



## wwPDB EM Validation Summary Report ⓘ

Sep 3, 2025 – 12:25 PM JST

PDB ID : 9LHD / pdb\_00009lhd  
EMDB ID : EMD-63094  
Title : human alpha 7 nicotinic acetylcholine receptor in complex with L-nicotine  
(one-nicotine-bound desensitized state)  
Authors : Liu, S.; Chen, H.; Tian, C.  
Deposited on : 2025-01-11  
Resolution : 3.24 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.45.1

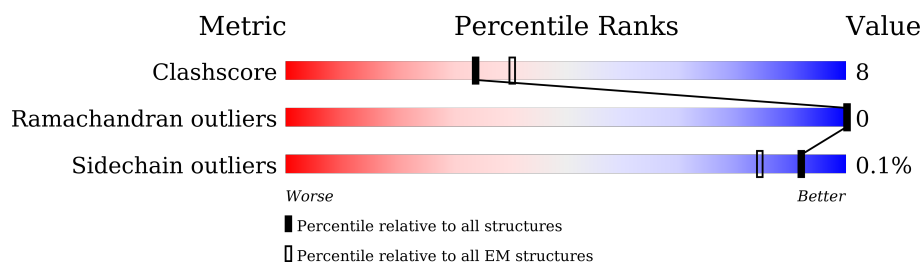
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.24 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.



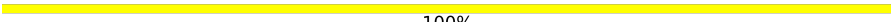

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	512	
1	B	512	
1	C	512	
1	D	512	
1	E	512	
2	F	2	
2	G	2	
2	H	2	

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Mol	Chain	Length	Quality of chain
2	I	2	 100%
2	J	2	 50%50%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16113 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 Neuronal acetylcholine receptor subunit alpha-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	400	Total	C	N	O	S	1	0
			3178	2070	513	572	23		
1	B	400	Total	C	N	O	S	1	0
			3172	2064	513	572	23		
1	C	400	Total	C	N	O	S	1	0
			3178	2070	513	572	23		
1	D	400	Total	C	N	O	S	1	0
			3184	2073	516	572	23		
1	E	400	Total	C	N	O	S	1	0
			3178	2070	513	572	23		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	GLY	-	expression tag	UNP P36544
A	504	GLY	-	expression tag	UNP P36544
A	505	ASP	-	expression tag	UNP P36544
A	506	TYR	-	expression tag	UNP P36544
A	507	LYS	-	expression tag	UNP P36544
A	508	ASP	-	expression tag	UNP P36544
A	509	ASP	-	expression tag	UNP P36544
A	510	ASP	-	expression tag	UNP P36544
A	511	ASP	-	expression tag	UNP P36544
A	512	LYS	-	expression tag	UNP P36544
B	503	GLY	-	expression tag	UNP P36544
B	504	GLY	-	expression tag	UNP P36544
B	505	ASP	-	expression tag	UNP P36544
B	506	TYR	-	expression tag	UNP P36544
B	507	LYS	-	expression tag	UNP P36544
B	508	ASP	-	expression tag	UNP P36544
B	509	ASP	-	expression tag	UNP P36544
B	510	ASP	-	expression tag	UNP P36544
B	511	ASP	-	expression tag	UNP P36544
B	512	LYS	-	expression tag	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
C	503	GLY	-	expression tag	UNP P36544
C	504	GLY	-	expression tag	UNP P36544
C	505	ASP	-	expression tag	UNP P36544
C	506	TYR	-	expression tag	UNP P36544
C	507	LYS	-	expression tag	UNP P36544
C	508	ASP	-	expression tag	UNP P36544
C	509	ASP	-	expression tag	UNP P36544
C	510	ASP	-	expression tag	UNP P36544
C	511	ASP	-	expression tag	UNP P36544
C	512	LYS	-	expression tag	UNP P36544
D	503	GLY	-	expression tag	UNP P36544
D	504	GLY	-	expression tag	UNP P36544
D	505	ASP	-	expression tag	UNP P36544
D	506	TYR	-	expression tag	UNP P36544
D	507	LYS	-	expression tag	UNP P36544
D	508	ASP	-	expression tag	UNP P36544
D	509	ASP	-	expression tag	UNP P36544
D	510	ASP	-	expression tag	UNP P36544
D	511	ASP	-	expression tag	UNP P36544
D	512	LYS	-	expression tag	UNP P36544
E	503	GLY	-	expression tag	UNP P36544
E	504	GLY	-	expression tag	UNP P36544
E	505	ASP	-	expression tag	UNP P36544
E	506	TYR	-	expression tag	UNP P36544
E	507	LYS	-	expression tag	UNP P36544
E	508	ASP	-	expression tag	UNP P36544
E	509	ASP	-	expression tag	UNP P36544
E	510	ASP	-	expression tag	UNP P36544
E	511	ASP	-	expression tag	UNP P36544
E	512	LYS	-	expression tag	UNP P36544

