



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 05:44 AM EST

PDB ID : 7KWO  
EMDB ID : EMD-23057  
Title : rFVIIIIFc-VWF-XTEN (BIVV001)  
Authors : Fuller, J.R.; Batchelor, J.D.  
Deposited on : 2020-12-01  
Resolution : 2.90 Å(reported)  
Based on initial models : 6MF2, 6N29

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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

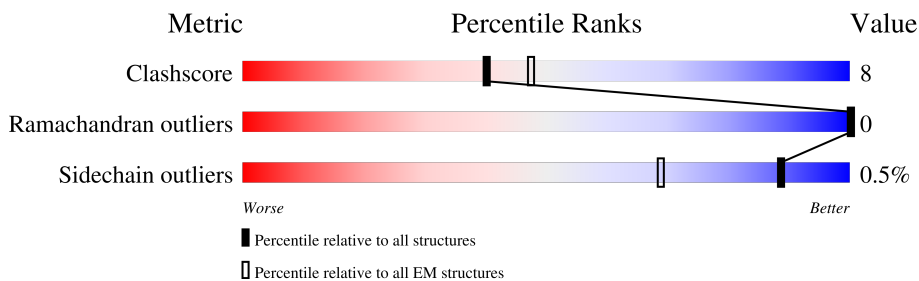
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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	1965	
2	V	1646	
3	B	3	

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 13469 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 Coagulation factor FVIII-Fc-XTEN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1200	9743	6288	1640	1759	56	0	0

- Molecule 2 is a protein called von Willebrand factor-XTEN-Fc.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	478	3641	2244	632	707	58	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	B	3	39	22	2	15	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	28	16	2	10	0
4	A	1	28	16	2	10	0
4	V	1	14	8	1	5	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
5	A	1	1	1	0
5	V	1	1	1	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
6	A	1	1	1	0

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
7	A	1	1	1	0







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

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

Chain B:  100%

MAG1  
MAG2  
B01A3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116200	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.036	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0145	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, CU, CA, ZN, NAG, TYS

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	0.27	0/10002	0.45	1/13549 (0.0%)
2	V	0.25	0/3717	0.43	0/5052
All	All	0.26	0/13719	0.44	1/18601 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1978	LEU	C-N-CA	5.29	134.91	121.70

