



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 01:55 AM UTC

PDB ID : 8C8T / pdb_00008c8t
EMDB ID : EMD-16493
Title : cryo-EM structure of BG505 SOSIP.664 HIV-1 Env trimer in complex with bNAbs EPTC112 and 3BNC117
Authors : Baquero, E.; Molinos-Albert, L.; Mouquet, H.
Deposited on : 2023-01-21
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary 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

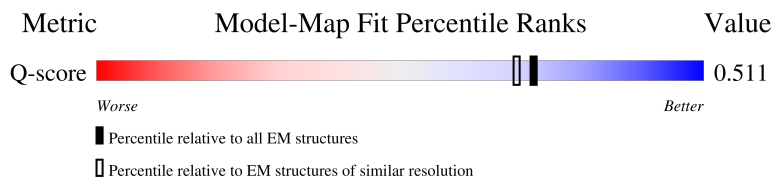
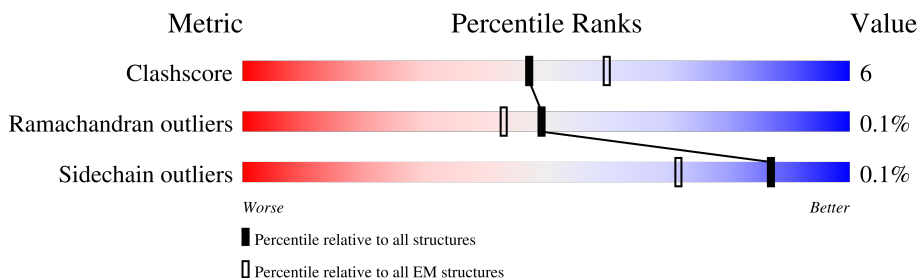
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



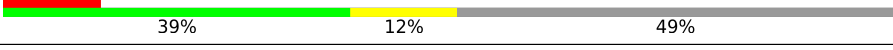
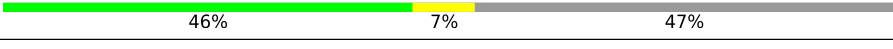
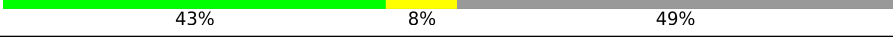
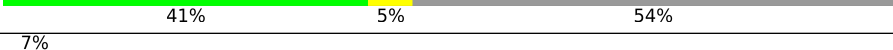
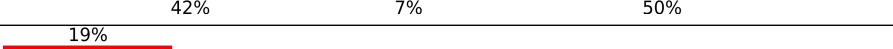
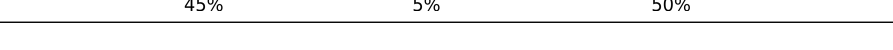
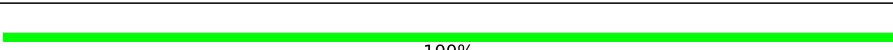
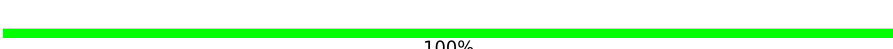
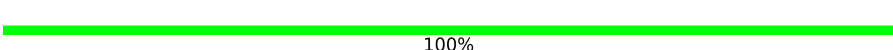
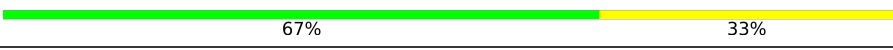
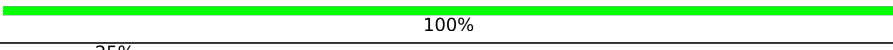
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	469	
1	F	469	
1	G	469	
2	B	145	

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Mol	Chain	Length	Quality of chain
2	I	145	
2	J	145	
3	C	233	
3	H	233	
4	R	226	
4	S	226	
5	T	206	
5	U	206	
6	D	216	
6	K	216	
7	E	2	
7	M	2	
7	N	2	
7	O	2	
7	P	2	
7	Q	2	
7	W	2	
7	Y	2	
7	Z	2	
7	a	2	
7	b	2	
8	L	3	
8	X	3	
9	V	4	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 19762 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	420	Total	C	N	O	S	0	0
			3254	2060	574	592	28		
1	F	426	Total	C	N	O	S	0	0
			3277	2070	575	604	28		
1	G	422	Total	C	N	O	S	0	0
			3246	2057	571	591	27		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S5
A	501	CYS	ALA	conflict	UNP Q2N0S5
F	332	ASN	THR	conflict	UNP Q2N0S5
F	501	CYS	ALA	conflict	UNP Q2N0S5
G	332	ASN	THR	conflict	UNP Q2N0S5
G	501	CYS	ALA	conflict	UNP Q2N0S5

- Molecule 2 is a protein called Gp41 Bg505 T332n Sosip.664.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	117	Total	C	N	O	S	0	0
			918	581	160	171	6		
2	I	118	Total	C	N	O	S	0	0
			906	578	160	163	5		
2	J	116	Total	C	N	O	S	0	0
			879	559	150	164	6		

- Molecule 3 is a protein called IgG EPTC112 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	0	0
			897	573	151	170	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	119	Total	C	N	O	S	0	0
			891	570	151	167	3		

- Molecule 4 is a protein called IgG 3BNC117 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	120	Total	C	N	O	S	0	0
			938	595	170	170	3		
4	S	116	Total	C	N	O	S	0	0
			894	570	158	163	3		

- Molecule 5 is a protein called IgG 3BNC117 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	95	Total	C	N	O	S	0	0
			680	436	112	129	3		
5	U	98	Total	C	N	O	S	0	0
			664	422	113	126	3		

- Molecule 6 is a protein called IgG EPTC112 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	108	Total	C	N	O	S	0	0
			773	479	125	167	2		
6	K	108	Total	C	N	O	S	0	0
			773	479	125	167	2		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



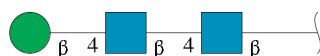
Mol	Chain	Residues	Atoms				AltConf	Trace
7	E	2	Total	C	N	O	0	0
			28	16	2	10		
7	M	2	Total	C	N	O	0	0
			28	16	2	10		
7	N	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	2	Total	C	N	O	0	0
			28	16	2	10		
7	P	2	Total	C	N	O	0	0
			28	16	2	10		
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 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
8	L	3	Total	C	N	O	0	0
			39	22	2	15		
8	X	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
9	V	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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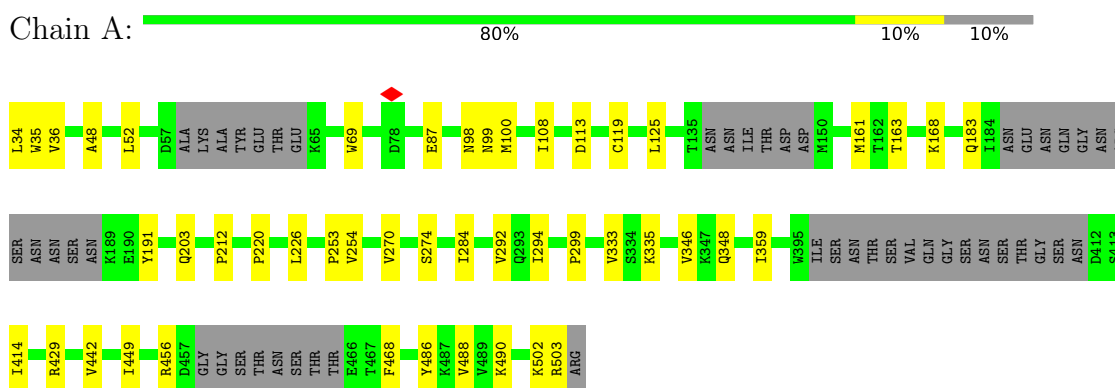
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Mol	Chain	Residues	Atoms				AltConf
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	T	1	Total 14	C 8	N 1	O 5	0

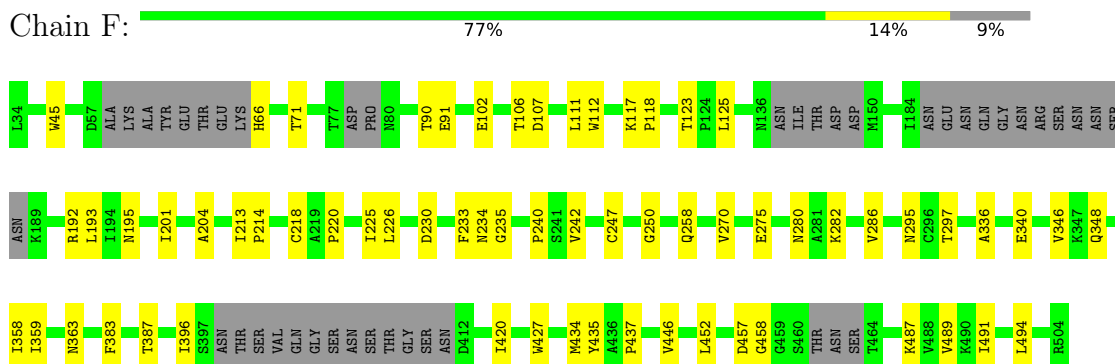
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

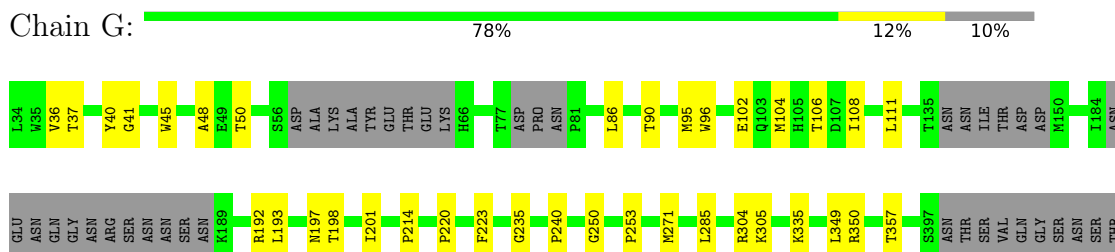
• Molecule 1: Envelope glycoprotein gp160



• Molecule 1: Envelope glycoprotein gp160

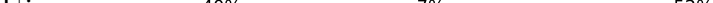


• Molecule 1: Envelope glycoprotein gp160



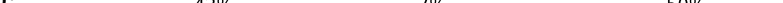
[illegible]

- Molecule 5: IgG 3BNC117 Fab Light Chain

Chain U:  7% 40% 7% 46%

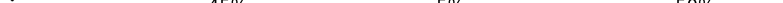
Residue	Position	Conservation	Phylogenetic Information
SER	1	0.00	D1
THR	2	0.00	S7
LEU	3	0.00	P8
THR	4	0.00	S9
SER	5	0.00	S10
LYS	6	0.00	L11
ALA	7	0.00	S12
ASP	8	0.00	A13
TYR	9	0.00	S14
GLU	10	0.00	D17
LYS	11	0.00	T22
HIS	12	0.00	C23
LYS	13	0.00	L33
THR	14	0.00	N34
VAL	15	0.00	W35
VAL	16	0.00	Q38
THR	17	0.00	G41
LEU	18	0.00	L47
SER	19	0.00	I48
PRO	20	0.00	G51
PRO	21	0.00	S52
THR	22	0.00	K53
LYS	23	0.00	G57
ASN	24	0.00	I75
ARG	25	0.00	Q79
GLY	26	0.00	P90
GLY	27	0.00	E81
ASN	28	0.00	A84
SER	29	0.00	T85
GLN	30	0.00	C88
GLU	31	0.00	Q89
SER	32	0.00	V98
THR	33	0.00	G101
GLN	34	0.00	L106
ASP	35	0.00	Lys
SER	36	0.00	ARG
LYS	37	0.00	THR
THR	38	0.00	VAL
THR	39	0.00	ALA
SER	40	0.00	ALA
LEU	41	0.00	PRO
VAL	42	0.00	VAL
THR	43	0.00	VAL
GLY	44	0.00	VAL
GLY	45	0.00	SER
GLY	46	0.00	VAL
GLY	47	0.00	THR
GLY	48	0.00	THR
GLY	49	0.00	THR
GLY	50	0.00	THR
GLY	51	0.00	THR
GLY	52	0.00	THR
GLY	53	0.00	THR
GLY	54	0.00	THR
GLY	55	0.00	THR
GLY	56	0.00	THR
GLY	57	0.00	THR
GLY	58	0.00	THR
GLY	59	0.00	THR
GLY	60	0.00	THR
GLY	61	0.00	THR
GLY	62	0.00	THR
GLY	63	0.00	THR
GLY	64	0.00	THR
GLY	65	0.00	THR
GLY	66	0.00	THR
GLY	67	0.00	THR
GLY	68	0.00	THR
GLY	69	0.00	THR
GLY	70	0.00	THR
GLY	71	0.00	THR
GLY	72	0.00	THR
GLY	73	0.00	THR
GLY	74	0.00	THR
GLY	75	0.00	THR
GLY	76	0.00	THR
GLY	77	0.00	THR
GLY	78	0.00	THR
GLY	79	0.00	THR
GLY	80	0.00	THR
GLY	81	0.00	THR
GLY	82	0.00	THR
GLY	83	0.00	THR
GLY	84	0.00	THR
GLY	85	0.00	THR
GLY	86	0.00	THR
GLY	87	0.00	THR
GLY	88	0.00	THR
GLY	89	0.00	THR
GLY	90	0.00	THR
GLY	91	0.00	THR
GLY	92	0.00	THR
GLY	93	0.00	THR
GLY	94	0.00	THR
GLY	95	0.00	THR
GLY	96	0.00	THR
GLY	97	0.00	THR
GLY	98	0.00	THR
GLY	99	0.00	THR
GLY	100	0.00	THR

- Molecule 6: IgG EPTC112 Fab Light Chain

Chain D: 

[illegible]

- Molecule 6: IgG EPTC112 Fab Light Chain

Chain K: 

[illegible]

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

MAG1
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 50%

MAG1
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 50%

MAG1
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50% 50%

MAG1
MAG2

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  67% 33%

MAG1
MAG2
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1
MAG2
BMA3

- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  25% 75% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251591	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)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.013	Depositor
Minimum map value	-2.374	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	0.14	0/3324	0.32	0/4520
1	F	0.14	0/3343	0.36	0/4543
1	G	0.13	0/3313	0.33	0/4500
2	B	0.12	0/934	0.26	0/1267
2	I	0.12	0/923	0.30	0/1255
2	J	0.13	0/893	0.32	0/1212
3	C	0.13	0/924	0.41	0/1269
3	H	0.15	0/918	0.42	0/1261
4	R	0.10	0/967	0.31	0/1321
4	S	0.11	0/921	0.32	0/1258
5	T	0.16	0/697	0.41	0/957
5	U	0.13	0/679	0.37	0/932
6	D	0.12	0/790	0.33	0/1079
6	K	0.11	0/790	0.34	0/1079
All	All	0.13	0/19416	0.34	0/26453

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	15	SER	Peptide
1	F	123	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3254	0	3169	29	0
1	F	3277	0	3169	38	0
1	G	3246	0	3159	37	0
2	B	918	0	884	19	0
2	I	906	0	873	15	0
2	J	879	0	836	14	0
3	C	897	0	830	16	0
3	H	891	0	819	23	0
4	R	938	0	855	9	0
4	S	894	0	805	13	0
5	T	680	0	591	5	0
5	U	664	0	547	10	0
6	D	773	0	729	13	0
6	K	773	0	729	8	0
7	E	28	0	25	0	0
7	M	28	0	25	1	0
7	N	28	0	25	2	0
7	O	28	0	25	2	0
7	P	28	0	25	0	0
7	Q	28	0	25	0	0
7	W	28	0	24	0	0
7	Y	28	0	25	0	0
7	Z	28	0	25	0	0
7	a	28	0	25	1	0
7	b	28	0	25	0	0
8	L	39	0	34	1	0
8	X	39	0	34	0	0
9	V	50	0	43	0	0
10	A	140	0	130	3	0
10	F	98	0	91	2	0
10	G	84	0	78	1	0
10	T	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19762	0	18692	230	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 6.