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



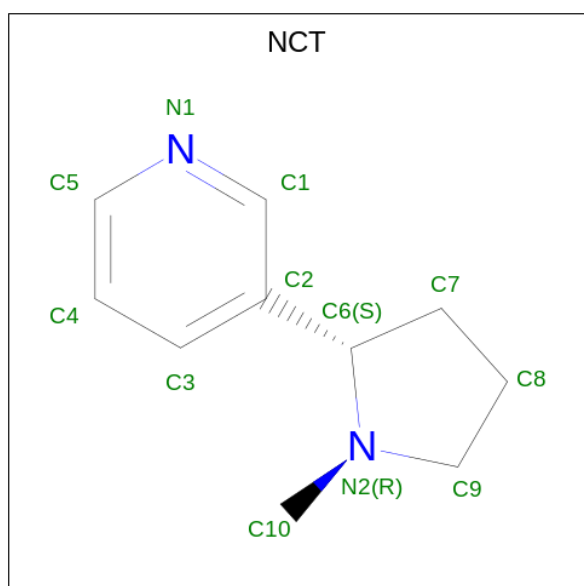
Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (CCD ID: NCT) (formula:  $C_{10}H_{14}N_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	N	0
			12	10	2	

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	O	0
			1	1	





Chain C:

62% 16% 22%

Conservation scores (bits) for Chain C:

Position	Amino Acid	Conservation Score (bits)
1	MET	0.00
2	ARG	0.00
3	CYS	0.00
4	SER	0.00
5	PRO	0.00
6	GLY	0.00
7	GLY	0.00
8	VAL	0.00
9	TRP	0.00
10	LEU	0.00
11	ALA	0.00
12	LEU	0.00
13	ALA	0.00
14	SER	0.00
15	LEU	0.00
16	HIS	0.00
17	VAL	0.00
18	SER	0.00
19	LEU	0.00
20	GLN	0.00
21	G23	0.00
22	L29	0.00
23	R42	0.00
24	P43	0.00
25	V44	0.00
26	S58	0.00
27	L59	0.00
28	L60	0.00
29	M63	0.00
30	D66	0.00
31	E67	0.00
32	V71	0.00
33	L72	0.00
34	T73	0.00
35	I76	0.00
36	W77	0.00
37	L78	0.00
38	W89	0.00
39	N90	0.00
40	E93	0.00
41	L113	0.00
42	L141	0.00
43	W171	0.00
44	G176	0.00
45	W176	0.00
46	S307	0.00
47	V308	0.00
48	V309	0.00
49	V310	0.00
50	V314	0.00
51	W330	0.00
52	I334	0.00
53	L335	0.00
54	L336	0.00
55	G349	0.00
56	G411	0.00
57	ASP	0.00
58	LYS	0.00
59	VAL	0.00
60	ARG	0.00
61	PRO	0.00
62	HIS	0.00
63	ALA	0.00
64	GLN	0.00
65	LYS	0.00
66	GLN	0.00
67	ARG	0.00
68	GLY	0.00
69	CYS	0.00
70	SER	0.00
71	VAL	0.00
72	PRO	0.00
73	ALA	0.00
74	HIS	0.00
75	ASP	0.00
76	GLU	0.00
77	LEU	0.00
78	LEU	0.00
79	HIS	0.00
80	GLY	0.00
81	GLY	0.00
82	ASP	0.00
83	ASP	0.00
84	ASP	0.00
85	ASP	0.00
86	ASP	0.00
87	ASP	0.00
88	ASP	0.00
89	ASP	0.00
90	ASP	0.00
91	ASP	0.00
92	ASP	0.00
93	ASP	0.00
94	ASP	0.00
95	ASP	0.00
96	ASP	0.00
97	ASP	0.00
98	ASP	0.00
99	ASP	0.00
100	ASP	0.00