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	9743	0	9487	150	0
2	V	3641	0	3445	56	0
3	B	39	0	34	0	0
4	A	28	0	26	0	0
4	V	14	0	13	0	0
5	A	1	0	0	0	0
5	V	1	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
All	All	13469	0	13005	202	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (202) 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)
2:V:870:ILE:O	2:V:874:HIS:HB2	1.78	0.82
1:A:265:GLU:H	1:A:290:PRO:HG3	1.47	0.79
1:A:1678:ASP:OD1	2:V:820:ARG:NH1	2.17	0.78
1:A:113:GLU:HB2	1:A:126:ASP:HB3	1.71	0.72
1:A:1936:GLN:NE2	1:A:1991:SER:O	2.22	0.71
2:V:1225:CYS:HB3	2:V:1232:LEU:HD11	1.74	0.69
1:A:2063:SER:OG	1:A:2159:ARG:NH1	2.27	0.67
2:V:870:ILE:HG22	2:V:1083:VAL:HG11	1.76	0.67
1:A:1965:VAL:HG12	1:A:1986:VAL:HG12	1.75	0.67
1:A:425:LYS:NZ	1:A:544:ALA:O	2.27	0.67
2:V:971:SER:HB2	2:V:983:VAL:HB	1.79	0.65
1:A:389:GLU:OE1	1:A:439:ARG:NH1	2.30	0.65
1:A:2246:GLN:NE2	1:A:2290:PHE:O	2.30	0.64
1:A:300:LEU:HD13	1:A:326:VAL:HG22	1.80	0.64
1:A:2264:SER:HB3	1:A:2301:LEU:HD21	1.80	0.64
1:A:389:GLU:OE2	1:A:431:TYR:OH	2.16	0.63
2:V:965:LEU:HD21	2:V:1166:PRO:HD3	1.81	0.62
1:A:1894:ASN:OD1	1:A:1897:ARG:NH2	2.32	0.62
2:V:1045:THR:OG1	2:V:1089:CYS:O	2.17	0.62
1:A:259:GLY:O	1:A:291:ILE:HA	2.00	0.62
1:A:532:TYR:HB3	1:A:640:LEU:HD21	1.80	0.62
1:A:1680:TYS:O1	1:A:1680:TYS:HE1	1.98	0.62
1:A:1962:VAL:HG12	1:A:1974:ALA:HB2	1.82	0.61
1:A:2255:MET:HA	1:A:2314:VAL:O	2.01	0.61
1:A:1927:ASP:HA	1:A:2012:THR:HA	1.84	0.60
1:A:272:GLU:HG2	1:A:307:LEU:H	1.65	0.60
2:V:844:ILE:O	2:V:847:ASN:ND2	2.35	0.59
2:V:788:CYS:SG	2:V:801:SER:OG	2.59	0.59
1:A:2025:LEU:HD12	1:A:2166:LEU:HB3	1.84	0.59
1:A:2206:SER:O	1:A:2209:ARG:NH1	2.34	0.59
2:V:1143:GLU:OE1	2:V:1145:ARG:NH2	2.36	0.59
1:A:293:PHE:CE2	1:A:1975:LEU:HD12	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:O	1:A:421:ARG:NH2	2.34	0.58
1:A:2185:ILE:O	1:A:2209:ARG:NH2	2.35	0.58
1:A:471:ARG:HG2	1:A:472:PRO:HD2	1.86	0.57
2:V:1229:VAL:HG12	2:V:1230:VAL:HG23	1.86	0.57
1:A:4:ARG:HD2	1:A:85:VAL:HB	1.85	0.57
1:A:53:GLU:HB2	1:A:74:PRO:HG3	1.87	0.56
1:A:2196:PHE:N	1:A:2220:ARG:O	2.31	0.56
2:V:1123:ALA:HA	2:V:1127:PRO:HB3	1.88	0.56
1:A:1975:LEU:HD11	1:A:2001:LEU:HD12	1.87	0.56
1:A:66:PRO:HG2	1:A:69:MET:HG3	1.87	0.56
1:A:2076:LEU:O	1:A:2147:ARG:NH1	2.38	0.56
1:A:616:SER:HB3	1:A:621:VAL:HG22	1.89	0.55
1:A:687:LEU:HB3	1:A:1802:PRO:HB3	1.88	0.55
1:A:196:ILE:HD13	1:A:256:HIS:HB2	1.88	0.55
2:V:1206:PHE:HD2	2:V:1210:LYS:HB3	1.71	0.55
2:V:1208:SER:OG	2:V:1228:ASP:O	2.22	0.55
2:V:1148:SER:HA	2:V:1171:GLU:HG3	1.89	0.55
1:A:417:GLN:NE2	1:A:600:GLY:O	2.40	0.55
1:A:2169:CYS:SG	1:A:2173:SER:HA	2.46	0.55
1:A:2205:PRO:HA	1:A:2219:TRP:HB2	1.87	0.55
1:A:648:PHE:CZ	1:A:1953:ILE:HD11	2.42	0.54
1:A:650:SER:HB2	1:A:693:HIS:HB2	1.90	0.54
1:A:399:VAL:HB	1:A:421:ARG:HH12	1.72	0.54
1:A:658:PHE:HB2	1:A:678:VAL:CG1	2.37	0.54
1:A:2093:PHE:HZ	2:V:989:GLN:OE1	1.91	0.54
2:V:960:ARG:HE	2:V:1128:GLN:HE22	1.55	0.54
1:A:2198:ASN:OD1	1:A:2201:ALA:N	2.34	0.54
2:V:889:CYS:HB2	2:V:891:TYR:CZ	2.42	0.54
1:A:2249:LYS:NZ	2:V:1078:GLU:OE2	2.40	0.54
1:A:15:ASP:HB3	1:A:45:VAL:HG22	1.88	0.54
2:V:1056:VAL:HG13	2:V:1088:THR:HB	1.89	0.53
2:V:791:THR:HG22	2:V:793:GLN:H	1.73	0.53
1:A:113:GLU:OE1	1:A:127:LYS:NZ	2.32	0.53
1:A:2117:GLY:HA2	1:A:2142:PRO:HD2	1.90	0.53
1:A:467:ASN:ND2	1:A:503:ILE:O	2.42	0.52
2:V:977:HIS:ND1	2:V:1102:ASP:OD2	2.42	0.52
2:V:1158:GLN:HE21	2:V:1186:LEU:HG	1.73	0.52
1:A:449:LEU:HD22	1:A:550:PRO:HD3	1.91	0.52
1:A:4:ARG:NH2	1:A:87:THR:OG1	2.42	0.52
1:A:632:HIS:ND1	1:A:683:GLU:OE1	2.40	0.51
1:A:1881:THR:OG1	1:A:1947:MET:O	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1767:VAL:CG2	1:A:1860:THR:HG23	2.40	0.51
1:A:2180:MET:HG2	1:A:2185:ILE:HD12	1.93	0.51
1:A:264:PRO:HA	1:A:290:PRO:HG2	1.92	0.51
1:A:426:VAL:HG22	1:A:547:LEU:HD21	1.93	0.51
2:V:881:LEU:HD23	2:V:1006:ASP:HB2	1.92	0.50
2:V:1214:LEU:O	2:V:1222:CYS:HA	2.10	0.50
1:A:1759:LEU:HD23	1:A:1852:ILE:HG23	1.92	0.50
1:A:1789:LEU:HD11	1:A:1835:TRP:CD1	2.47	0.50
2:V:1211:LYS:HE3	2:V:1226:HIS:HE1	1.76	0.50
1:A:2237:THR:HA	1:A:2304:ARG:HG2	1.94	0.50
1:A:1859:HIS:O	1:A:1862:THR:OG1	2.27	0.50
1:A:382:TRP:HB2	1:A:461:LEU:HD23	1.92	0.50
1:A:2070:TRP:HA	1:A:2151:LEU:O	2.12	0.50
1:A:386:ILE:O	1:A:465:PHE:HA	2.13	0.49
2:V:1215:ASN:HB3	2:V:1218:ASP:HB3	1.94	0.49
1:A:199:PHE:HZ	1:A:308:LEU:HD21	1.78	0.49
1:A:90:ASN:ND2	1:A:128:VAL:O	2.30	0.49
1:A:1749:ARG:HG3	1:A:1753:ASN:HB2	1.95	0.48
1:A:1944:LEU:HB3	1:A:1978:LEU:HD21	1.94	0.48
1:A:2244:THR:HB	1:A:2322:GLU:HB3	1.94	0.48
1:A:2229:TRP:HA	1:A:2308:ILE:O	2.14	0.48
1:A:656:TYR:HE1	1:A:682:MET:HA	1.77	0.48
1:A:396:ALA:O	1:A:421:ARG:NH1	2.47	0.48
2:V:1158:GLN:NE2	2:V:1184:ASP:OD1	2.45	0.48
1:A:581:GLU:HB2	1:A:612:ASN:HB3	1.95	0.48
1:A:550:PRO:HB3	1:A:573:VAL:HG11	1.95	0.48
2:V:1008:THR:HA	2:V:1014:VAL:HA	1.96	0.48
1:A:2048:PRO:HA	1:A:2062:TRP:HB2	1.96	0.47
1:A:1927:ASP:HB3	1:A:2013:LEU:HG	1.96	0.47
1:A:122:GLU:OE2	1:A:2239:LYS:NZ	2.36	0.47
1:A:443:GLN:HG2	1:A:445:GLU:H	1.79	0.47
1:A:2089:ALA:HB3	1:A:2161:THR:HG21	1.95	0.47
1:A:2223:VAL:O	1:A:2225:ASN:ND2	2.48	0.47
1:A:467:ASN:HD21	1:A:472:PRO:HA	1.80	0.47
1:A:2186:SER:HB3	1:A:2189:GLN:HG3	1.96	0.47
1:A:571:ARG:HA	1:A:638:TYR:HE2	1.80	0.47
1:A:2241:THR:HG22	1:A:2325:GLY:HA2	1.95	0.47
1:A:1886:THR:HA	1:A:1891:PHE:CD1	2.50	0.46
1:A:157:SER:HG	1:A:293:PHE:HZ	1.63	0.46
2:V:960:ARG:NE	2:V:1128:GLN:HE22	2.13	0.46
2:V:973:VAL:HB	2:V:981:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1046:CYS:O	2:V:1053:GLN:NE2	2.48	0.46
2:V:1122:THR:HG23	2:V:1125:LEU:H	1.79	0.46
1:A:417:GLN:O	1:A:418:ARG:NH1	2.44	0.46
1:A:533:TYR:CZ	1:A:549:GLY:HA3	2.51	0.46
1:A:582:ASN:HA	1:A:587:LEU:HD22	1.98	0.46
1:A:2207:LYS:NZ	1:A:2215:ARG:O	2.46	0.46
2:V:1208:SER:HA	2:V:1227:CYS:HB3	1.97	0.46
1:A:1899:CYS:SG	1:A:1916:TYR:OH	2.73	0.46
1:A:2313:TRP:HB2	1:A:2316:GLN:O	2.15	0.46
1:A:2026:GLY:HA3	1:A:2031:HIS:HB3	1.98	0.46
1:A:2179:GLY:HA3	1:A:2184:ALA:HB3	1.96	0.46
1:A:2194:SER:HB3	1:A:2222:GLN:HG2	1.97	0.46
1:A:666:ASP:HB2	1:A:1835:TRP:HZ3	1.81	0.45
1:A:2275:PHE:HA	1:A:2280:VAL:HA	1.98	0.45
1:A:260:MET:HA	1:A:291:ILE:HD13	1.98	0.45
1:A:427:ARG:HD2	1:A:448:ILE:HA	1.98	0.45
2:V:1184:ASP:O	2:V:1188:GLN:N	2.50	0.45
1:A:175:ALA:HB2	1:A:196:ILE:HG21	1.98	0.45
1:A:452:LEU:HD11	1:A:552:LEU:HG	1.98	0.45
1:A:577:SER:HA	1:A:642:ILE:O	2.17	0.45
1:A:430:ALA:HB2	1:A:451:PRO:HB3	1.99	0.45
2:V:829:CYS:SG	2:V:836:TYR:HB2	2.57	0.45
2:V:925:VAL:HB	2:V:936:LEU:HB2	1.99	0.45
1:A:1929:LEU:HD12	1:A:1930:PRO:HD2	1.99	0.44
1:A:2021:CYS:SG	1:A:2175:SER:HB2	2.58	0.44
2:V:1043:PRO:O	2:V:1047:HIS:N	2.50	0.44
1:A:242:LEU:HD12	1:A:243:PRO:HD2	1.98	0.44
1:A:2071:ILE:HG21	1:A:2162:LEU:HD23	1.98	0.44
1:A:641:SER:HB2	1:A:670:LEU:HD13	1.99	0.44
2:V:907:ILE:HG12	2:V:927:ILE:HG23	1.98	0.44
1:A:438:THR:HG23	1:A:438:THR:O	2.17	0.44
1:A:634:VAL:CG1	1:A:679:PHE:CE2	3.01	0.44
1:A:2093:PHE:HZ	2:V:989:GLN:CD	2.21	0.44
1:A:647:ASP:HB2	1:A:1950:ASN:ND2	2.32	0.43
2:V:897:TYR:HE1	2:V:906:ARG:HB2	1.83	0.43
2:V:1109:HIS:O	2:V:1113:GLN:HG2	2.18	0.43
1:A:1700:ILE:O	1:A:1775:PHE:HA	2.18	0.43
1:A:389:GLU:OE2	1:A:468:GLN:NE2	2.51	0.43
1:A:1737:GLU:HB2	1:A:1761:PRO:CG	2.49	0.43
1:A:591:ILE:HG23	1:A:601:VAL:HG21	2.00	0.43
1:A:1870:GLN:OE1	1:A:1941:ARG:NH1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1837:TYR:CZ	1:A:1853:GLY:HA3	2.53	0.43
1:A:521:PRO:HG2	1:A:555:TYR:HB2	2.01	0.43
1:A:1929:LEU:HB3	1:A:2012:THR:OG1	2.18	0.43
1:A:1946:SER:O	1:A:1980:PRO:HA	2.19	0.43
2:V:791:THR:HG23	2:V:816:ARG:O	2.19	0.43
1:A:8:GLY:HA3	1:A:54:PHE:HE2	1.82	0.42
1:A:1738:PHE:HA	1:A:1746:PRO:HA	2.00	0.42
1:A:1789:LEU:HD13	1:A:1823:MET:HB3	2.01	0.42
2:V:1150:ALA:HB3	2:V:1174:HIS:CE1	2.54	0.42
1:A:452:LEU:HA	1:A:550:PRO:HG2	2.02	0.42
1:A:2174:CYS:O	1:A:2241:THR:HG21	2.19	0.42
2:V:844:ILE:HG13	2:V:847:ASN:HD21	1.85	0.42
2:V:874:HIS:CG	2:V:1083:VAL:HG22	2.54	0.42
1:A:1945:LEU:HB2	1:A:1983:PHE:CE1	2.55	0.42
2:V:988:TYR:HB3	2:V:992:VAL:HG13	2.01	0.42
1:A:118:THR:HB	1:A:122:GLU:HB2	2.00	0.42
1:A:461:LEU:HB2	1:A:513:TRP:HB2	2.01	0.42
1:A:1846:ASP:OD1	1:A:1889:TRP:NE1	2.44	0.41
2:V:817:HIS:O	2:V:820:ARG:HG2	2.20	0.41
2:V:831:HIS:CG	2:V:832:GLN:H	2.38	0.41
2:V:879:ASP:HB2	2:V:1006:ASP:OD2	2.20	0.41
1:A:1785:PHE:HB3	1:A:1815:TYR:CE1	2.56	0.41
1:A:2105:TYR:HD2	1:A:2146:ALA:HB2	1.85	0.41
1:A:1764:ARG:HG2	1:A:1856:LEU:HB2	2.01	0.41
1:A:95:PRO:HG2	1:A:162:VAL:HG11	2.03	0.41
1:A:2054:HIS:NE2	1:A:2135:ILE:HD11	2.36	0.41
1:A:2150:ARG:HD3	1:A:2152:HIS:NE2	2.35	0.41
1:A:240:ARG:HD3	1:A:323:TYR:CZ	2.56	0.41
2:V:846:CYS:SG	2:V:863:CYS:N	2.93	0.41
1:A:264:PRO:HA	1:A:290:PRO:CG	2.51	0.41
1:A:1965:VAL:HG11	1:A:1976:TYR:CE1	2.56	0.41
2:V:1198:VAL:HG22	2:V:1207:ALA:HA	2.01	0.41
1:A:656:TYR:CE1	1:A:682:MET:HA	2.56	0.41
1:A:101:VAL:HG13	1:A:1957:HIS:CE1	2.56	0.41
1:A:634:VAL:HG13	1:A:679:PHE:CZ	2.55	0.41
1:A:1938:GLN:O	1:A:1990:PRO:HD2	2.20	0.41
2:V:831:HIS:HB3	2:V:836:TYR:HE2	1.86	0.41
2:V:849:CYS:HA	2:V:858:CYS:HA	2.03	0.41
1:A:289:SER:OG	1:A:1979:TYR:OH	2.33	0.41
1:A:146:PRO:HB3	1:A:154:LEU:HG	2.03	0.40
1:A:232:HIS:CG	1:A:318:ASP:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:PRO:HD3	1:A:498:LEU:HD11	2.03	0.40
2:V:954:GLU:OE2	2:V:1210:LYS:NZ	2.54	0.40
1:A:181:GLU:OE1	1:A:181:GLU:N	2.36	0.40
1:A:1946:SER:HB2	1:A:1978:LEU:HB3	2.02	0.40
2:V:1100:PHE:HE2	2:V:1125:LEU:HD11	1.85	0.40
1:A:1998:VAL:O	1:A:1998:VAL:HG13	2.22	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	1173/1965 (60%)	1141 (97%)	32 (3%)	0	100	100
2	V	476/1646 (29%)	457 (96%)	19 (4%)	0	100	100
All	All	1649/3611 (46%)	1598 (97%)	51 (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	1066/1722 (62%)	1063 (100%)	3 (0%)	92	98
2	V	420/1415 (30%)	416 (99%)	4 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1486/3137 (47%)	1479 (100%)	7 (0%)	89 96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	TYR
1	A	497	HIS
1	A	1983	PHE
2	V	882	LYS
2	V	999	PHE
2	V	1149	CYS
2	V	1165	CYS

