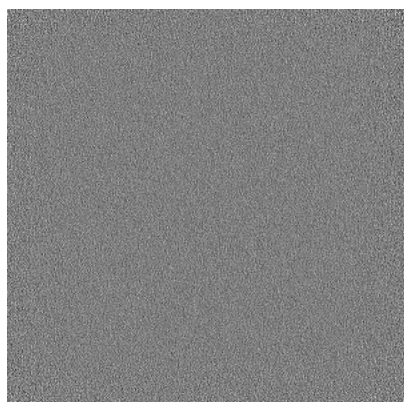


Y Index: 282

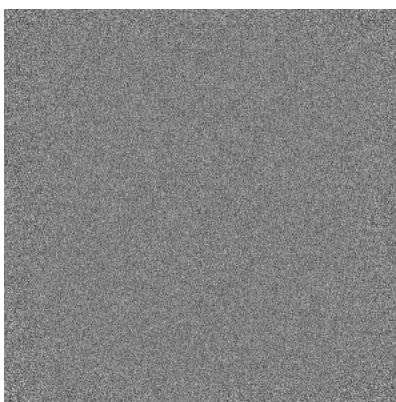


Z Index: 197

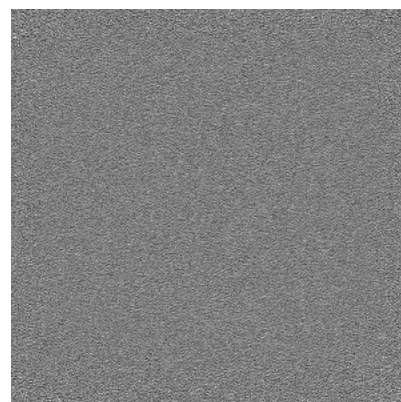
### 6.3.2 Raw map



X Index: 0



Y Index: 0

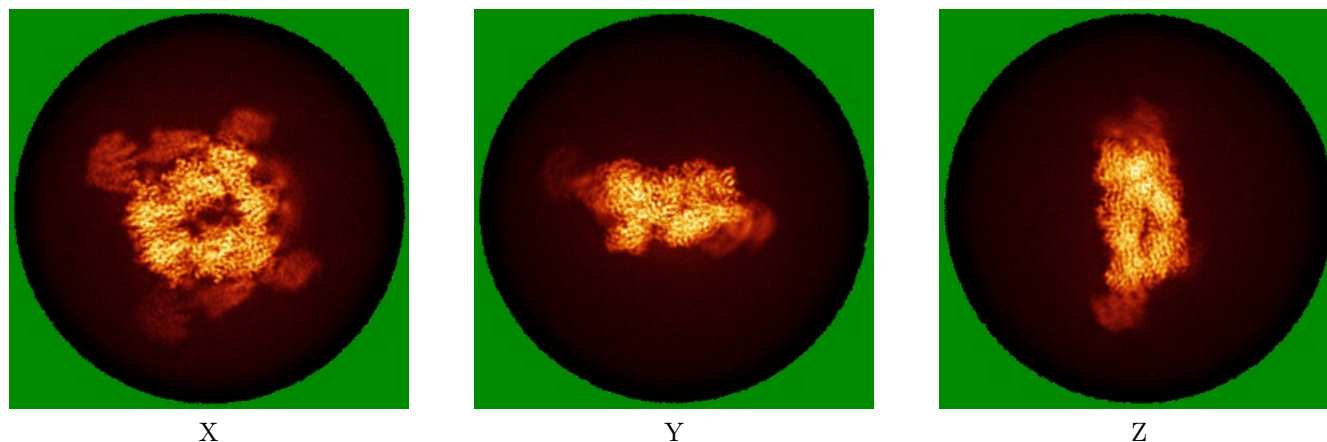


Z Index: 0

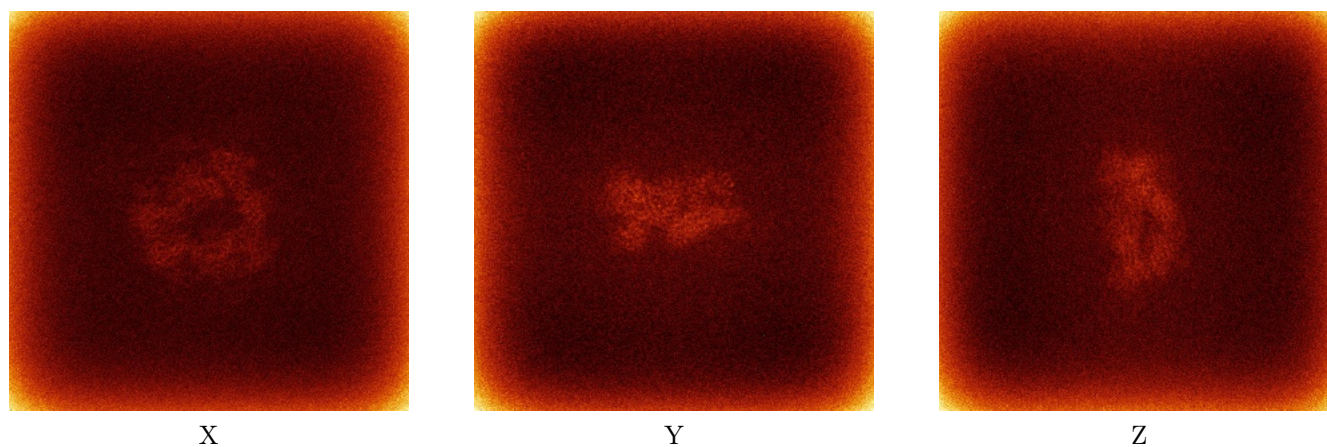