Chain D:

64% 14% 22%

Y210  
E215  
P218  
R227  
T230  
V242  
L243  
A248  
L249  
L250  
V251  
F252  
V268  
L272  
L278  
V279  
M283  
S287  
D288  
S289  
Y296  
F297  
M301  
V309  
L315  
M327  
P328  
W330  
T331  
R332  
V333  
I334  
L335  
L336  
N337  
R347  
P348  
GLU  
G349  
ASP  
LYS

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

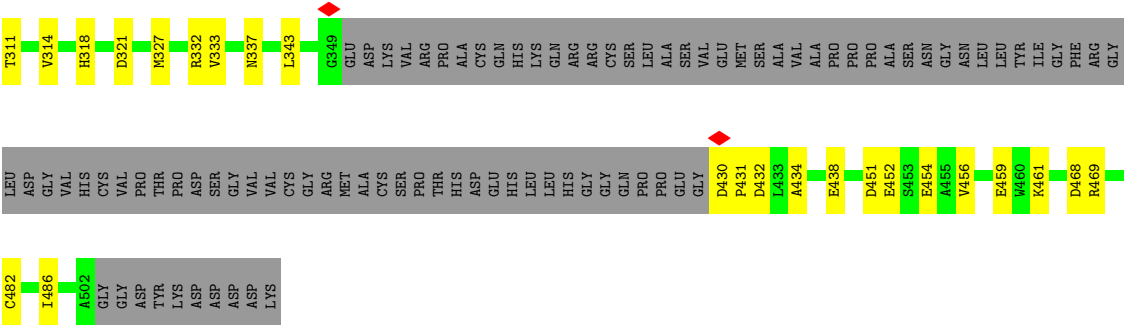
PRO  
THR  
GLU  
ASP  
HIS  
LEU  
LEU  
HIS  
GLY  
GLN  
GLN  
PRO  
PRO  
GLU  
GLY  
D430  
P431  
D432  
K435  
I436  
L437  
E438  
E439  
V440  
R441  
L472  
F475  
S476  
T479  
I480  
I481  
I486  
A490  
D500  
F501  
A502  
GLY  
GLY  
ASP  
TYR  
LYS  
ASP  
ASP  
ASP  
LYS

Chain E:

63% 15% 22%

Residue	Category
MET	Grey
ARG	Grey
CYS	Grey
SER	Grey
PRO	Grey
GLY	Grey
VAL	Grey
TRP	Grey
LEU	Grey
ALA	Grey
LEU	Grey
ALA	Grey
SER	Grey
LEU	Grey
LEU	Grey
HIS	Grey
VAL	Grey
SER	Grey
LEU	Grey
GLN	Grey
G23	Yellow
Q26	Yellow
K35	Yellow
N36	Yellow
R42	Yellow
P43	Yellow
V44	Yellow
A45	Green
N46	Yellow
T52	Yellow
S58	Yellow
L59	Green
L60	Yellow
W77	Yellow
L78	Yellow
S81	Yellow
D84	Yellow
H85	Green
Y86	Yellow
D119	Yellow
E120	Green
R121	Yellow
T125	Yellow
S135	Yellow
G136	Green
H137	Yellow

Residue	Category
P142	Yellow
K147	Yellow
D160	Yellow
K167	Yellow
W176	Yellow
D179	Yellow
C212	Yellow
C213	Yellow
K214	Green
E215	Yellow
D219	Yellow
R228	Yellow
L231	Yellow
G234	Yellow
L235	Yellow
L238	Yellow
C241	Yellow
A248	Yellow
L249	Green
L250	Yellow
T262	Yellow
L266	Yellow
T267	Green
V268	Yellow
T273	Yellow
L277	Yellow
L278	Yellow
E281	Yellow
I282	Yellow
S287	Yellow
Y286	Yellow
F297	Yellow
A298	Yellow
K301	Green
I302	Yellow
V308	Yellow
V309	Yellow
V310	Yellow



