



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:43 AM UTC

PDB ID : 9NJ3 / pdb_00009nj3
EMDB ID : EMD-49463
Title : Computationally optimized broadly reactive influenza B hemagglutinin BC2 bound by antibodies #46 and #3978
Authors : Dzimianski, J.V.; Kunkel, I.; Balasco Serrao, V.H.; DuBois, R.M.
Deposited on : 2025-02-26
Resolution : 2.48 Å(reported)
Based on initial model : .

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

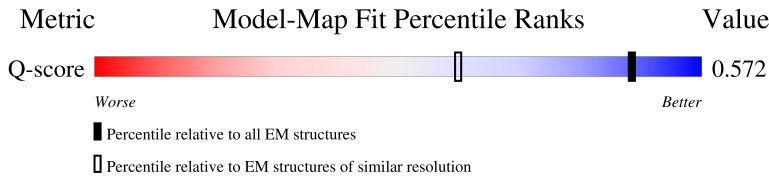
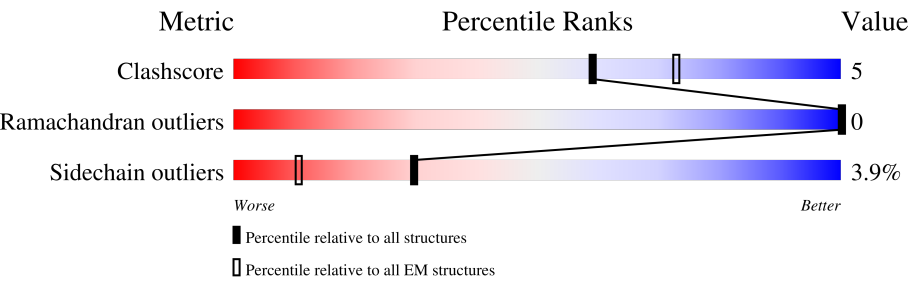
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.48 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.



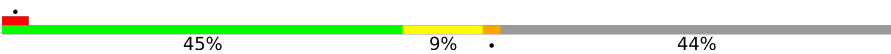
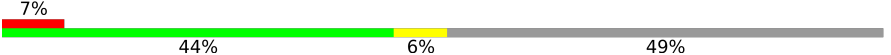

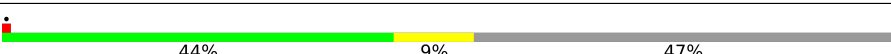
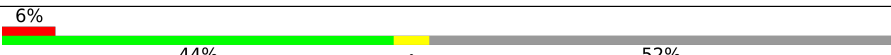

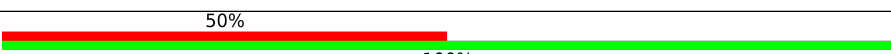
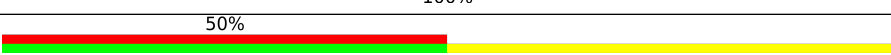
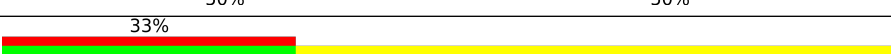
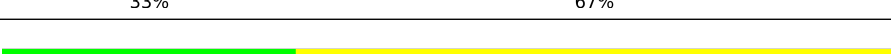
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6178 (1.98 - 2.98)

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 $\leq 5\%$. 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	530	<div><div></div><div>43%9%48%</div></div>
1	B	530	<div><div></div><div>44%8%48%</div></div>
1	C	530	<div><div></div><div>47%5%48%</div></div>
2	H	239	<div><div></div><div>45%10%44%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	239	
3	K	217	
3	L	217	
4	Q	233	
5	P	218	
6	D	2	
6	E	2	
6	G	2	
7	F	3	
7	I	3	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11862 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	275	Total	C	N	O	S	0	0
			2082	1302	374	391	15		
1	B	275	Total	C	N	O	S	0	0
			2084	1303	375	391	15		
1	C	277	Total	C	N	O	S	0	0
			2101	1314	379	393	15		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	ARG	LYS	conflict	UNP P17504
A	116	ASN	HIS	conflict	UNP P17504
A	129	LYS	THR	conflict	UNP P17504
A	136	ARG	LYS	conflict	UNP P17504
A	137	ILE	VAL	conflict	UNP P17504
A	199	THR	ALA	conflict	UNP P17504
A	202	LYS	VAL	conflict	UNP P17504
A	235	THR	ALA	conflict	UNP P17504
A	262	VAL	THR	conflict	UNP P17504
A	293	ALA	ARG	conflict	UNP P17504
A	524	SER	-	expression tag	UNP P17504
A	525	GLY	-	expression tag	UNP P17504
A	526	ARG	-	expression tag	UNP P17504
A	527	LEU	-	expression tag	UNP P17504
A	528	VAL	-	expression tag	UNP P17504
A	529	PRO	-	expression tag	UNP P17504
A	530	ARG	-	expression tag	UNP P17504
B	88	ARG	LYS	conflict	UNP P17504
B	116	ASN	HIS	conflict	UNP P17504
B	129	LYS	THR	conflict	UNP P17504
B	136	ARG	LYS	conflict	UNP P17504
B	137	ILE	VAL	conflict	UNP P17504
B	199	THR	ALA	conflict	UNP P17504
B	202	LYS	VAL	conflict	UNP P17504

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	235	THR	ALA	conflict	UNP P17504
B	262	VAL	THR	conflict	UNP P17504
B	293	ALA	ARG	conflict	UNP P17504
B	524	SER	-	expression tag	UNP P17504
B	525	GLY	-	expression tag	UNP P17504
B	526	ARG	-	expression tag	UNP P17504
B	527	LEU	-	expression tag	UNP P17504
B	528	VAL	-	expression tag	UNP P17504
B	529	PRO	-	expression tag	UNP P17504
B	530	ARG	-	expression tag	UNP P17504
C	88	ARG	LYS	conflict	UNP P17504
C	116	ASN	HIS	conflict	UNP P17504
C	129	LYS	THR	conflict	UNP P17504
C	136	ARG	LYS	conflict	UNP P17504
C	137	ILE	VAL	conflict	UNP P17504
C	199	THR	ALA	conflict	UNP P17504
C	202	LYS	VAL	conflict	UNP P17504
C	235	THR	ALA	conflict	UNP P17504
C	262	VAL	THR	conflict	UNP P17504
C	293	ALA	ARG	conflict	UNP P17504
C	524	SER	-	expression tag	UNP P17504
C	525	GLY	-	expression tag	UNP P17504
C	526	ARG	-	expression tag	UNP P17504
C	527	LEU	-	expression tag	UNP P17504
C	528	VAL	-	expression tag	UNP P17504
C	529	PRO	-	expression tag	UNP P17504
C	530	ARG	-	expression tag	UNP P17504

- Molecule 2 is a protein called Fab A Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	133	Total	C	N	O	S	0	0
			1027	651	171	197	8		
2	J	133	Total	C	N	O	S	0	0
			1027	651	171	197	8		

- Molecule 3 is a protein called Fab A Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	110	Total	C	N	O	S	0	0
			807	503	137	165	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	109	Total	C	N	O	S	0	0
			799	497	136	164	2		

- Molecule 4 is a protein called Fab B Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	124	Total	C	N	O	S	0	0
			957	613	161	179	4		

- Molecule 5 is a protein called Fab B Light Chain.

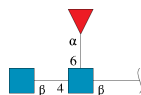
Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	104	Total	C	N	O	S	0	0
			776	478	136	159	3		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	2	Total	C	N	O	0	0
			28	16	2	10		
6	E	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
7	F	3	Total	C	N	O	0	0
			38	22	2	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	3	Total	C	N	O	0	0
			38	22	2	14		

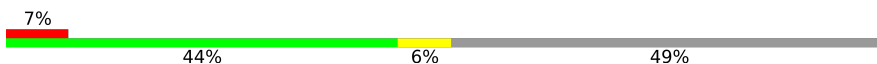
- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

GLY
THR
GLN
THR
TYR
ILE
CYS
ASN
VAL
HIS
HIS
LYS
PRO
SER
ASN
THR
LYS
VAL
GLU
PRO
LYS
SER
CYS
LYS
THR
HIS

• Molecule 3: Fab A Light Chain

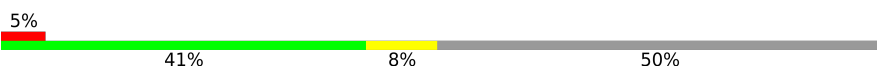
Chain K: 

GLN
S2
S9
V11
G13
A14
P15
G16
Q17
G18
H34
V35
V36
Q37
H38
K42
A43
P44
K45
L46
L47
L48
Y49
D50
P55
I58
L73
G77
L78
Q79
G80
E81
D82
E83
L104
T105
V106
L106A
LEU
GLY
GLN
PRO
LYS
ALA
ALA
TYR
PRO
SER
VAL
THR
LEU
PHE

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

SER
LEU
THR
PRO
GLU
GLU
TRP
LYS
LYS
HIS
ARG
HIS
SER
TYR
SER
CYS
GLN
VAL
THR
HIS
GLU
SER
THR
VAL
GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS

• Molecule 3: Fab A Light Chain

Chain L: 

GLN
S2
S12
G13
A14
P15
G16
G17
G18
V33
H34
V35
V36
Q37
H38
K42
A43
P44
L47
L48
P55
I58
P59
D60
L73
A74
I75
G80
E81
D82
E83
C88
Q89
H94
H96
S96
V106
LEU
LEU
GLY
GLN
PRO
LYS
ALA
ALA
PRO
PRO
PRO
VAL
THR

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

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

• Molecule 4: Fab B Heavy Chain


Chain Q: 

GLN
V2
Q3
L4
K12
V18
K19
A24
N35
W36
V37
R38
M48
T55
M69
Y79
L80
E81
E85
D86
T87
A88
A93
E94
E95
W99
P100
G100D
F100I
T110
V111
S112
SER
ALA
SER
SER
LYS
GLY
PRO
SER
SER
VAL
VAL
PHE
PRO
LEU
PRO
PRO

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

SER
SER
GLY
THR
THR
TYR
ILE
CYS
ASN
VAL
ASN
HIS
LYS
PRO
SER
ASN
THR
LYS
VAL
VAL
LYS
ASP
VAL
VAL
GLU
PRO
LYS
SER
CYS
ASP
LYS
HIS

• Molecule 5: Fab B Light Chain

Chain P: 

GLN
LEU
ALA
ASN
GLY
GLY
SER
GLU
E9
V19
S20
G22
Q23
T24
A25
E30
L52
V55
R60
P65
E66
R67
T84
Q85
T86
M87
D88
E89
Q95
V102
L112
GLY
GLN
PRO
LYS
ALA
ALA
SER
SER
TYR
TYR
ALA
ALA
SER
SER
VAL
SER
THR
THR
PHE
PRO
PRO
PRO
GLN
GLU
SER