The worst 5 of 230 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:VAL:HG11	3:C:76:TYR:HA	1.69	0.75
3:C:47:TRP:NE1	6:D:98:LEU:O	2.21	0.74
1:F:218:CYS:HA	1:F:247:CYS:HB3	1.70	0.73
1:A:294:ILE:HG22	1:A:333:VAL:HG22	1.71	0.72
1:F:204:ALA:HB3	1:F:437:PRO:HD3	1.72	0.71

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	408/469 (87%)	393 (96%)	15 (4%)	0	100	100
1	F	412/469 (88%)	400 (97%)	12 (3%)	0	100	100
1	G	408/469 (87%)	398 (98%)	10 (2%)	0	100	100
2	B	111/145 (77%)	108 (97%)	3 (3%)	0	100	100
2	I	114/145 (79%)	111 (97%)	3 (3%)	0	100	100
2	J	110/145 (76%)	109 (99%)	1 (1%)	0	100	100
3	C	117/233 (50%)	107 (92%)	9 (8%)	1 (1%)	14	47
3	H	117/233 (50%)	107 (92%)	10 (8%)	0	100	100
4	R	118/226 (52%)	117 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S	112/226 (50%)	112 (100%)	0	0	100	100
5	T	93/206 (45%)	89 (96%)	4 (4%)	0	100	100
5	U	96/206 (47%)	93 (97%)	3 (3%)	0	100	100
6	D	106/216 (49%)	104 (98%)	1 (1%)	1 (1%)	14	47
6	K	106/216 (49%)	104 (98%)	2 (2%)	0	100	100
All	All	2428/3604 (67%)	2352 (97%)	74 (3%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	52	VAL
3	C	29	VAL

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	359/418 (86%)	359 (100%)	0	100	100
1	F	360/418 (86%)	360 (100%)	0	100	100
1	G	354/418 (85%)	354 (100%)	0	100	100
2	B	95/125 (76%)	95 (100%)	0	100	100
2	I	90/125 (72%)	89 (99%)	1 (1%)	65	79
2	J	87/125 (70%)	87 (100%)	0	100	100
3	C	94/203 (46%)	94 (100%)	0	100	100
3	H	92/203 (45%)	92 (100%)	0	100	100
4	R	93/193 (48%)	93 (100%)	0	100	100
4	S	87/193 (45%)	87 (100%)	0	100	100
5	T	61/183 (33%)	60 (98%)	1 (2%)	55	75
5	U	53/183 (29%)	53 (100%)	0	100	100
6	D	86/181 (48%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	K	86/181 (48%)	86 (100%)	0	100	100
All	All	1997/3149 (63%)	1995 (100%)	2 (0%)	87	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	543	ASN
5	T	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	S	60	ASN
6	D	39	GLN
1	F	302	ASN
1	F	315	GLN
1	F	374	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

32 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	E	1	1,7	14,14,15	0.38	0	17,19,21	0.49	0
7	NAG	E	2	7	14,14,15	0.20	0	17,19,21	0.40	0
8	NAG	L	1	1,8	14,14,15	0.22	0	17,19,21	0.46	0
8	NAG	L	2	8	14,14,15	0.17	0	17,19,21	0.43	0
8	BMA	L	3	8	11,11,12	0.53	0	15,15,17	0.69	0
7	NAG	M	1	1,7	14,14,15	0.39	0	17,19,21	1.36	2 (11%)
7	NAG	M	2	7	14,14,15	0.29	0	17,19,21	0.45	0
7	NAG	N	1	1,7	14,14,15	0.20	0	17,19,21	0.51	0
7	NAG	N	2	7	14,14,15	0.41	0	17,19,21	1.43	2 (11%)
7	NAG	O	1	1,7	14,14,15	0.37	0	17,19,21	1.37	2 (11%)
7	NAG	O	2	7	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	P	1	1,7	14,14,15	1.01	1 (7%)	17,19,21	1.00	1 (5%)
7	NAG	P	2	7	14,14,15	0.25	0	17,19,21	0.56	0
7	NAG	Q	1	1,7	14,14,15	0.26	0	17,19,21	0.55	0
7	NAG	Q	2	7	14,14,15	0.26	0	17,19,21	0.45	0
9	NAG	V	1	1,9	14,14,15	0.36	0	17,19,21	0.49	0
9	NAG	V	2	9	14,14,15	0.24	0	17,19,21	0.45	0
9	BMA	V	3	9	11,11,12	0.55	0	15,15,17	0.80	0
9	MAN	V	4	9	11,11,12	0.64	0	15,15,17	1.20	2 (13%)
7	NAG	W	1	1,7	14,14,15	0.26	0	17,19,21	0.43	0
7	NAG	W	2	7	14,14,15	0.19	0	17,19,21	0.45	0
8	NAG	X	1	1,8	14,14,15	0.24	0	17,19,21	0.52	0
8	NAG	X	2	8	14,14,15	0.19	0	17,19,21	0.45	0
8	BMA	X	3	8	11,11,12	0.54	0	15,15,17	0.70	0
7	NAG	Y	1	1,7	14,14,15	0.27	0	17,19,21	0.40	0
7	NAG	Y	2	7	14,14,15	0.20	0	17,19,21	0.47	0
7	NAG	Z	1	1,7	14,14,15	0.28	0	17,19,21	0.62	1 (5%)
7	NAG	Z	2	7	14,14,15	0.25	0	17,19,21	0.41	0
7	NAG	a	1	1,7	14,14,15	0.44	0	17,19,21	1.43	2 (11%)
7	NAG	a	2	7	14,14,15	0.25	0	17,19,21	0.44	0
7	NAG	b	1	1,7	14,14,15	0.68	1 (7%)	17,19,21	0.74	0
7	NAG	b	2	7	14,14,15	0.28	0	17,19,21	0.40	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
7	NAG	E	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	L	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	L	2	8	-	0/6/23/26	0/1/1/1
8	BMA	L	3	8	-	1/2/19/22	0/1/1/1
7	NAG	M	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
7	NAG	N	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	6/6/23/26	0/1/1/1
7	NAG	O	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	NAG	P	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
9	NAG	V	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	0/6/23/26	0/1/1/1
9	BMA	V	3	9	-	0/2/19/22	0/1/1/1
9	MAN	V	4	9	-	0/2/19/22	0/1/1/1
7	NAG	W	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	4/6/23/26	0/1/1/1
8	NAG	X	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	0/2/19/22	0/1/1/1
7	NAG	Y	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	2/6/23/26	0/1/1/1
7	NAG	Z	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
7	NAG	a	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	a	2	7	-	0/6/23/26	0/1/1/1
7	NAG	b	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	b	2	7	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	1	NAG	O5-C1	-3.58	1.37	1.43
7	b	1	NAG	O5-C1	-2.45	1.39	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	2	NAG	C2-N2-C7	4.81	129.35	122.90
7	a	1	NAG	C2-N2-C7	4.71	129.21	122.90
7	O	1	NAG	C2-N2-C7	4.64	129.12	122.90
7	M	1	NAG	C2-N2-C7	4.60	129.07	122.90
9	V	4	MAN	C1-O5-C5	3.59	116.99	112.19

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

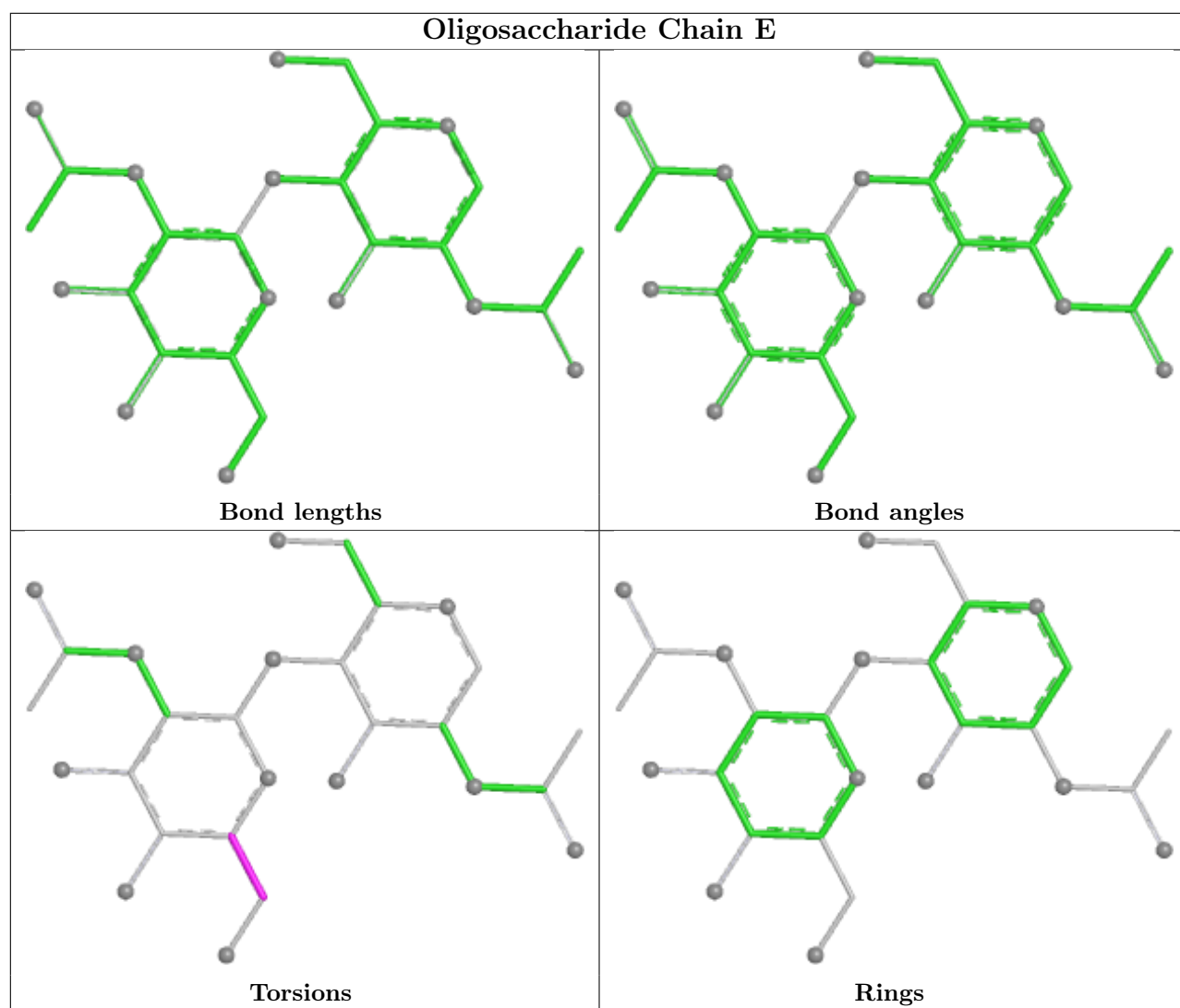
Mol	Chain	Res	Type	Atoms
7	Y	2	NAG	C4-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6

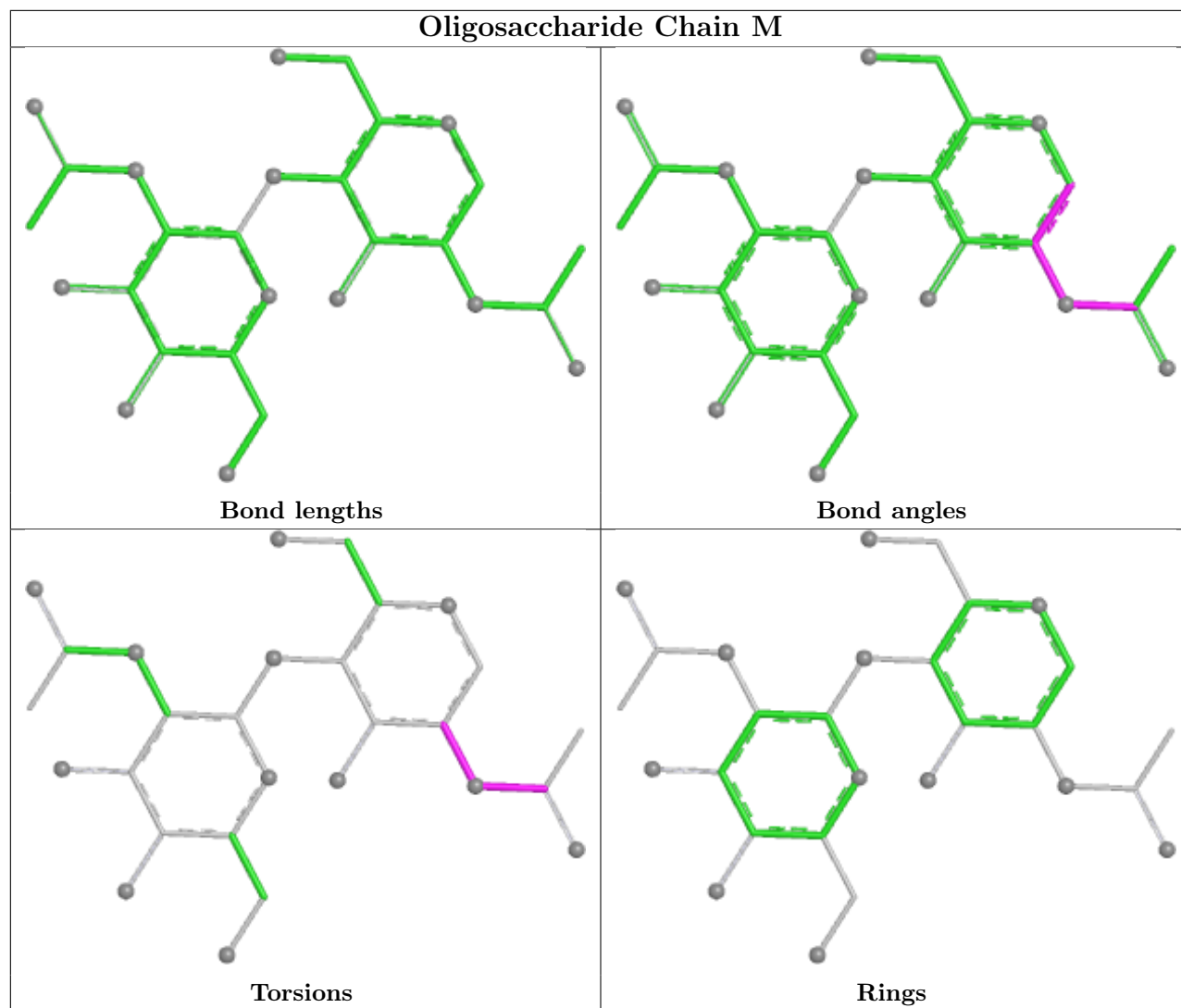
There are no ring outliers.