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

Chain F: 100%



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

Chain G: 100%



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

Chain H: 100%



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

Chain I: 100%



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

Chain J: 50% 50%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7980	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 ( $e^-/\text{\AA}^2$ )	56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.624	Depositor
Minimum map value	-0.610	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	242.4, 242.4, 242.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	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: NCT, 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	0.23	0/3269	0.31	0/4462
1	B	0.23	0/3262	0.34	0/4453
1	C	0.23	0/3269	0.33	0/4462
1	D	0.24	0/3275	0.35	0/4469
1	E	0.23	0/3269	0.33	0/4462
All	All	0.23	0/16344	0.33	0/22308

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	3178	0	3110	49	0
1	B	3172	0	3103	64	0
1	C	3178	0	3110	55	0
1	D	3184	0	3121	58	0
1	E	3178	0	3110	58	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	28	0	25	0	0
2	J	28	0	25	3	0
3	A	12	0	14	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	1	0
4	E	14	0	13	1	0
5	A	1	0	0	0	0
All	All	16113	0	15758	255	0

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

The worst 5 of 255 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:D:272:LEU:HD22	1:D:301:MET:HE3	1.39	1.02
1:D:155:ARG:HG3	1:D:156:TRP:CE3	1.96	1.00
1:D:155:ARG:CG	1:D:156:TRP:CZ3	2.56	0.89
1:A:86:TYR:HH	1:B:23:GLY:N	1.73	0.85
1:C:212:CYS:SG	1:C:213:CYS:N	2.50	0.85

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	397/512 (78%)	385 (97%)	12 (3%)	0	100	100
1	B	397/512 (78%)	384 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	397/512 (78%)	386 (97%)	11 (3%)	0	100	100
1	D	397/512 (78%)	388 (98%)	9 (2%)	0	100	100
1	E	397/512 (78%)	386 (97%)	11 (3%)	0	100	100
All	All	1985/2560 (78%)	1929 (97%)	56 (3%)	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	350/449 (78%)	350 (100%)	0	100	100
1	B	349/449 (78%)	349 (100%)	0	100	100
1	C	350/449 (78%)	350 (100%)	0	100	100
1	D	351/449 (78%)	350 (100%)	1 (0%)	91	95
1	E	350/449 (78%)	350 (100%)	0	100	100
All	All	1750/2245 (78%)	1749 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	283	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	337	ASN
1	D	49	GLN
1	E	295	GLN
1	E	49	GLN
1	B	163	HIS

### 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 ⓘ

10 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	F	1	2,1	14,14,15	1.82	3 (21%)	17,19,21	2.17	5 (29%)
2	NAG	F	2	2	14,14,15	1.96	3 (21%)	17,19,21	1.23	2 (11%)
2	NAG	G	1	2,1	14,14,15	2.02	6 (42%)	17,19,21	1.47	3 (17%)
2	NAG	G	2	2	14,14,15	1.99	4 (28%)	17,19,21	1.16	2 (11%)
2	NAG	H	1	2,1	14,14,15	1.99	6 (42%)	17,19,21	1.37	3 (17%)
2	NAG	H	2	2	14,14,15	2.01	4 (28%)	17,19,21	1.37	3 (17%)
2	NAG	I	1	2,1	14,14,15	2.02	6 (42%)	17,19,21	1.44	3 (17%)
2	NAG	I	2	2	14,14,15	2.00	4 (28%)	17,19,21	1.19	2 (11%)
2	NAG	J	1	2,1	14,14,15	1.98	6 (42%)	17,19,21	1.52	3 (17%)
2	NAG	J	2	2	14,14,15	1.96	4 (28%)	17,19,21	1.25	2 (11%)