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



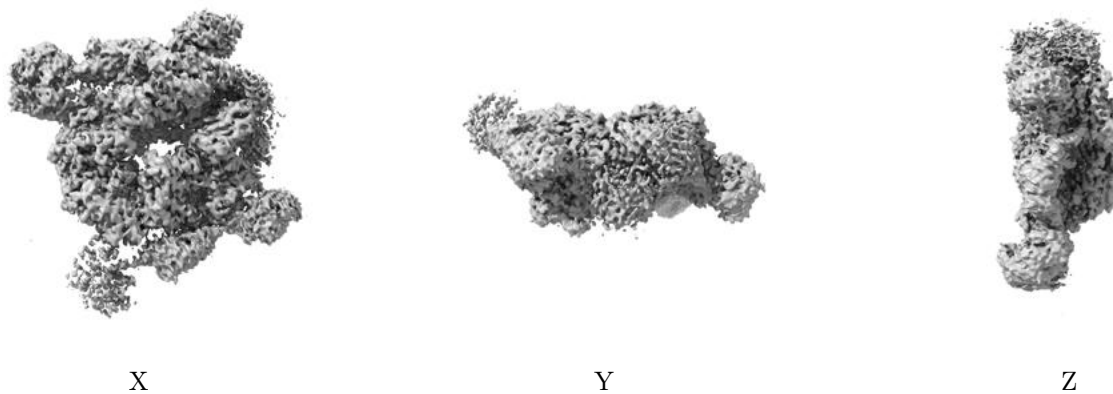
### 6.4.2 Raw map



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.

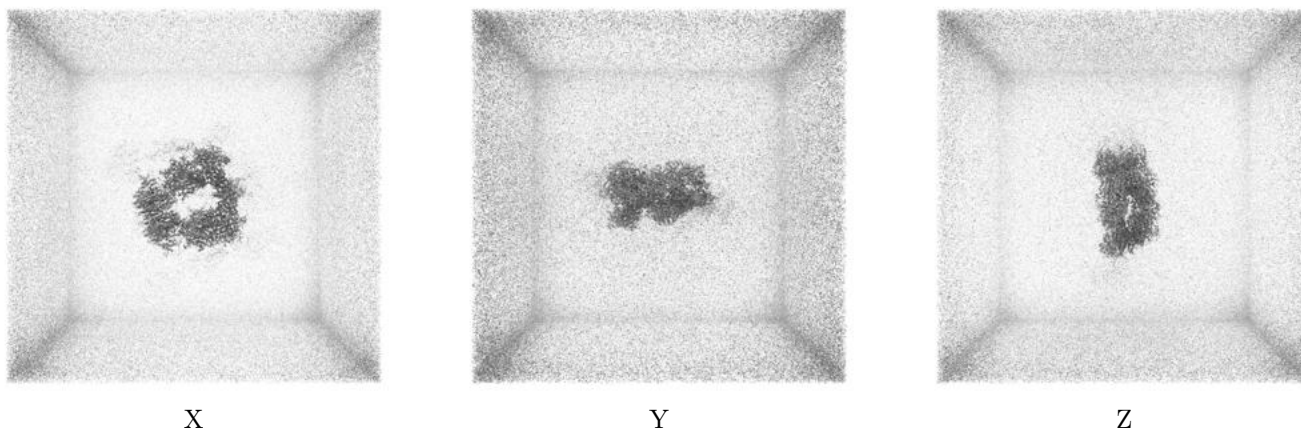
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