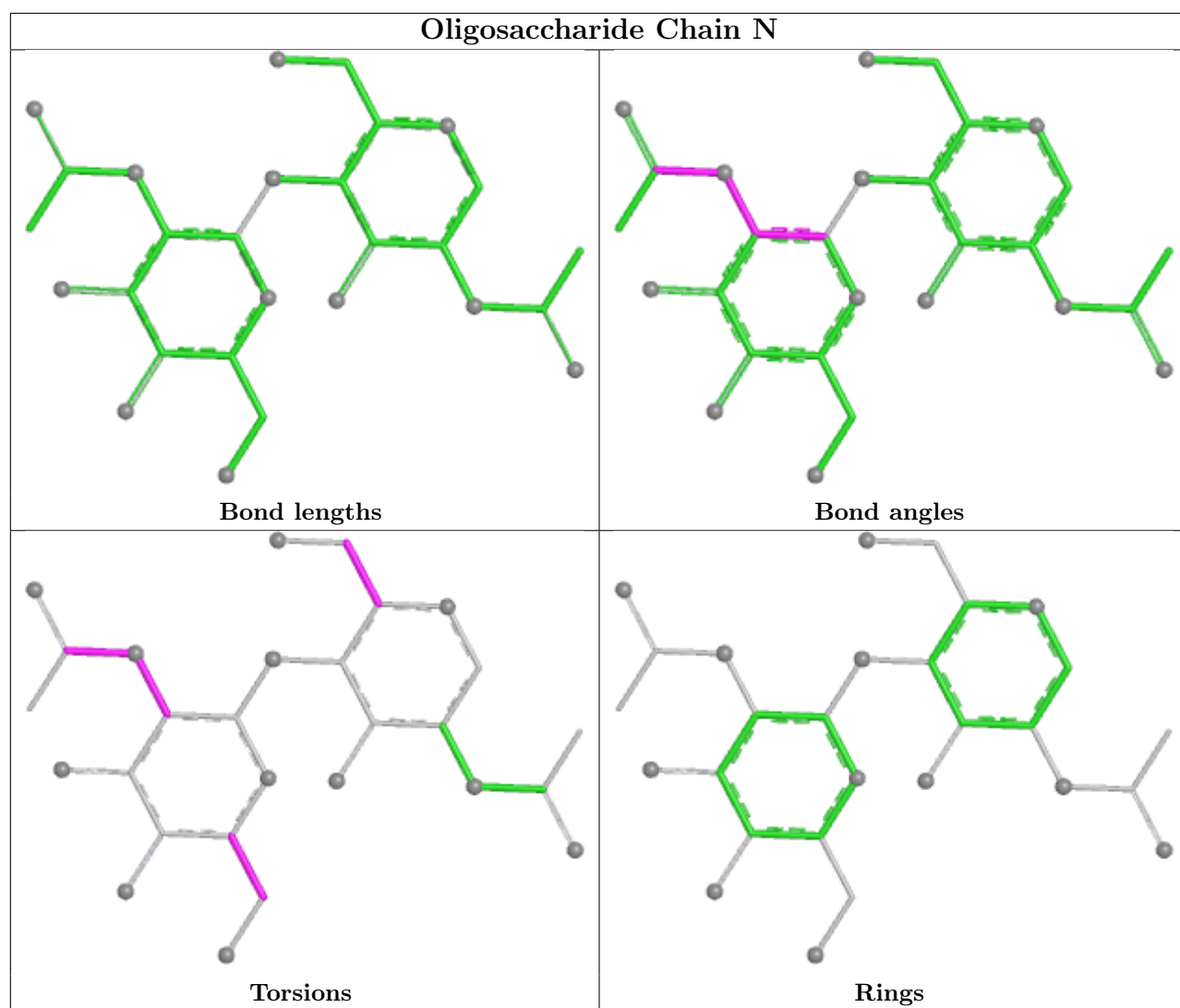
5 monomers are involved in 7 short contacts:

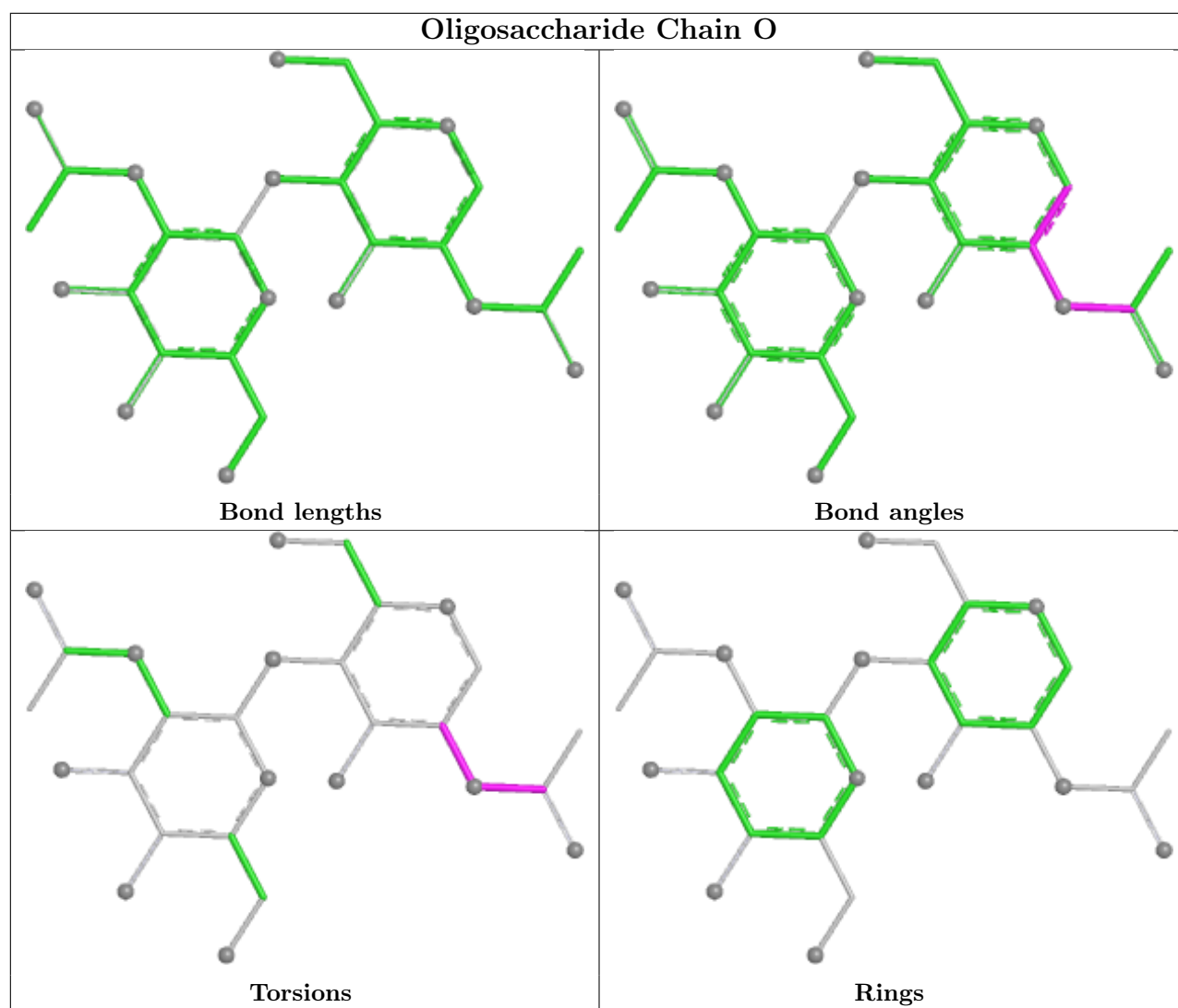
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	O	1	NAG	2	0
7	N	2	NAG	2	0
7	M	1	NAG	1	0
7	a	1	NAG	1	0
8	L	1	NAG	1	0

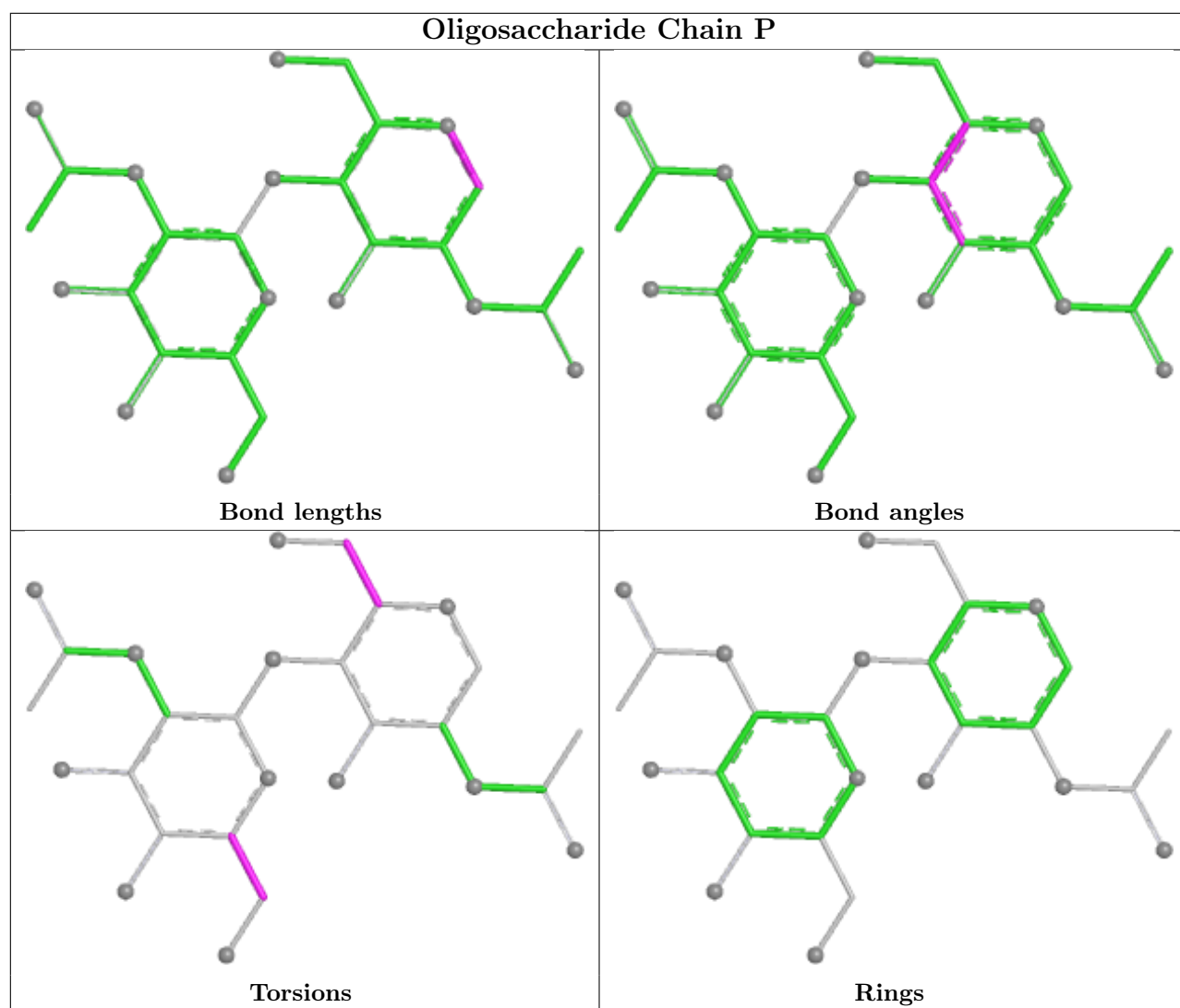
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