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	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	NAG	O5-C1	4.76	1.51	1.43
2	G	2	NAG	O5-C1	4.74	1.51	1.43
2	G	1	NAG	O5-C1	4.71	1.51	1.43
2	I	1	NAG	O5-C1	4.68	1.51	1.43
2	J	1	NAG	O5-C1	4.65	1.51	1.43

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C3-C4-C5	5.14	119.40	110.24
2	F	1	NAG	C4-C3-C2	4.29	117.30	111.02
2	J	1	NAG	C2-N2-C7	-3.97	117.25	122.90
2	H	2	NAG	C2-N2-C7	-3.41	118.05	122.90
2	G	1	NAG	C2-N2-C7	-3.37	118.10	122.90

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6

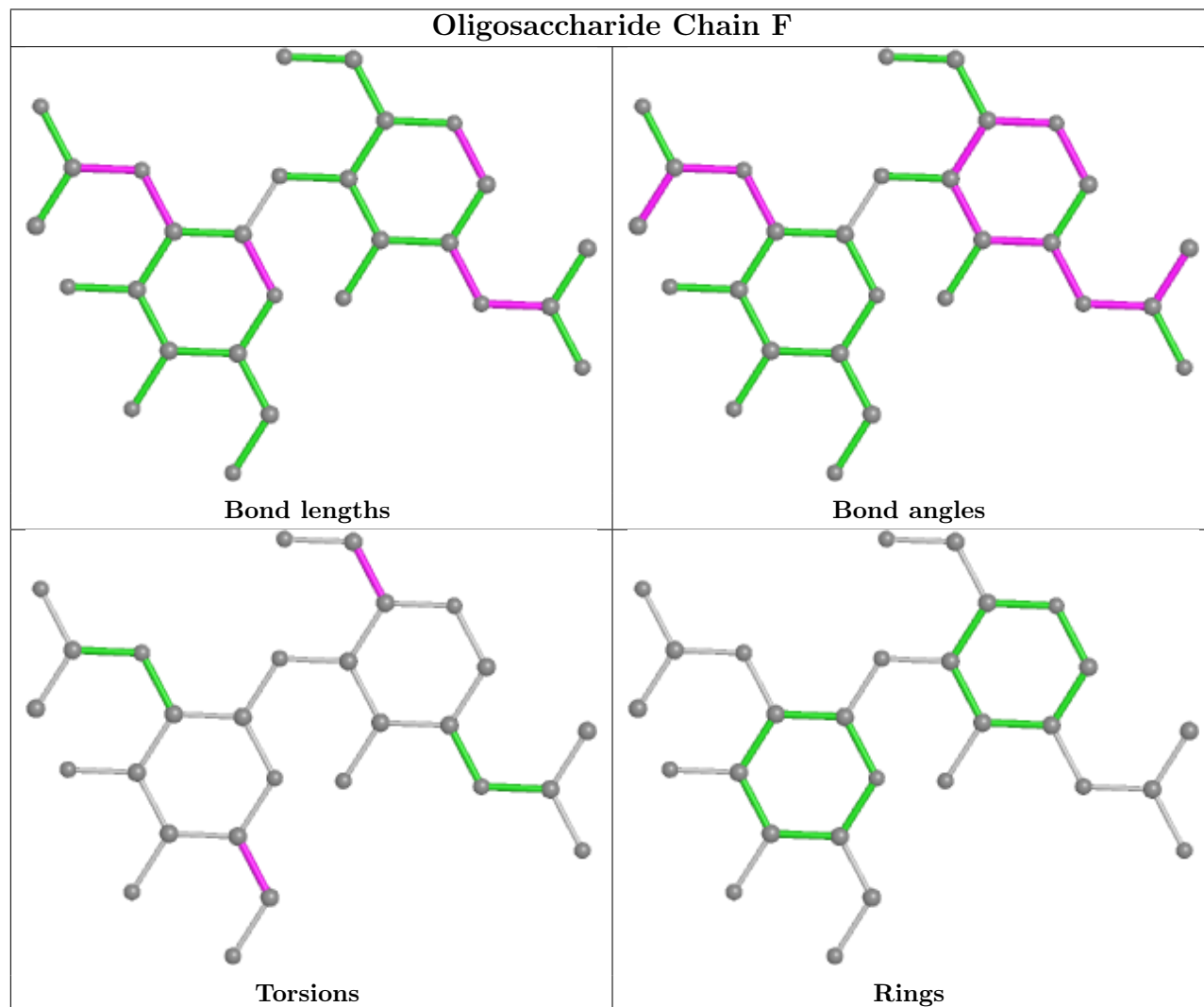
There are no ring outliers.