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

TRP
LYS
SER
HIS
ARG
SER
TYR
SER
CYS
GLN
VAL
THR
HIS
GLU
GLY
SER
THR
VAL
GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
FUC3

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
FUC3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	356503	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	3.157	Depositor
Minimum map value	-1.927	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	329.8752, 329.8752, 329.8752	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5727, 0.5727, 0.5727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	0.24	0/2126	0.36	0/2878
1	B	0.23	0/2127	0.36	0/2877
1	C	0.23	0/2146	0.35	0/2904
2	H	0.20	0/1054	0.38	0/1426
2	J	0.18	0/1054	0.34	0/1426
3	K	0.18	0/828	0.33	0/1128
3	L	0.19	0/820	0.39	0/1117
4	Q	0.22	0/983	0.37	0/1336
5	P	0.18	0/790	0.43	0/1073
All	All	0.22	0/11928	0.36	0/16165

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2082	0	2071	25	0
1	B	2084	0	2077	21	0
1	C	2101	0	2089	13	0
2	H	1027	0	965	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1027	0	965	9	0
3	K	807	0	765	9	0
3	L	799	0	754	11	0
4	Q	957	0	928	12	0
5	P	776	0	751	4	0
6	D	28	0	25	0	0
6	E	28	0	25	0	0
6	G	28	0	25	0	0
7	F	38	0	34	0	0
7	I	38	0	34	1	0
8	A	14	0	13	0	0
8	C	28	0	26	0	0
All	All	11862	0	11547	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (108) 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:J:82:MET:HB3	2:J:82(C):LEU:HD21	1.73	0.71
1:C:164:ASP:HA	1:C:167:LYS:HE2	1.73	0.70
1:A:90:VAL:HG23	1:A:105:ARG:HH12	1.60	0.67
2:J:40:ALA:HB3	2:J:43:LYS:HB2	1.78	0.65
1:B:164:ASP:HA	1:B:167:LYS:HE2	1.79	0.63
1:A:185:GLU:HG2	1:A:277:SER:HB3	1.80	0.62
1:A:73:MET:HE1	1:A:154:ALA:HB2	1.83	0.60
5:P:95:GLN:HE21	5:P:102:VAL:HG13	1.67	0.59
2:H:82:MET:HE2	2:H:82(C):LEU:HD21	1.84	0.59
2:J:34:MET:HB3	2:J:78:LEU:HD22	1.85	0.58
1:A:83:ILE:HD11	1:A:296:LEU:HD13	1.85	0.58
1:B:49:THR:HG22	1:B:81:ALA:HB3	1.86	0.57
3:L:55:PRO:HG2	3:L:58:ILE:HD13	1.85	0.57
1:B:185:GLU:HG2	1:B:277:SER:HB3	1.87	0.56
3:K:11:VAL:HG23	3:K:104:LEU:HD13	1.88	0.55
4:Q:19:LYS:HE2	4:Q:79:TYR:HB3	1.88	0.55
4:Q:87:THR:HG23	4:Q:110:THR:HA	1.88	0.55
3:K:46:LEU:HD21	3:K:49:TYR:HB3	1.87	0.55
1:A:70:PRO:HA	1:A:73:MET:HE2	1.89	0.54
1:A:136:ARG:HD3	4:Q:100(D):GLY:HA3	1.91	0.53
1:A:124:VAL:HG23	1:A:125:ILE:HG12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:HG22	1:B:178:PRO:HD2	1.91	0.53
3:K:55:PRO:HD2	3:K:58:ILE:HG13	1.91	0.53
1:A:198:GLU:HG2	1:A:208:SER:HB2	1.92	0.52
5:P:65:PRO:HB2	5:P:67:ARG:HG2	1.91	0.52
5:P:52:LEU:HD21	5:P:55:TYR:HB3	1.92	0.52
1:A:205:TYR:HB3	1:A:265:ARG:HB3	1.92	0.51
1:A:91:THR:O	1:A:236:GLU:HB3	2.10	0.51
3:K:35:TRP:CE2	3:K:73:LEU:HB2	2.46	0.51
3:L:38:HIS:HB2	3:L:44:PRO:HB3	1.93	0.51
1:B:116:ASN:O	1:B:276:ALA:HA	2.11	0.50
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.94	0.50
1:A:50:ARG:HH11	1:A:112:ARG:HA	1.76	0.50
1:B:67:LEU:O	1:B:153:PHE:HB3	2.12	0.50
1:B:109:ASN:O	1:B:112:ARG:HB3	2.11	0.49
2:J:93:ALA:HB1	2:J:100(O):MET:HB3	1.94	0.49
4:Q:35:ASN:ND2	4:Q:95:GLU:HB2	2.28	0.48
1:C:83:ILE:HD11	1:C:296:LEU:HD13	1.95	0.48
4:Q:38:ARG:HB2	4:Q:48:MET:SD	2.54	0.48
1:A:240:LEU:HD12	1:A:241:PRO:HD2	1.95	0.48
3:L:18:GLY:HA2	3:L:75:ILE:O	2.14	0.48
1:B:50:ARG:HD3	1:B:53:LEU:HD23	1.95	0.47
2:J:100(M):TYR:OH	3:K:50:ASP:HA	2.13	0.47
1:B:91:THR:O	1:B:236:GLU:HB2	2.14	0.47
1:A:123:ASN:HA	1:A:271:GLN:O	2.14	0.47
4:Q:19:LYS:HG3	4:Q:81:GLU:HB3	1.96	0.47
1:B:124:VAL:HG13	1:B:125:ILE:HG13	1.96	0.47
1:B:198:GLU:HG2	1:B:208:SER:HB2	1.97	0.47
1:B:196:ASP:HB3	1:B:200:GLN:HB3	1.97	0.47
4:Q:36:TRP:CG	4:Q:80:LEU:HD13	2.50	0.47
1:A:221:THR:HG21	1:C:223:HIS:O	2.15	0.47
4:Q:69:MET:HG2	4:Q:80:LEU:HD12	1.98	0.46
2:J:100(E):CYS:SG	2:J:100(K):TYR:HB3	2.55	0.46
1:A:90:VAL:HG21	1:A:236:GLU:HG3	1.97	0.46
4:Q:99:TRP:CD2	4:Q:100:PRO:HA	2.51	0.46
1:C:90:VAL:HG12	1:C:105:ARG:HH12	1.80	0.46
1:A:188:ILE:HB	1:A:274:TRP:HB2	1.95	0.46
3:K:37:GLN:HB2	3:K:47:LEU:HD11	1.98	0.46
3:L:89:GLN:HE21	3:L:96:SER:HB3	1.80	0.46
1:B:235:THR:O	1:B:236:GLU:HG2	2.15	0.45
1:A:50:ARG:NH1	1:A:112:ARG:HA	2.31	0.45
1:C:185:GLU:HG2	1:C:277:SER:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:HE3	1:B:145:ASN:O	2.16	0.45
3:L:94:HIS:HB3	7:I:2:NAG:H82	1.99	0.45
4:Q:93:ALA:HB1	4:Q:100(I):PHE:HB3	1.99	0.45
1:C:124:VAL:HG22	1:C:180:ILE:HD13	1.98	0.45
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.98	0.45
2:J:103:TRP:CE3	3:K:44:PRO:HD2	2.51	0.45
1:A:86:GLU:HG3	1:A:89:PRO:HG3	1.98	0.44
1:C:173:LEU:O	1:C:262:VAL:HA	2.16	0.44
1:B:114:TYR:CG	1:B:276:ALA:HB1	2.53	0.44
1:A:173:LEU:O	1:A:262:VAL:HA	2.18	0.44
1:C:188:ILE:HB	1:C:274:TRP:HB2	2.00	0.44
1:C:71:LYS:HE3	1:C:71:LYS:HB2	1.88	0.44
1:A:139:THR:HB	1:A:150:ASN:HB3	1.98	0.43
2:H:93:ALA:HB1	2:H:100(O):MET:HB3	1.99	0.43
3:L:34:HIS:O	3:L:88:CYS:HA	2.18	0.43
1:C:198:GLU:HG2	1:C:208:SER:HB3	2.00	0.43
2:H:82(C):LEU:HB3	2:H:111:VAL:HG21	2.00	0.43
1:B:194:HIS:HB2	1:B:246:ILE:HG22	1.99	0.43
1:A:114:TYR:CG	1:A:276:ALA:HB1	2.53	0.43
4:Q:12:LYS:HG3	4:Q:18:VAL:HB	2.01	0.43
2:J:100(N):ALA:HB2	3:K:34:HIS:CG	2.54	0.43
1:B:69:ARG:HG3	1:B:70:PRO:HD2	2.00	0.43
1:C:124:VAL:HG21	1:C:273:VAL:HG13	2.00	0.43
5:P:19:VAL:HG11	5:P:25:ALA:HB2	2.00	0.42
1:C:69:ARG:HD3	1:C:72:CYS:SG	2.59	0.42
2:J:83:ARG:HD2	2:J:85:GLU:OE2	2.19	0.42
4:Q:4:LEU:HD23	4:Q:24:ALA:HA	2.00	0.42
1:A:102:THR:HG22	1:A:224:TYR:CE1	2.54	0.42
1:C:185:GLU:OE1	1:C:275:CYS:HB3	2.20	0.42
2:H:52(A):TRP:HB3	2:H:98:GLU:HB2	2.02	0.42
3:K:38:HIS:CD2	3:K:44:PRO:HG3	2.55	0.41
3:L:35:TRP:CE2	3:L:73:LEU:HB2	2.55	0.41
3:L:15:PRO:HG3	3:L:106:VAL:HG22	2.03	0.41
1:A:135:TYR:CG	1:A:159:ALA:HB1	2.55	0.41
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	2.01	0.41
1:A:123:ASN:HB2	2:H:100(J):TYR:HE2	1.86	0.41
1:B:63:LEU:HD13	1:B:108:PRO:HD3	2.03	0.41
2:H:6:GLU:H	2:H:105:GLN:HE22	1.69	0.41
2:H:52(A):TRP:CD1	2:H:98:GLU:HB2	2.55	0.41
1:B:97:ILE:HB	1:B:99:HIS:CE1	2.56	0.40
1:B:123:ASN:HA	1:B:271:GLN:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HG2	1:A:143:CYS:HB3	2.02	0.40
1:B:84:LEU:HB3	1:B:284:LYS:HA	2.04	0.40
2:H:100(N):ALA:HB2	3:L:34:HIS:CG	2.57	0.40
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.03	0.40
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.03	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	271/530 (51%)	263 (97%)	8 (3%)	0	100	100
1	B	271/530 (51%)	261 (96%)	10 (4%)	0	100	100
1	C	273/530 (52%)	268 (98%)	5 (2%)	0	100	100
2	H	131/239 (55%)	130 (99%)	1 (1%)	0	100	100
2	J	131/239 (55%)	127 (97%)	4 (3%)	0	100	100
3	K	108/217 (50%)	105 (97%)	3 (3%)	0	100	100
3	L	107/217 (49%)	104 (97%)	3 (3%)	0	100	100
4	Q	122/233 (52%)	120 (98%)	2 (2%)	0	100	100
5	P	102/218 (47%)	99 (97%)	3 (3%)	0	100	100
All	All	1516/2953 (51%)	1477 (97%)	39 (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	229/441 (52%)	221 (96%)	8 (4%)	32	55
1	B	229/441 (52%)	224 (98%)	5 (2%)	45	70
1	C	231/441 (52%)	227 (98%)	4 (2%)	53	75
2	H	105/198 (53%)	91 (87%)	14 (13%)	4	7
2	J	105/198 (53%)	91 (87%)	14 (13%)	4	7
3	K	89/181 (49%)	89 (100%)	0	100	100
3	L	88/181 (49%)	86 (98%)	2 (2%)	44	69
4	Q	100/195 (51%)	99 (99%)	1 (1%)	68	84
5	P	86/183 (47%)	85 (99%)	1 (1%)	63	81
All	All	1262/2459 (51%)	1213 (96%)	49 (4%)	30	52