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

Mol	Chain	Res	Type
2	V	847	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	TYS	A	1680	1	15,16,17	0.64	0	18,22,24	0.86	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
1	TYS	A	1680	1	-	2/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1680	TYS	CE1-CZ-OH-S
1	A	1680	TYS	CE2-CZ-OH-S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1680	TYS	1	0

## 5.5 Carbohydrates [i](#)

3 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	B	1	1,3	14,14,15	0.40	0	17,19,21	0.53	0
3	NAG	B	2	3	14,14,15	0.17	0	17,19,21	0.43	0
3	BMA	B	3	3	11,11,12	0.51	0	15,15,17	0.82	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	B	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

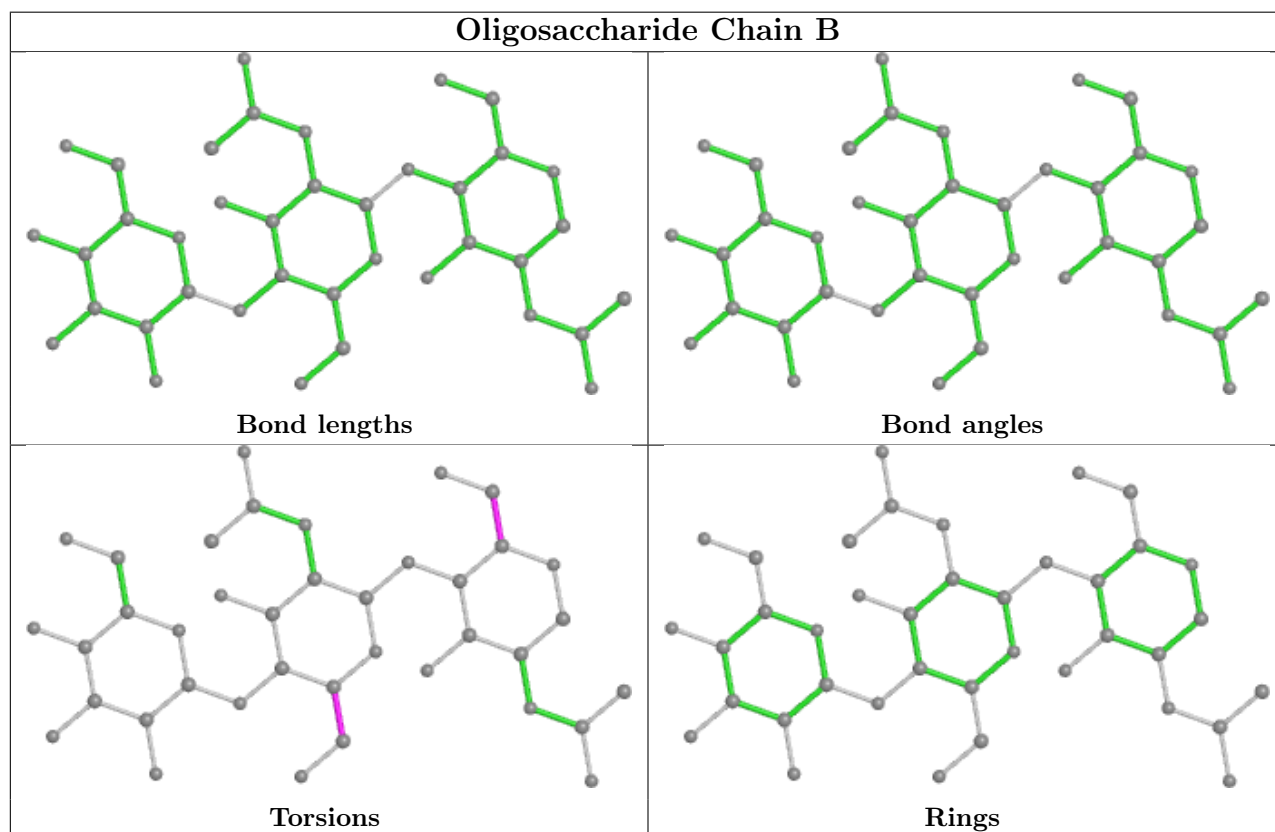
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	NAG	O5-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	B	2	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

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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	V	1701	2	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	A	2602	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	A	2601	1	14,14,15	0.23	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	V	1701	2	-	3/6/23/26	0/1/1/1
4	NAG	A	2602	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2601	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2601	NAG	O5-C5-C6-O6
4	A	2601	NAG	C4-C5-C6-O6
4	A	2602	NAG	C8-C7-N2-C2
4	A	2602	NAG	O7-C7-N2-C2
4	A	2602	NAG	O5-C5-C6-O6
4	A	2602	NAG	C4-C5-C6-O6
4	V	1701	NAG	C4-C5-C6-O6
4	V	1701	NAG	O5-C5-C6-O6
4	A	2601	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	V	1701	NAG	C3-C2-N2-C7

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.