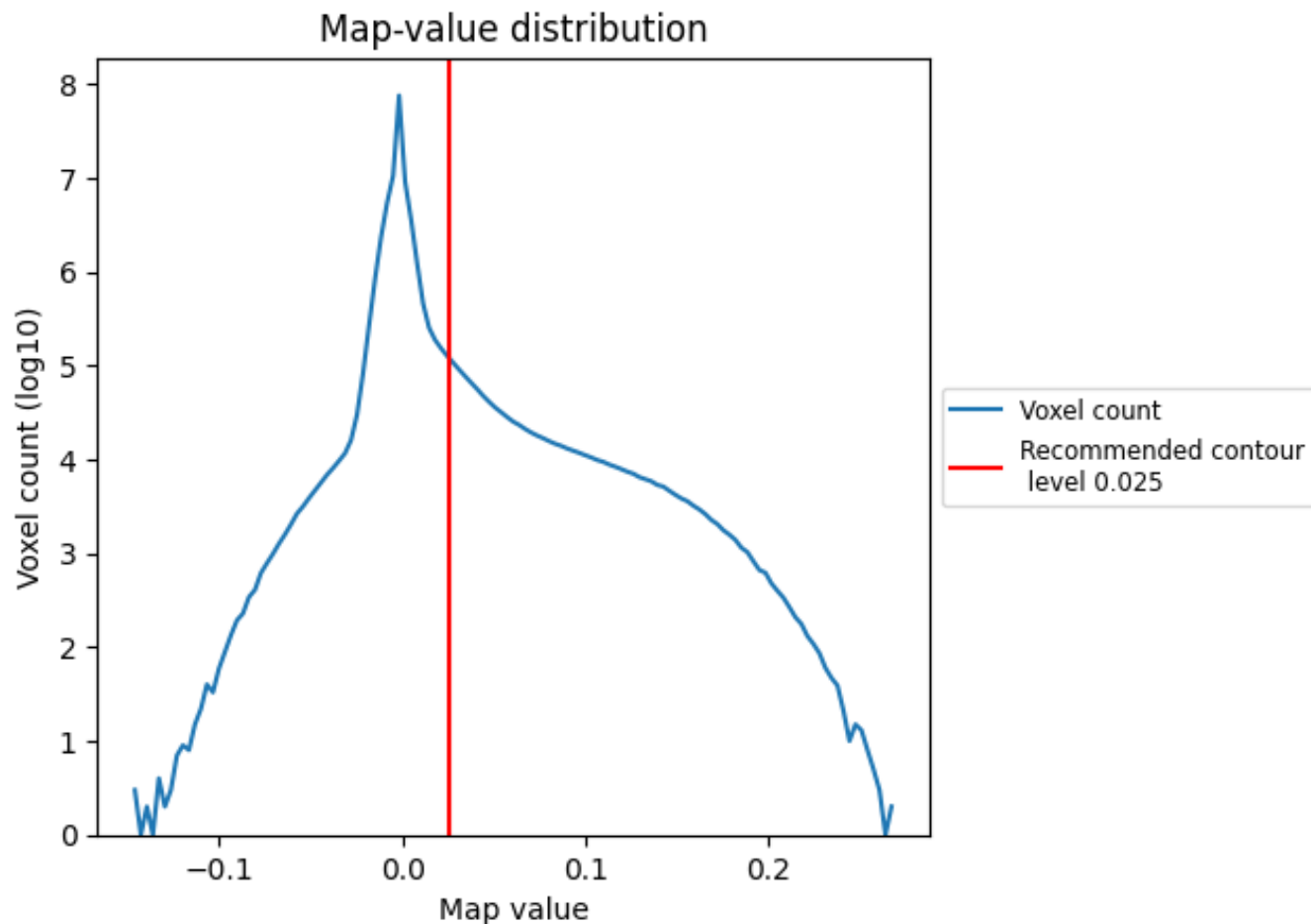
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