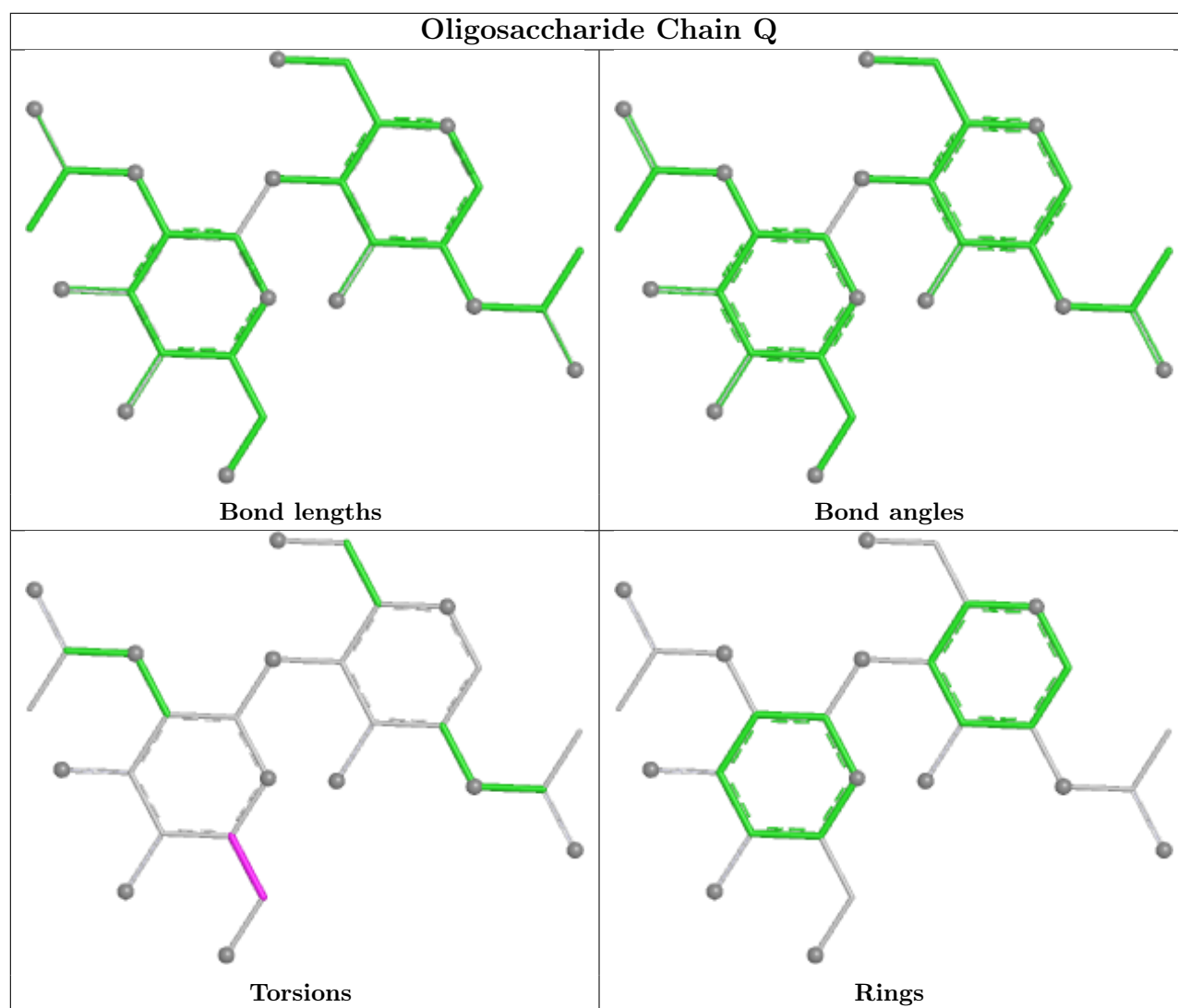


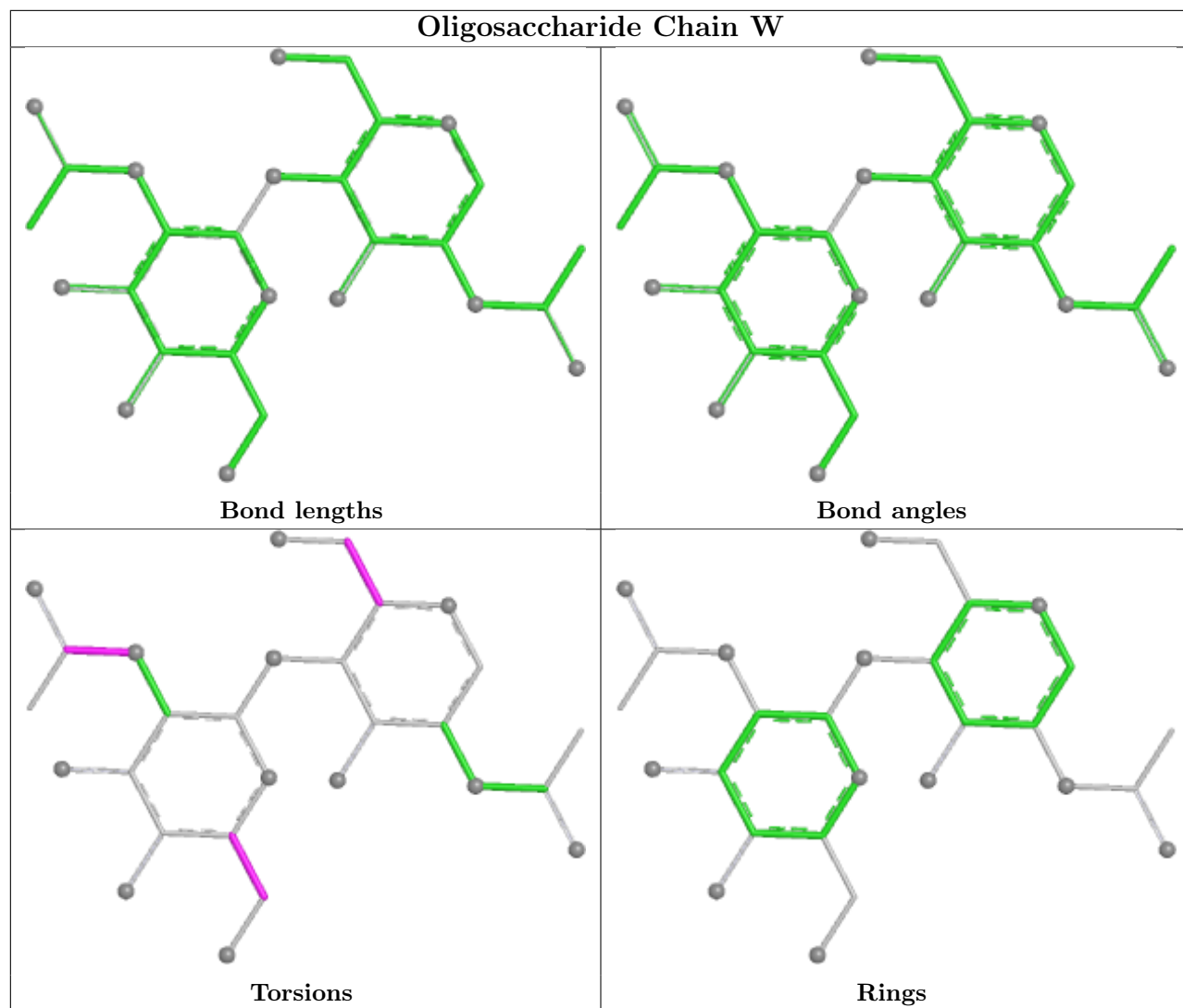


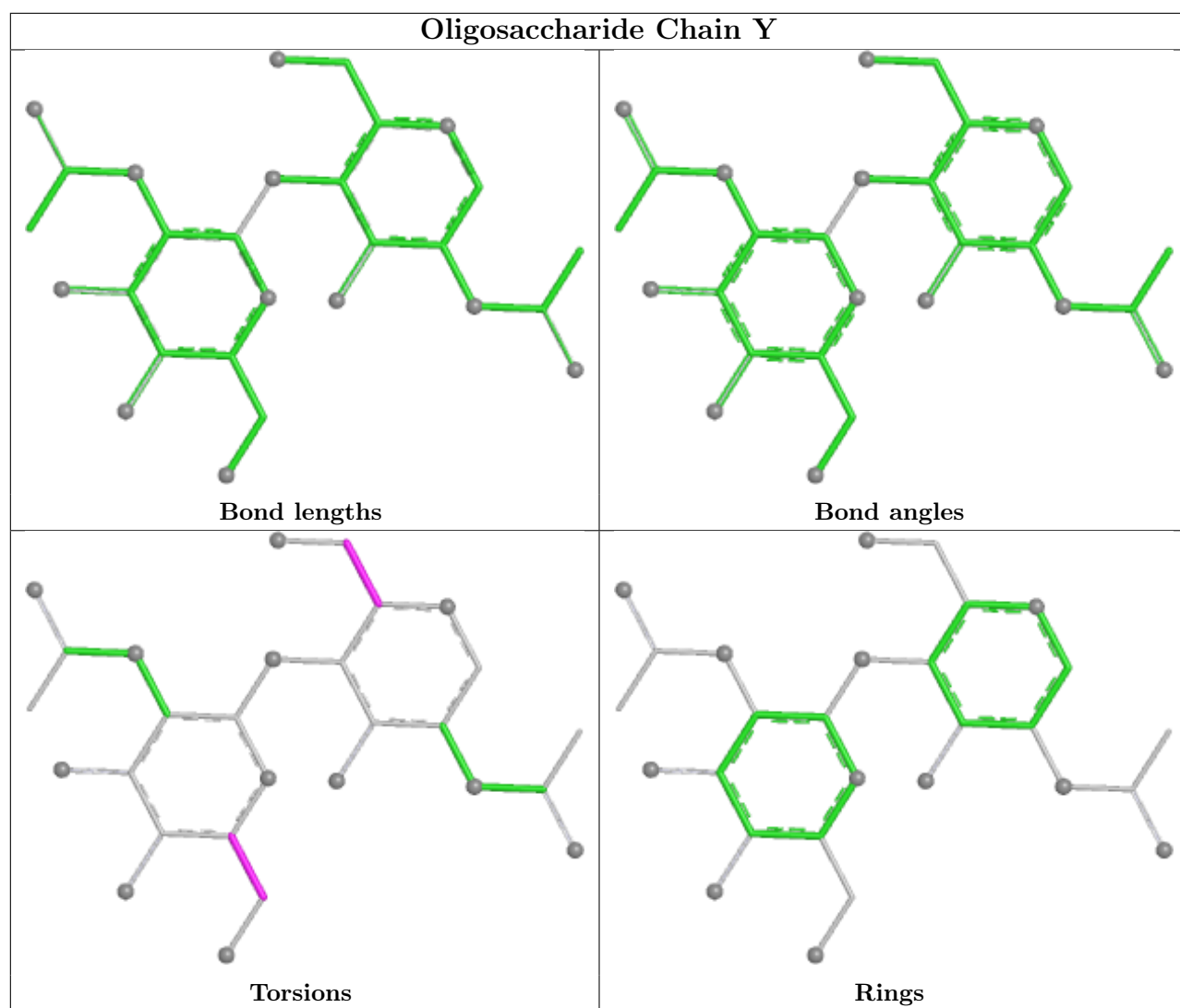


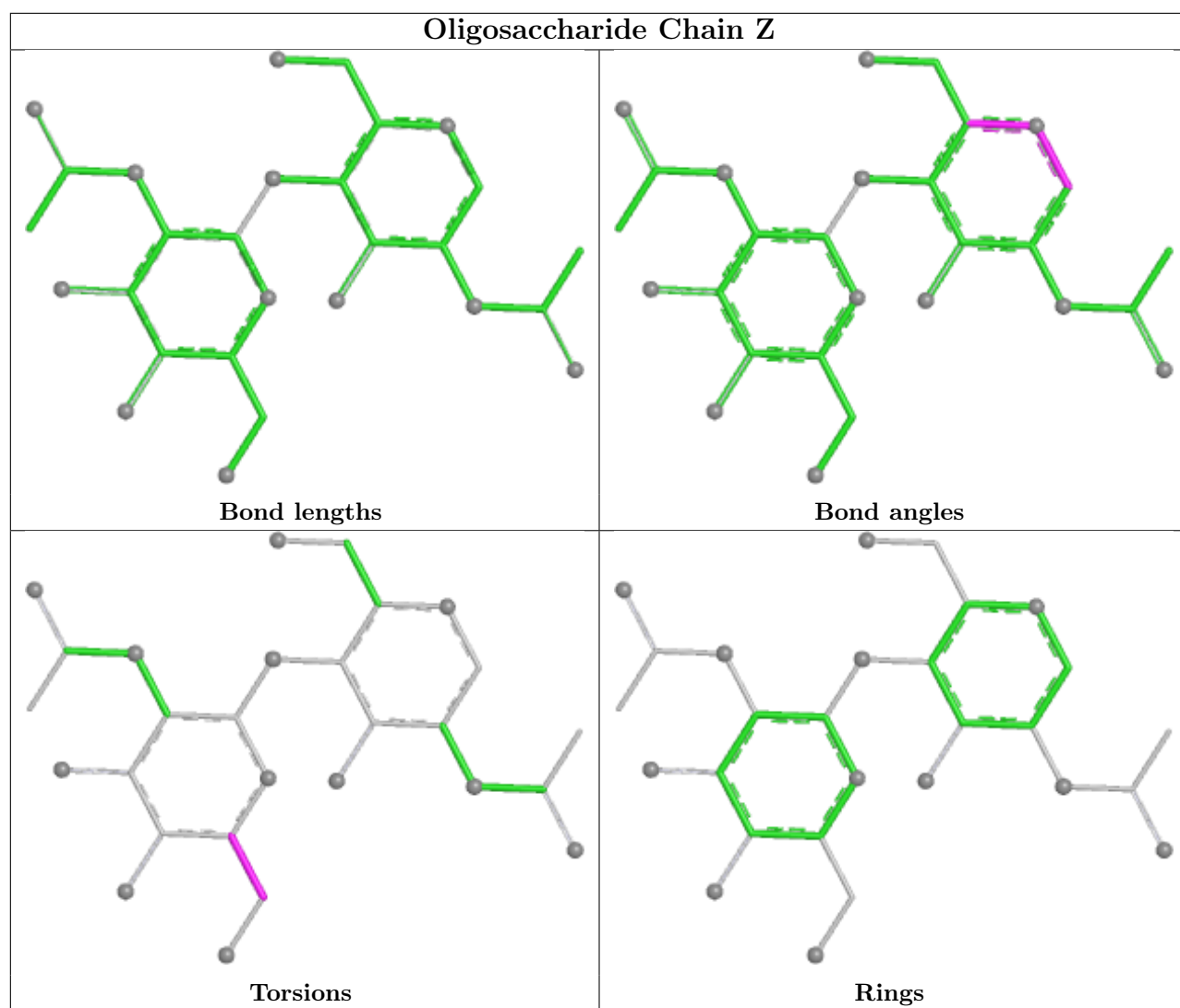