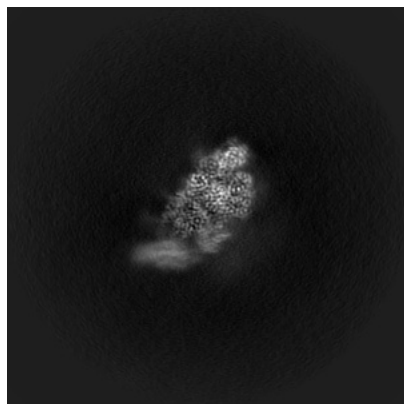
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23057. These allow visual inspection of the internal detail of the map and identification of artifacts.

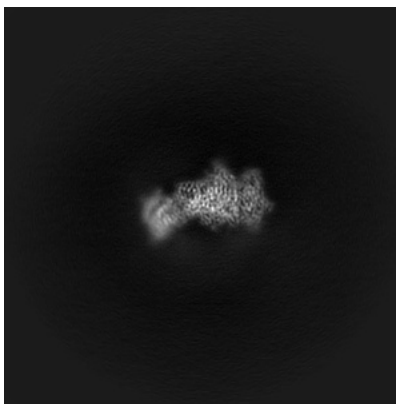
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

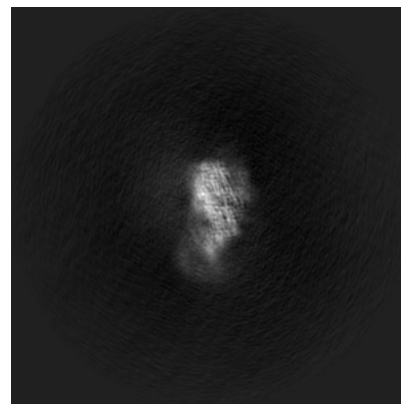
#### 6.1.1 Primary map



X

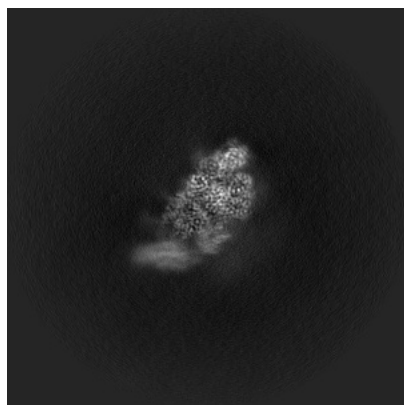


Y

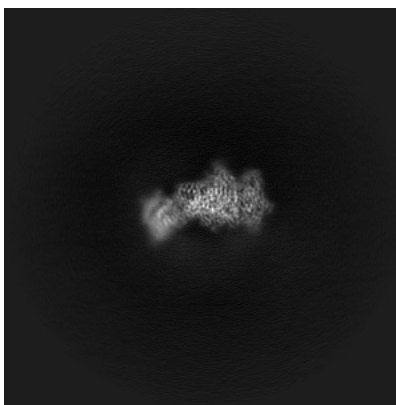


Z

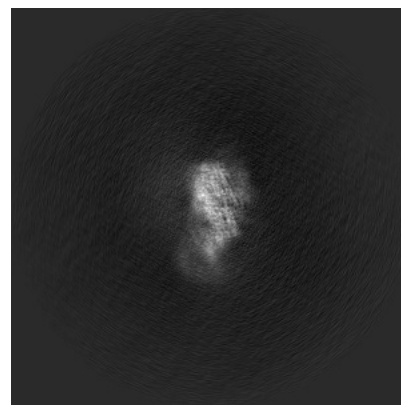
#### 6.1.2 Raw map



X



Y

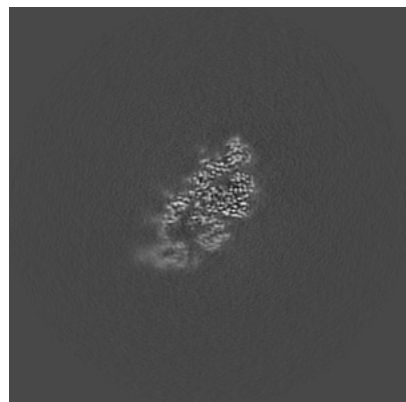


Z

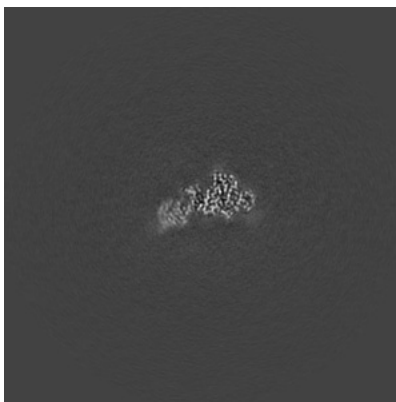
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

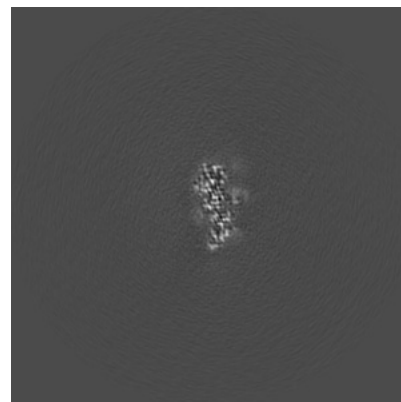
### 6.2.1 Primary map



X Index: 192

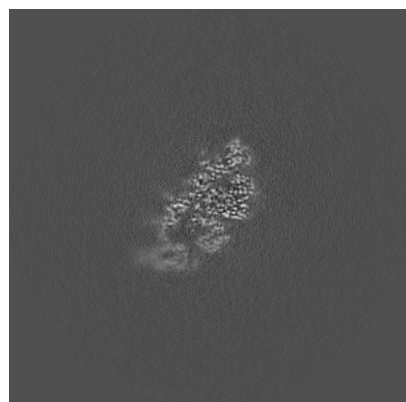


Y Index: 192

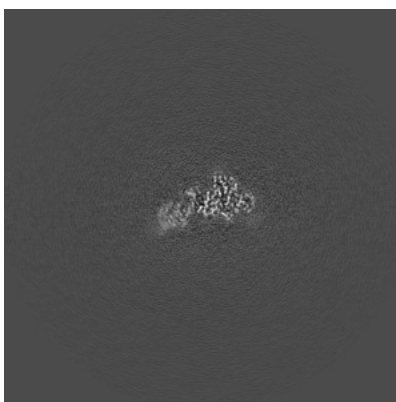


Z Index: 192

### 6.2.2 Raw map



X Index: 192



Y Index: 192

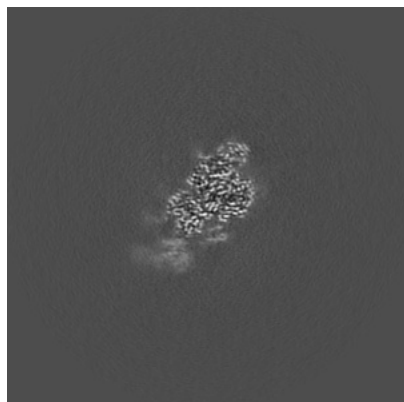


Z Index: 192

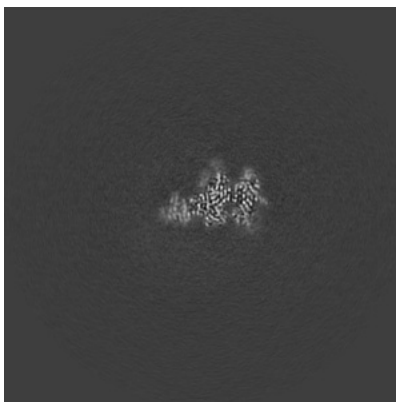
The images above show central slices of the map in three orthogonal directions.

