



## Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 06:18 AM JST

PDB ID : 8Y8J  
EMDB ID : EMD-39048  
Title : Local structure of HCoV-HKU1C spike in complex with glycan  
Authors : Lu, Y.C.; Zhang, X.; Wang, H.F.; Sun, L.; Yang, H.T.  
Deposited on : 2024-02-06  
Resolution : 3.57 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>.

---

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

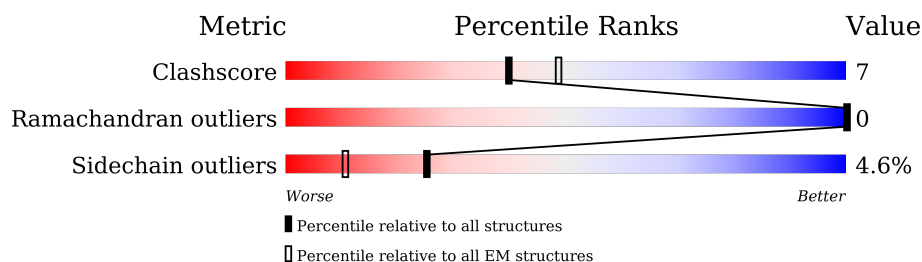
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.57 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1263	
1	B	1263	
2	C	3	
3	D	2	
3	E	2	
3	F	2	
3	G	2	
3	H	2	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5069 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	271	Total	C	N	O	S	0	0
			2197	1429	345	413	10		
1	B	337	Total	C	N	O	S	0	0
			2612	1646	443	501	22		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	GLY	ARG	engineered mutation	UNP Q0ZME7
A	753	GLY	ARG	engineered mutation	UNP Q0ZME7
A	754	SER	LYS	engineered mutation	UNP Q0ZME7
A	755	GLY	ARG	engineered mutation	UNP Q0ZME7
A	756	SER	ARG	engineered mutation	UNP Q0ZME7
A	902	PRO	LEU	engineered mutation	UNP Q0ZME7
A	980	PRO	SER	engineered mutation	UNP Q0ZME7
A	1023	PRO	ASN	engineered mutation	UNP Q0ZME7
A	1067	PRO	ASN	engineered mutation	UNP Q0ZME7
A	1068	PRO	LEU	engineered mutation	UNP Q0ZME7
B	752	GLY	ARG	engineered mutation	UNP Q0ZME7
B	753	GLY	ARG	engineered mutation	UNP Q0ZME7
B	754	SER	LYS	engineered mutation	UNP Q0ZME7
B	755	GLY	ARG	engineered mutation	UNP Q0ZME7
B	756	SER	ARG	engineered mutation	UNP Q0ZME7
B	902	PRO	LEU	engineered mutation	UNP Q0ZME7
B	980	PRO	SER	engineered mutation	UNP Q0ZME7
B	1023	PRO	ASN	engineered mutation	UNP Q0ZME7
B	1067	PRO	ASN	engineered mutation	UNP Q0ZME7
B	1068	PRO	LEU	engineered mutation	UNP Q0ZME7

- Molecule 2 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.



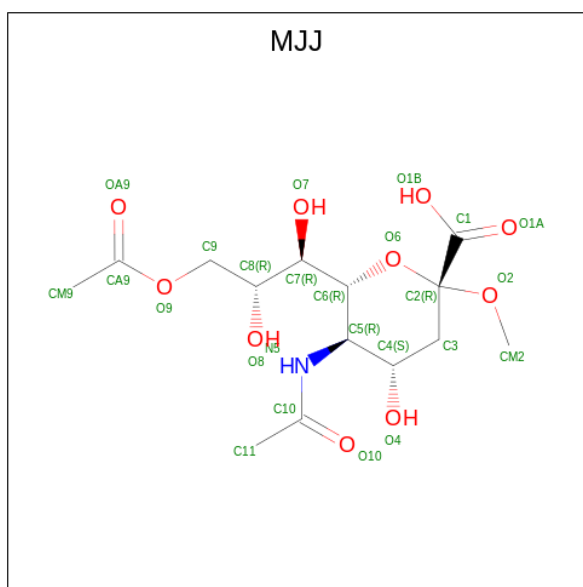
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	3	Total	C	N	O	0	0
			39	22	2	15		

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



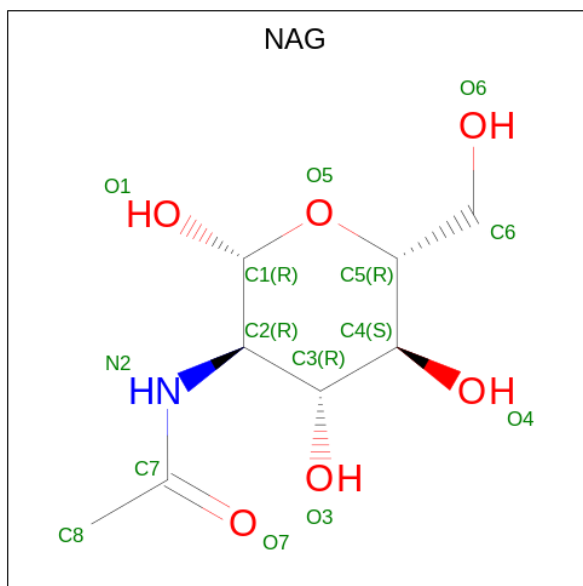
Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is methyl 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid (three-letter code: MJJ) (formula: C<sub>14</sub>H<sub>23</sub>NO<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			25	14	1	10	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

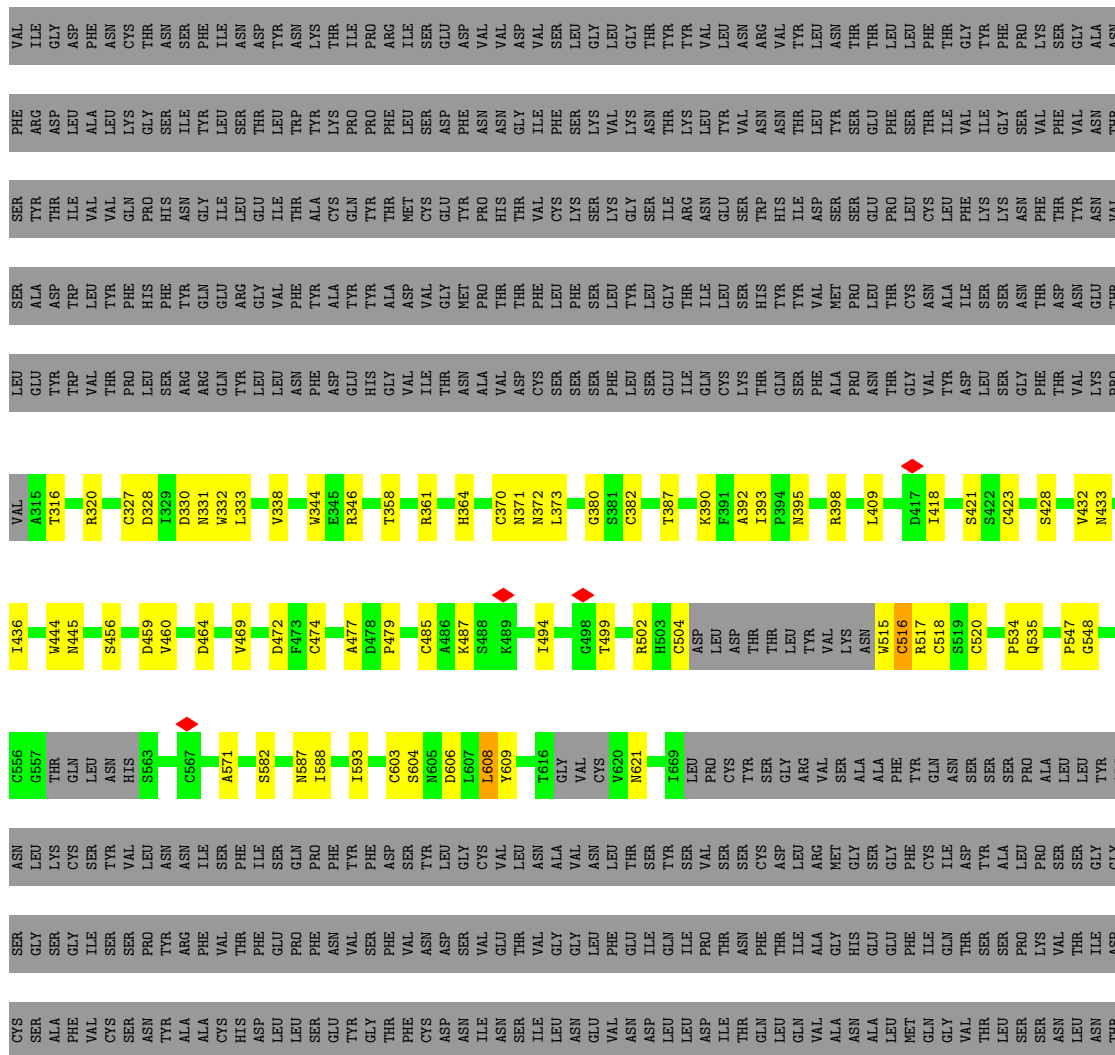
*Continued on next page...*

*Continued from previous page...*

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



- Molecule 1: Spike glycoprotein





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

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

Chain C: 100%



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

Chain D:  100%



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

Chain E:  100%



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

Chain F:  50% 100%



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120295	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	14.576	Depositor
Minimum map value	-0.137	Depositor
Average map value	-0.034	Depositor
Map value standard deviation	0.251	Depositor
Recommended contour level	2	Depositor
Map size ( $\text{\AA}$ )	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82, 0.82, 0.82	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: MJJ, NAG, BMA

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	0/2261	0.46	0/3086
1	B	0.24	0/2679	0.41	0/3645
All	All	0.26	0/4940	0.43	0/6731

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2197	0	2102	29	0
1	B	2612	0	2420	39	0
2	C	39	0	34	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	3	0
4	A	25	0	0	0	0
5	A	28	0	26	1	0
5	B	28	0	26	0	0
All	All	5069	0	4733	68	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 7.