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	CYS
1	A	136	ARG
1	A	163	ASN
1	A	195	SER
1	A	222	THR
1	A	245	ARG
1	A	258	THR
1	A	260	THR
1	B	94	CYS
1	B	168	THR
1	B	200	GLN
1	B	236	GLU
1	B	260	THR
1	C	94	CYS
1	C	214	THR
1	C	233	ASN
1	C	260	THR
2	H	100	CYS
2	H	100(A)	SER
2	H	100(C)	THR
2	H	100(D)	ASN
2	H	100(E)	CYS
2	H	100(F)	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	100(G)	SER
2	H	100(H)	TYR
2	H	100(I)	TYR
2	H	100(J)	TYR
2	H	100(K)	TYR
2	H	100(L)	PHE
2	H	100(M)	TYR
2	H	100(O)	MET
2	J	100	CYS
2	J	100(A)	SER
2	J	100(C)	THR
2	J	100(D)	ASN
2	J	100(E)	CYS
2	J	100(F)	TYR
2	J	100(G)	SER
2	J	100(H)	TYR
2	J	100(I)	TYR
2	J	100(J)	TYR
2	J	100(K)	TYR
2	J	100(L)	PHE
2	J	100(M)	TYR
2	J	100(O)	MET
3	L	33	VAL
3	L	75	ILE
4	Q	55	THR
5	P	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	109	ASN
1	A	116	ASN
1	A	122	HIS
1	B	166	ASN
1	B	223	HIS
2	H	100(D)	ASN
2	J	10	HIS
2	J	35	HIS
2	J	81	GLN
2	J	82(A)	ASN
2	J	100(D)	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	105	GLN
3	K	37	GLN
4	Q	39	GLN
5	P	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	$\# Z > 2$
6	NAG	D	1	6,1	14,14,15	0.78	0	17,19,21	1.11	1 (5%)
6	NAG	D	2	6	14,14,15	0.74	0	17,19,21	0.88	0
6	NAG	E	1	6,1	14,14,15	0.72	0	17,19,21	0.95	0
6	NAG	E	2	6	14,14,15	0.74	0	17,19,21	0.84	0
7	NAG	F	1	1,7	14,14,15	0.72	0	17,19,21	1.30	1 (5%)
7	NAG	F	2	7	14,14,15	0.74	0	17,19,21	0.81	0
7	FUC	F	3	7	10,10,11	0.94	1 (10%)	14,14,16	1.18	1 (7%)
6	NAG	G	1	6,1	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
6	NAG	G	2	6	14,14,15	0.72	0	17,19,21	0.87	0
7	NAG	I	1	1,7	14,14,15	0.70	0	17,19,21	1.36	1 (5%)
7	NAG	I	2	7	14,14,15	0.77	0	17,19,21	0.96	0
7	FUC	I	3	7	10,10,11	0.78	0	14,14,16	0.99	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
6	NAG	D	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	NAG	E	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
7	NAG	F	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	F	2	7	-	0/6/23/26	0/1/1/1
7	FUC	F	3	7	-	-	0/1/1/1
6	NAG	G	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1
7	NAG	I	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	FUC	I	3	7	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	3	FUC	O5-C1	-2.17	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	1	NAG	C2-N2-C7	3.50	127.58	122.90
7	I	1	NAG	C2-N2-C7	3.43	127.49	122.90
7	F	3	FUC	C1-C2-C3	-2.16	106.49	109.64
6	D	1	NAG	O3-C3-C4	2.09	115.30	110.38
6	G	1	NAG	O5-C1-C2	-2.08	108.07	111.29

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	1	NAG	O5-C5-C6-O6
7	F	1	NAG	C4-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
6	E	1	NAG	C4-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

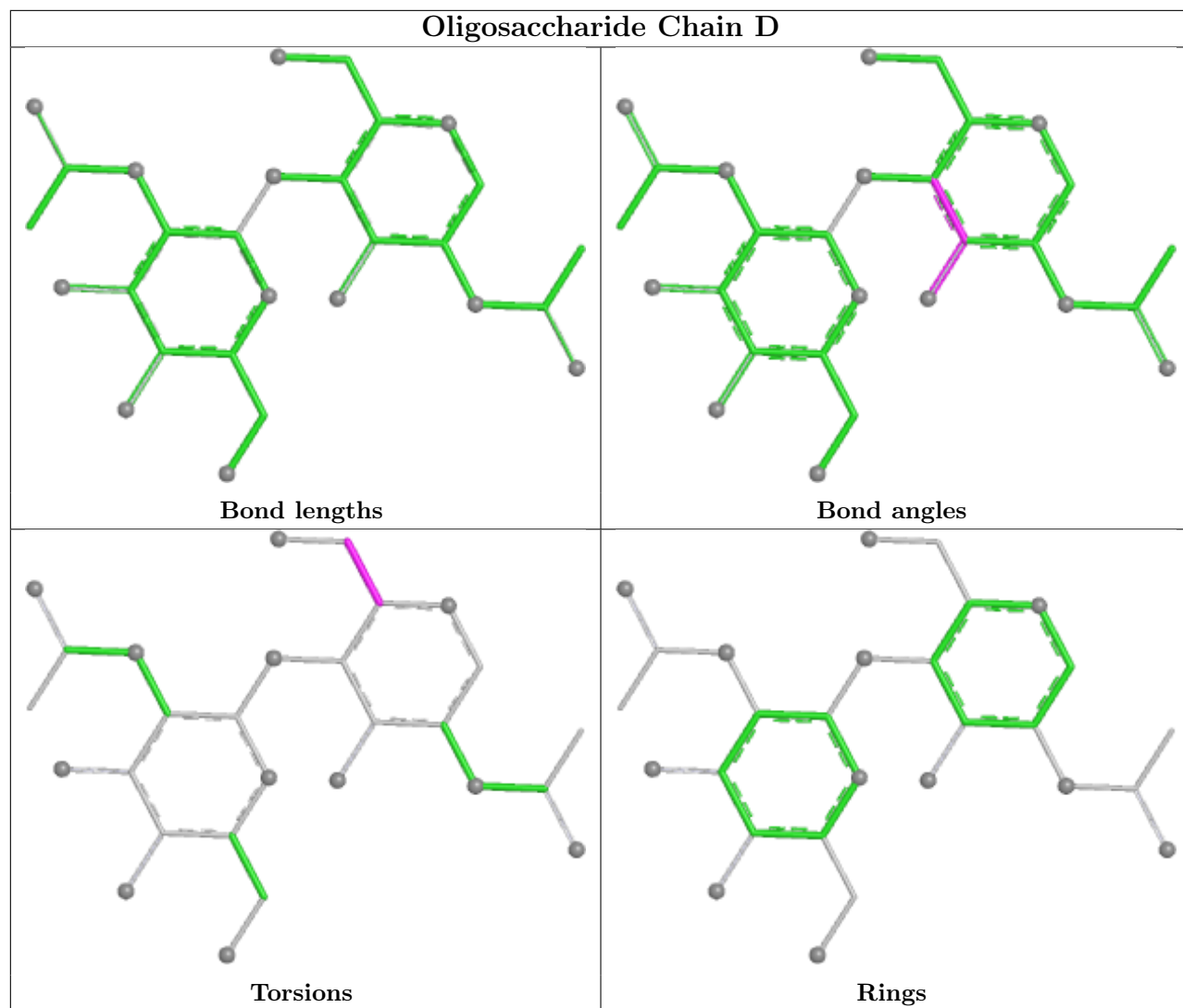
Mol	Chain	Res	Type	Atoms
6	E	1	NAG	O5-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
7	I	1	NAG	C3-C2-N2-C7
7	F	1	NAG	C1-C2-N2-C7
7	I	1	NAG	C1-C2-N2-C7
6	D	1	NAG	O5-C5-C6-O6
7	F	1	NAG	C3-C2-N2-C7