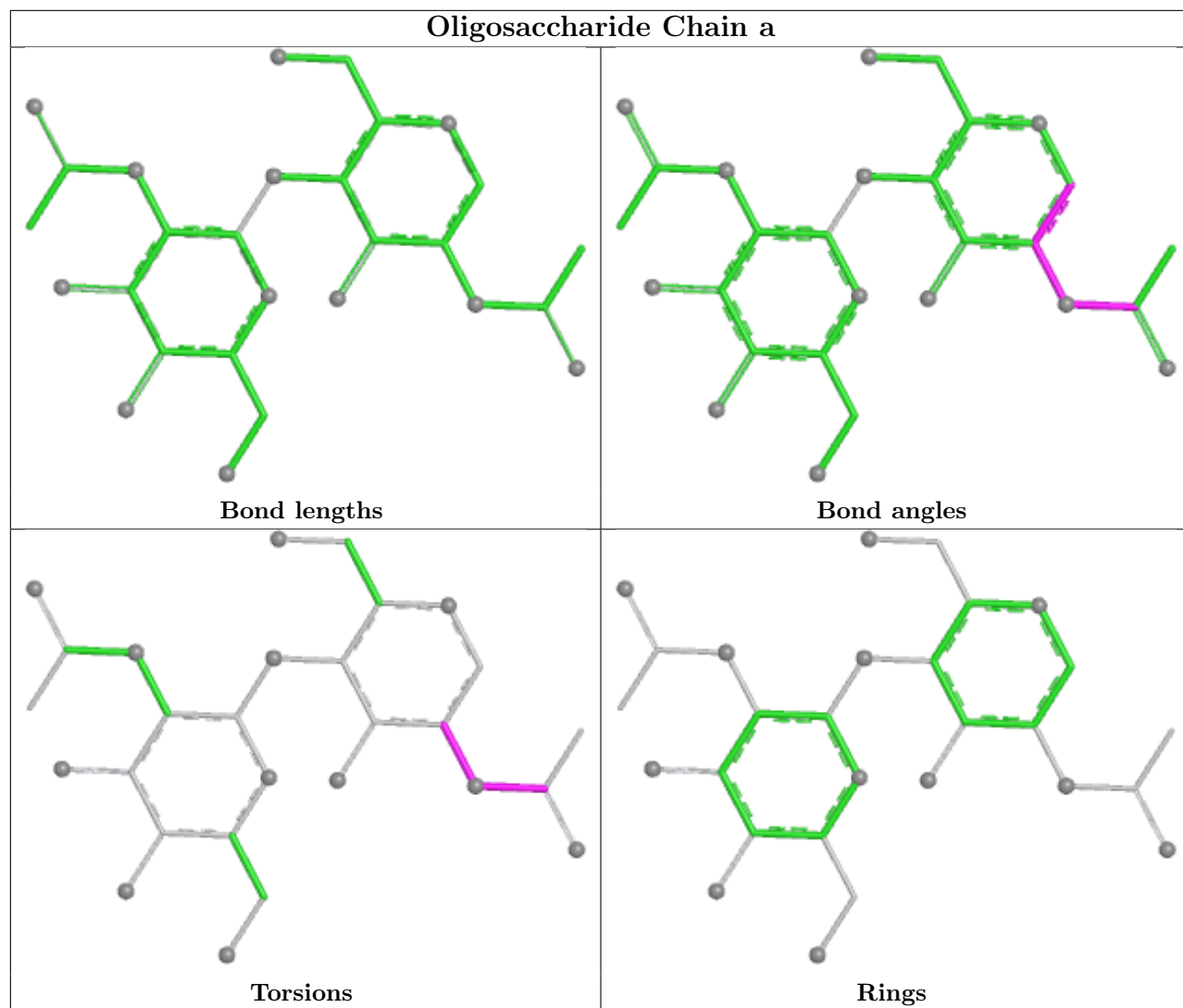


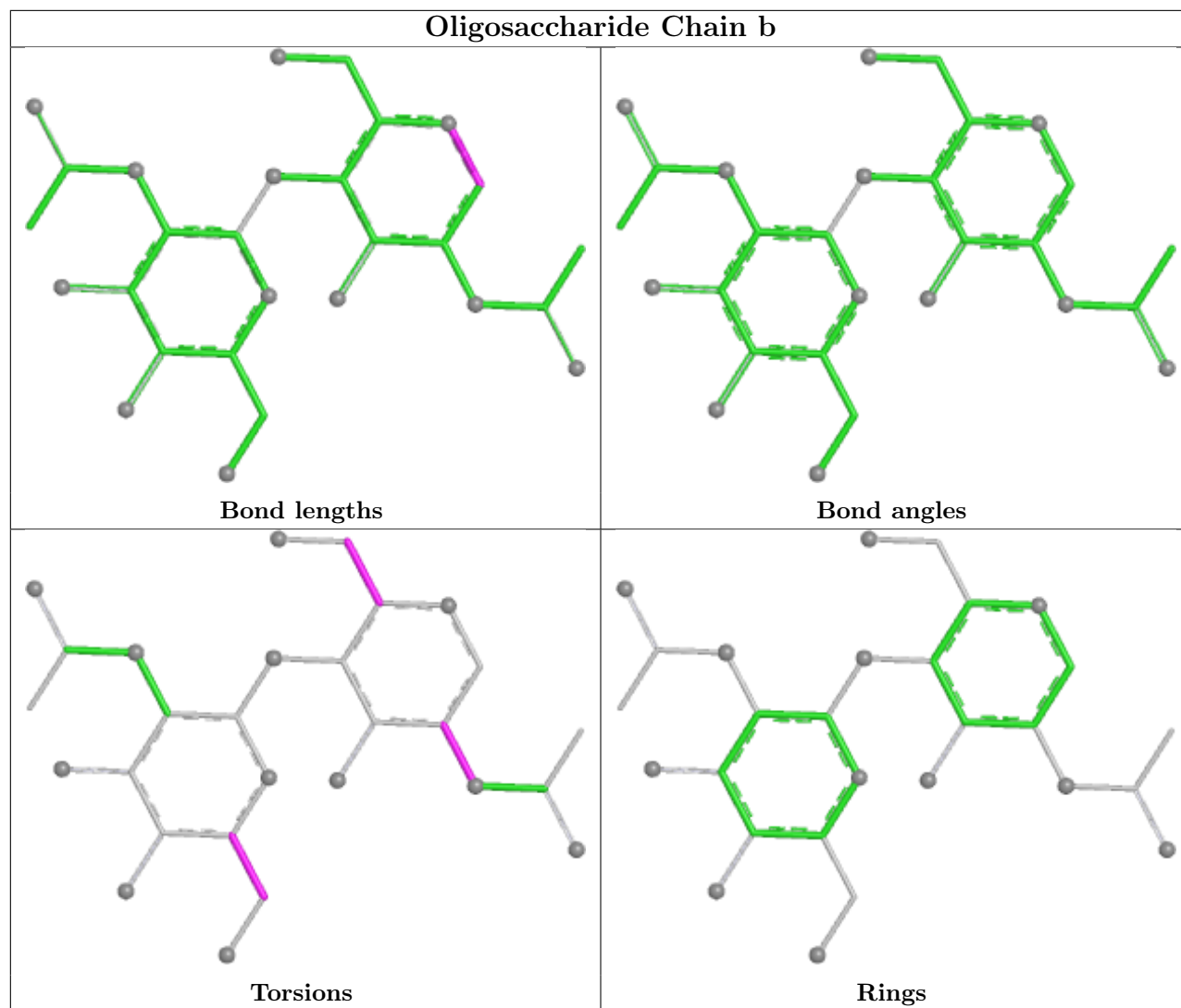


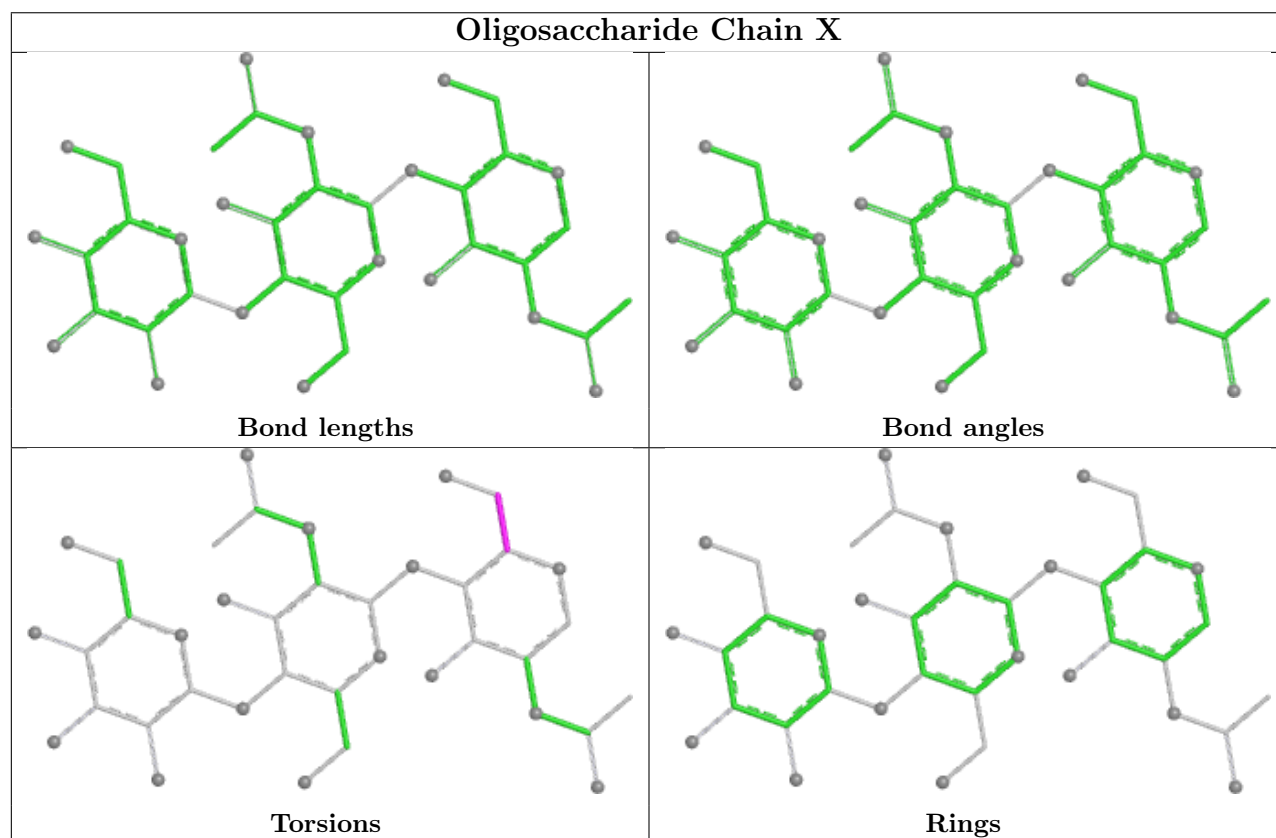
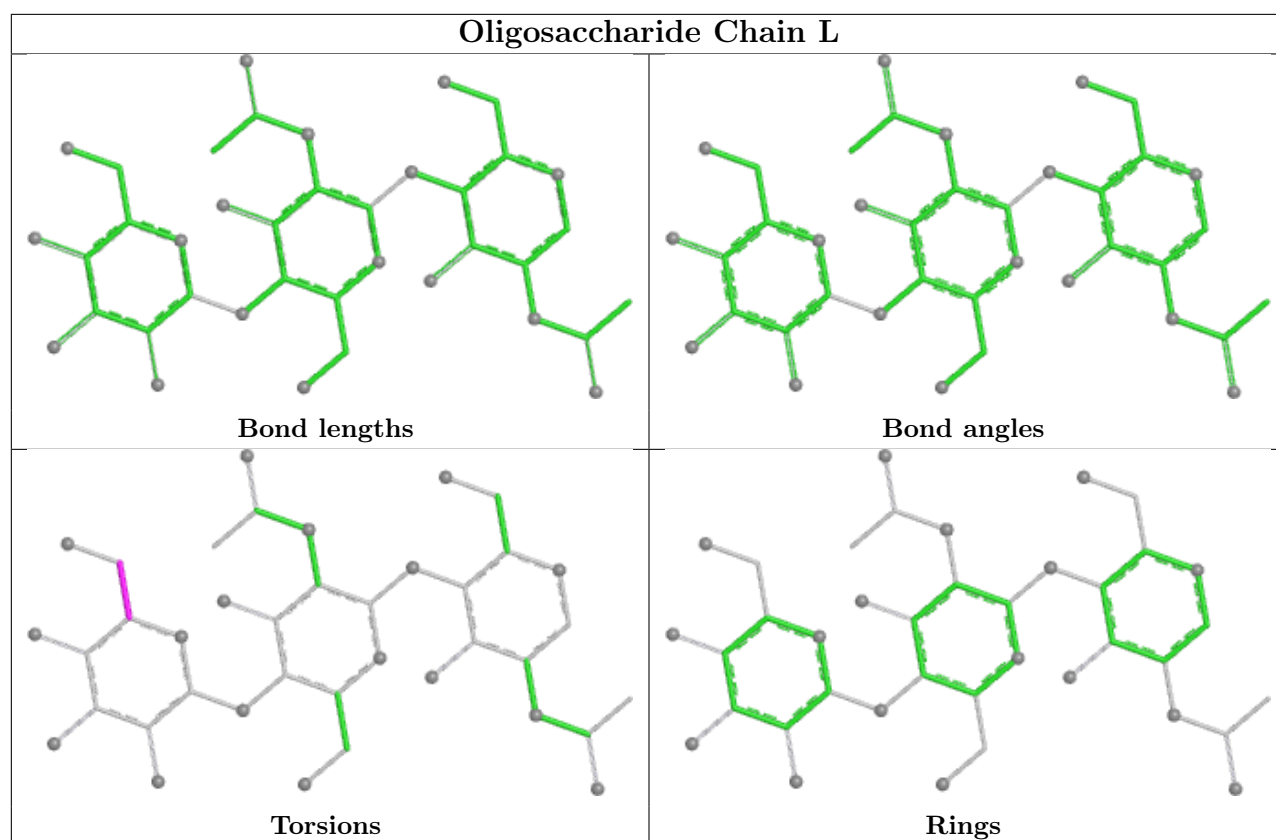