All (68) 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:214:ALA:HB2	1:A:220:THR:HA	1.69	0.75
1:A:123:THR:HG22	1:A:141:PRO:HD2	1.72	0.71
1:B:432:VAL:HG22	1:B:433:ASN:HD22	1.60	0.67
1:B:371:ASN:ND2	1:B:372:ASN:OD1	2.28	0.67
1:A:166:LYS:HD3	1:A:244:ALA:HB3	1.82	0.62
1:B:582:SER:HB3	1:B:587:ASN:HD21	1.67	0.60
1:B:444:TRP:NE1	1:B:547:PRO:O	2.35	0.60
1:B:395:ASN:HD22	1:B:398:ARG:HD2	1.68	0.59
1:A:14:VAL:N	1:A:157:GLU:O	2.36	0.58
1:A:125:VAL:HG12	1:A:138:VAL:HG22	1.84	0.58
1:A:156:CYS:SG	1:A:157:GLU:N	2.78	0.56
1:B:332:TRP:O	1:B:390:LYS:NZ	2.36	0.56
1:B:485:CYS:HB3	1:B:516:CYS:H	1.73	0.54
1:A:108:ASN:ND2	1:A:119:SER:OG	2.38	0.53
1:B:316:THR:HA	1:B:621:ASN:O	2.09	0.53
1:B:555:LYS:HD2	1:B:571:ALA:HA	1.90	0.52
1:B:364:HIS:ND1	1:B:428:SER:OG	2.42	0.52
1:B:392:ALA:HB3	1:B:460:VAL:HG11	1.92	0.52
1:B:504:CYS:HA	1:B:518:CYS:HA	1.91	0.52
1:B:328:ASP:HB3	1:B:331:ASN:HB2	1.92	0.52
1:B:606:ASP:HB3	3:H:1:NAG:H62	1.93	0.51
1:B:456:SER:OG	1:B:459:ASP:OD2	2.28	0.50
1:A:74:PHE:HB3	1:A:257:TRP:HB3	1.95	0.49
1:A:17:ASP:N	1:A:17:ASP:OD1	2.45	0.49
1:A:24:PHE:O	1:A:170:ARG:NH2	2.46	0.49
1:B:604:SER:OG	1:B:606:ASP:OD1	2.30	0.49
1:A:51:VAL:HB	1:A:54:ARG:HB2	1.95	0.48
1:A:32:ILE:H	1:A:32:ILE:HG12	1.45	0.47
1:B:393:ILE:HD12	1:B:587:ASN:HB3	1.96	0.47
1:B:361:ARG:NH1	3:H:2:NAG:O6	2.48	0.47
1:A:51:VAL:HG21	1:A:56:TYR:HE2	1.80	0.46
1:B:382:CYS:HA	1:B:603:CYS:HA	1.98	0.46
1:B:479:PRO:HD3	1:B:494:ILE:HA	1.98	0.46
1:A:76:ASP:HB2	1:A:257:TRP:CZ3	2.51	0.45
1:B:358:THR:OG1	3:H:1:NAG:O7	2.35	0.45
1:B:344:TRP:HZ3	1:B:346:ARG:HE	1.65	0.45
1:A:219:PRO:HG2	1:A:276:ILE:HB	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:HG13	1:A:168:SER:HB3	1.99	0.44
1:B:380:GLY:H	1:B:604:SER:HB3	1.83	0.44
1:B:370:CYS:HA	1:B:423:CYS:HA	1.98	0.44
1:B:487:LYS:HB2	1:B:515:TRP:CD1	2.52	0.43
1:B:373:LEU:HD22	1:B:421:SER:HB2	1.99	0.43
1:A:113:VAL:O	1:A:116:THR:HG22	2.18	0.43
1:A:170:ARG:HA	5:A:1303:NAG:H82	2.00	0.43
1:A:271:ASP:OD1	1:A:275:VAL:N	2.51	0.43
1:A:105:LYS:HE2	1:A:199:TYR:HE1	1.82	0.43
1:B:330:ASP:OD1	1:B:330:ASP:N	2.51	0.43
1:B:320:ARG:O	1:B:609:TYR:OH	2.36	0.43
1:B:445:ASN:HD21	1:B:548:GLY:HA3	1.82	0.43
1:A:164:LYS:HE3	1:A:164:LYS:HB3	1.90	0.43
1:B:469:VAL:HG12	1:B:535:GLN:HG2	2.01	0.43
1:B:338:VAL:HB	1:B:436:ILE:HD13	2.01	0.42
1:B:392:ALA:HA	1:B:588:ILE:HG13	2.00	0.42
1:A:148:ILE:HG21	1:A:224:PHE:CE1	2.54	0.42
1:B:372:ASN:HB2	1:B:421:SER:HA	2.02	0.42
1:B:472:ASP:HA	1:B:499:THR:HG22	2.02	0.42
1:B:608:LEU:H	1:B:608:LEU:HD23	1.85	0.42
1:A:79:LEU:HD13	1:A:89:TRP:HB3	2.02	0.41
1:B:333:LEU:HD23	1:B:390:LYS:HD3	2.02	0.41
1:A:213:TYR:HB3	1:A:223:LEU:HD11	2.02	0.41
1:B:387:THR:OG1	1:B:593:ILE:HB	2.19	0.41
1:B:477:ALA:HB2	1:B:502:ARG:HB3	2.02	0.41
1:A:36:SER:HB3	1:A:257:TRP:CZ3	2.56	0.41
1:A:109:THR:HB	1:A:120:GLU:O	2.21	0.41
1:A:281:ASP:OD1	1:A:282:CYS:N	2.53	0.41
1:B:520:CYS:SG	1:B:534:PRO:HD2	2.60	0.41
1:A:104:SER:OG	1:A:200:PHE:HB2	2.21	0.40
1:A:53:ASN:OD1	1:A:53:ASN:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	269/1263 (21%)	255 (95%)	14 (5%)	0	100	100
1	B	329/1263 (26%)	312 (95%)	17 (5%)	0	100	100
All	All	598/2526 (24%)	567 (95%)	31 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	249/1132 (22%)	232 (93%)	17 (7%)	13	40
1	B	299/1132 (26%)	291 (97%)	8 (3%)	40	65
All	All	548/2264 (24%)	523 (95%)	25 (5%)	25	51

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	CYS
1	A	28	TYR
1	A	29	ASN
1	A	30	LYS
1	A	32	ILE
1	A	35	ILE
1	A	61	LEU
1	A	69	LYS
1	A	80	LYS
1	A	116	THR
1	A	156	CYS
1	A	162	VAL
1	A	163	CYS
1	A	164	LYS
1	A	213	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	215	ASP
1	A	246	SER
1	B	327	CYS
1	B	409	LEU
1	B	418	ILE
1	B	464	ASP
1	B	474	CYS
1	B	516	CYS
1	B	517	ARG
1	B	608	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	29	ASN
1	A	108	ASN
1	B	343	ASN
1	B	351	ASN
1	B	371	ASN
1	B	372	ASN
1	B	395	ASN
1	B	413	ASN
1	B	445	ASN
1	B	552	ASN
1	B	587	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](#)

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

## 5.5 Carbohydrates [i](#)

13 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	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	C	2	2	14,14,15	0.20	0	17,19,21	0.40	0
2	BMA	C	3	2	11,11,12	0.58	0	15,15,17	0.79	0
3	NAG	D	1	1,3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	D	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	E	1	1,3	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	E	2	3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	F	1	1,3	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	G	1	1,3	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	G	2	3	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	H	1	1,3	14,14,15	0.25	0	17,19,21	0.37	0
3	NAG	H	2	3	14,14,15	0.22	0	17,19,21	0.43	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

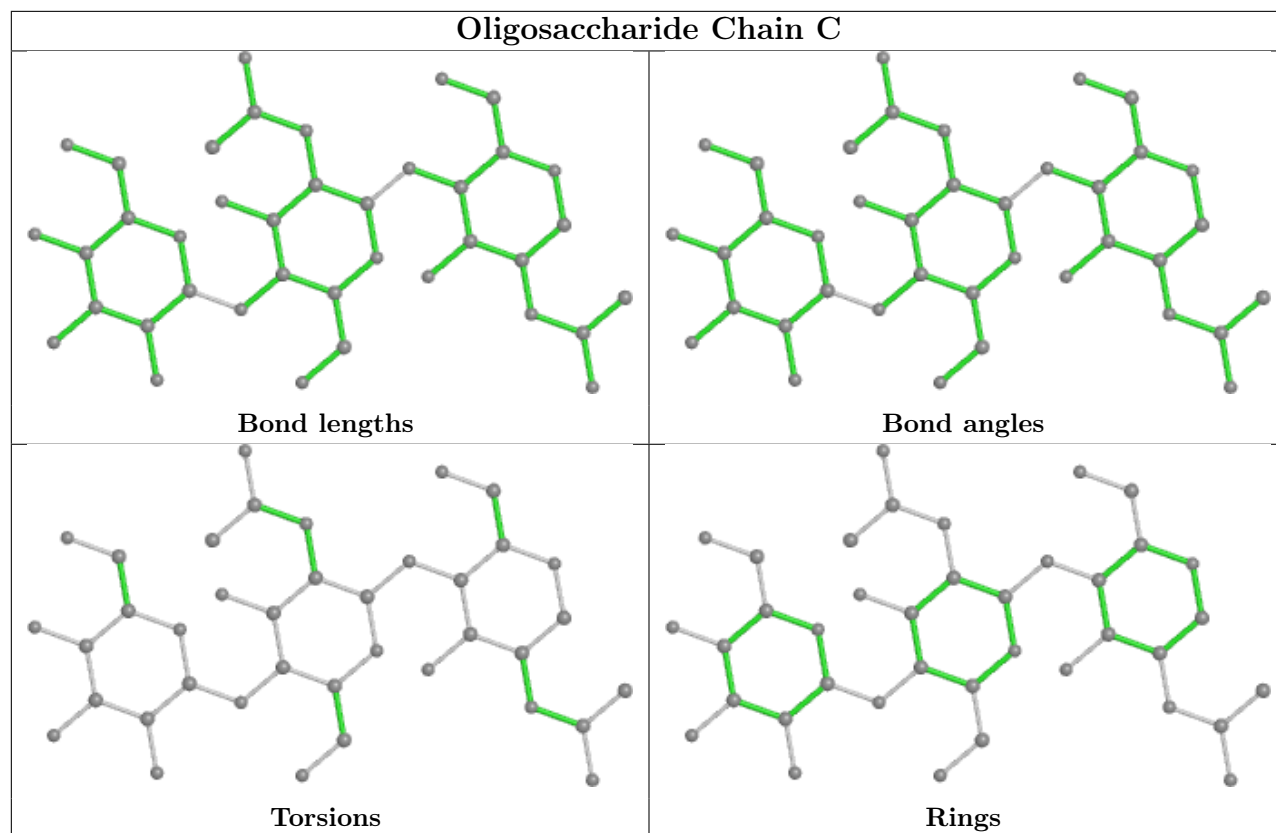
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