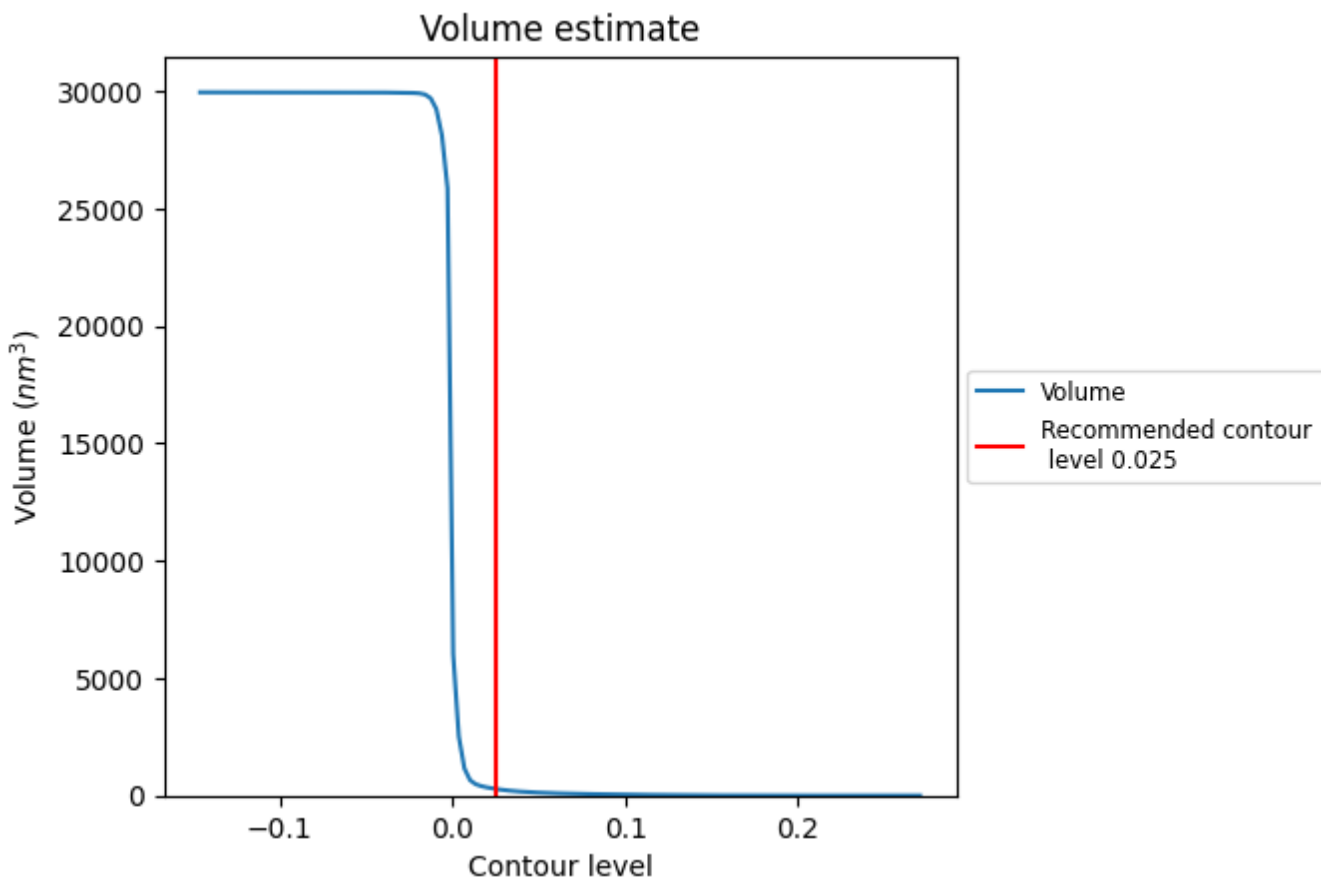
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