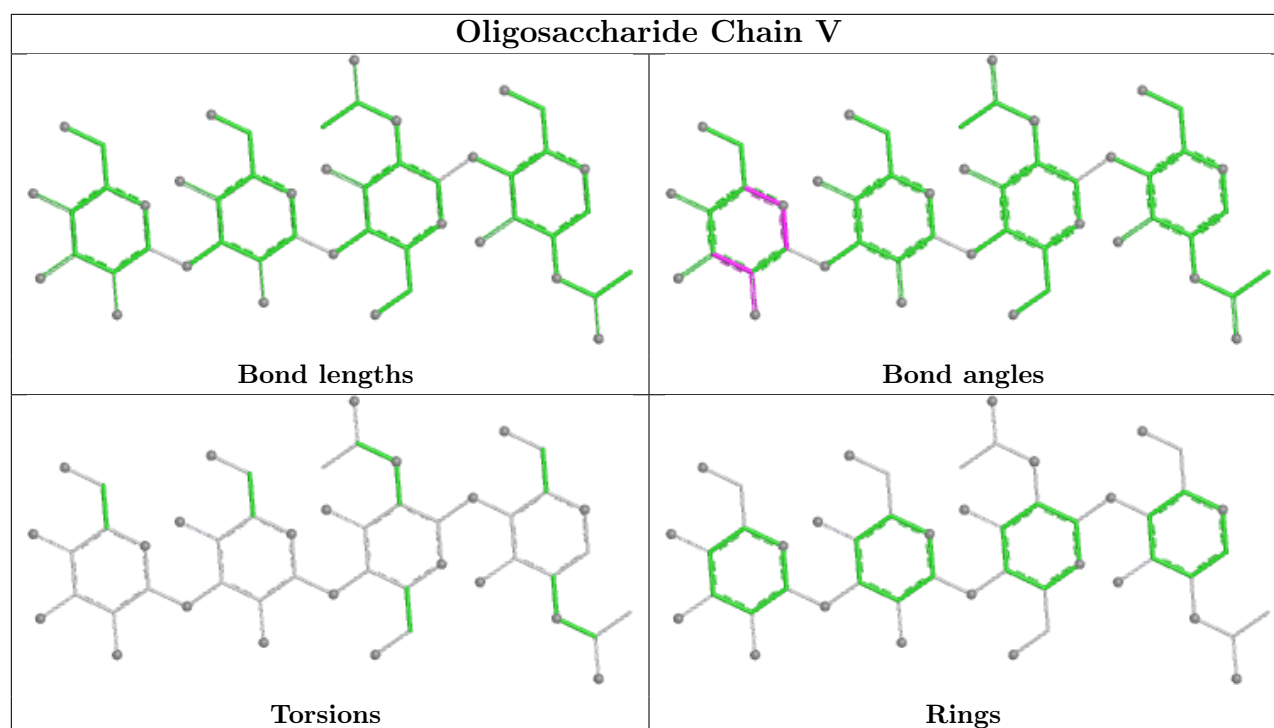












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
10	NAG	F	607	1	14,14,15	0.30	0	17,19,21	0.41	0
10	NAG	G	601	1	14,14,15	0.45	0	17,19,21	1.36	2 (11%)
10	NAG	G	605	1	14,14,15	0.29	0	17,19,21	0.45	0
10	NAG	F	604	1	14,14,15	0.20	0	17,19,21	0.44	0
10	NAG	A	601	1	14,14,15	0.22	0	17,19,21	0.46	0
10	NAG	T	301	5	14,14,15	1.05	2 (14%)	17,19,21	0.94	1 (5%)
10	NAG	A	603	1	14,14,15	0.50	0	17,19,21	1.37	2 (11%)
10	NAG	A	610	1	14,14,15	0.26	0	17,19,21	0.49	0
10	NAG	G	602	1	14,14,15	0.27	0	17,19,21	0.47	0
10	NAG	A	608	1	14,14,15	0.27	0	17,19,21	0.51	0
10	NAG	A	602	1	14,14,15	0.27	0	17,19,21	0.51	0
10	NAG	G	606	1	14,14,15	0.19	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	F	605	1	14,14,15	0.35	0	17,19,21	0.61	1 (5%)
10	NAG	G	604	1	14,14,15	0.17	0	17,19,21	0.50	0
10	NAG	F	602	1	14,14,15	0.28	0	17,19,21	0.50	0
10	NAG	A	606	1	14,14,15	0.21	0	17,19,21	0.44	0
10	NAG	A	607	1	14,14,15	0.23	0	17,19,21	0.49	0
10	NAG	G	603	1	14,14,15	0.21	0	17,19,21	0.45	0
10	NAG	A	604	1	14,14,15	0.23	0	17,19,21	0.44	0
10	NAG	F	601	1	14,14,15	0.43	0	17,19,21	1.34	2 (11%)
10	NAG	A	605	1	14,14,15	0.20	0	17,19,21	0.43	0
10	NAG	F	606	1	14,14,15	0.51	0	17,19,21	1.33	2 (11%)
10	NAG	A	609	1	14,14,15	0.25	0	17,19,21	0.50	0
10	NAG	F	603	1	14,14,15	0.29	0	17,19,21	0.47	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
10	NAG	F	607	1	-	0/6/23/26	0/1/1/1
10	NAG	G	601	1	-	4/6/23/26	0/1/1/1
10	NAG	G	605	1	-	0/6/23/26	0/1/1/1
10	NAG	F	604	1	-	2/6/23/26	0/1/1/1
10	NAG	A	601	1	-	2/6/23/26	0/1/1/1
10	NAG	T	301	5	-	0/6/23/26	0/1/1/1
10	NAG	A	603	1	-	6/6/23/26	0/1/1/1
10	NAG	A	610	1	-	2/6/23/26	0/1/1/1
10	NAG	G	602	1	-	0/6/23/26	0/1/1/1
10	NAG	A	608	1	-	0/6/23/26	0/1/1/1
10	NAG	A	602	1	-	4/6/23/26	0/1/1/1
10	NAG	G	606	1	-	2/6/23/26	0/1/1/1
10	NAG	F	605	1	-	2/6/23/26	0/1/1/1
10	NAG	G	604	1	-	0/6/23/26	0/1/1/1
10	NAG	F	602	1	-	2/6/23/26	0/1/1/1
10	NAG	A	606	1	-	2/6/23/26	0/1/1/1
10	NAG	A	607	1	-	1/6/23/26	0/1/1/1
10	NAG	G	603	1	-	0/6/23/26	0/1/1/1
10	NAG	A	604	1	-	2/6/23/26	0/1/1/1
10	NAG	F	601	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	605	1	-	2/6/23/26	0/1/1/1
10	NAG	F	606	1	-	6/6/23/26	0/1/1/1
10	NAG	A	609	1	-	1/6/23/26	0/1/1/1
10	NAG	F	603	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	T	301	NAG	O5-C1	2.93	1.48	1.43
10	T	301	NAG	C1-C2	2.51	1.55	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	601	NAG	C2-N2-C7	4.62	129.09	122.90
10	F	601	NAG	C2-N2-C7	4.62	129.09	122.90
10	A	603	NAG	C2-N2-C7	4.58	129.04	122.90
10	F	606	NAG	C2-N2-C7	4.53	128.97	122.90
10	T	301	NAG	C1-O5-C5	3.57	116.97	112.19

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	606	NAG	O5-C5-C6-O6
10	A	605	NAG	O5-C5-C6-O6
10	A	602	NAG	O5-C5-C6-O6
10	F	602	NAG	O5-C5-C6-O6
10	A	603	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G	601	NAG	1	0
10	A	601	NAG	1	0
10	A	603	NAG	1	0
10	A	610	NAG	1	0
10	F	601	NAG	1	0
10	F	606	NAG	1	0

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.

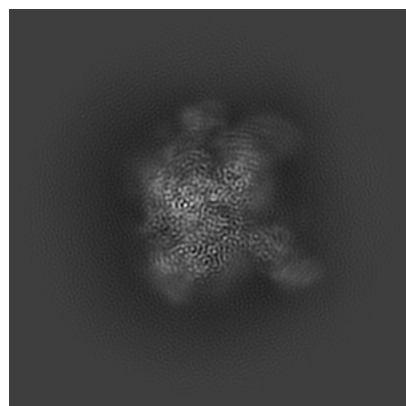
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16493. These allow visual inspection of the internal detail of the map and identification of artifacts.

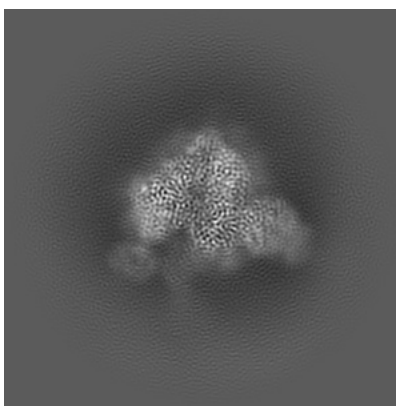
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

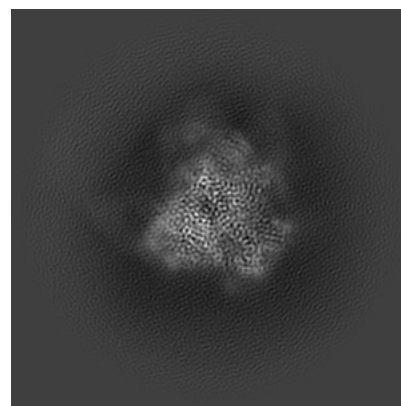
6.1.1 Primary map



X

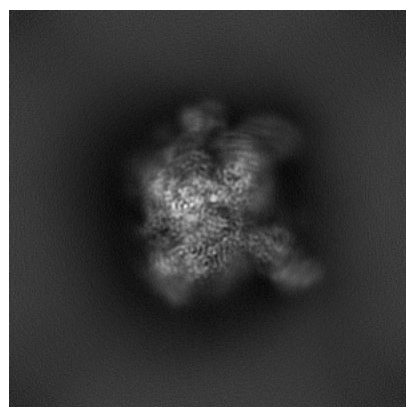


Y

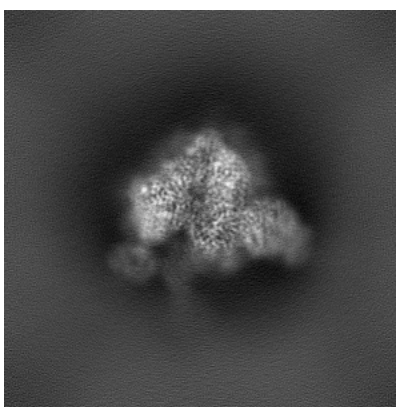


Z

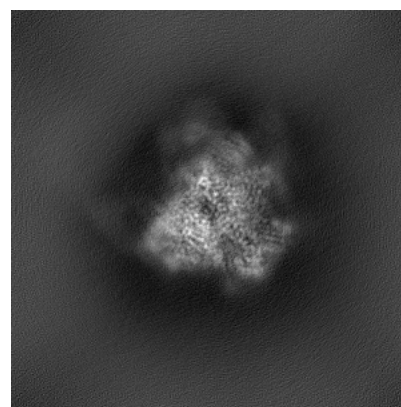
6.1.2 Raw map



X



Y

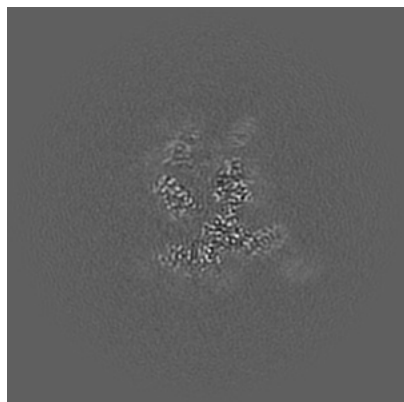


Z

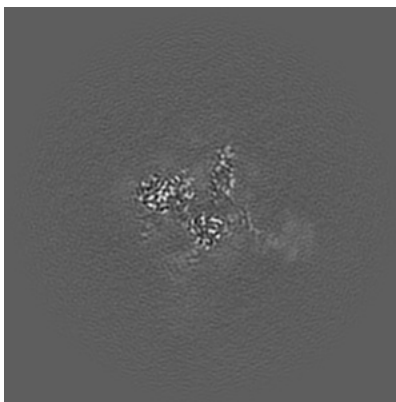
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

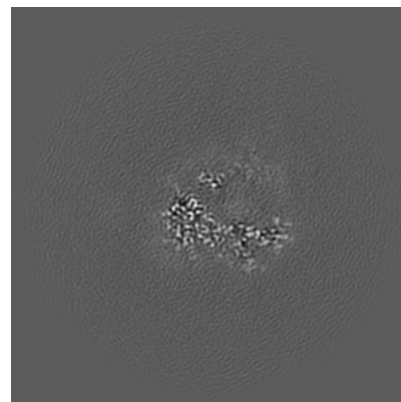
6.2.1 Primary map



X Index: 200

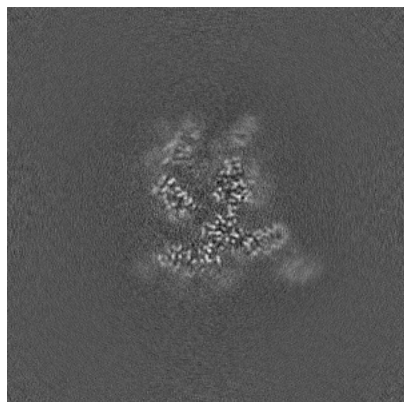


Y Index: 200

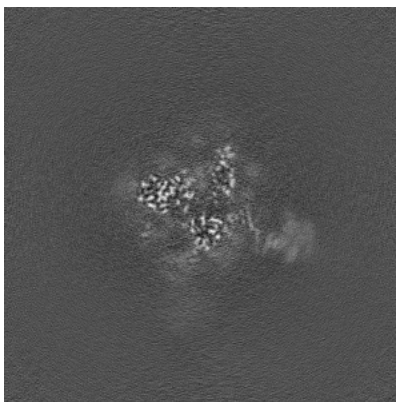


Z Index: 200

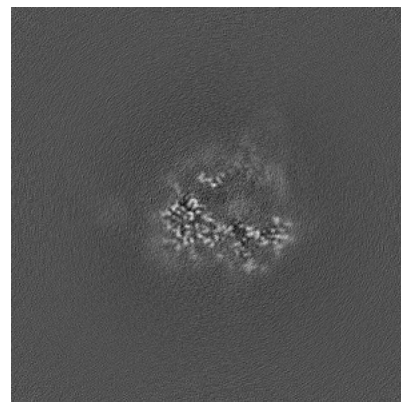
6.2.2 Raw map



X Index: 200



Y Index: 200

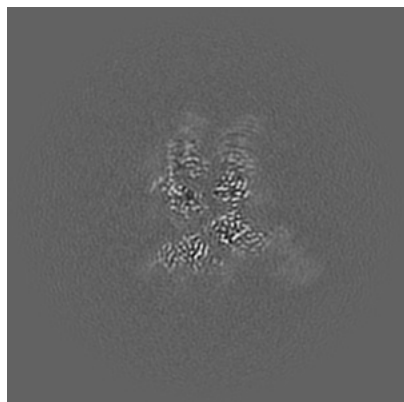


Z Index: 200

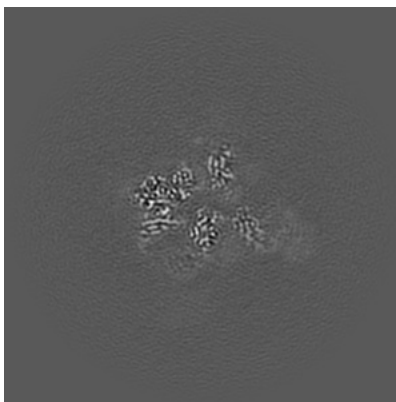
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

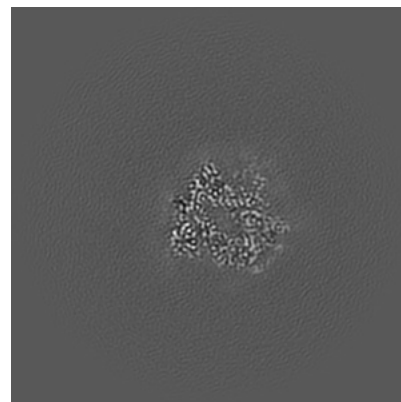
6.3.1 Primary map



X Index: 194

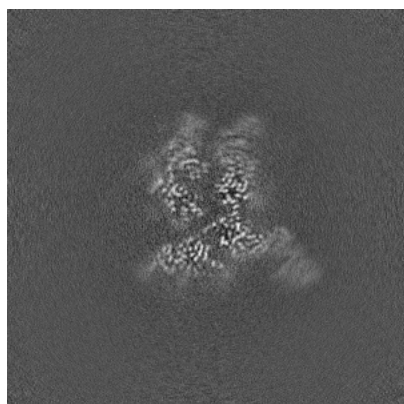


Y Index: 194

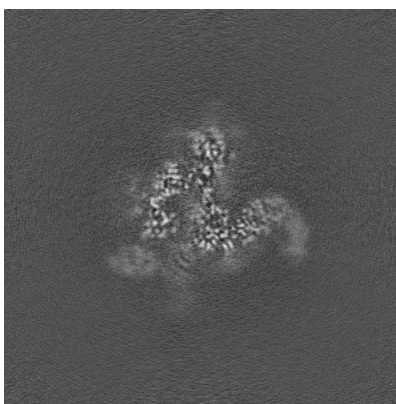


Z Index: 212

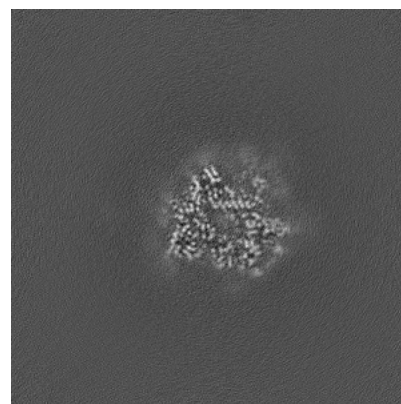
6.3.2 Raw map



X Index: 195



Y Index: 177

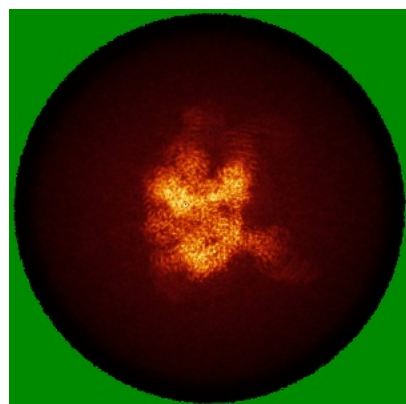


Z Index: 211

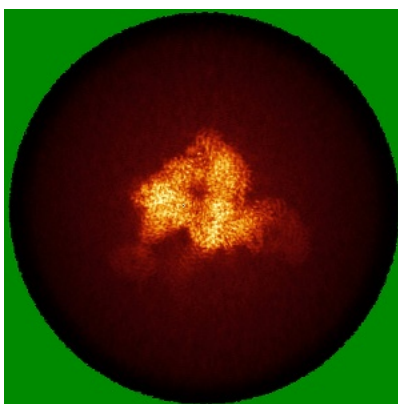
The images above show the largest variance slices of the map in three orthogonal directions.