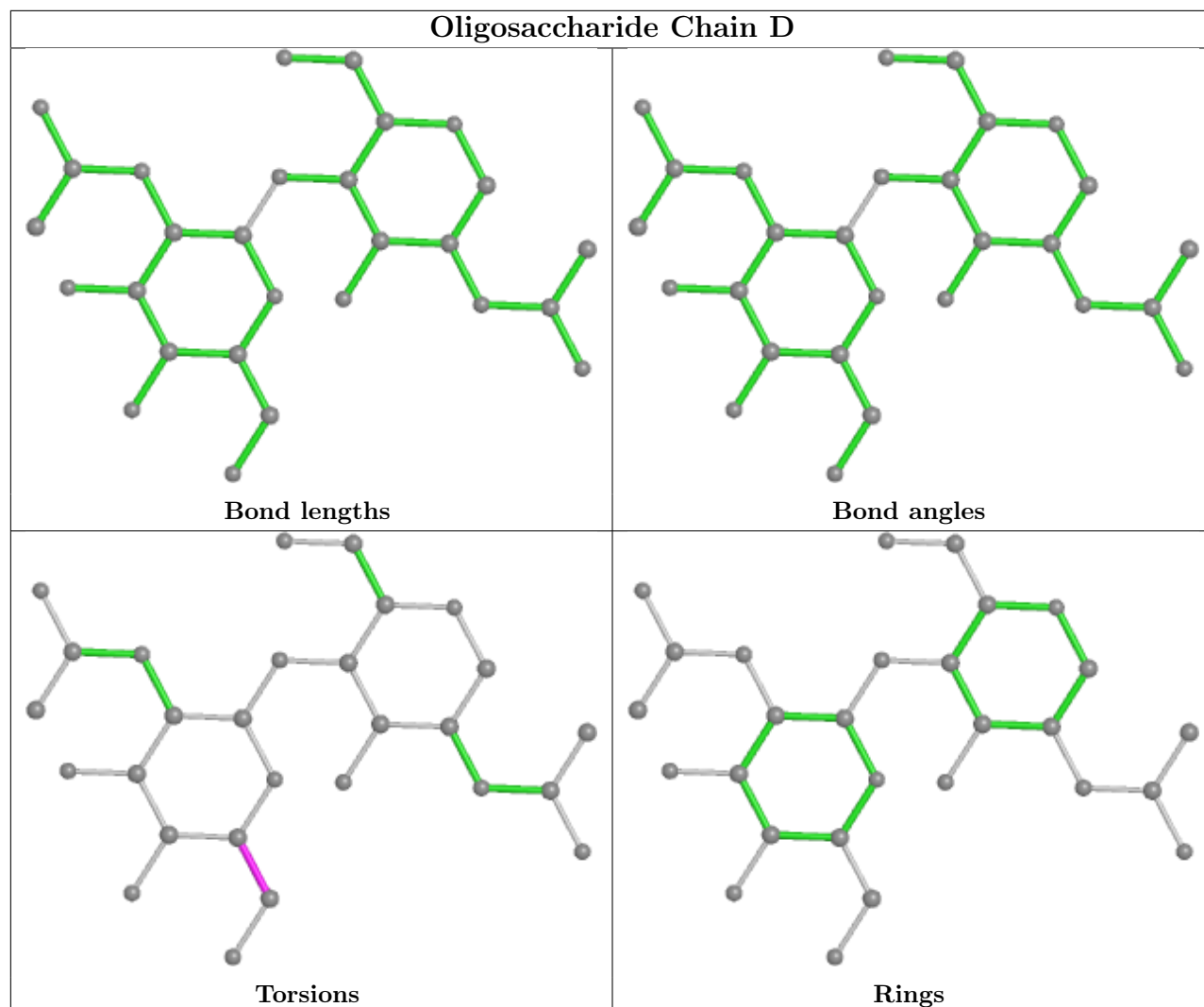
There are no ring outliers.

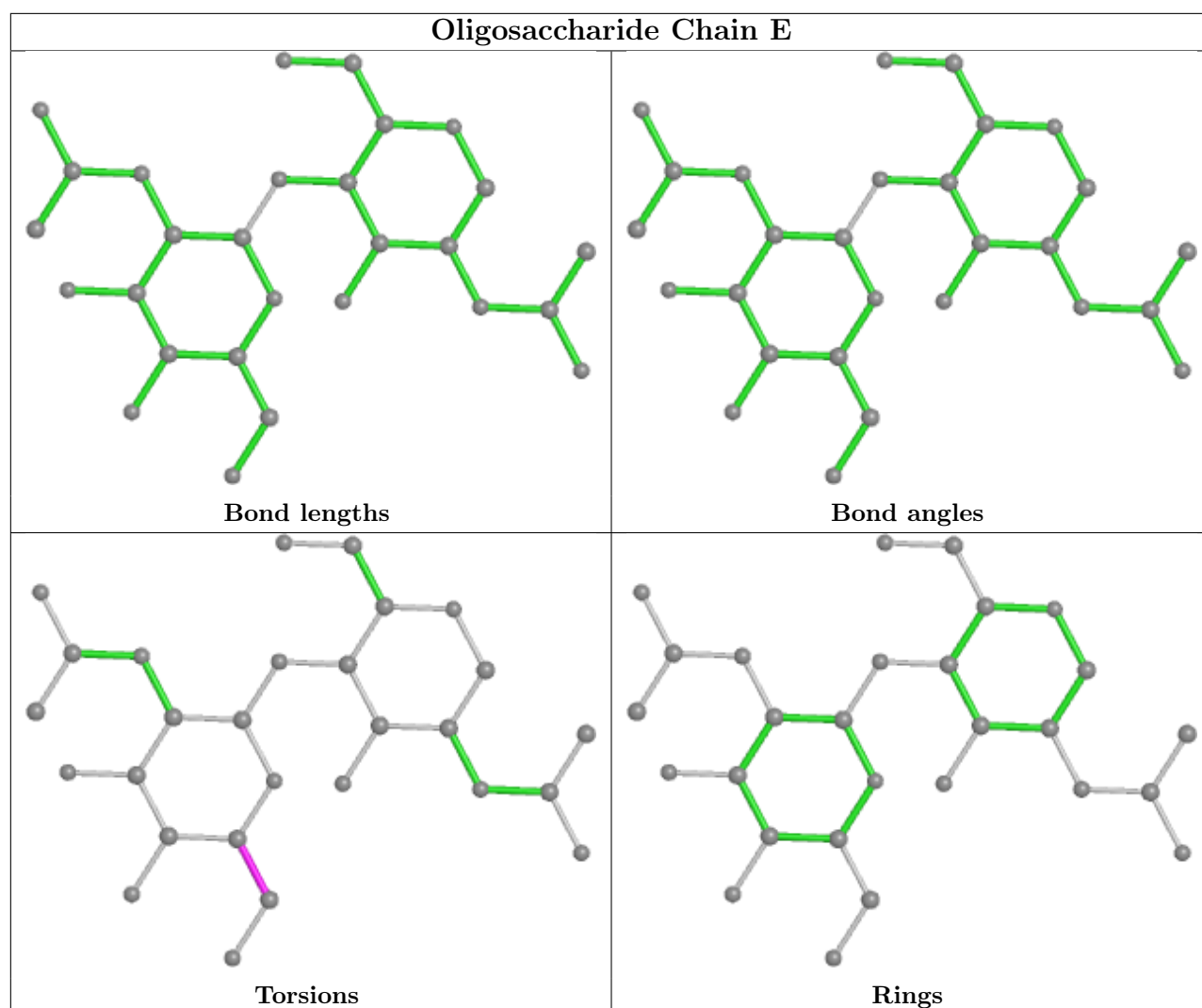
2 monomers are involved in 3 short contacts:

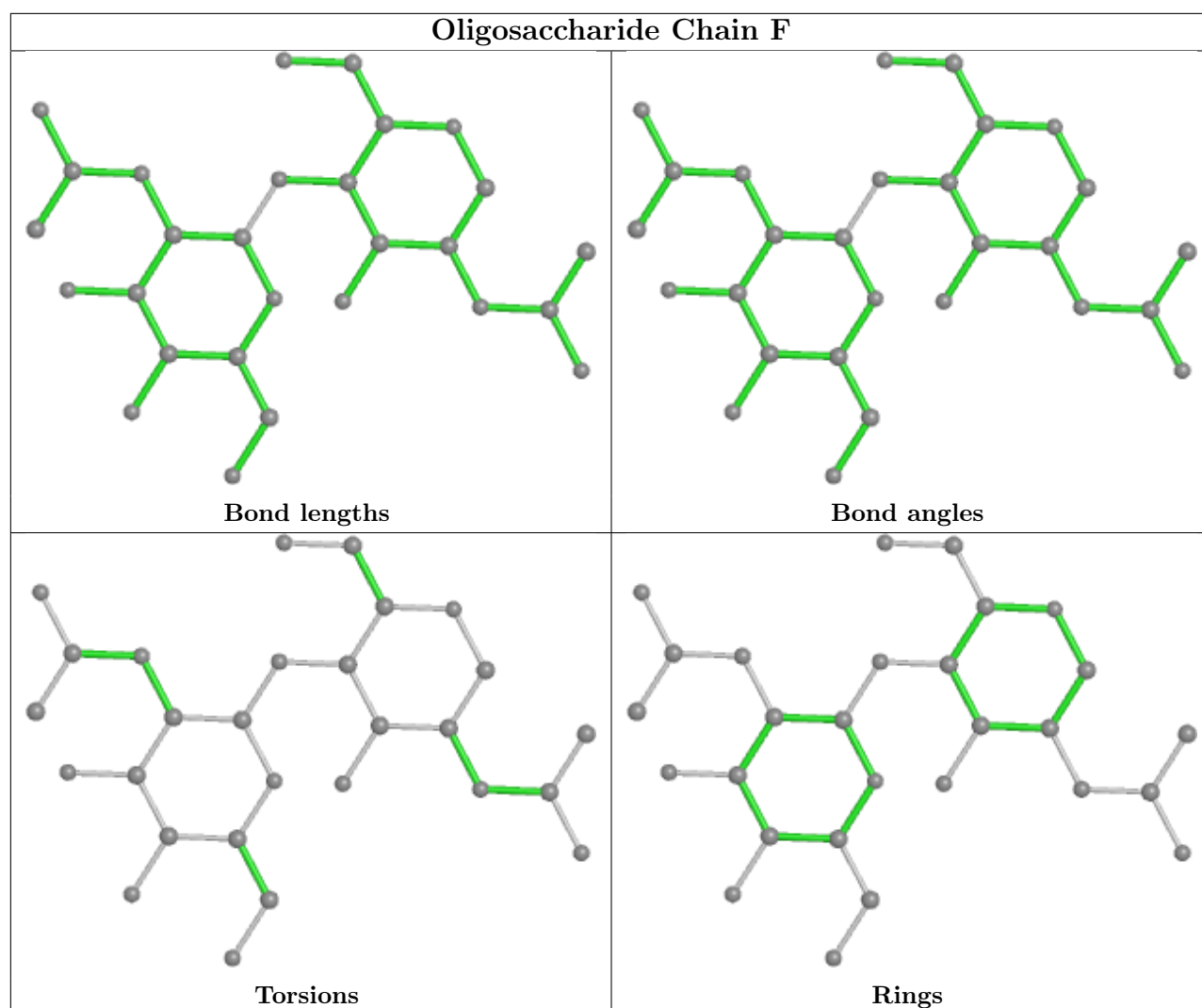
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	2	0
3	H	2	NAG	1	0