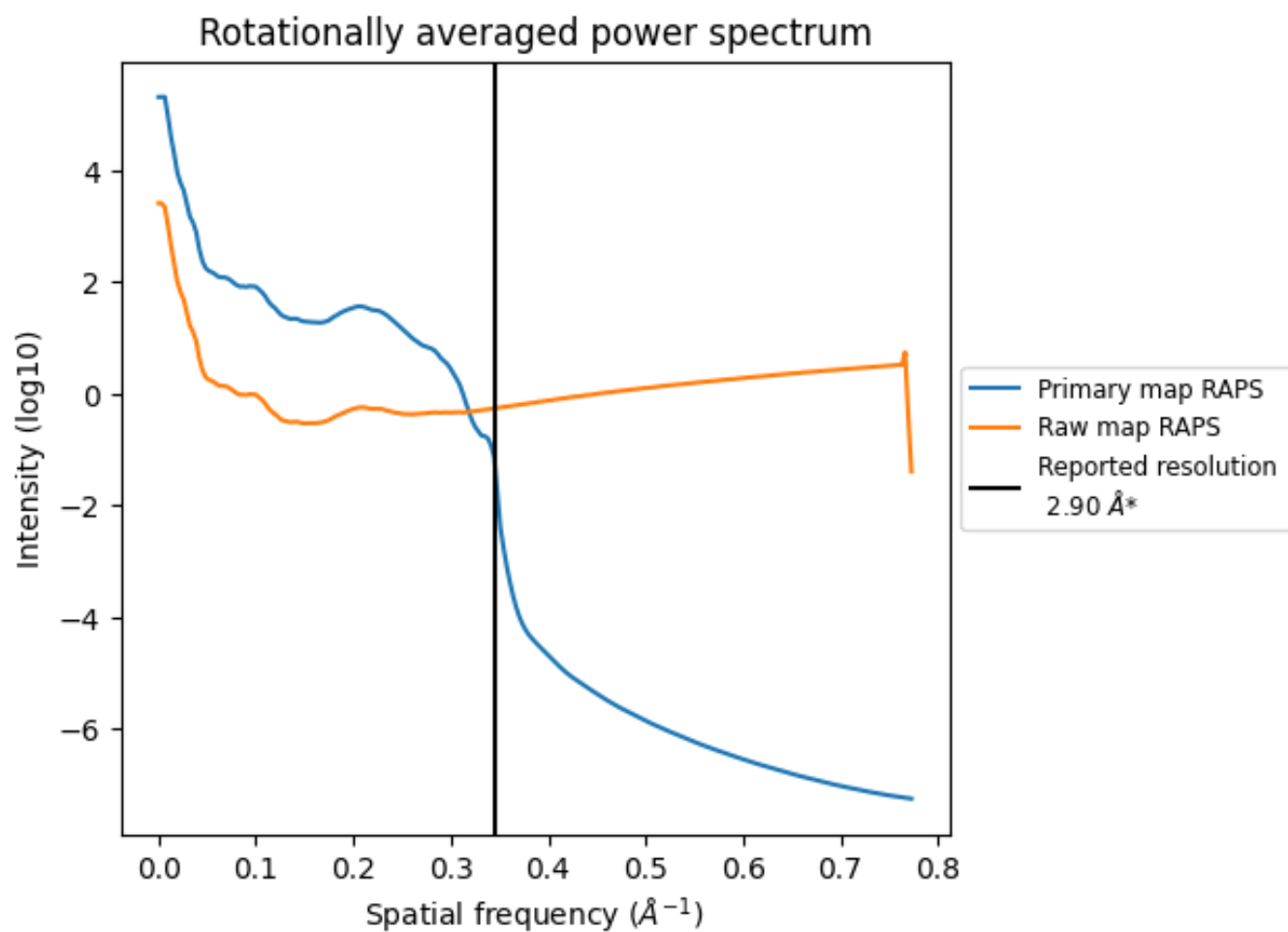


The volume at the recommended contour level is 282  $\text{nm}^3$ ; this corresponds to an approximate mass of 255 kDa.