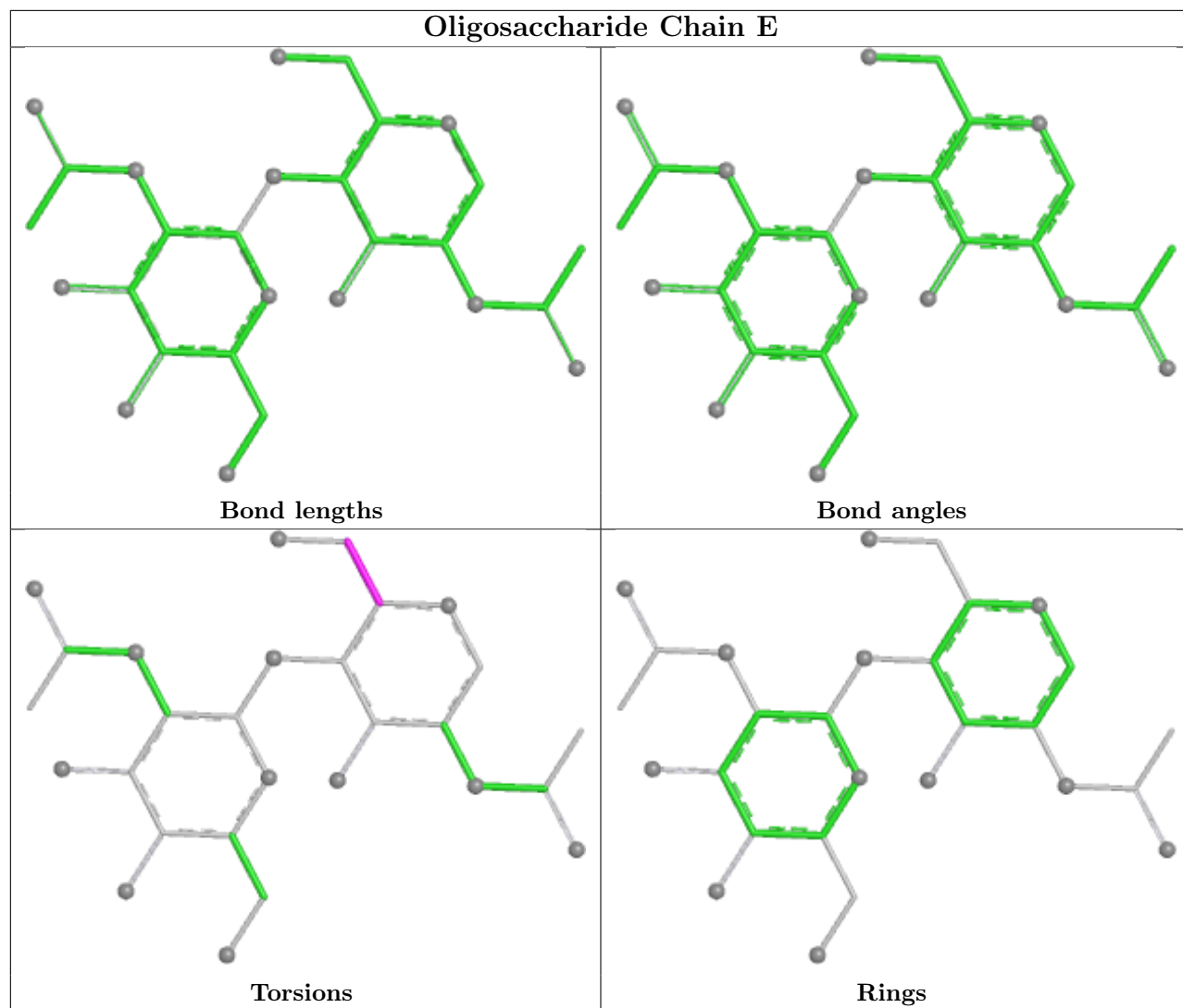
There are no ring outliers.

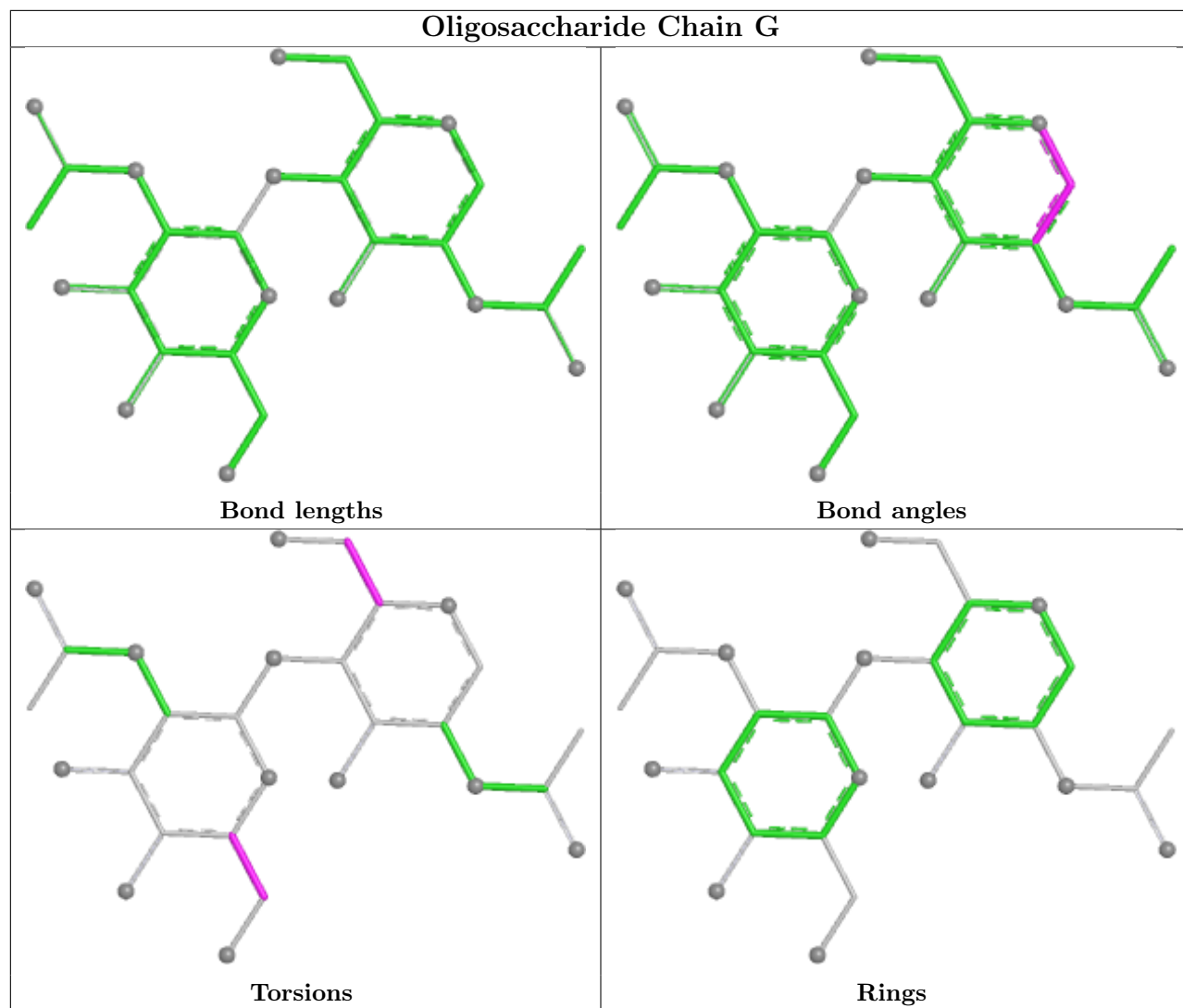
1 monomer is involved in 1 short contact:

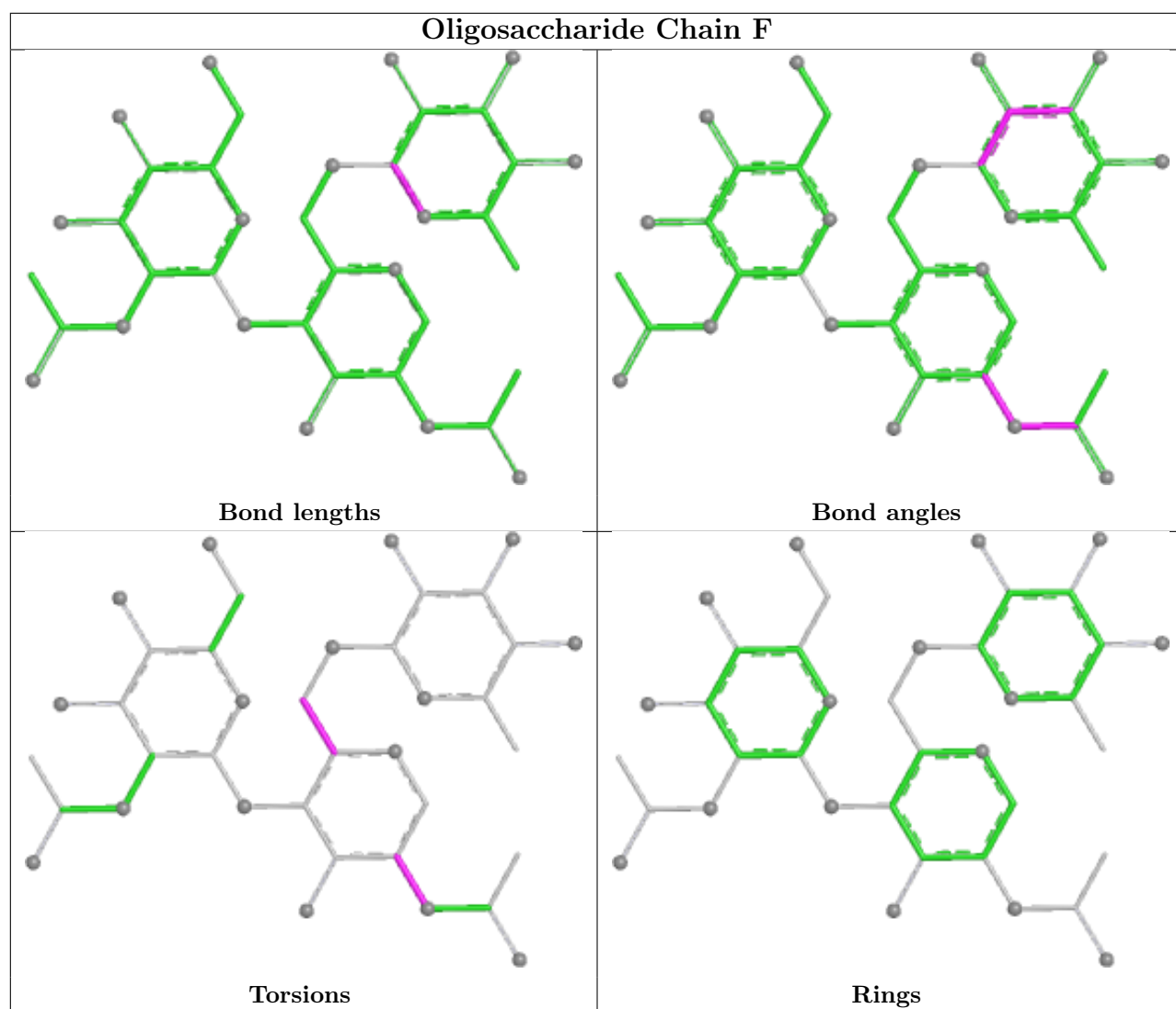
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	2	NAG	1	0