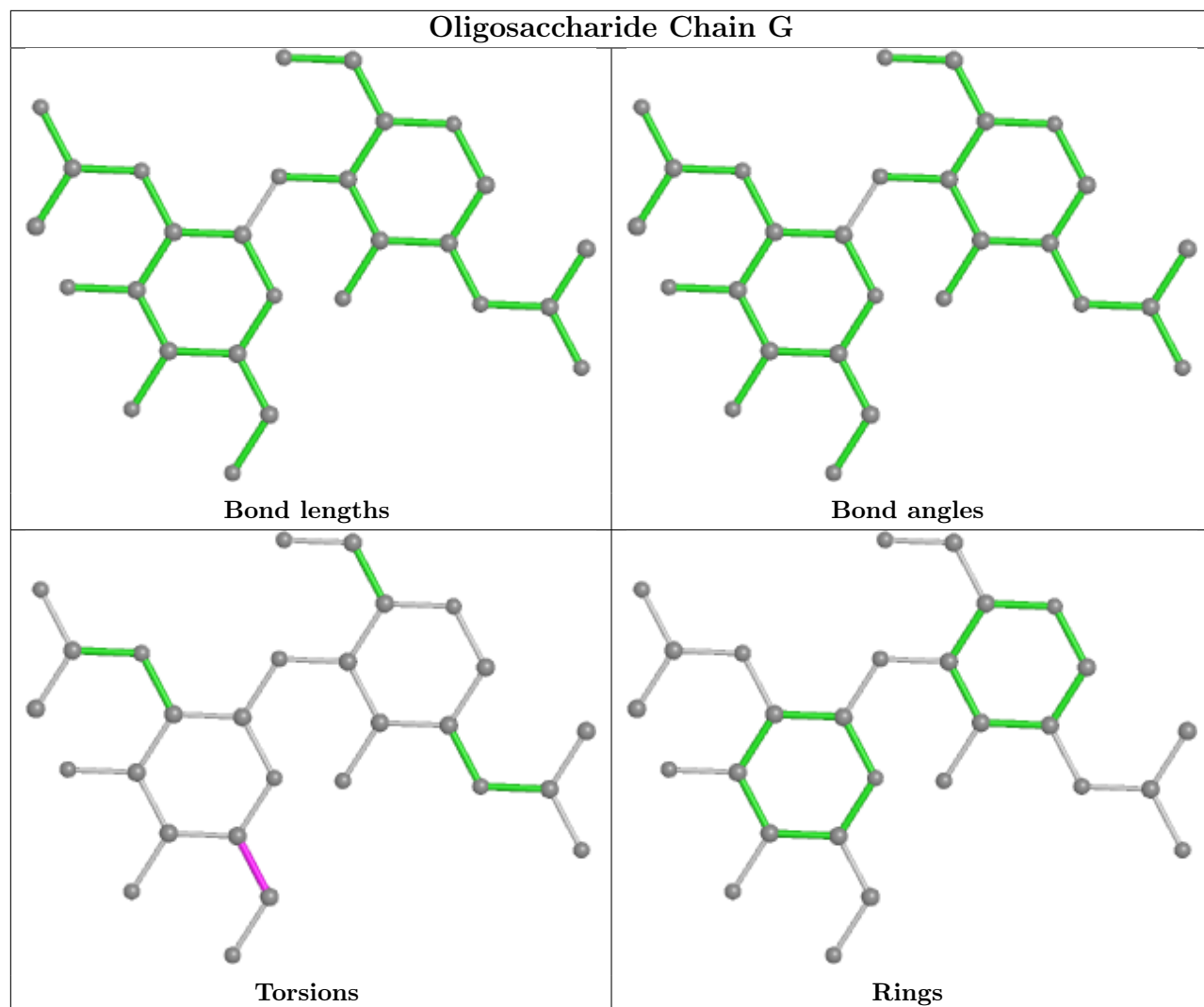
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

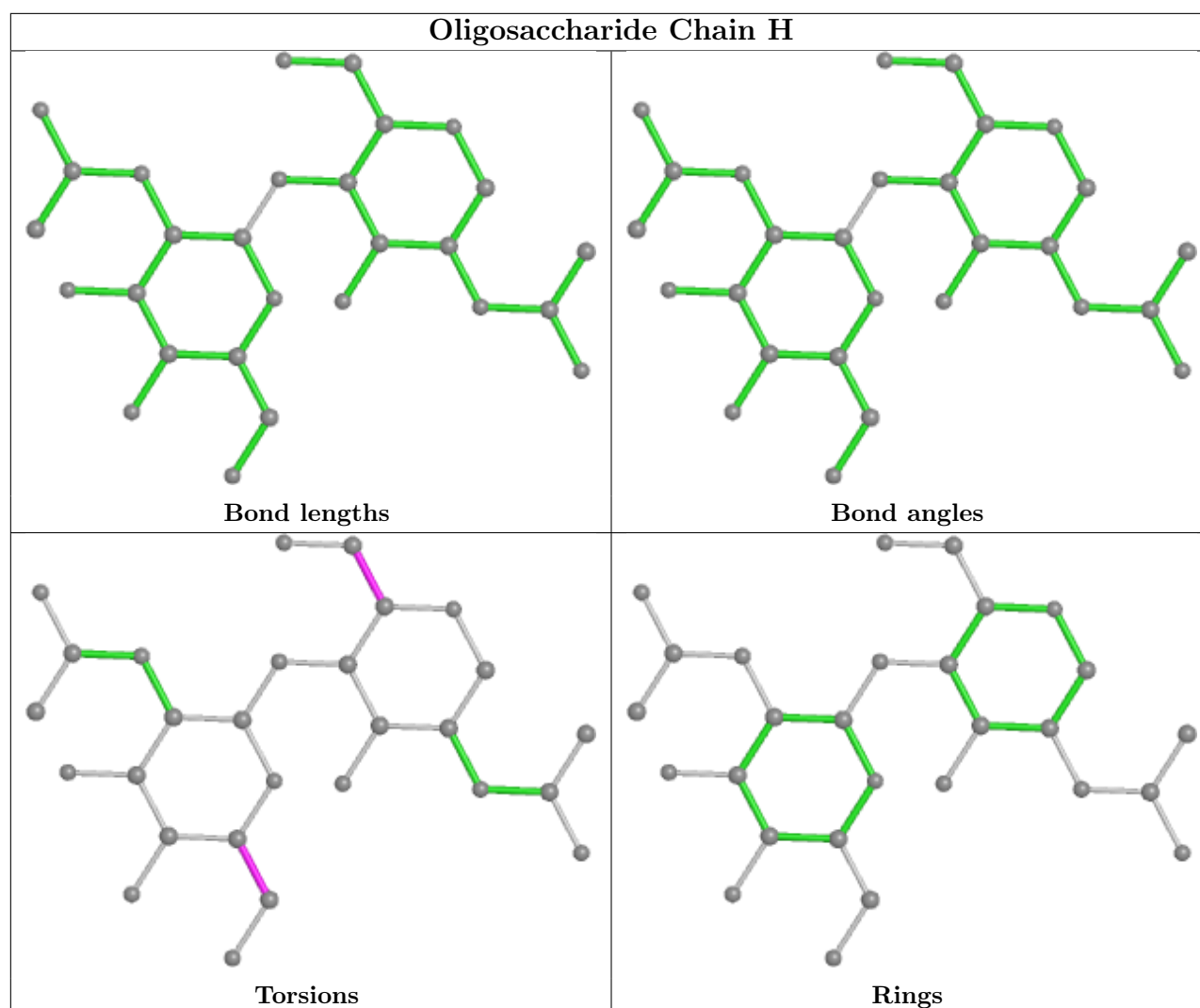












## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
5	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.42	0
4	MJJ	A	1301	-	25,25,25	2.04	5 (20%)	31,36,36	2.19	8 (25%)
5	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.41	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	B	1301	1	14,14,15	0.21	0	17,19,21	0.42	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
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	MJJ	A	1301	-	-	8/26/44/44	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	MJJ	O6-C2	6.17	1.50	1.42
4	A	1301	MJJ	C3-C4	-4.17	1.46	1.53
4	A	1301	MJJ	C10-N5	3.28	1.45	1.34
4	A	1301	MJJ	C4-C5	-2.24	1.51	1.53
4	A	1301	MJJ	O9-C9	-2.15	1.40	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	MJJ	O6-C2-C3	5.60	119.30	111.24
4	A	1301	MJJ	CM2-O2-C2	5.23	122.54	115.42
4	A	1301	MJJ	O6-C6-C5	4.72	114.38	109.78
4	A	1301	MJJ	C3-C2-C1	4.28	121.05	111.19
4	A	1301	MJJ	O6-C2-C1	3.00	119.06	107.08
4	A	1301	MJJ	C11-C10-N5	2.37	120.12	116.10
4	A	1301	MJJ	C4-C5-C6	2.30	114.92	109.10
4	A	1301	MJJ	C3-C4-C5	2.22	113.40	109.98

There are no chirality outliers.