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

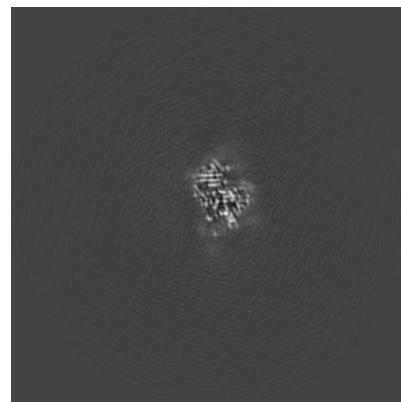
### 6.3.1 Primary map



X Index: 198

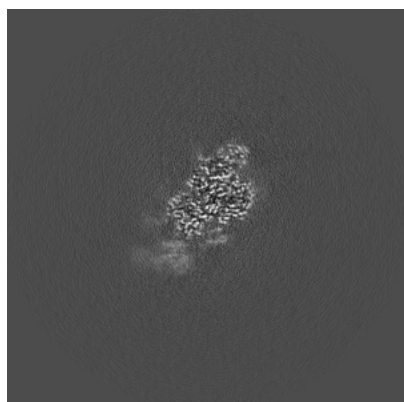


Y Index: 205

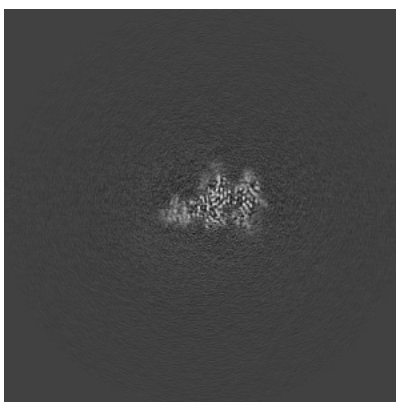


Z Index: 208

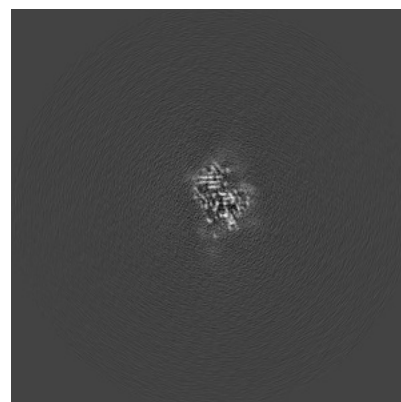
### 6.3.2 Raw map



X Index: 198



Y Index: 205



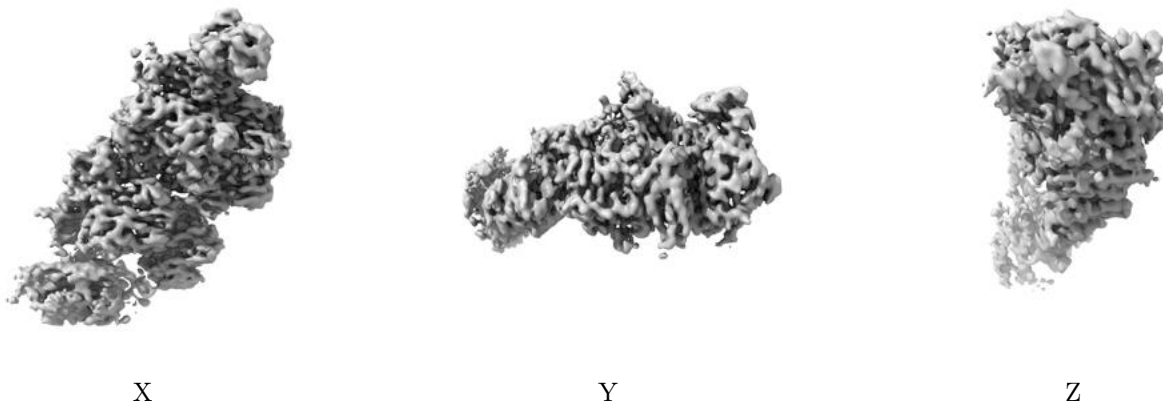
Z Index: 208

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



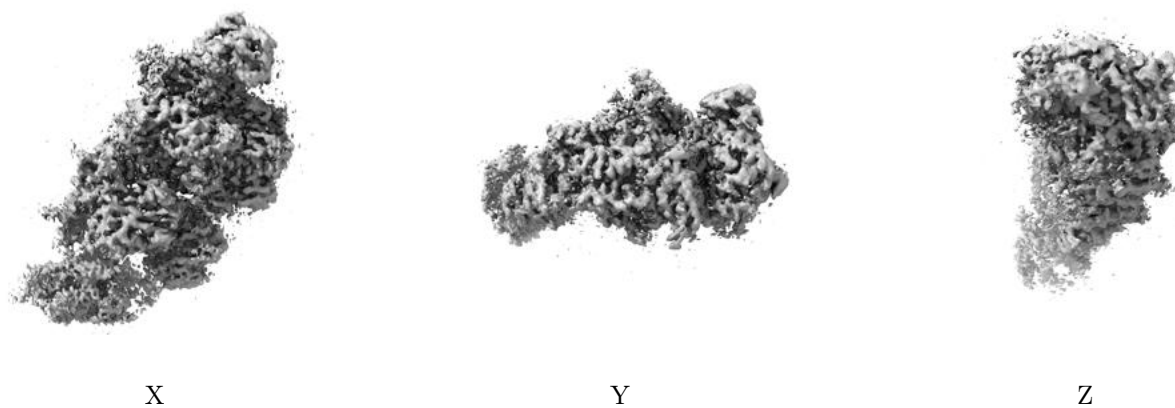
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0145. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

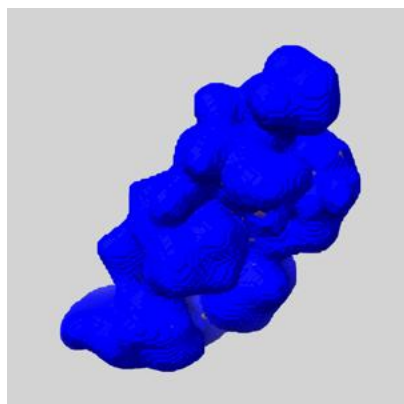
## 6.5 Mask visualisation [i](#)

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

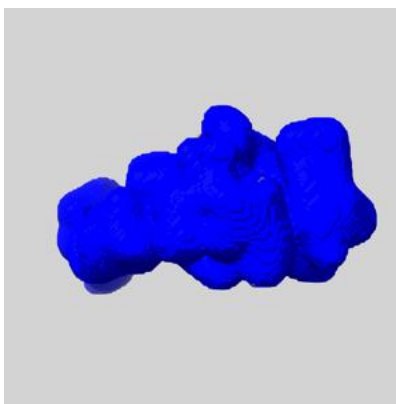
A mask typically either:

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

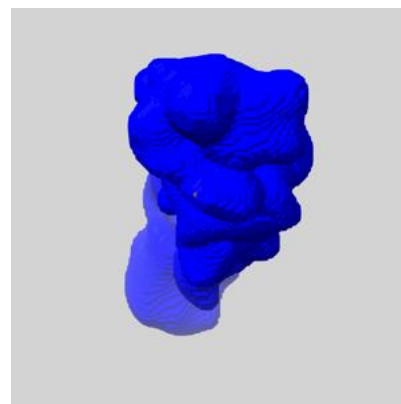
### 6.5.1 emd\_23057\_msk\_1.map [i](#)