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

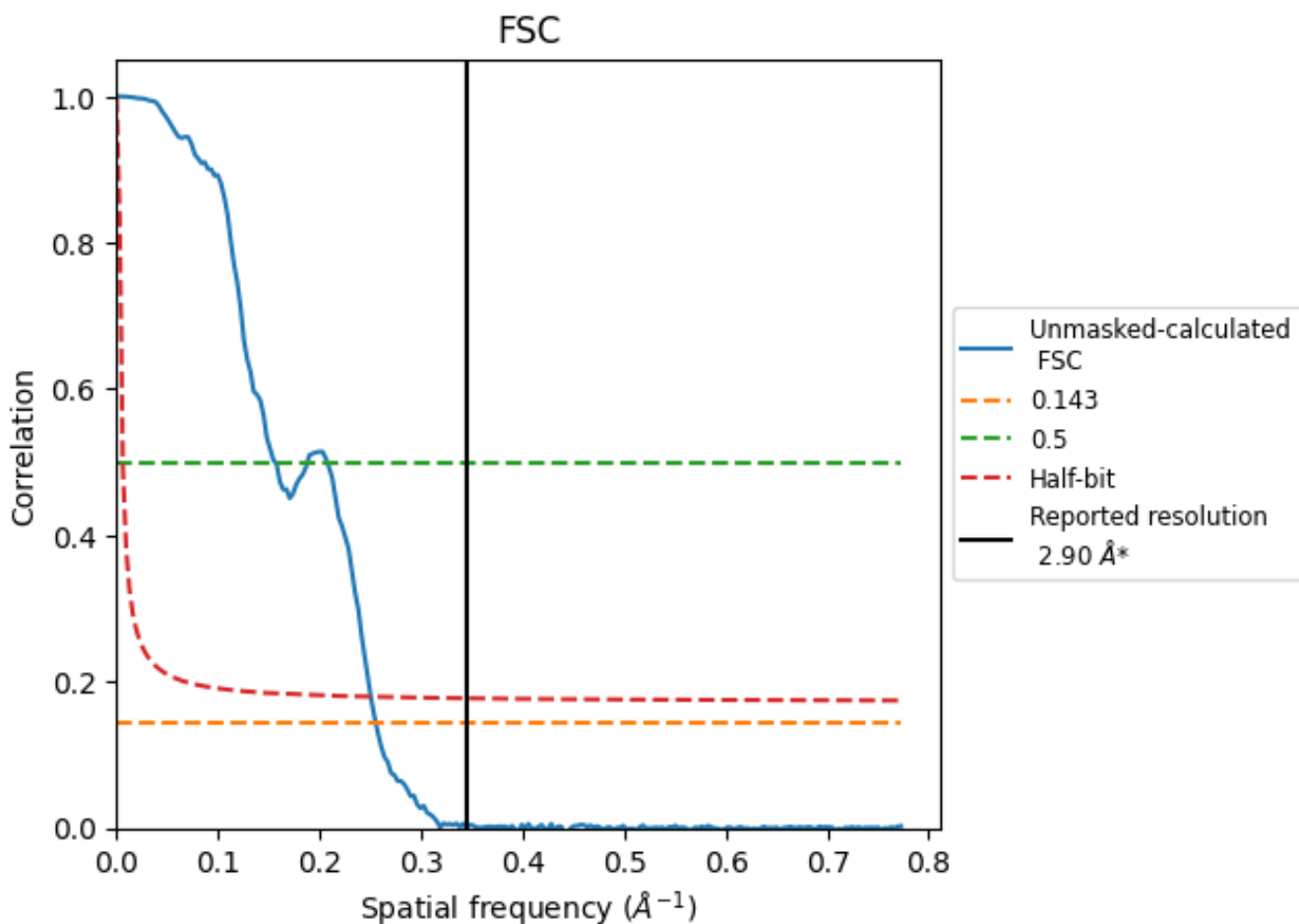


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

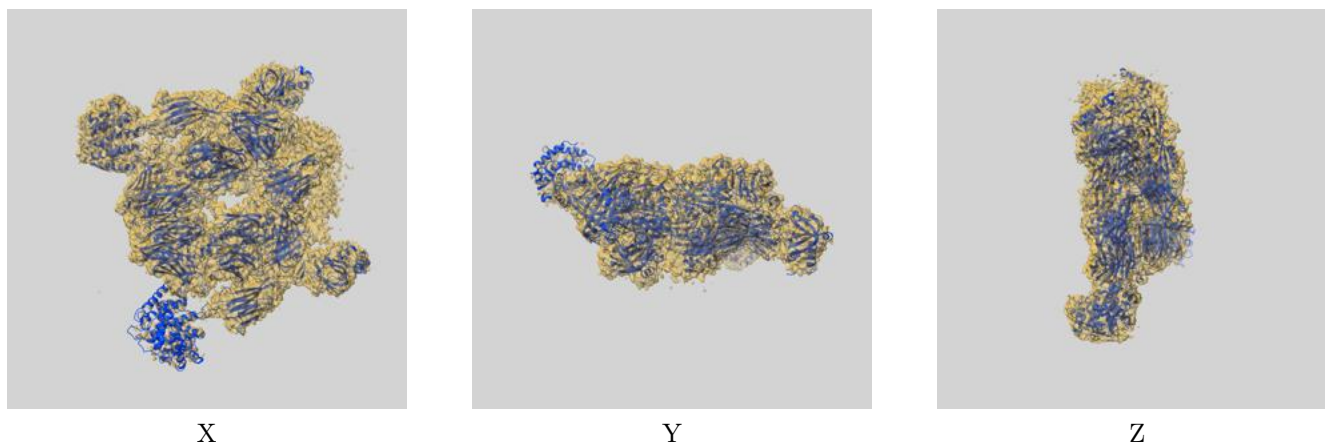
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	6.41	3.99