All (14) torsion outliers are listed below:

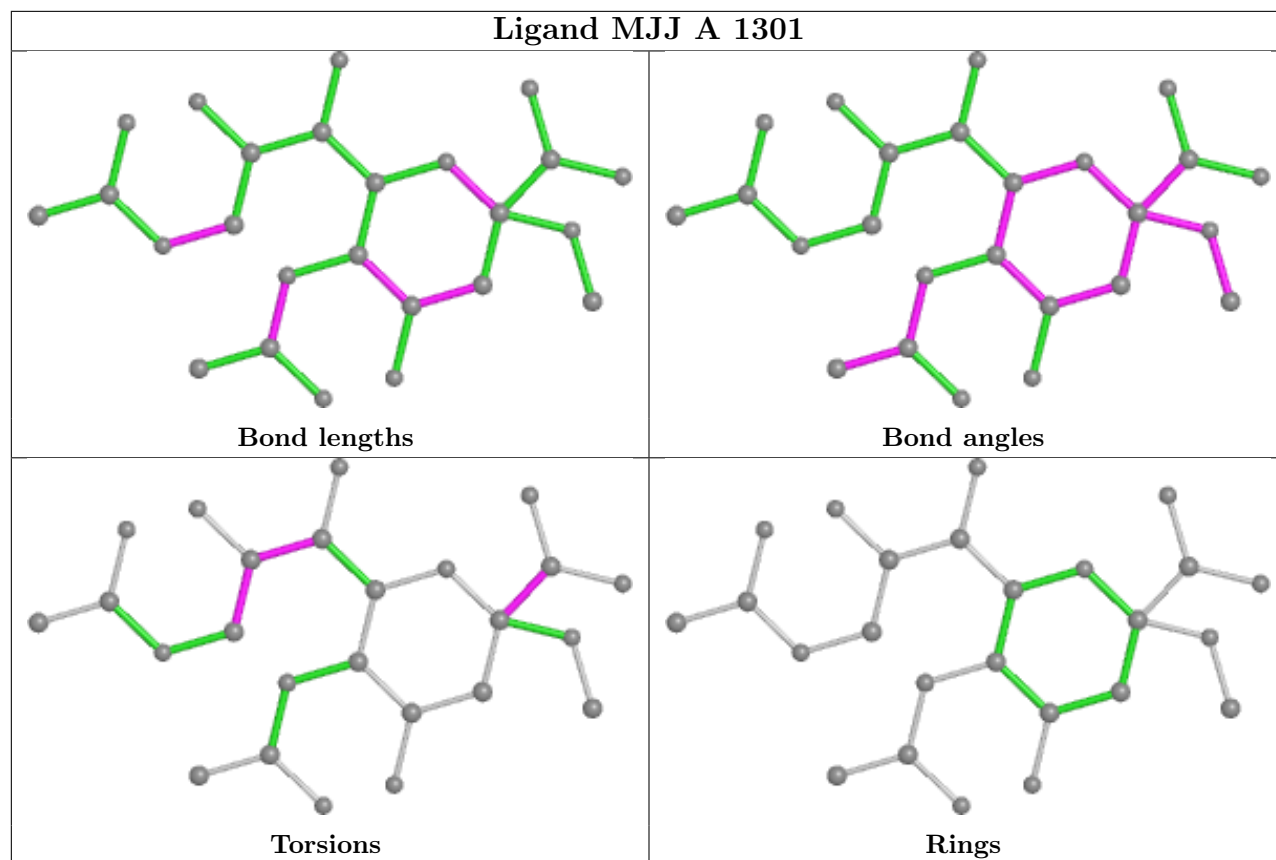
Mol	Chain	Res	Type	Atoms
4	A	1301	MJJ	O1B-C1-C2-O2
5	A	1303	NAG	C4-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	A	1302	NAG	C8-C7-N2-C2
5	A	1302	NAG	O7-C7-N2-C2
5	A	1303	NAG	O5-C5-C6-O6
4	A	1301	MJJ	O7-C7-C8-C9
4	A	1301	MJJ	C6-C7-C8-C9
4	A	1301	MJJ	C6-C7-C8-O8
4	A	1301	MJJ	O7-C7-C8-O8
4	A	1301	MJJ	C7-C8-C9-O9
4	A	1301	MJJ	O1A-C1-C2-O2
4	A	1301	MJJ	O8-C8-C9-O9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1303	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

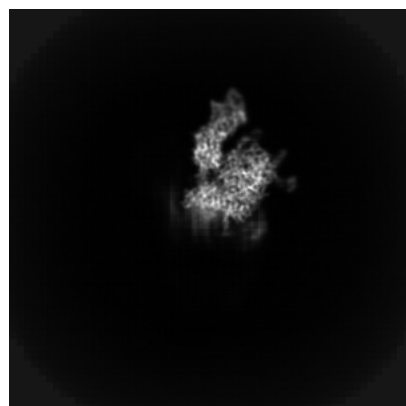
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39048. These allow visual inspection of the internal detail of the map and identification of artifacts.

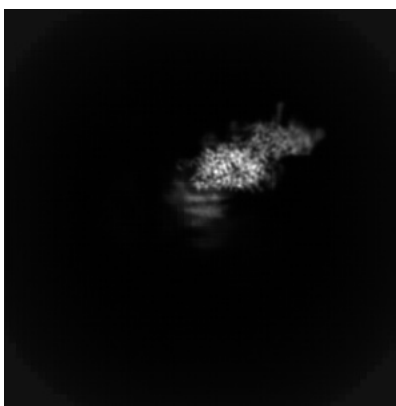
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

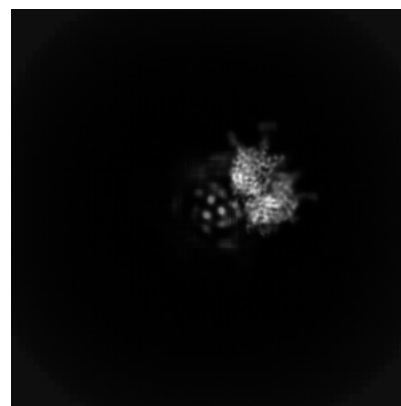
#### 6.1.1 Primary map



X

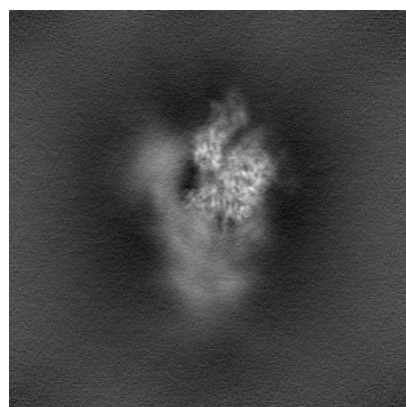


Y

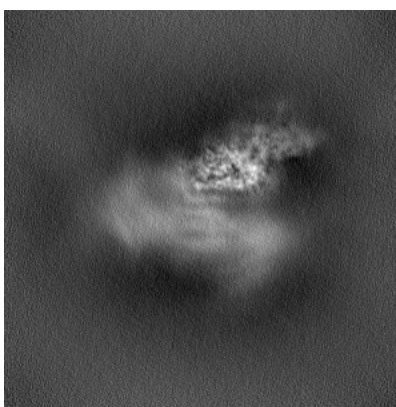


Z

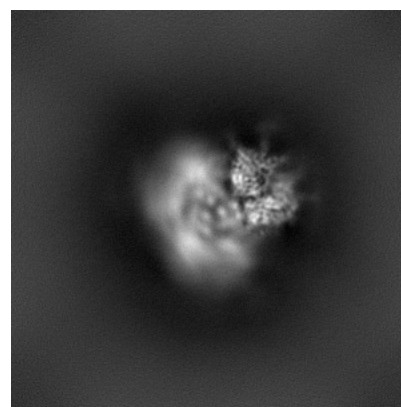
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

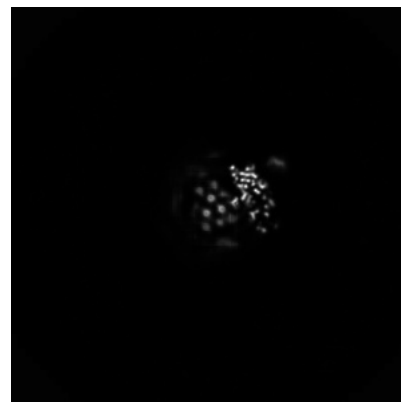
### 6.2.1 Primary map



X Index: 200



Y Index: 200

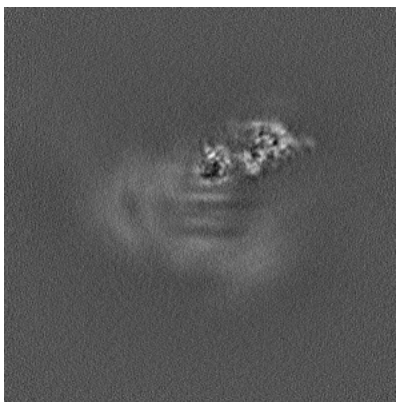


Z Index: 200

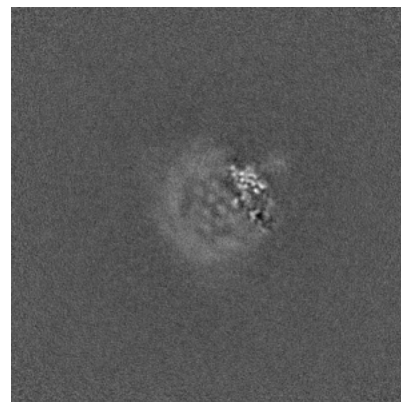
### 6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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: 243