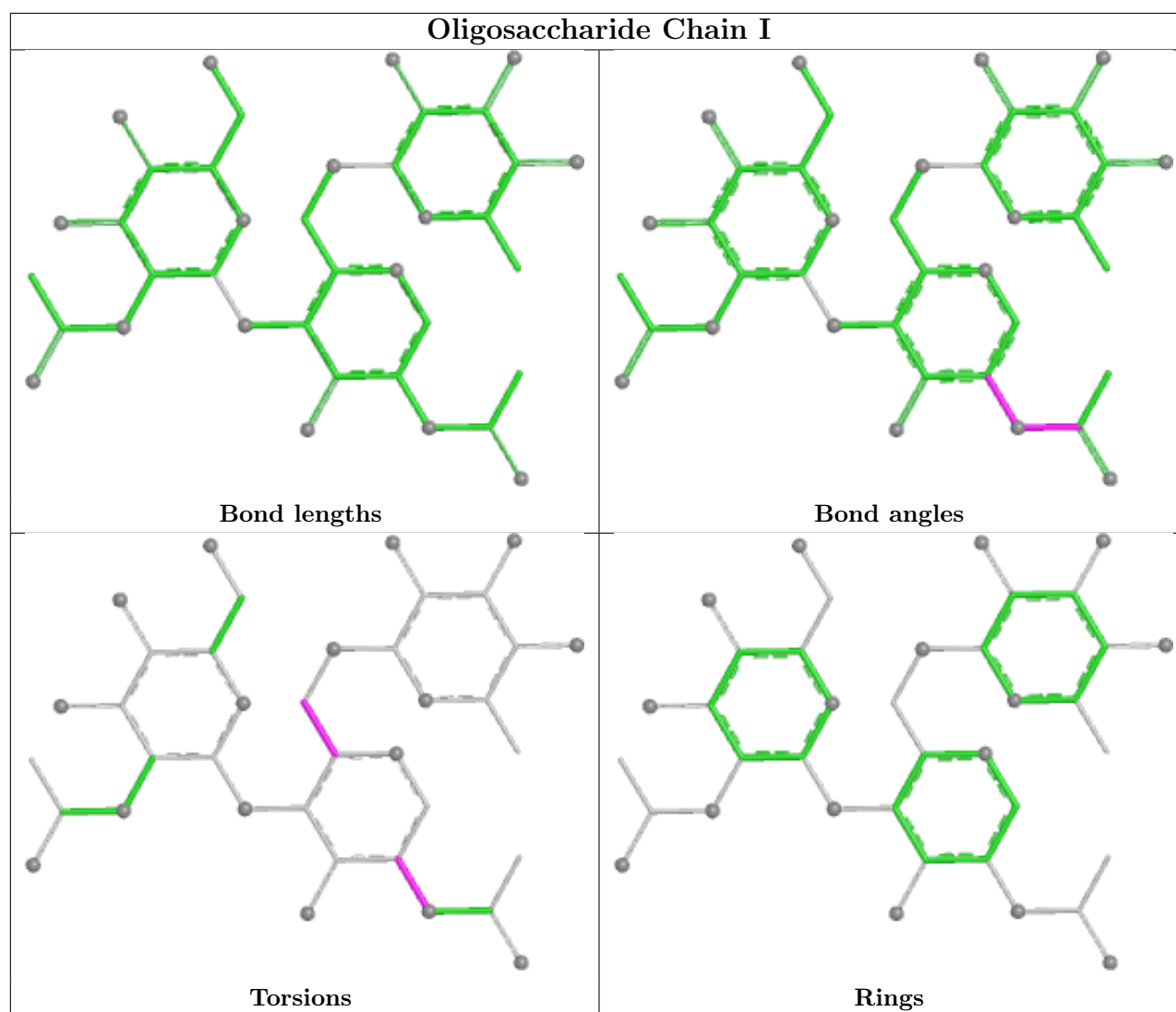
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
8	NAG	C	601	1	14,14,15	0.70	0	17,19,21	0.92	0
8	NAG	C	602	1	14,14,15	0.68	0	17,19,21	0.83	0
8	NAG	A	601	1	14,14,15	0.72	0	17,19,21	0.75	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
8	NAG	C	601	1	-	0/6/23/26	0/1/1/1
8	NAG	C	602	1	-	0/6/23/26	0/1/1/1
8	NAG	A	601	1	-	0/6/23/26	0/1/1/1

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.

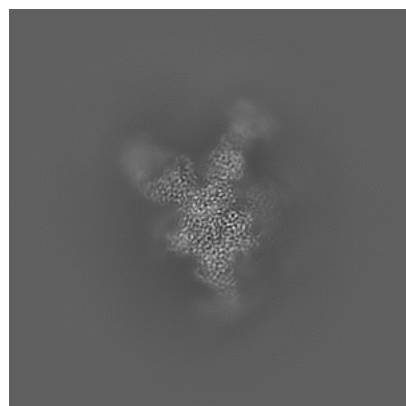
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49463. These allow visual inspection of the internal detail of the map and identification of artifacts.

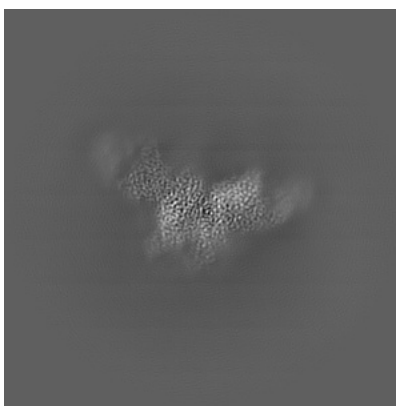
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

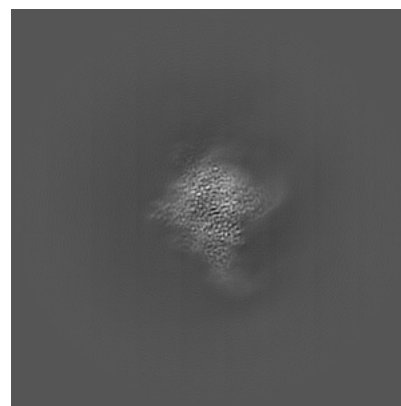
6.1.1 Primary map



X

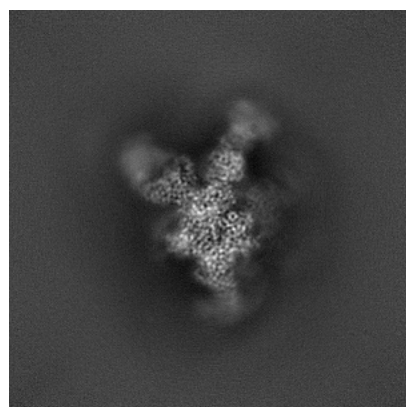


Y

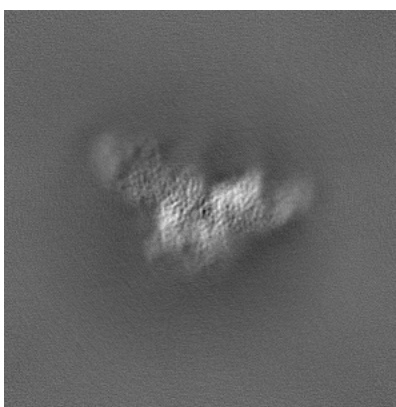


Z

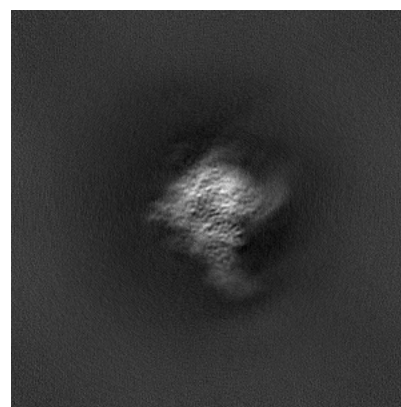
6.1.2 Raw map



X



Y

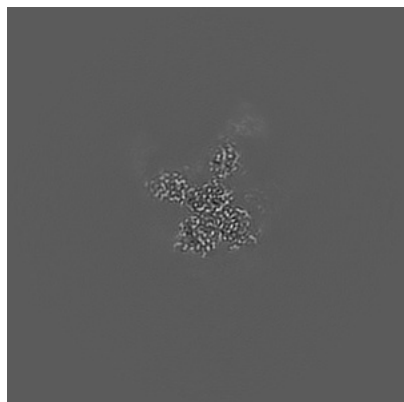


Z

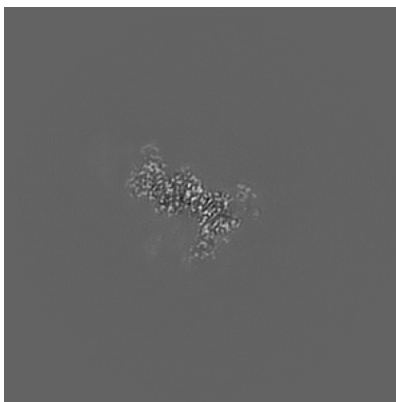
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

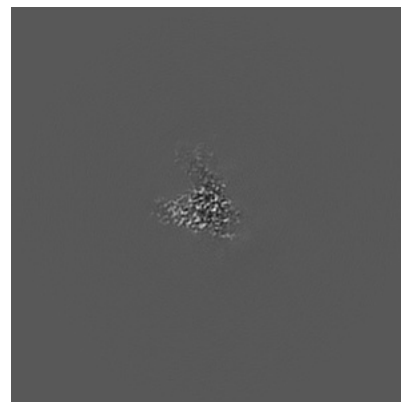
6.2.1 Primary map



X Index: 288

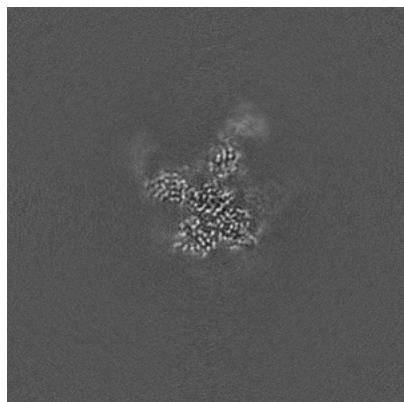


Y Index: 288

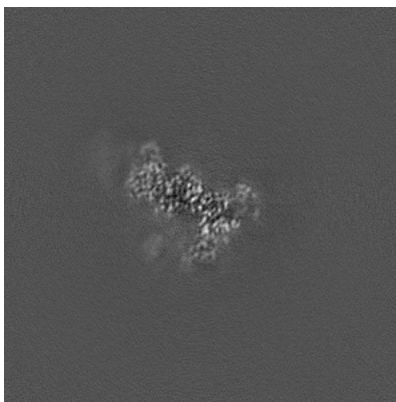


Z Index: 288

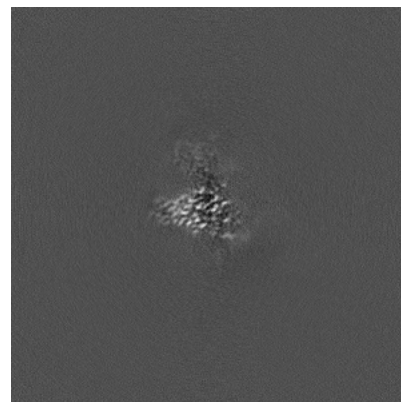
6.2.2 Raw map



X Index: 288



Y Index: 288

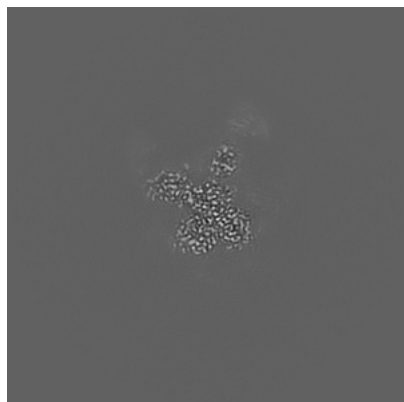


Z Index: 288

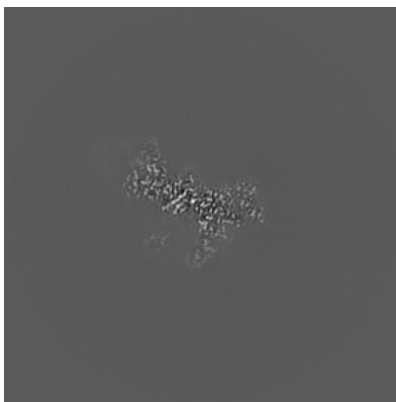
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