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 2.9 by more than 10 %

## 9 Map-model fit [i](#)

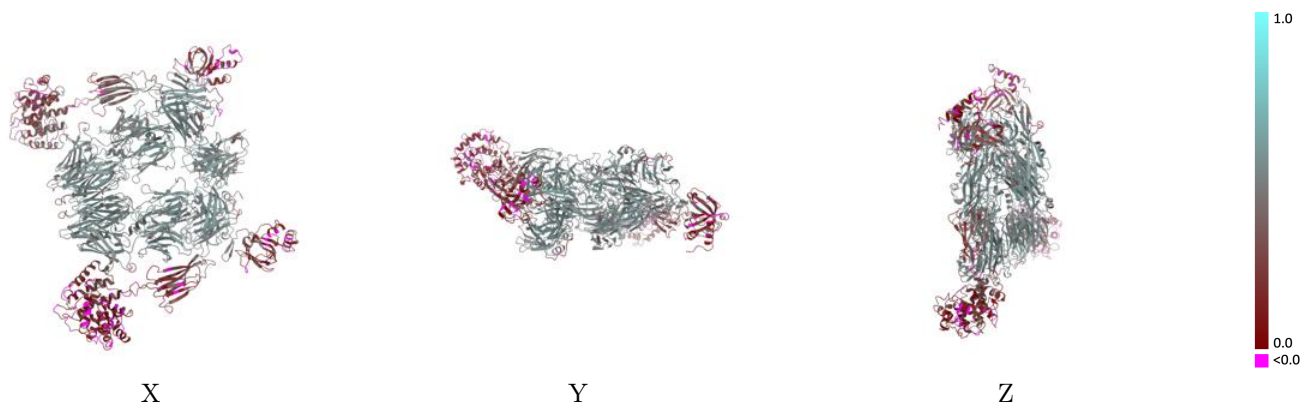
This section contains information regarding the fit between EMDB map EMD-17103 and PDB model 8OQ3. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



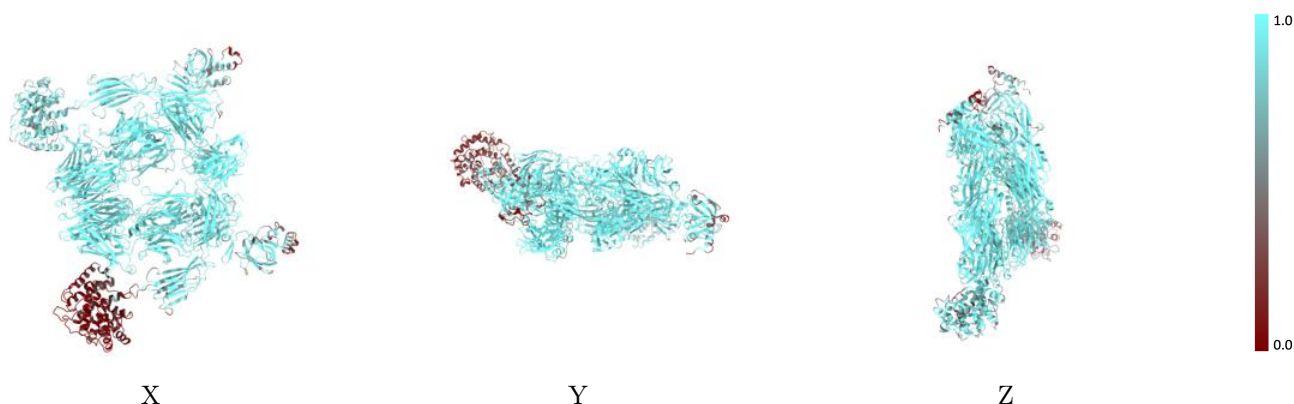
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