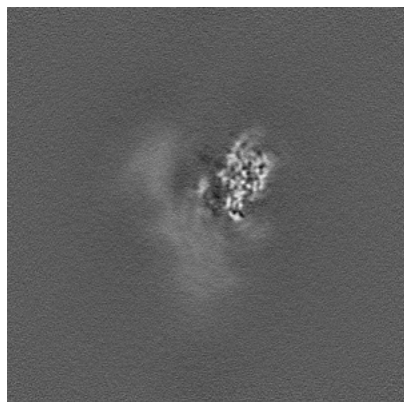


Y Index: 204

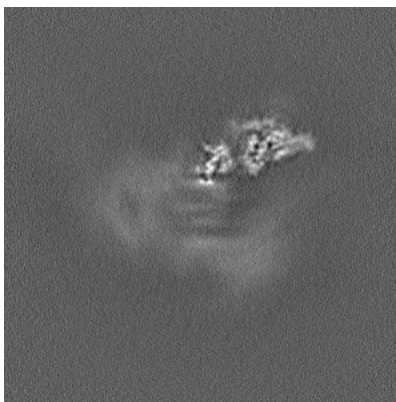


Z Index: 235

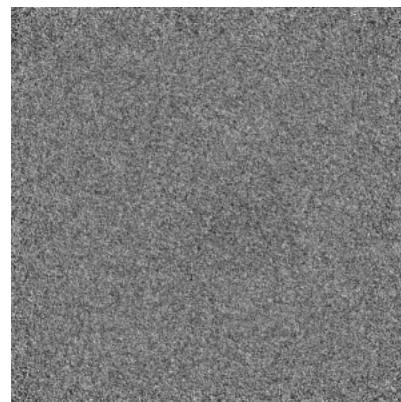
### 6.3.2 Raw map



X Index: 229



Y Index: 204



Z Index: 399

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

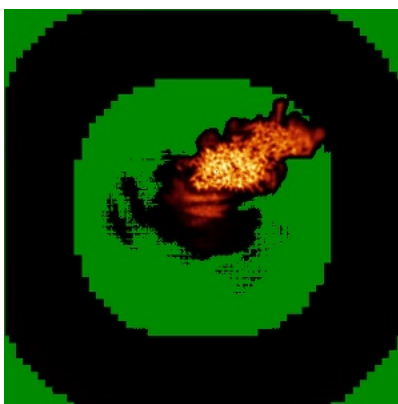


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

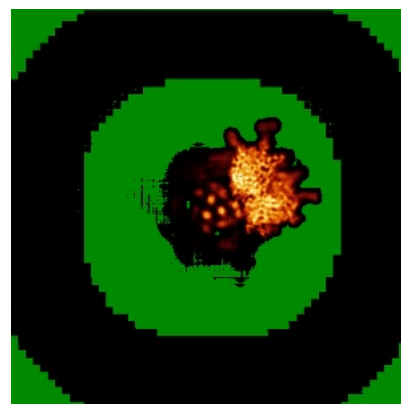
### 6.4.1 Primary map



X

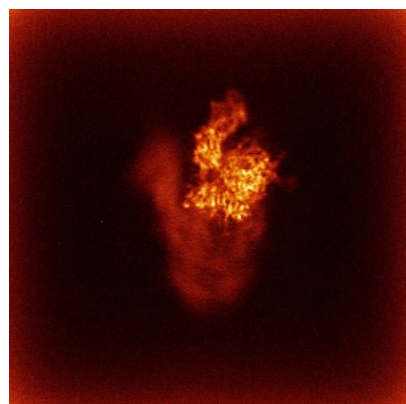


Y

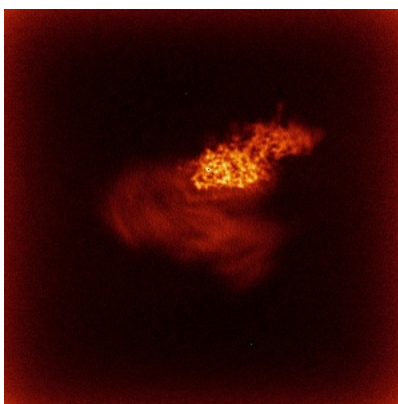


Z

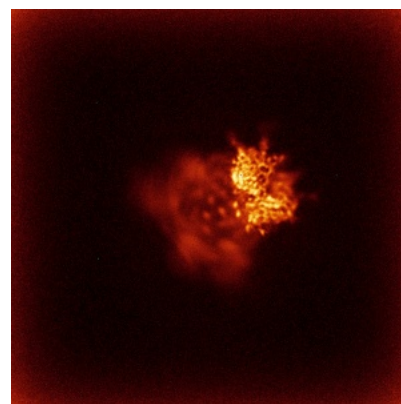
### 6.4.2 Raw map



X



Y

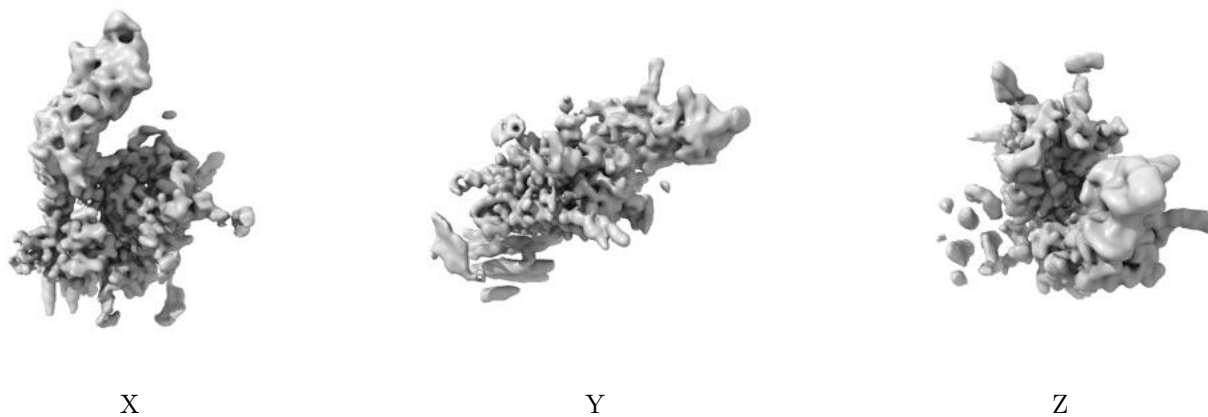


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. 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](#)

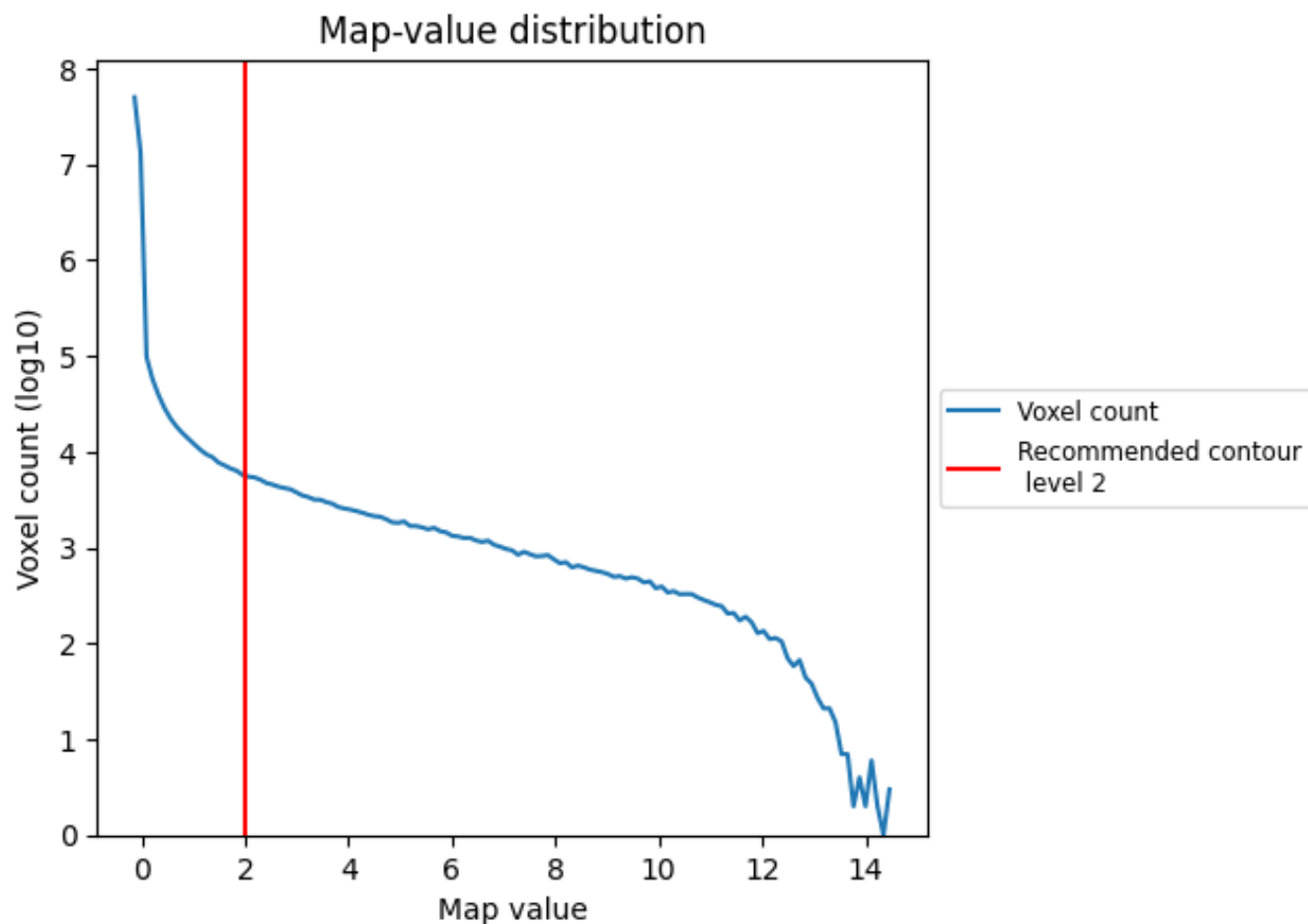
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