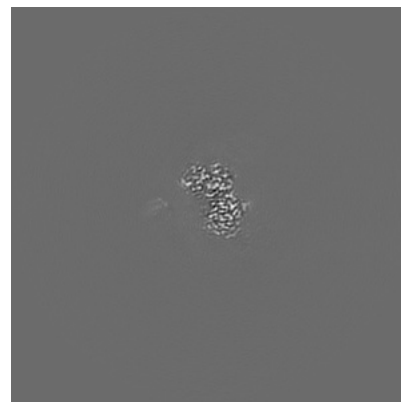
6.3.1 Primary map



X Index: 292

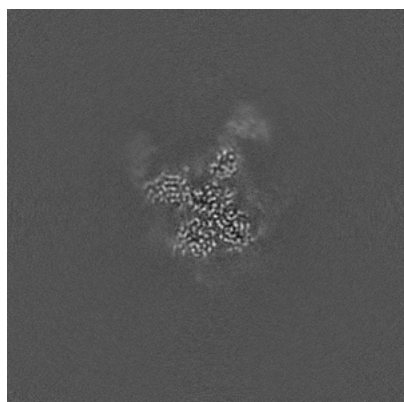


Y Index: 296

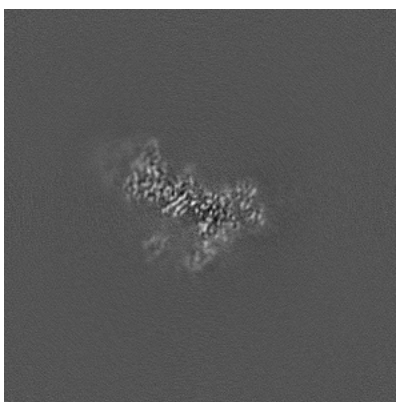


Z Index: 266

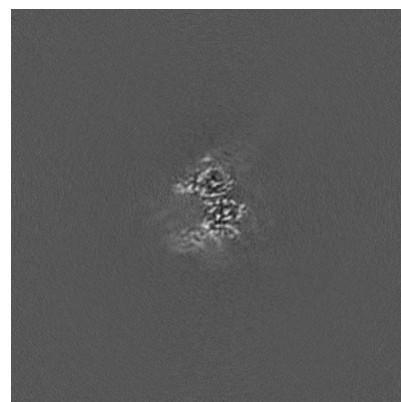
6.3.2 Raw map



X Index: 291



Y Index: 296



Z Index: 248

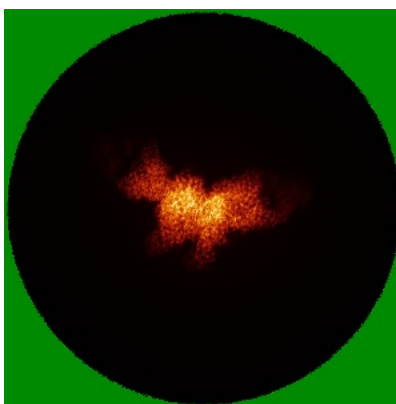
The images above show the largest variance slices of the map in three orthogonal directions.

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

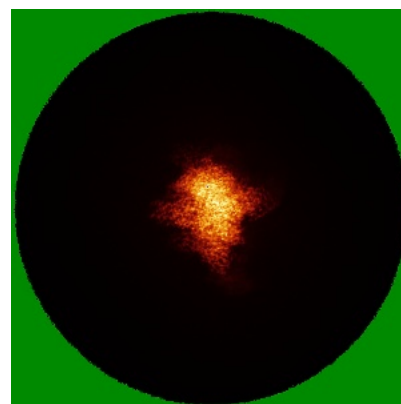
6.4.1 Primary map



X

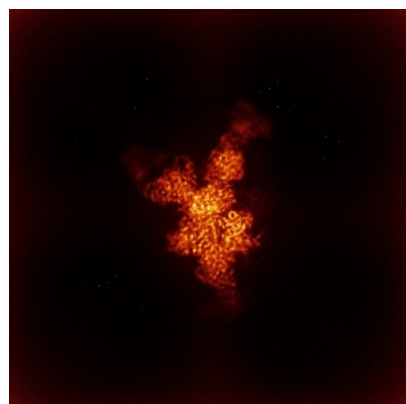


Y

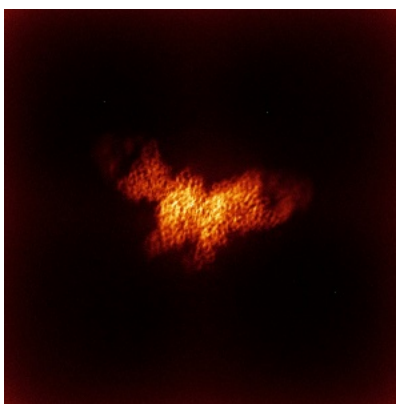


Z

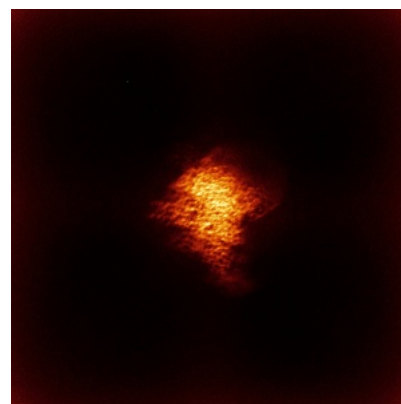
6.4.2 Raw map



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](#)

This section was not generated.

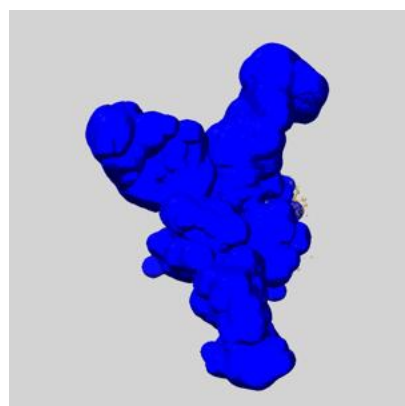
6.6 Mask visualisation [i](#)

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

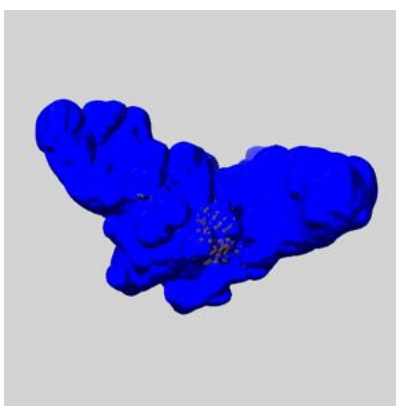
A mask typically either:

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

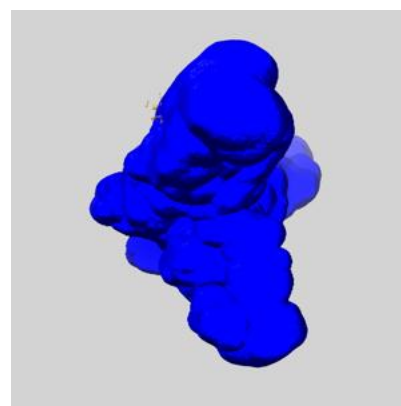
6.6.1 emd_49463_msk_1.map [i](#)