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

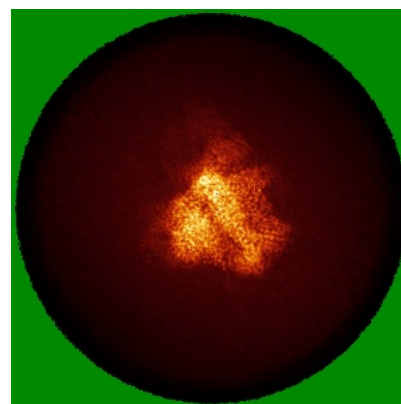
6.4.1 Primary map



X

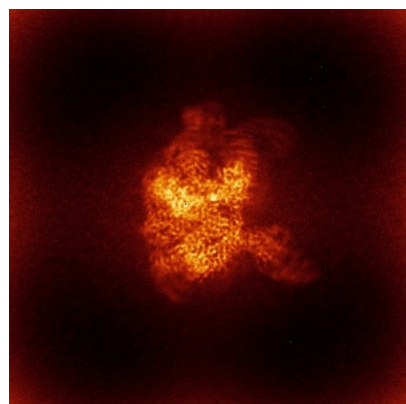


Y

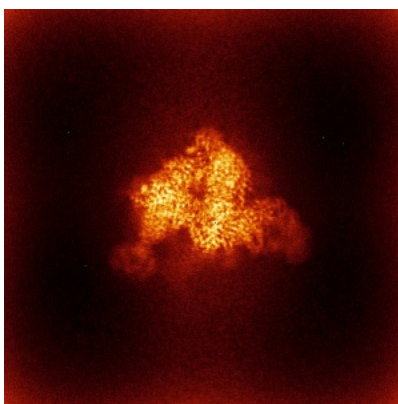


Z

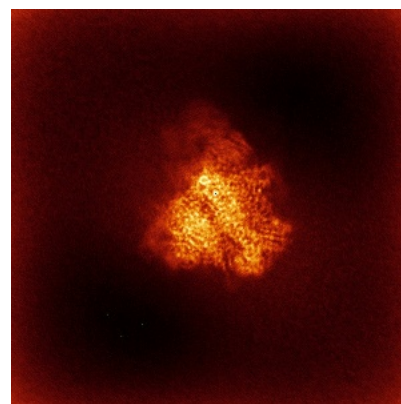
6.4.2 Raw map



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.

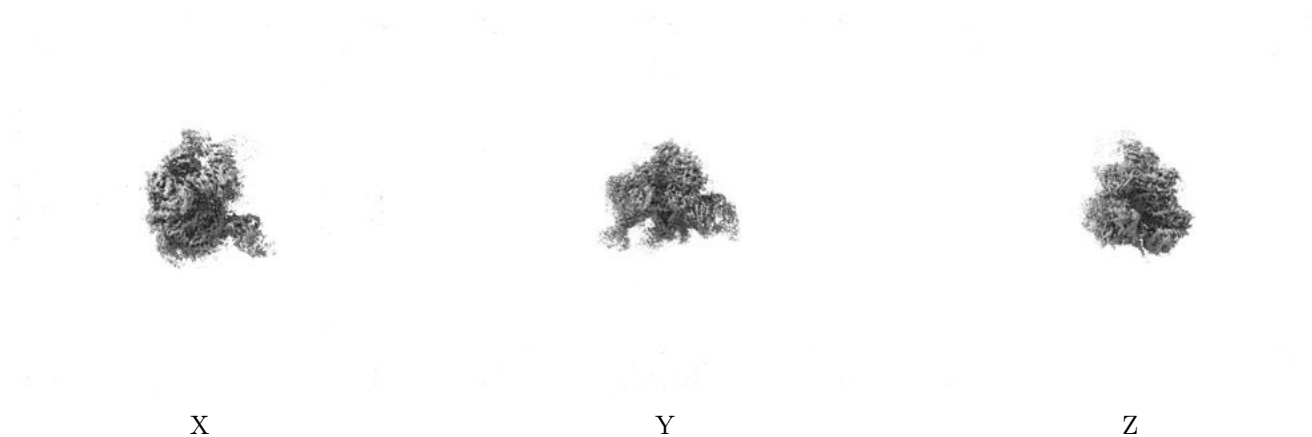
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

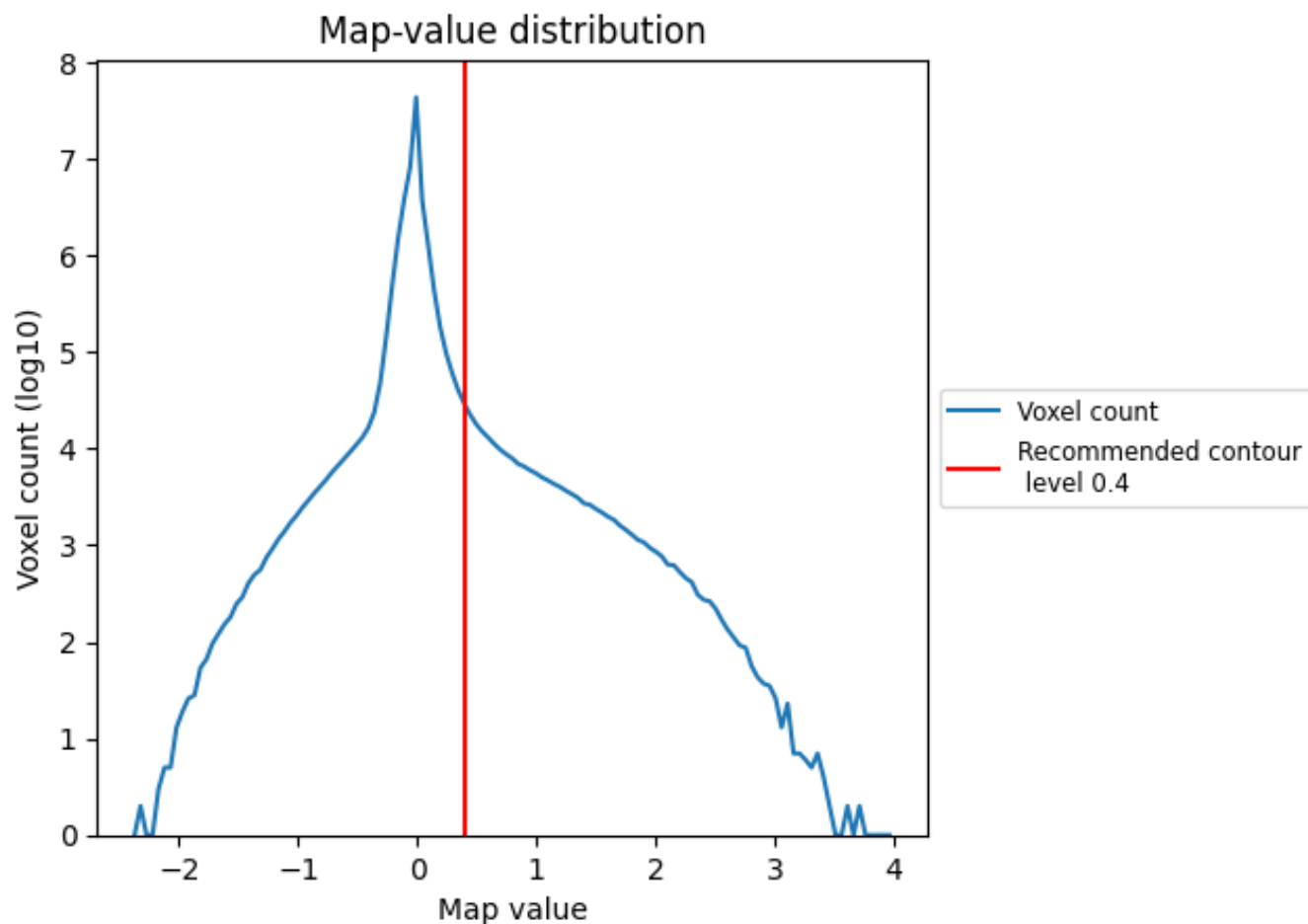
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

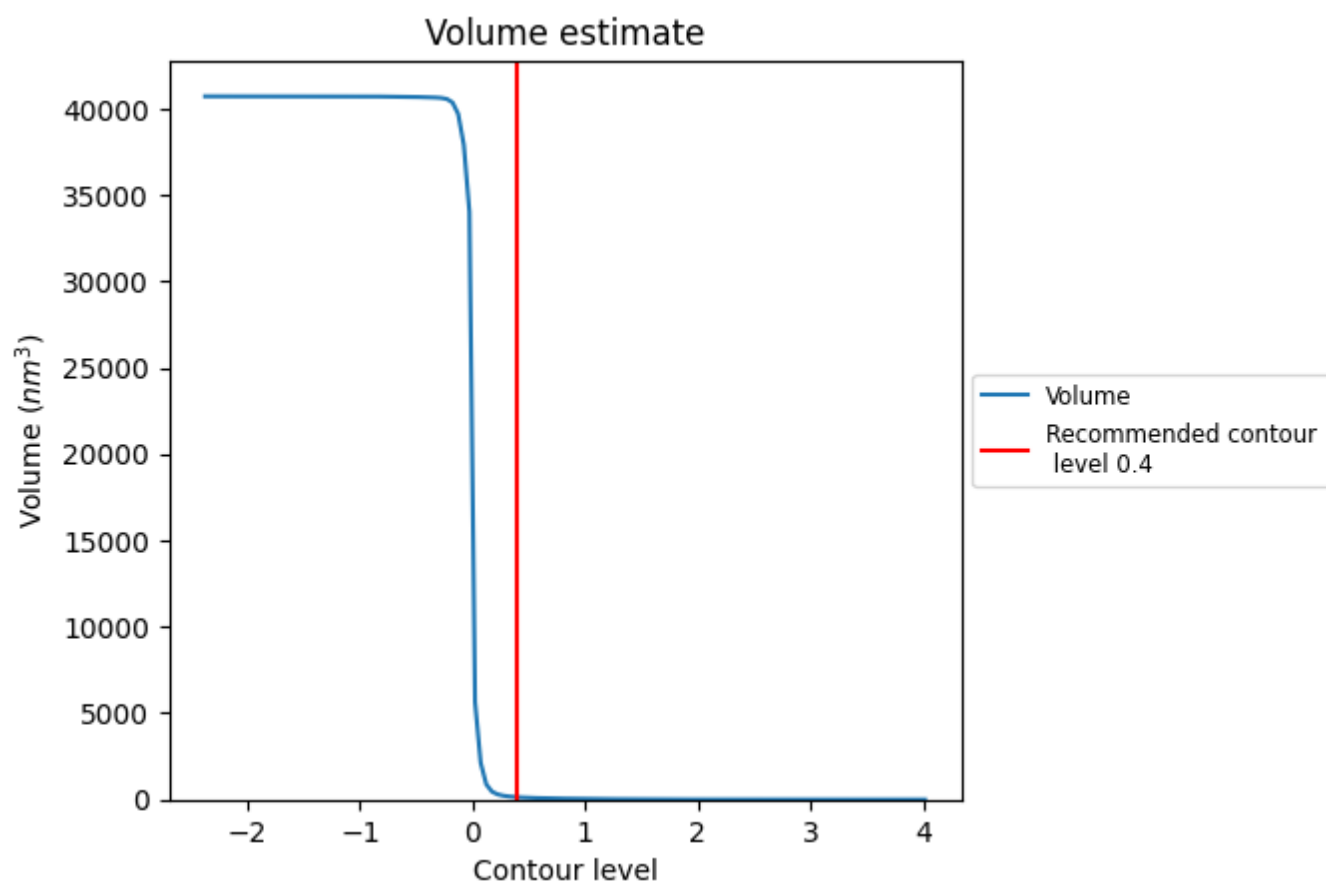
This section contains the results of statistical analysis of the map.

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.

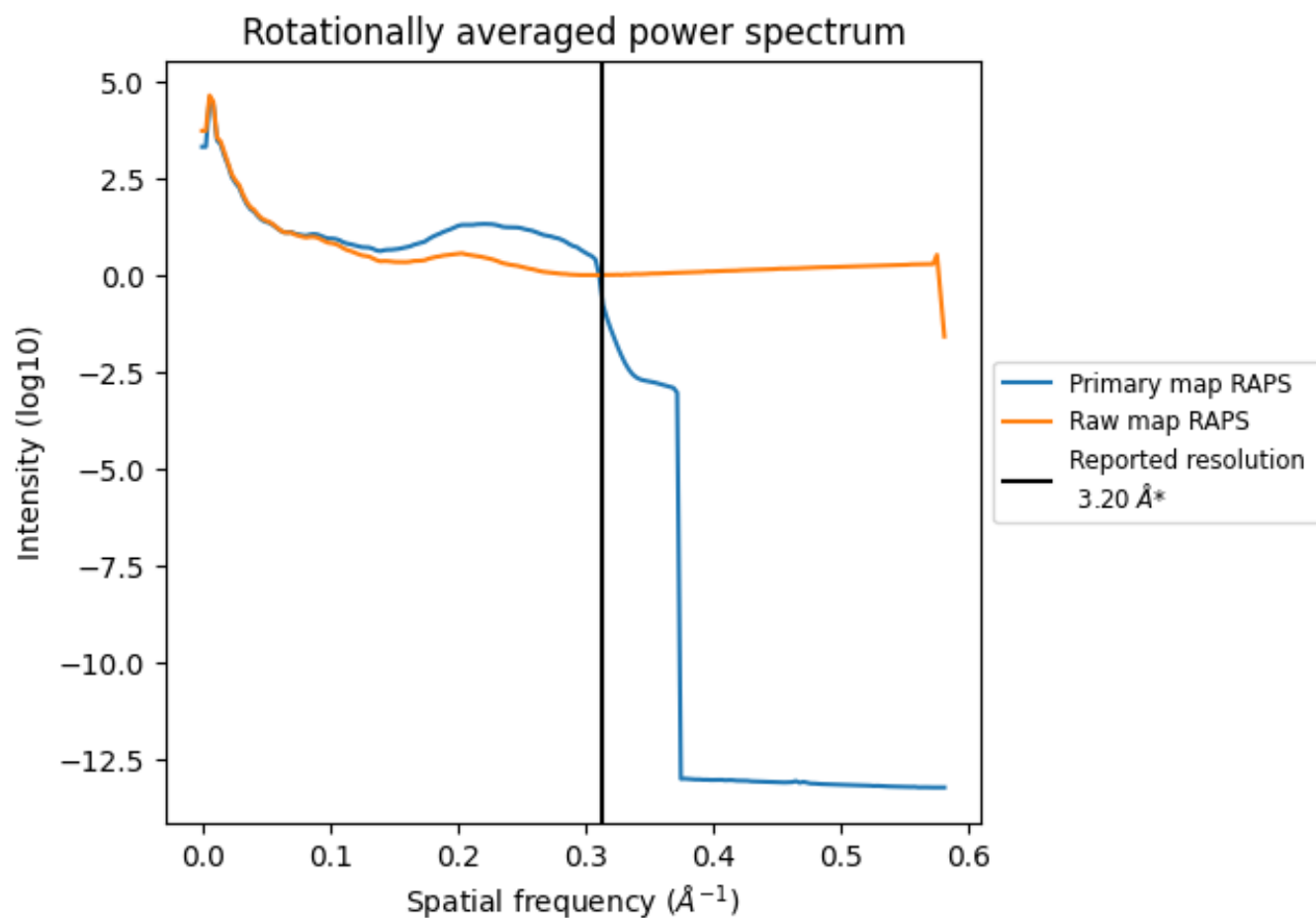
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm^3 ; this corresponds to an approximate mass of 122 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 ⓘ