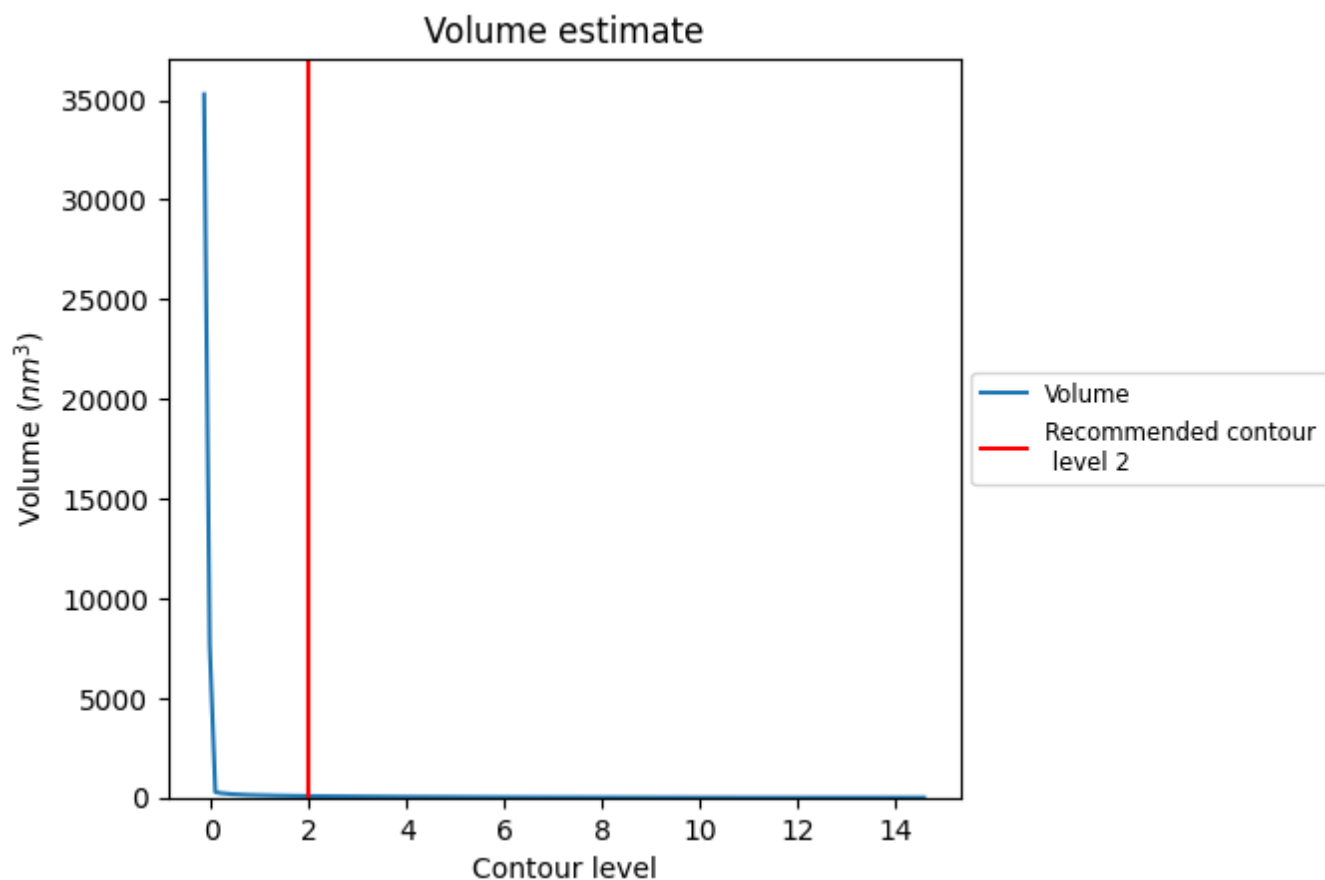
This section contains the results of statistical analysis of the map.

### 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.

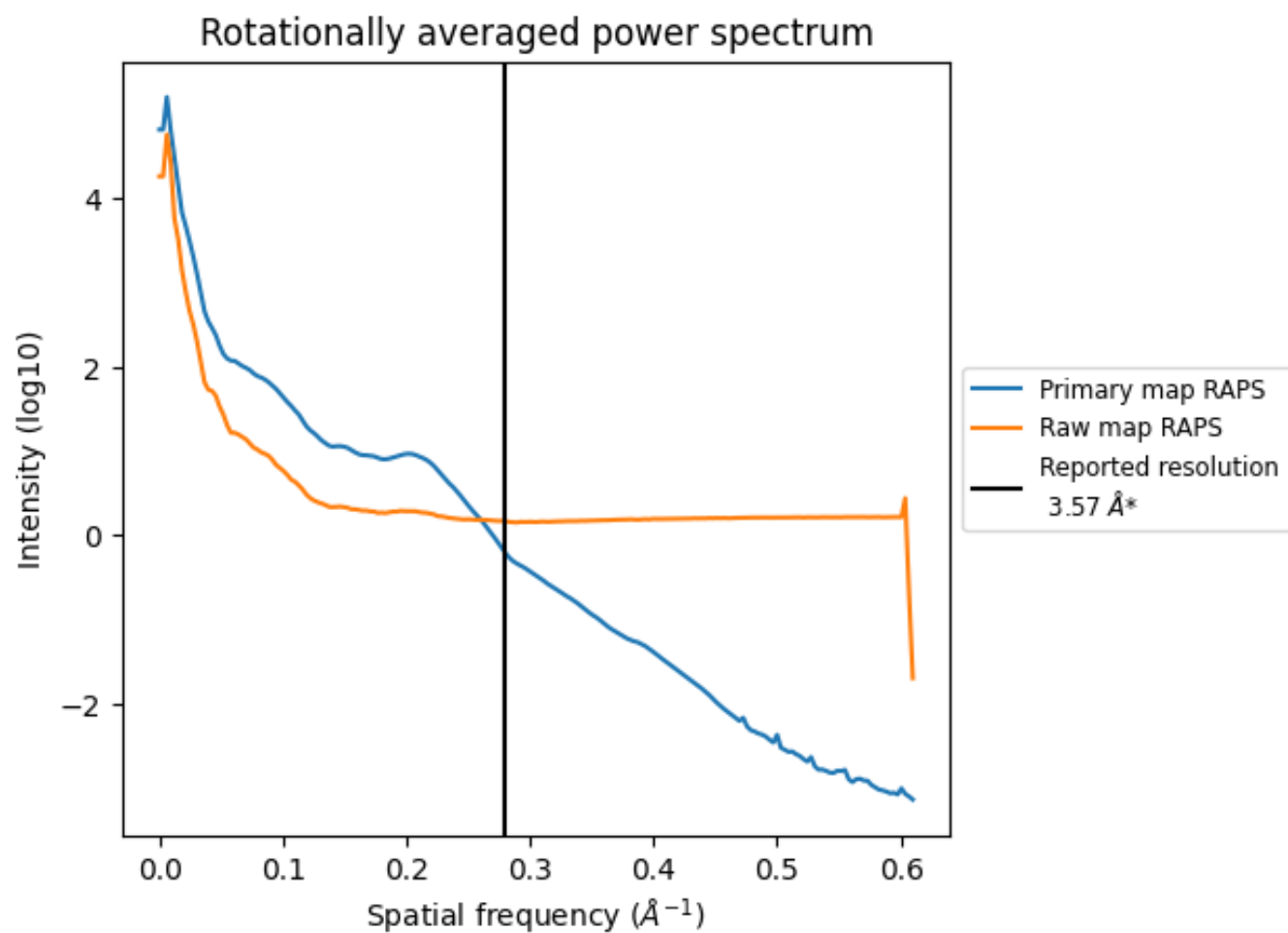
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74  $\text{nm}^3$ ; this corresponds to an approximate mass of 67 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 ⓘ

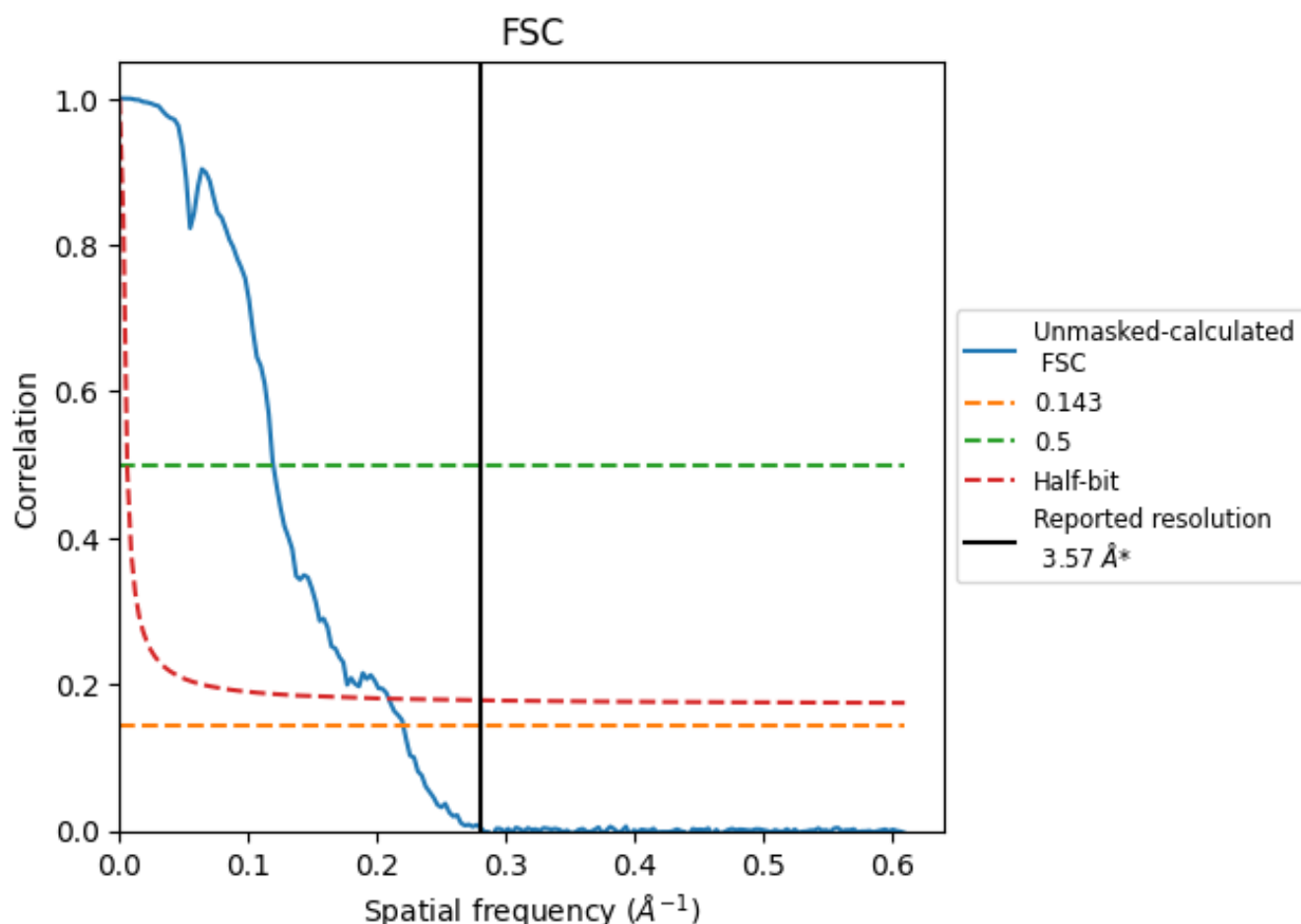


\*Reported resolution corresponds to spatial frequency of 0.280  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