X



Y

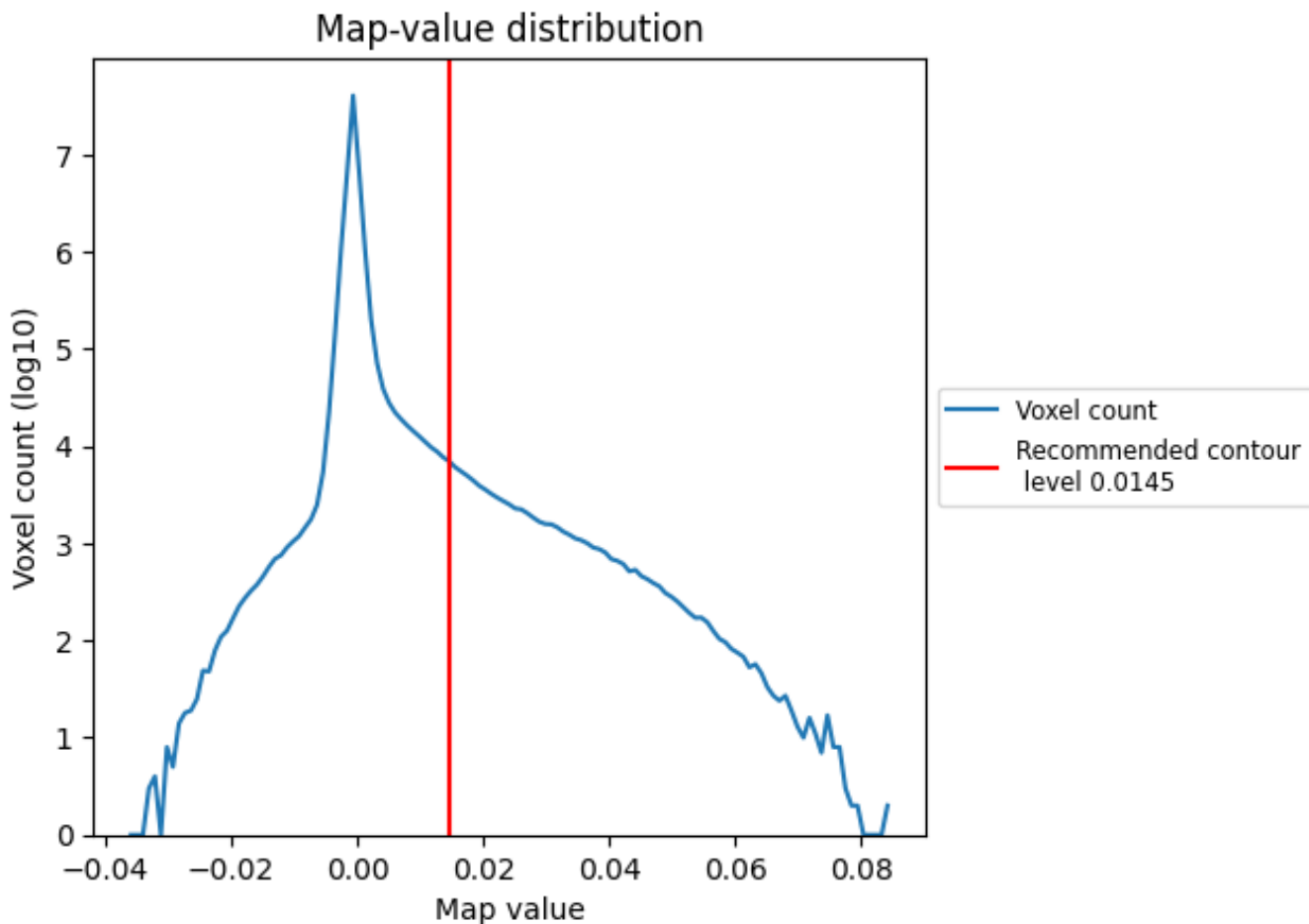


Z

## 7 Map analysis [i](#)

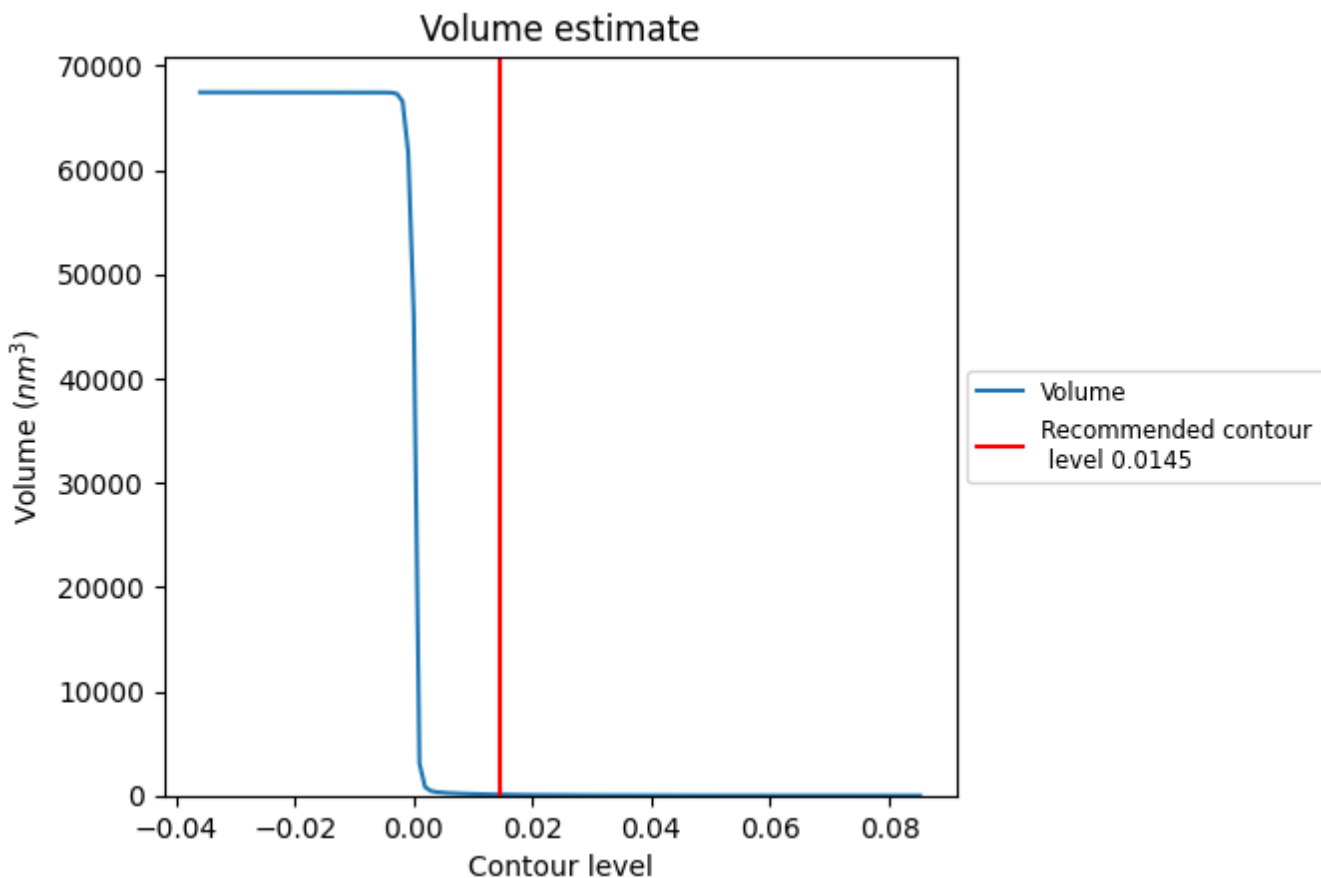
This section contains the results of statistical analysis of the map.