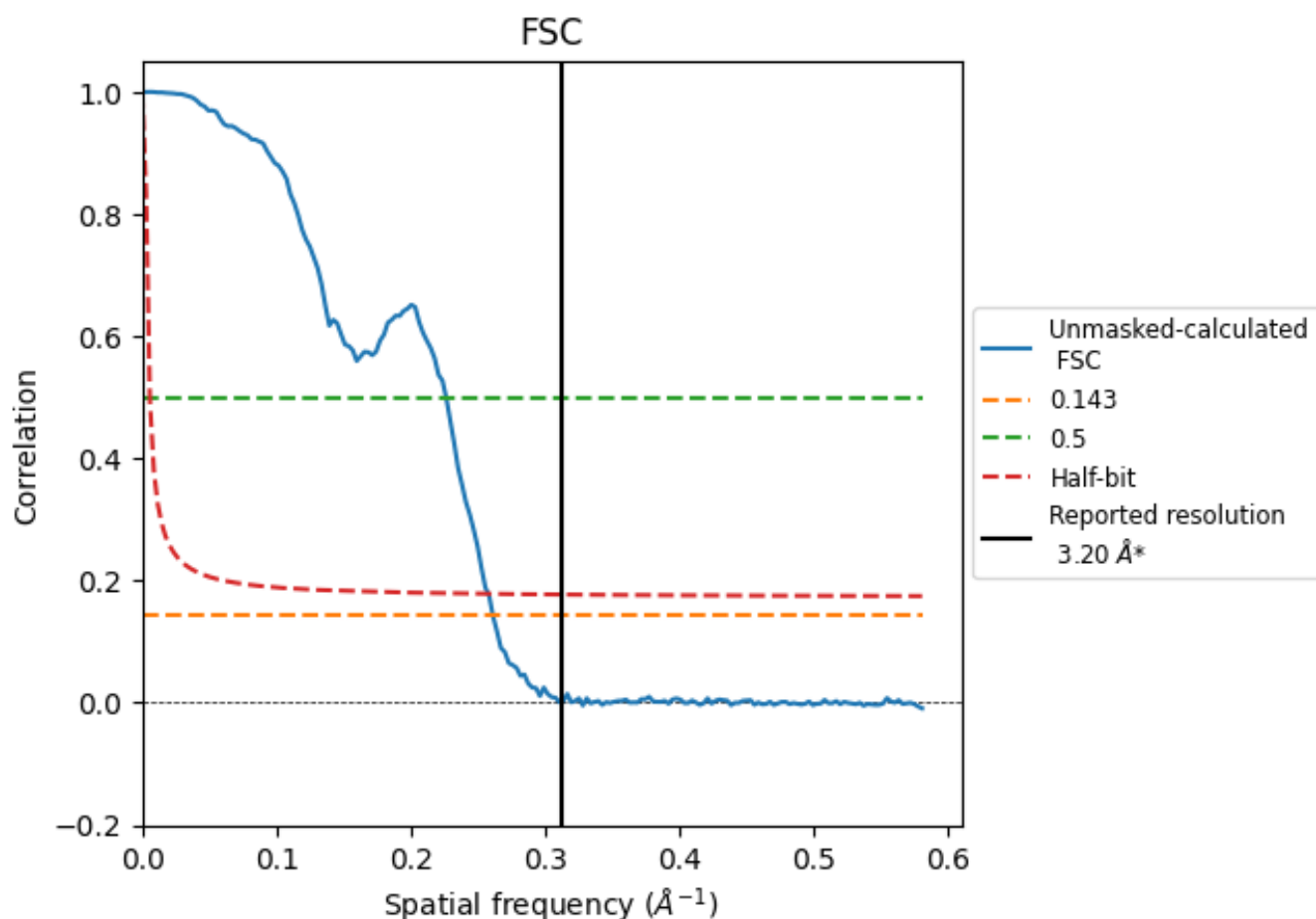


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

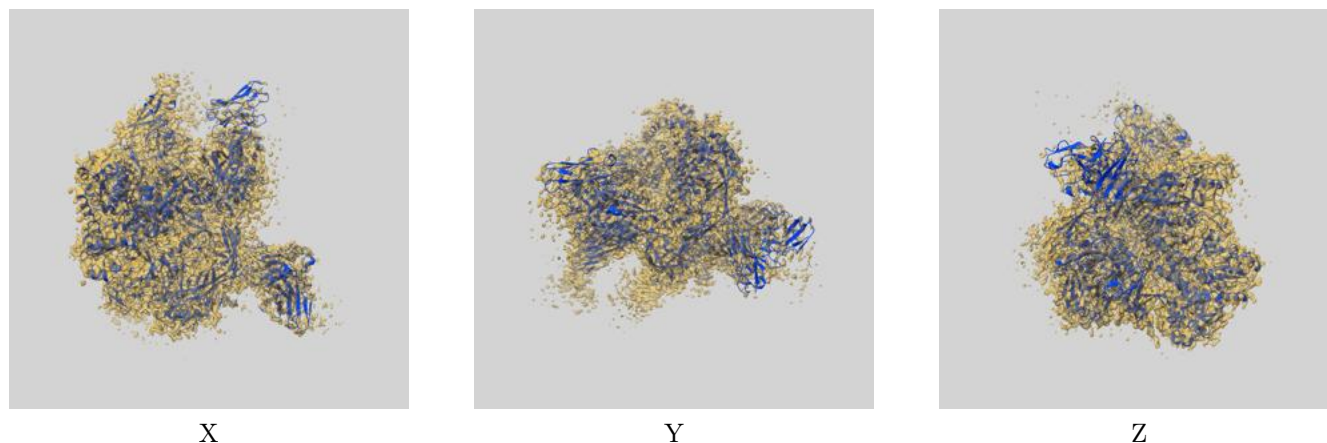
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	4.41	3.88

*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 3.83 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

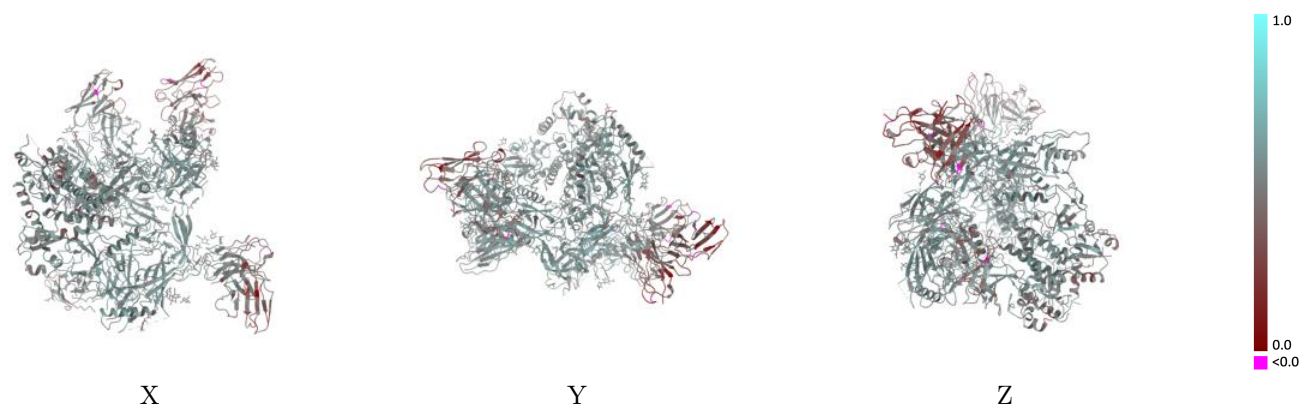
This section contains information regarding the fit between EMDB map EMD-16493 and PDB model 8C8T. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



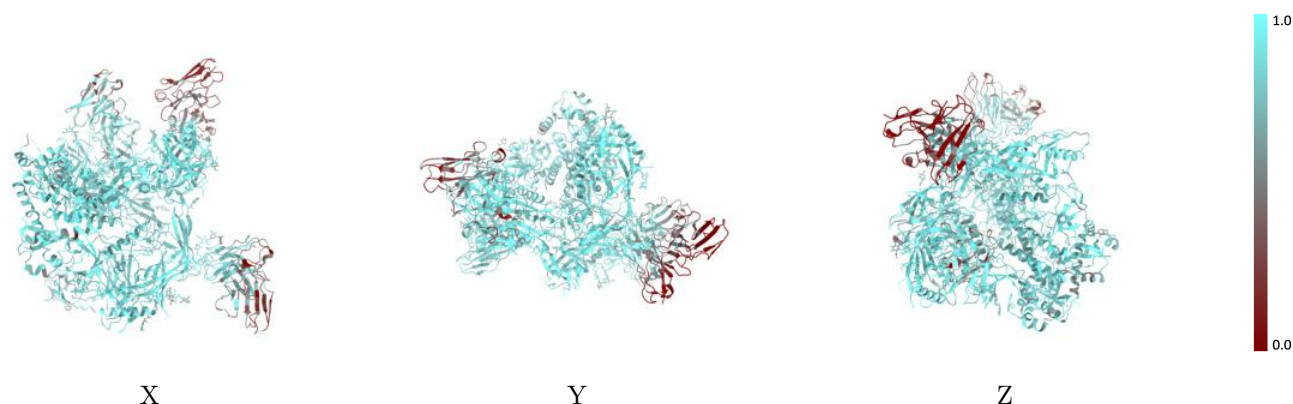
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



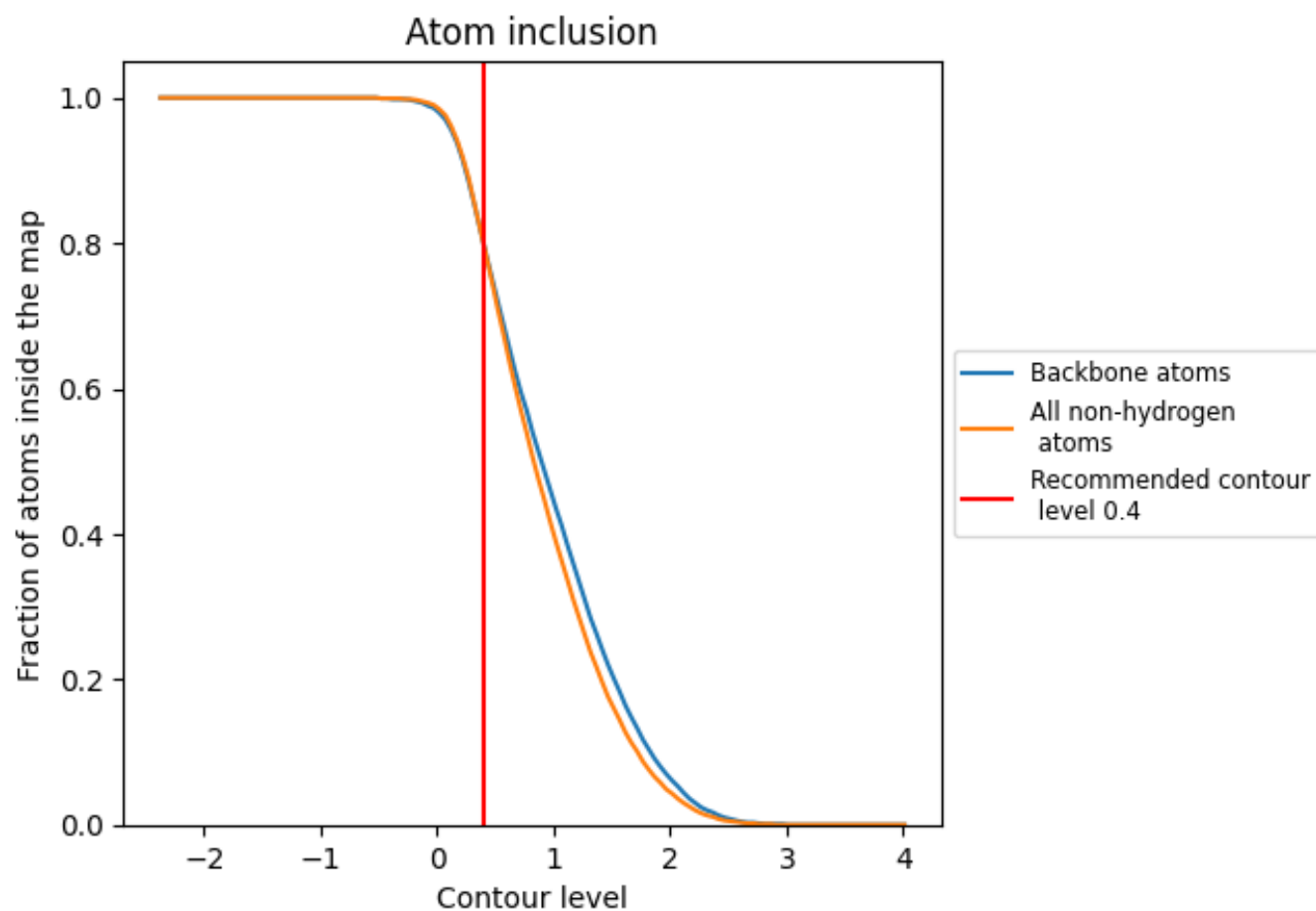
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7980	 0.5110
A	 0.8820	 0.5410
B	 0.8400	 0.5120
C	 0.4700	 0.3720
D	 0.1840	 0.3160
E	 0.9640	 0.5500
F	 0.9040	 0.5600
G	 0.8950	 0.5550
H	 0.6990	 0.4550
I	 0.8730	 0.5280
J	 0.8360	 0.5080
K	 0.4700	 0.3860
L	 0.8720	 0.5360
M	 0.6070	 0.4730
N	 0.8570	 0.4520
O	 0.7860	 0.4810
P	 0.8210	 0.4950
Q	 0.8210	 0.5450
R	 0.8660	 0.5480
S	 0.8390	 0.5280
T	 0.7900	 0.4990
U	 0.6750	 0.4420
V	 0.7600	 0.5120
W	 0.7860	 0.4830
X	 0.9230	 0.5460
Y	 0.8570	 0.5170
Z	 0.7860	 0.5210
a	 0.8210	 0.5210
b	 0.6430	 0.3770