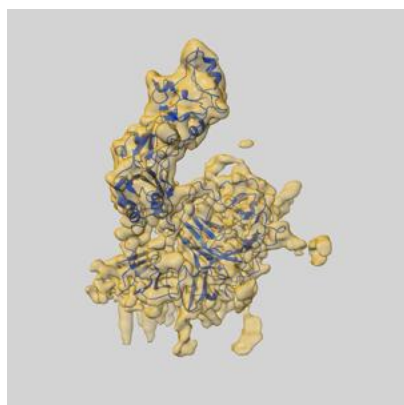
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.54	8.38	4.78

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.54 differs from the reported value 3.57 by more than 10 %

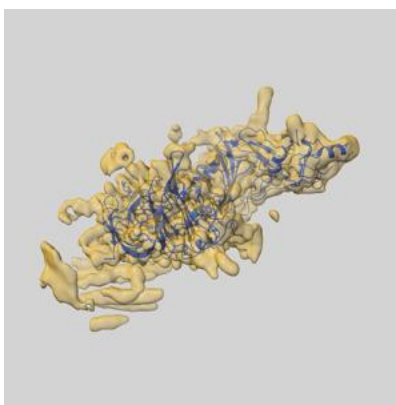
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39048 and PDB model 8Y8J. Per-residue inclusion information can be found in section [3](#) on page [7](#).

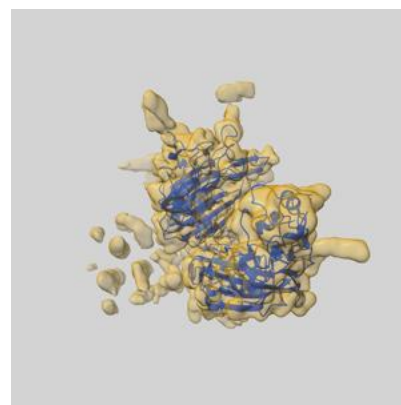
### 9.1 Map-model overlay [i](#)



X



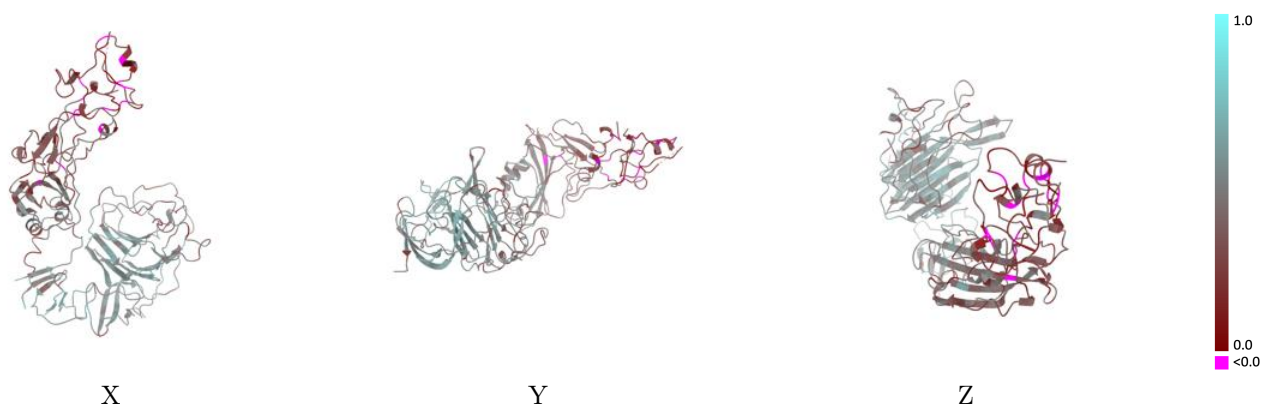
Y



Z

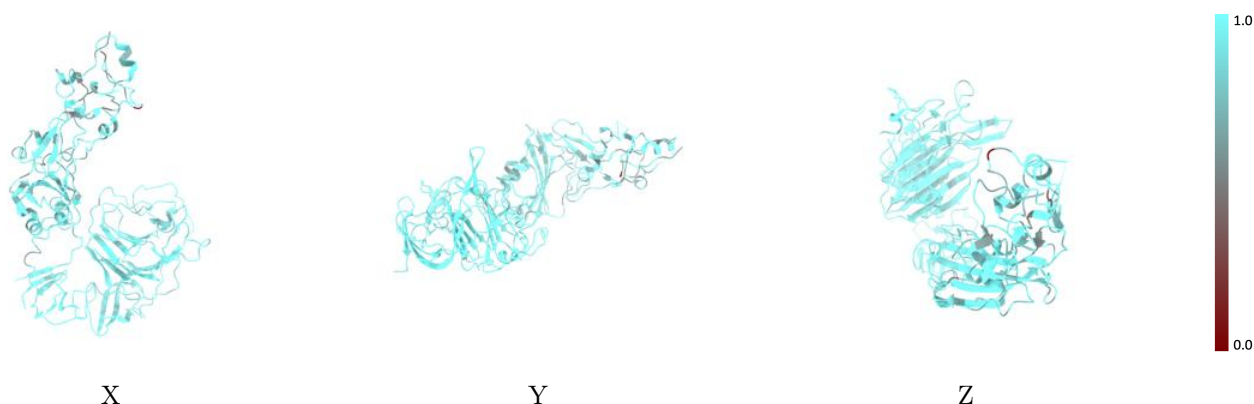
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



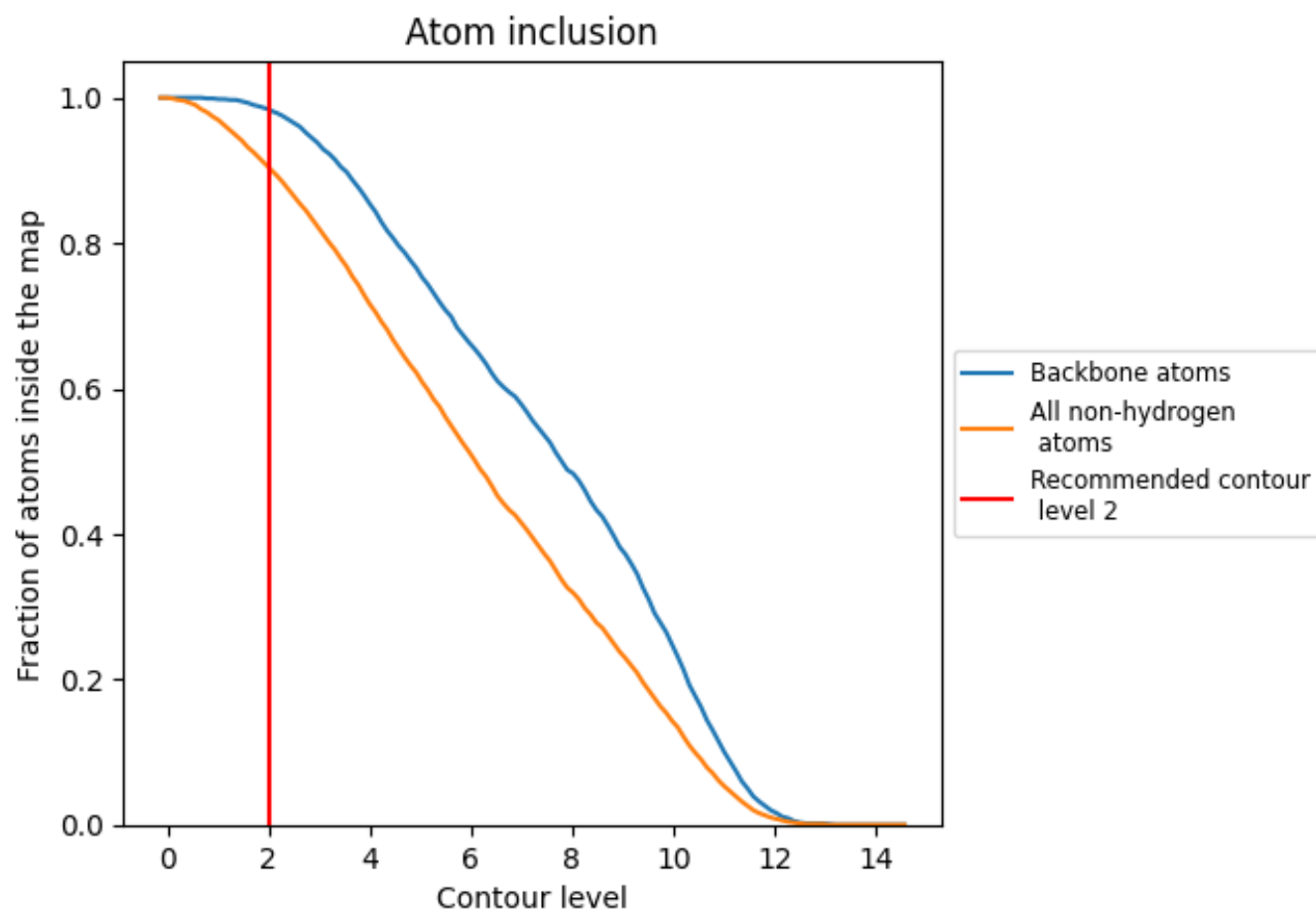
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 90% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9040</div>	<div><div></div>0.4090</div>
A	<div><div></div>0.9490</div>	<div><div></div>0.4880</div>
B	<div><div></div>0.8790</div>	<div><div></div>0.3480</div>
C	<div><div></div>0.9230</div>	<div><div></div>0.3740</div>
D	<div><div></div>0.7860</div>	<div><div></div>0.3860</div>
E	<div><div></div>0.7500</div>	<div><div></div>0.3710</div>
F	<div><div></div>0.5710</div>	<div><div></div>0.2710</div>
G	<div><div></div>0.5710</div>	<div><div></div>0.2820</div>
H	<div><div></div>0.6790</div>	<div><div></div>0.2720</div>

1.0

0.0

<0.0