X



Y

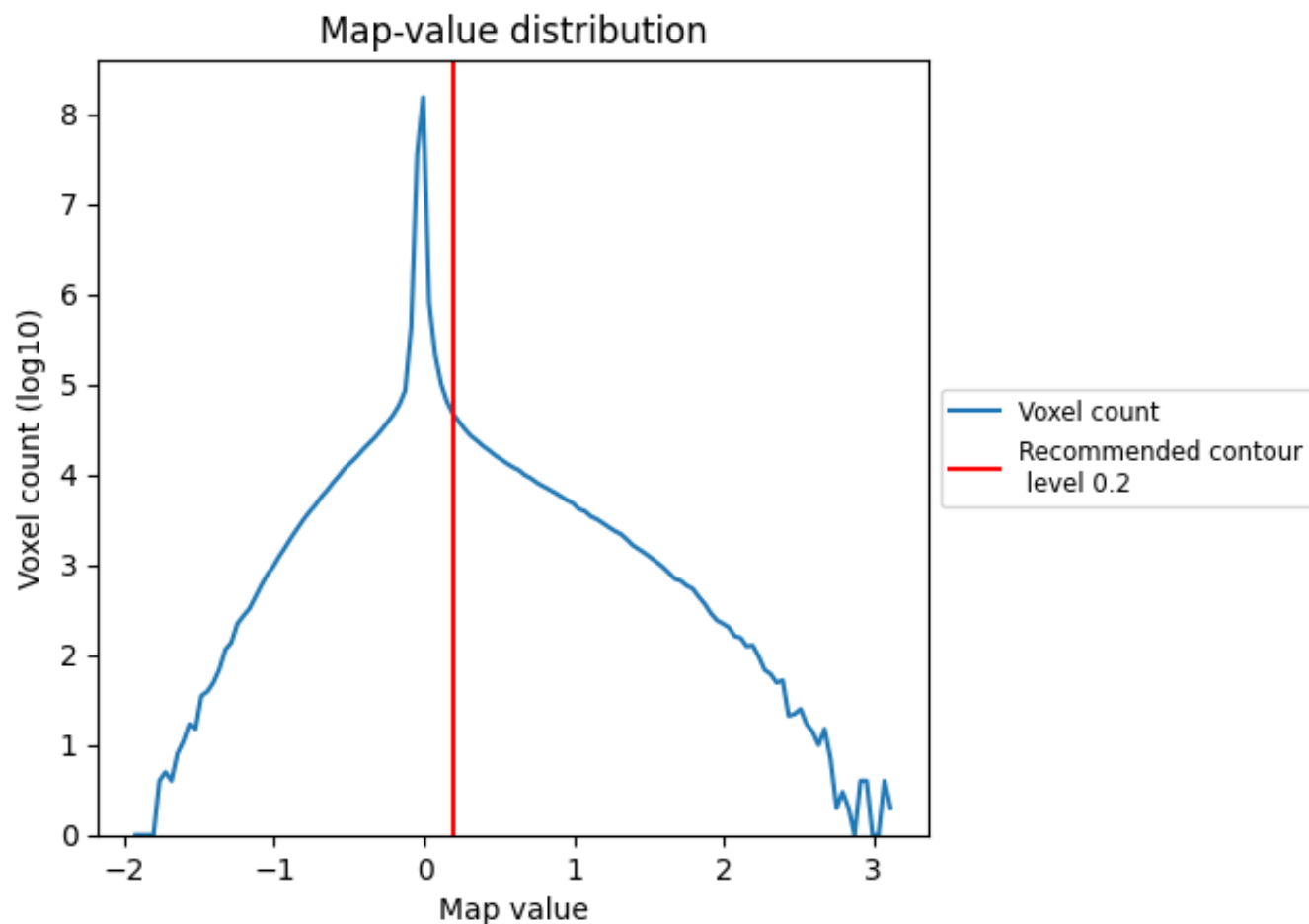


Z

7 Map analysis [i](#)

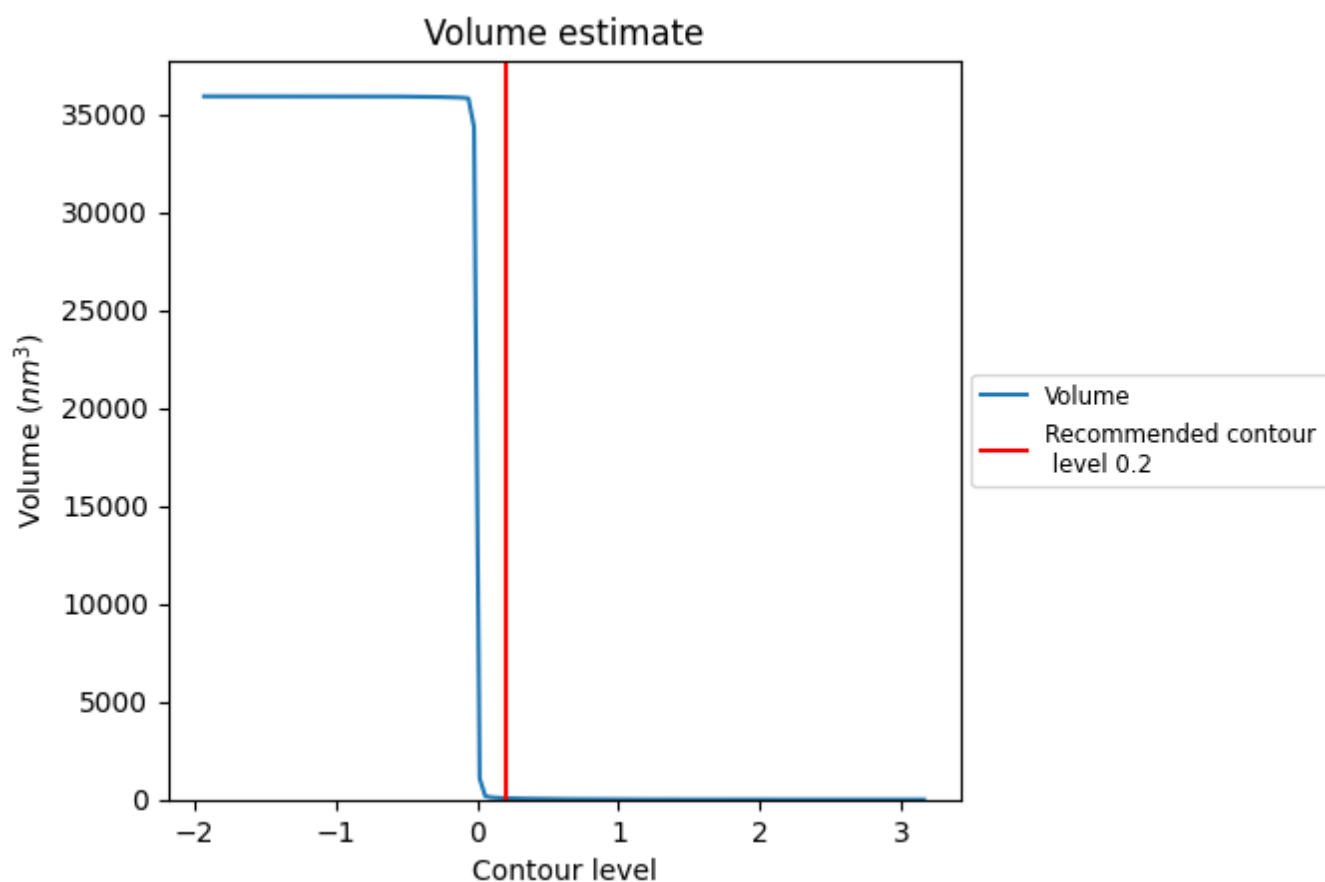
This section contains the results of statistical analysis of the map.

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.

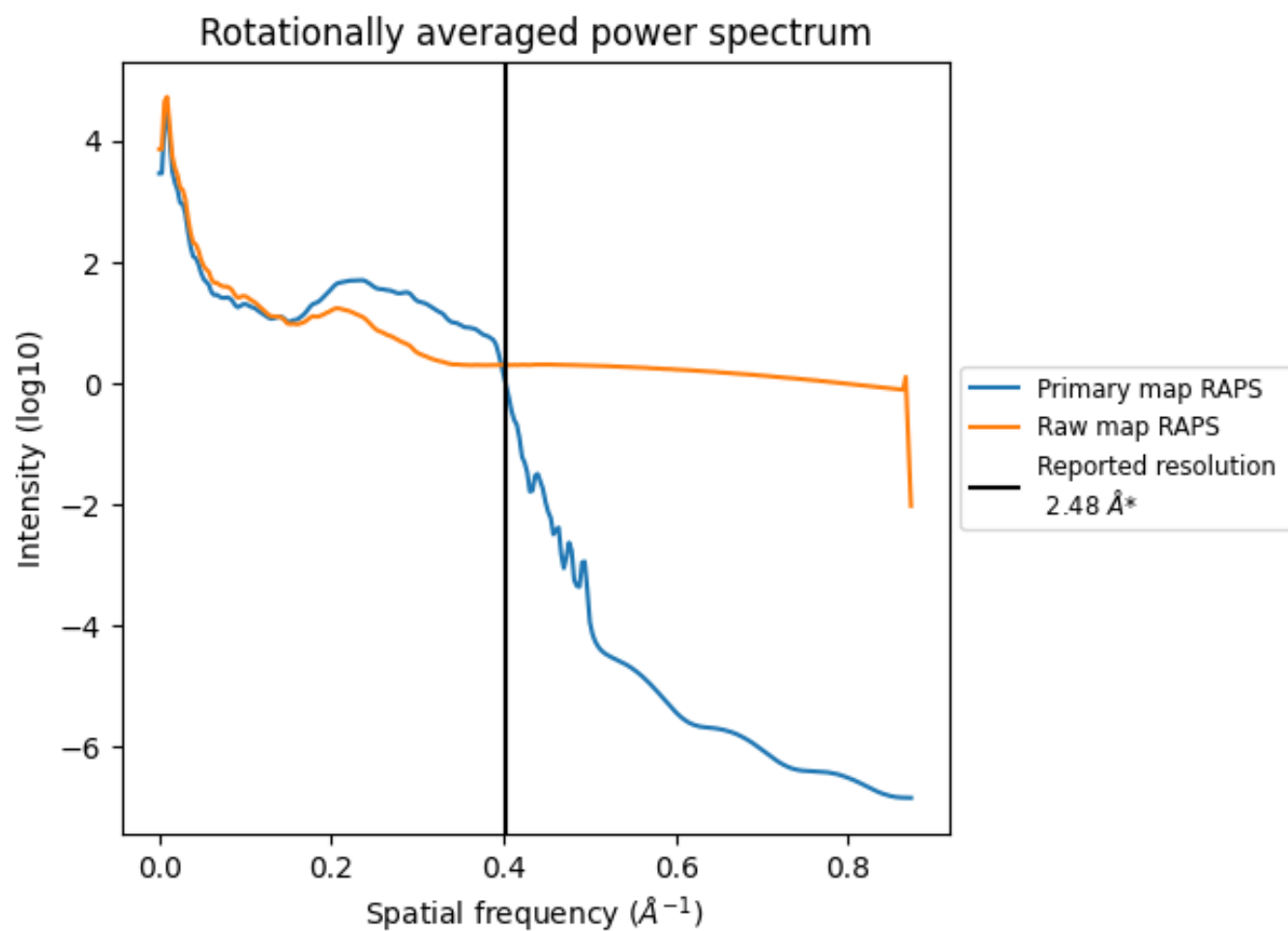
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm^3 ; this corresponds to an approximate mass of 63 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