### 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.

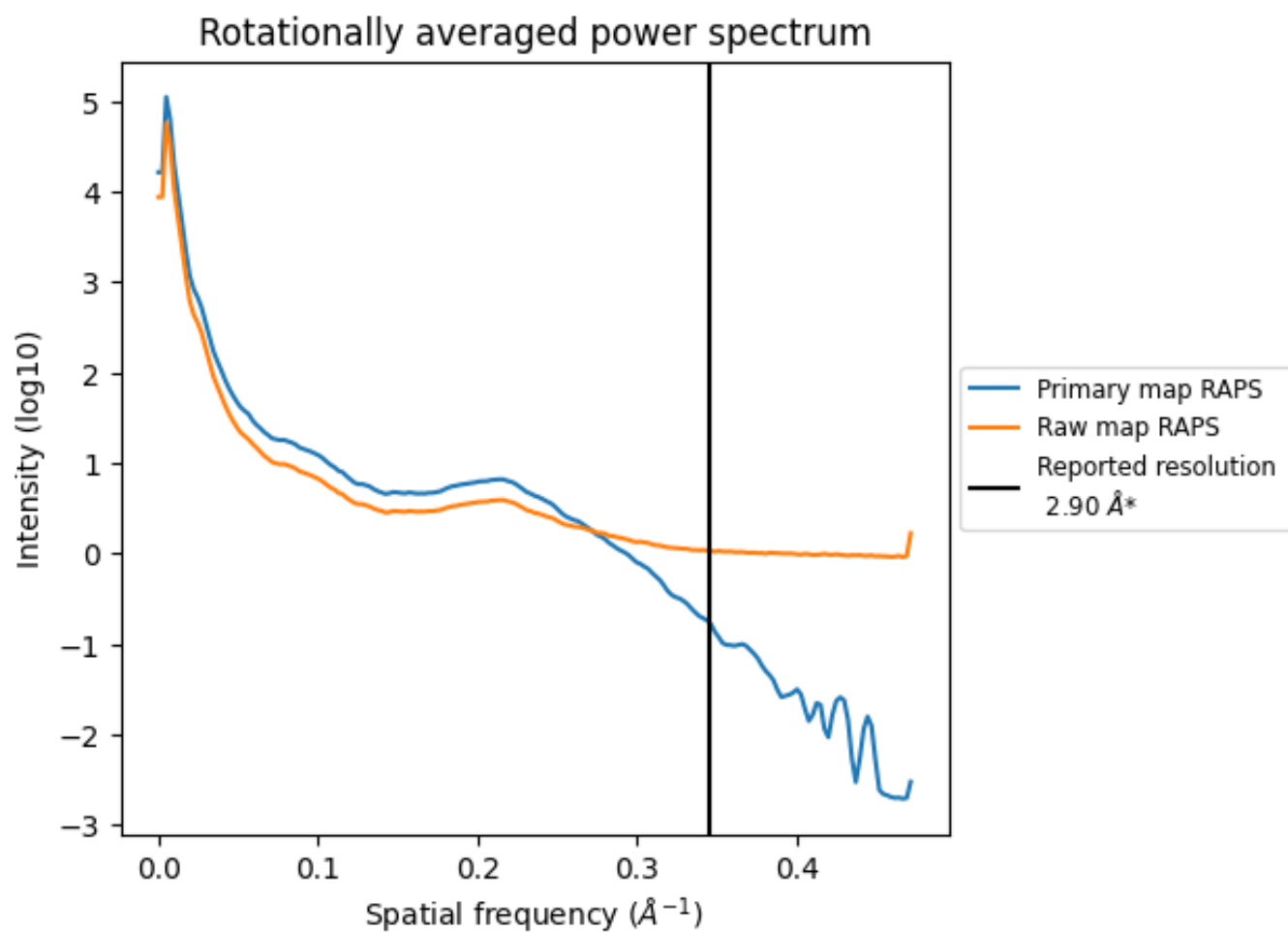
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 93 nm<sup>3</sup>; this corresponds to an approximate mass of 84 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

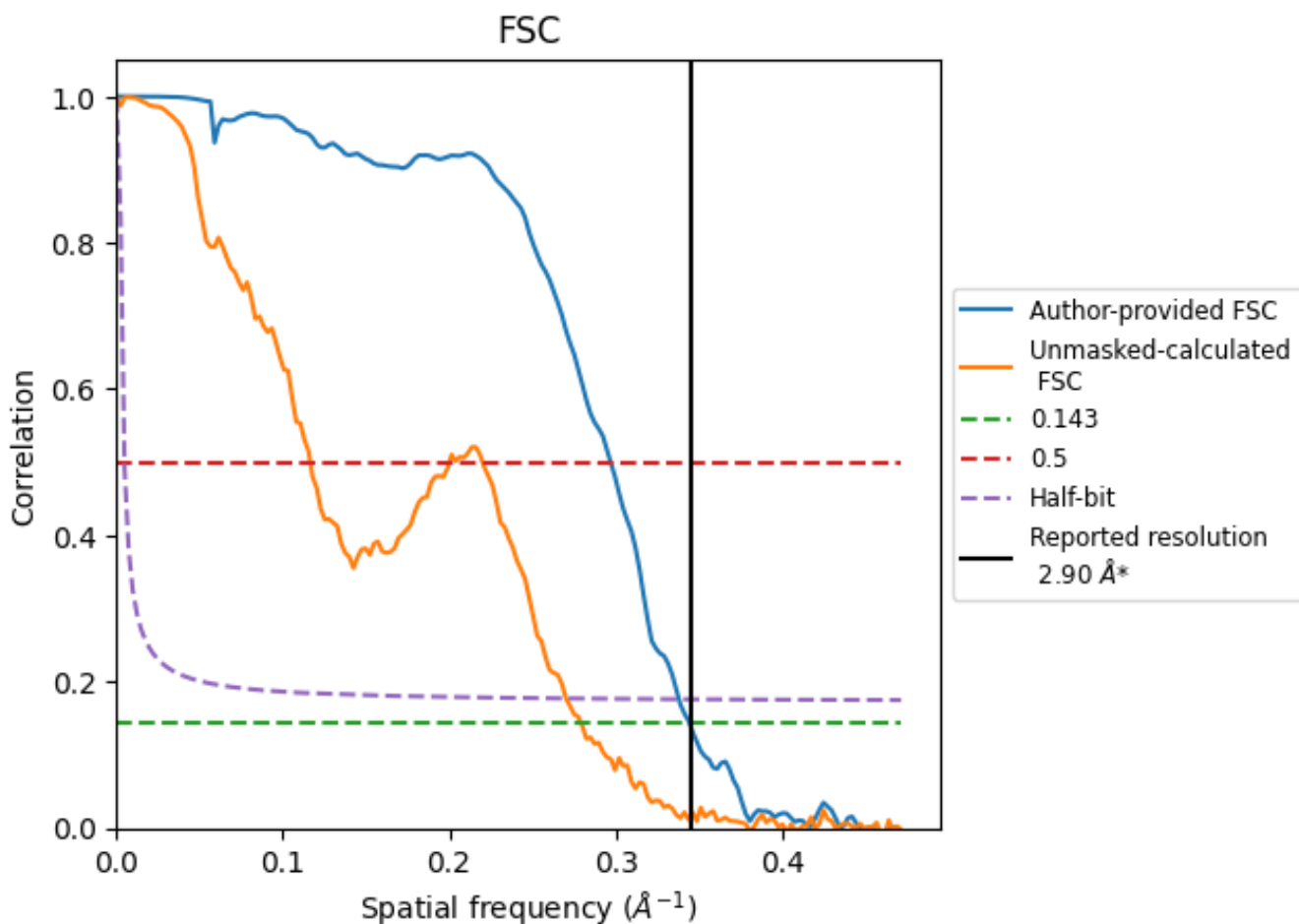


\*Reported resolution corresponds to spatial frequency of  $0.345 \text{ \AA}^{-1}$

## 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 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

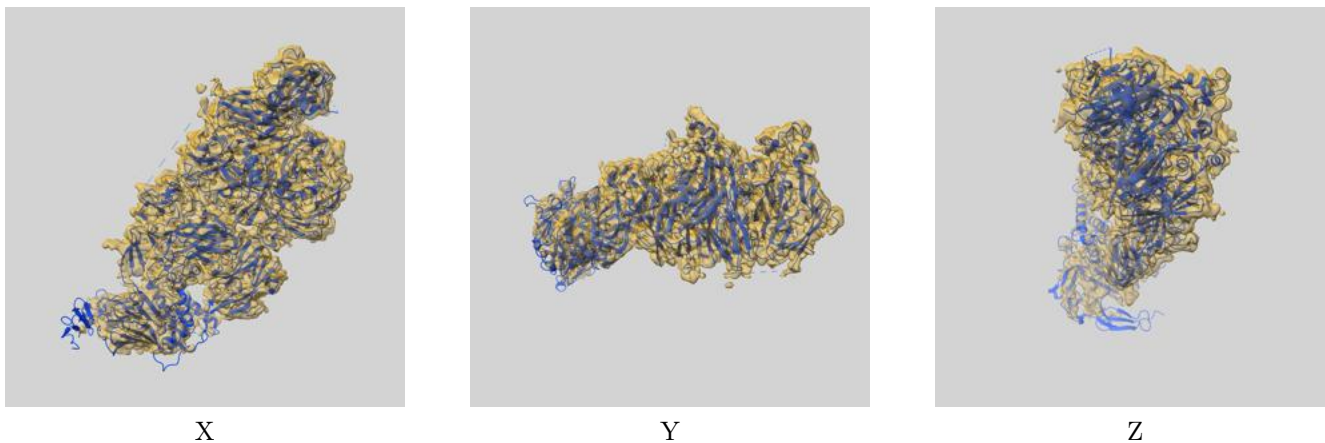
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.37	2.96
Unmasked-calculated*	3.58	8.58	3.70

\*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 3.58 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-23057 and PDB model 7KWO. Per-residue inclusion information can be found in section 3 on page 5.