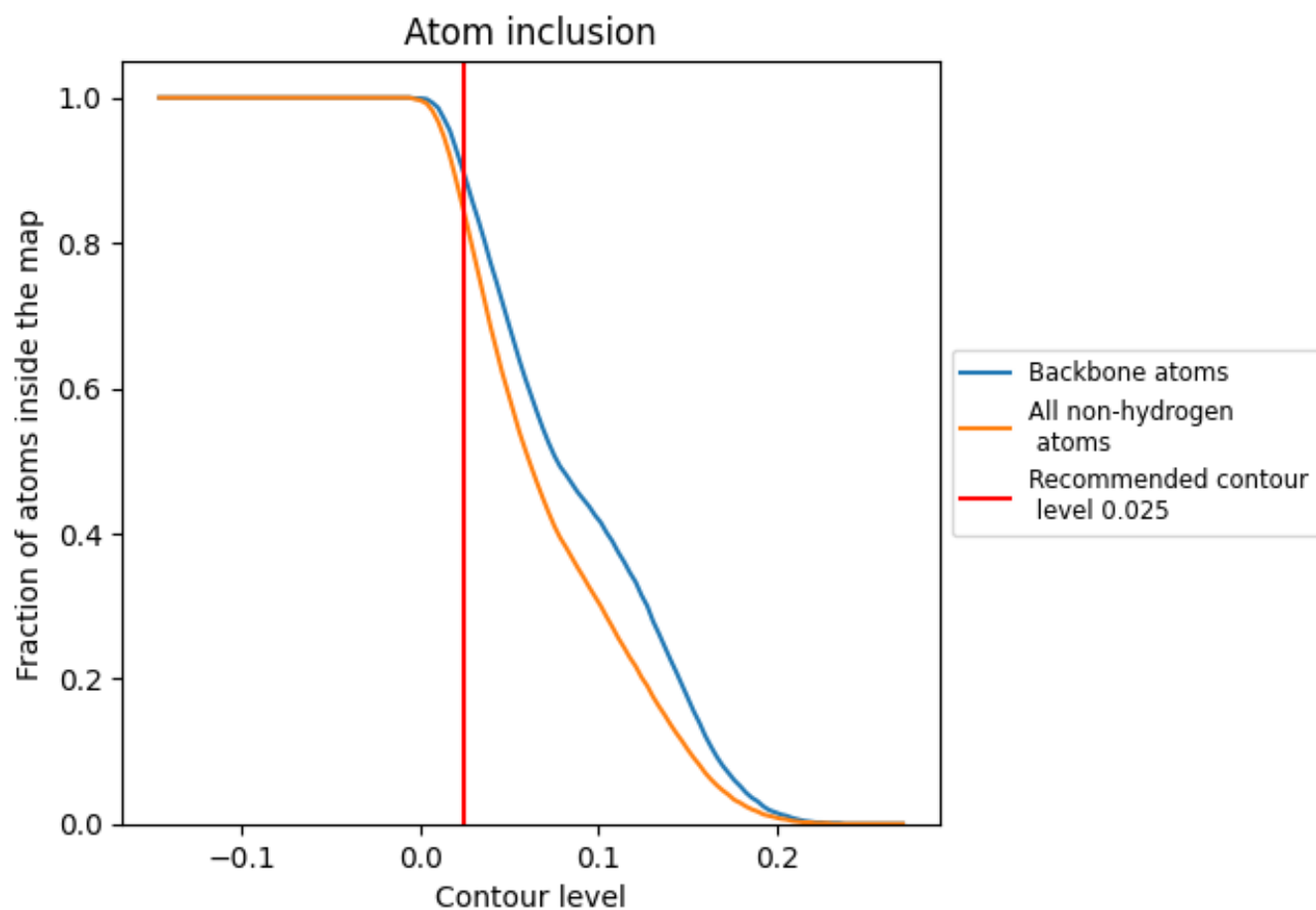
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.4120
A	 0.9000	 0.4170
C	 0.9710	 0.5110
D	 0.7580	 0.3920
F	 0.9800	 0.5120
G	 0.7180	 0.3050
H	 0.8970	 0.4100