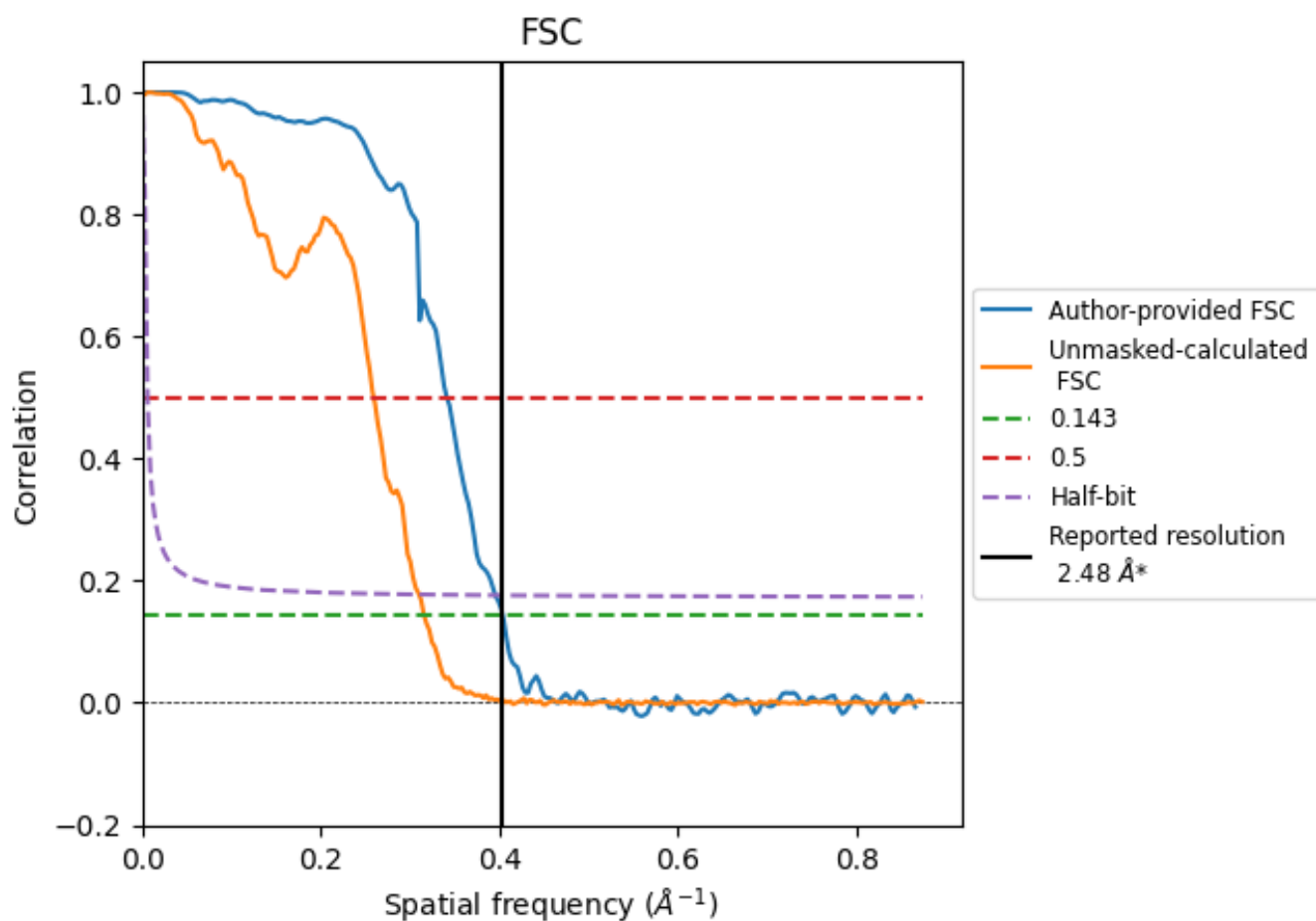


*Reported resolution corresponds to spatial frequency of 0.403 Å⁻¹

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 0.403 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.48	2.93	2.53
Unmasked-calculated*	3.17	3.86	3.23

*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 3.17 differs from the reported value 2.48 by more than 10 %

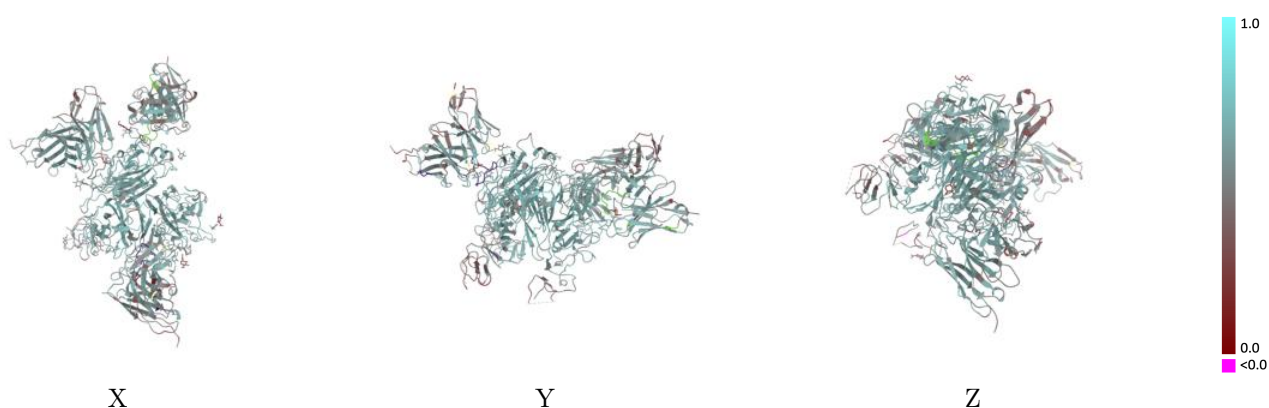
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-49463 and PDB model 9NJ3. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

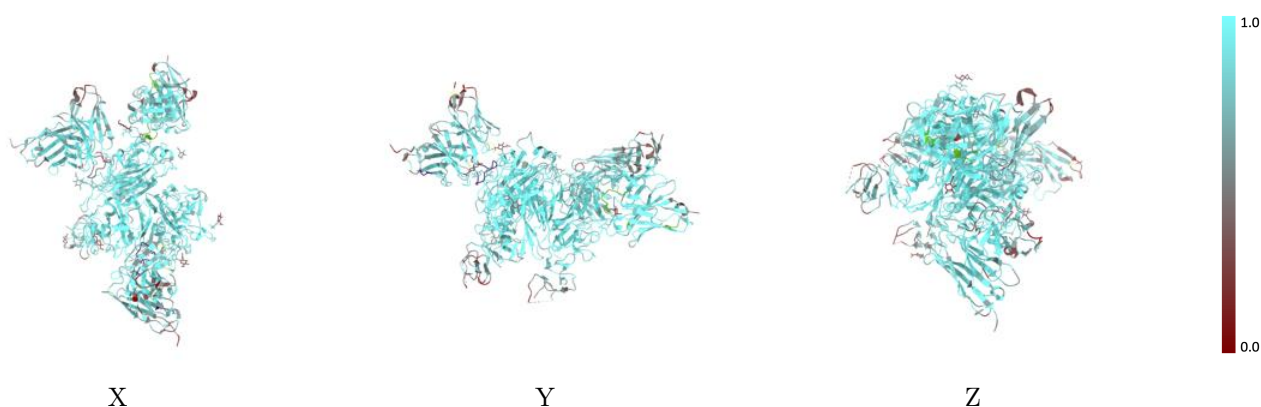
This section was not generated.

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



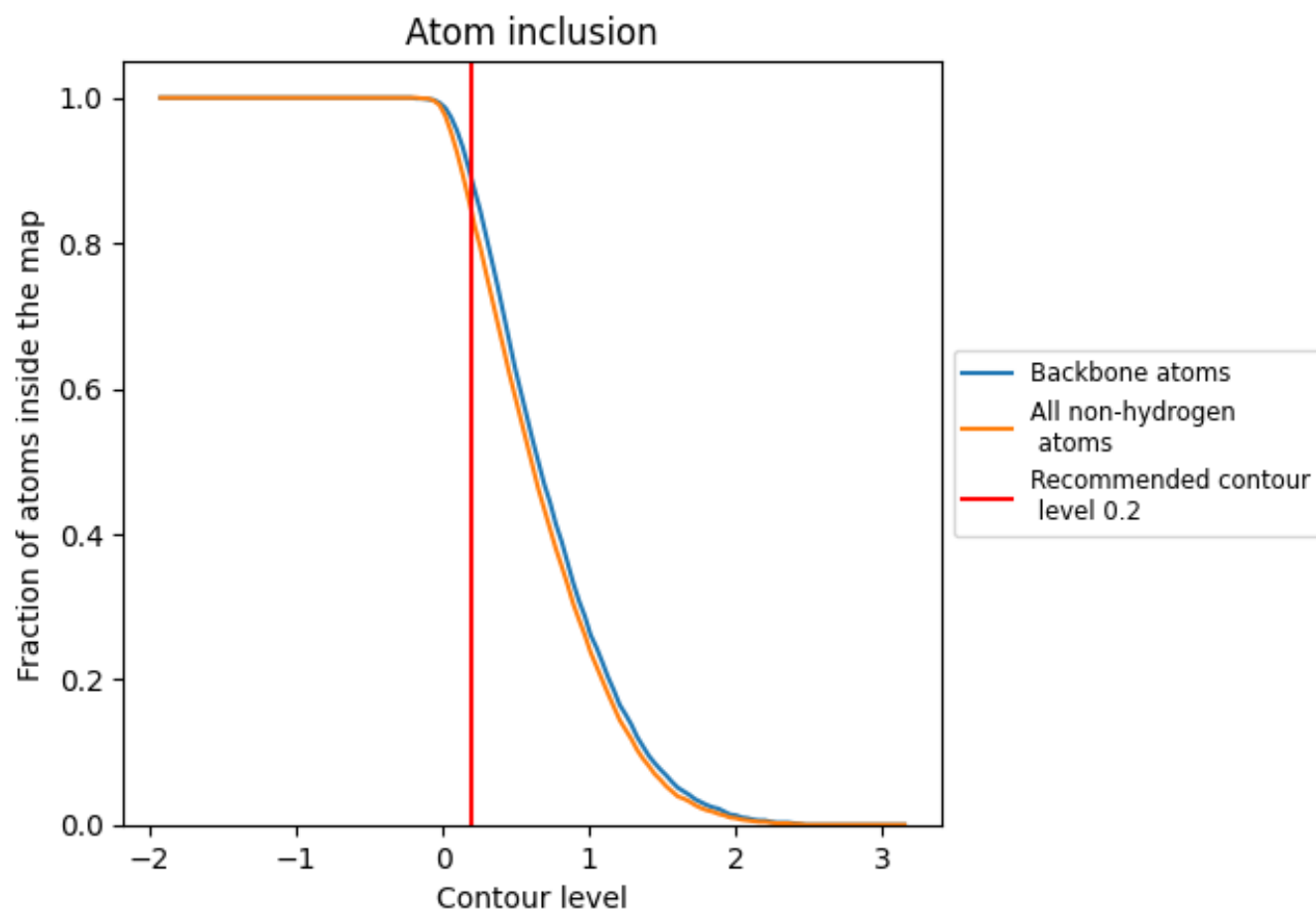
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).































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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5720
A	 0.8980	 0.6010
B	 0.8600	 0.5810
C	 0.8790	 0.5930
D	 0.5360	 0.3990
E	 0.5360	 0.3940
F	 0.5790	 0.4690
G	 0.5710	 0.5150
H	 0.8640	 0.5900
I	 0.7110	 0.5320
J	 0.8120	 0.5590
K	 0.7380	 0.5290
L	 0.7630	 0.5380
P	 0.7630	 0.5050
Q	 0.8650	 0.5730