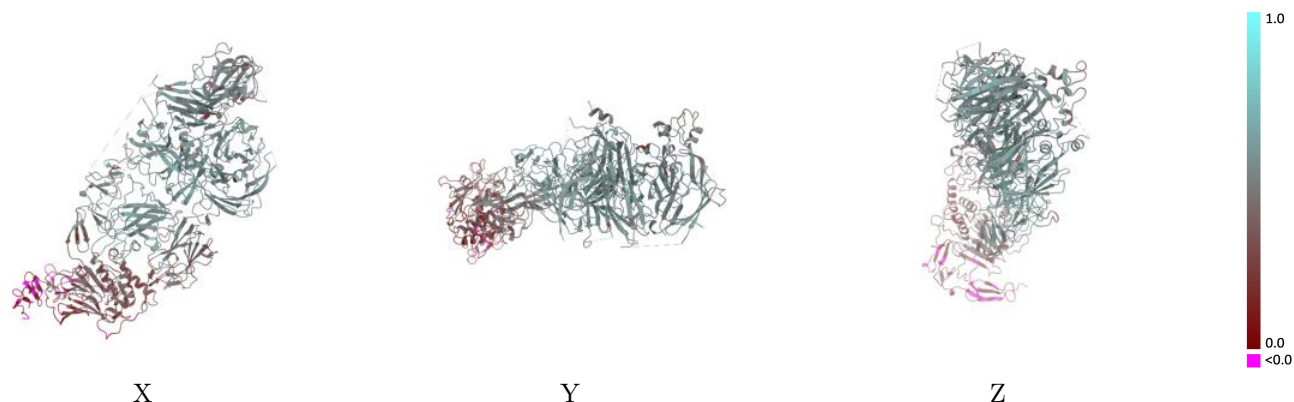
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0145 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.

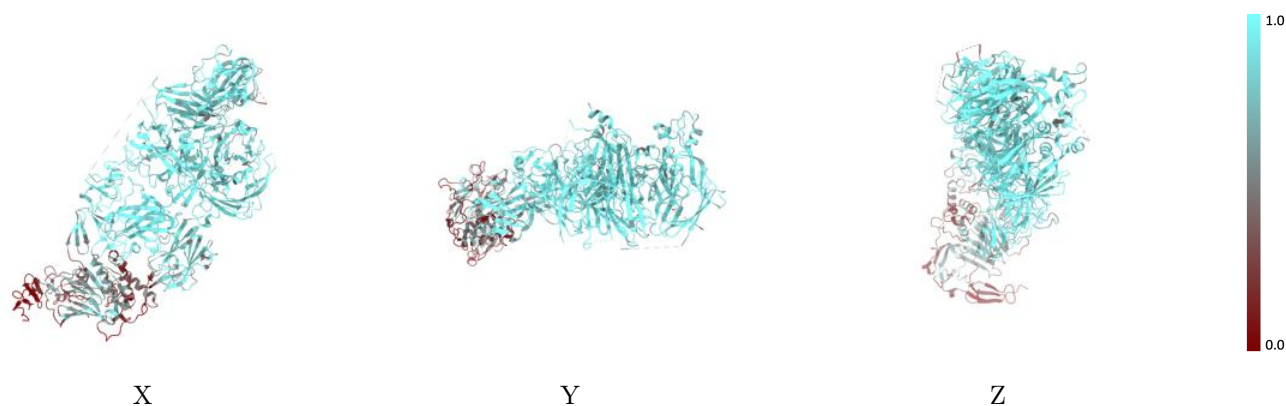


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



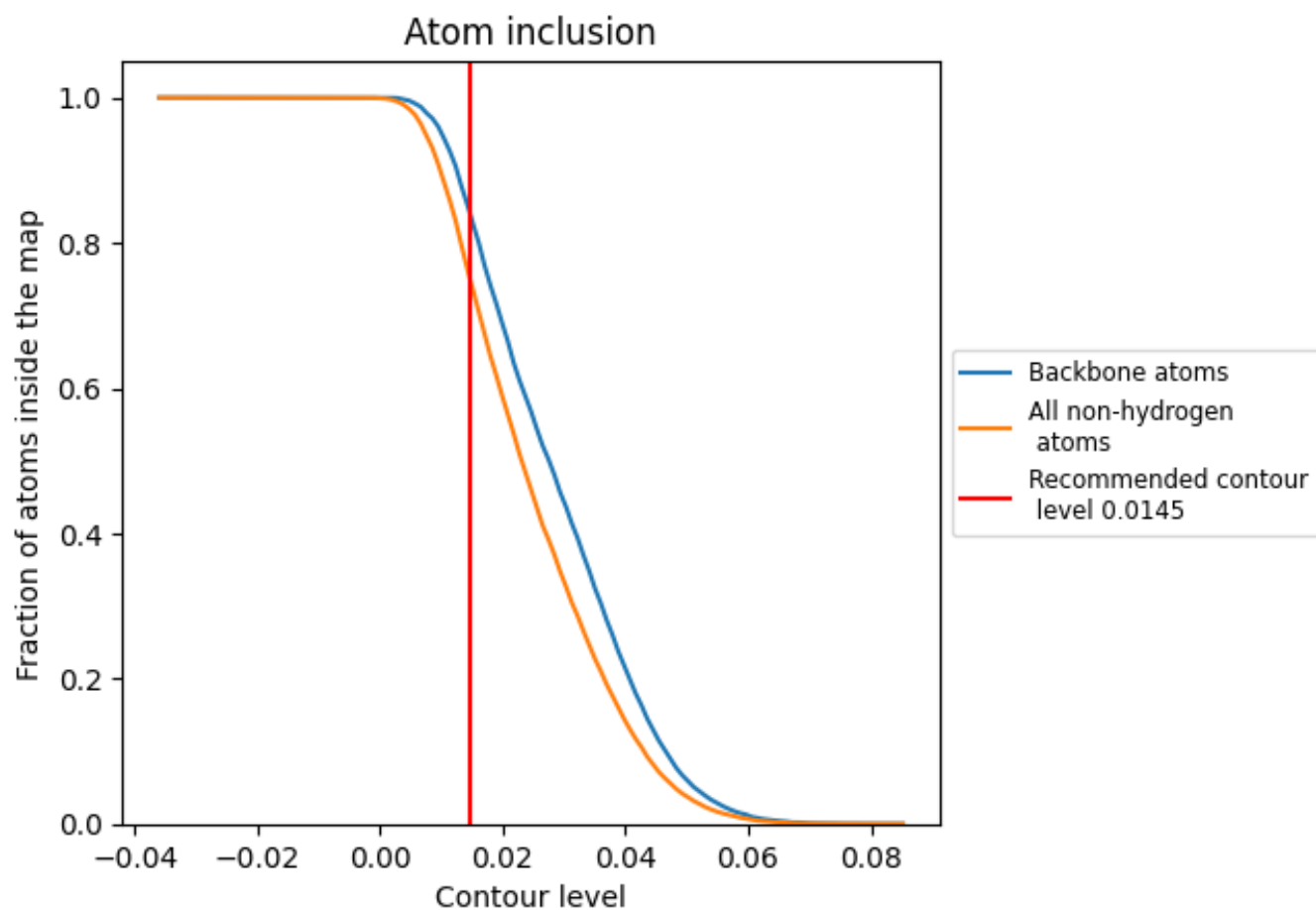
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0145).









## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 76% 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 (0.0145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7551	 0.4620
A	 0.8729	 0.5270
B	 0.8974	 0.5130
V	 0.4400	 0.2880