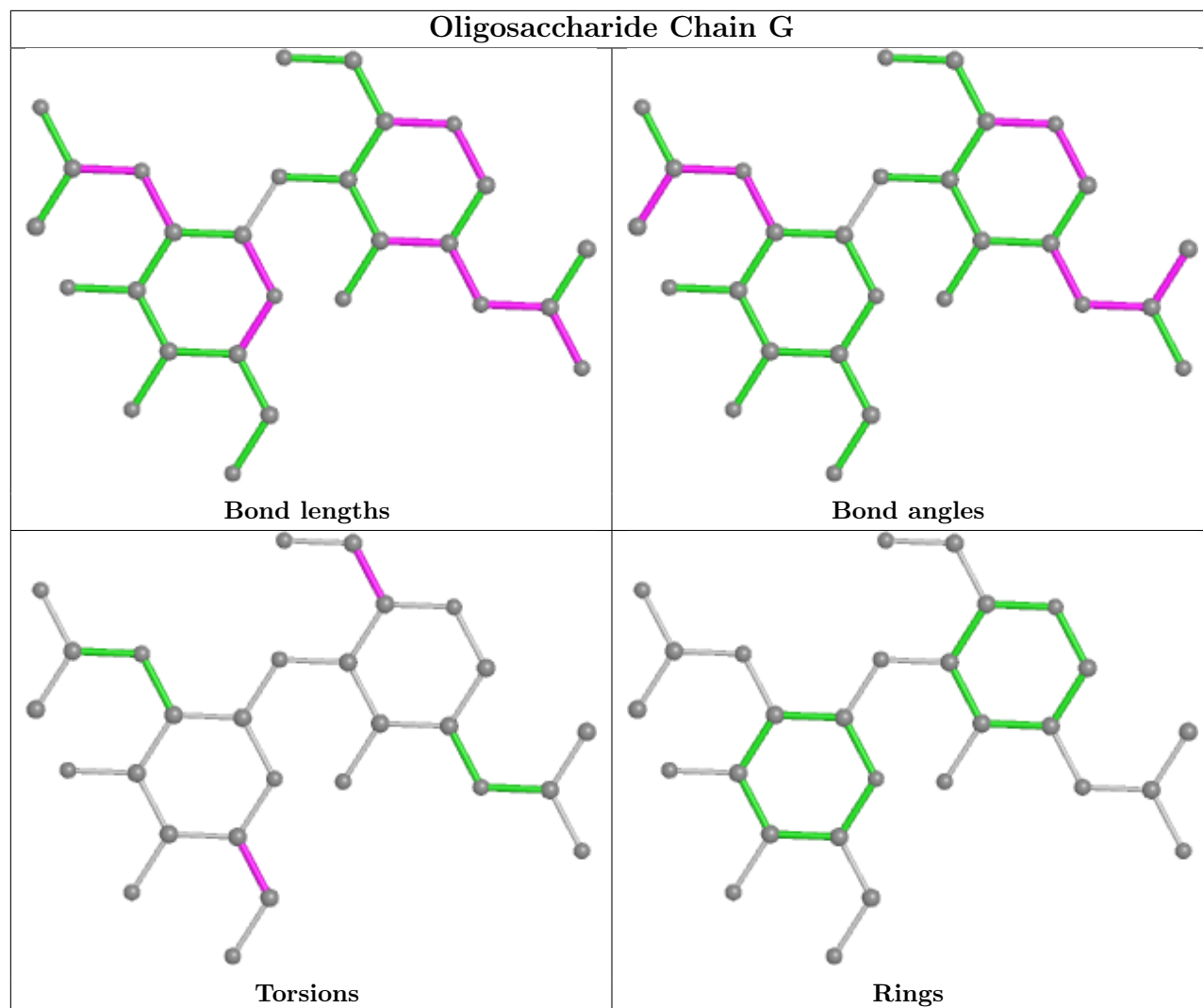
1 monomer is involved in 3 short contacts:

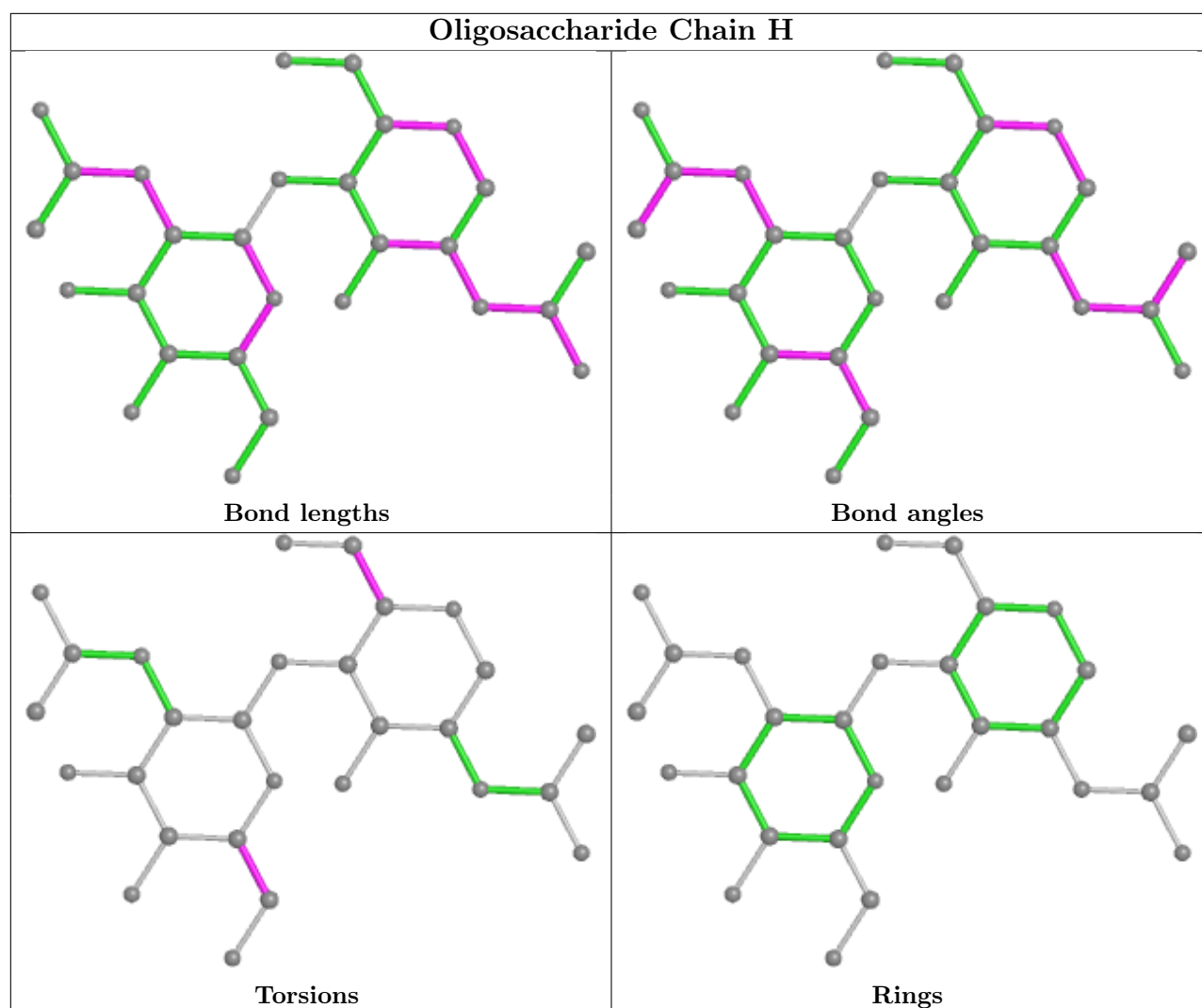


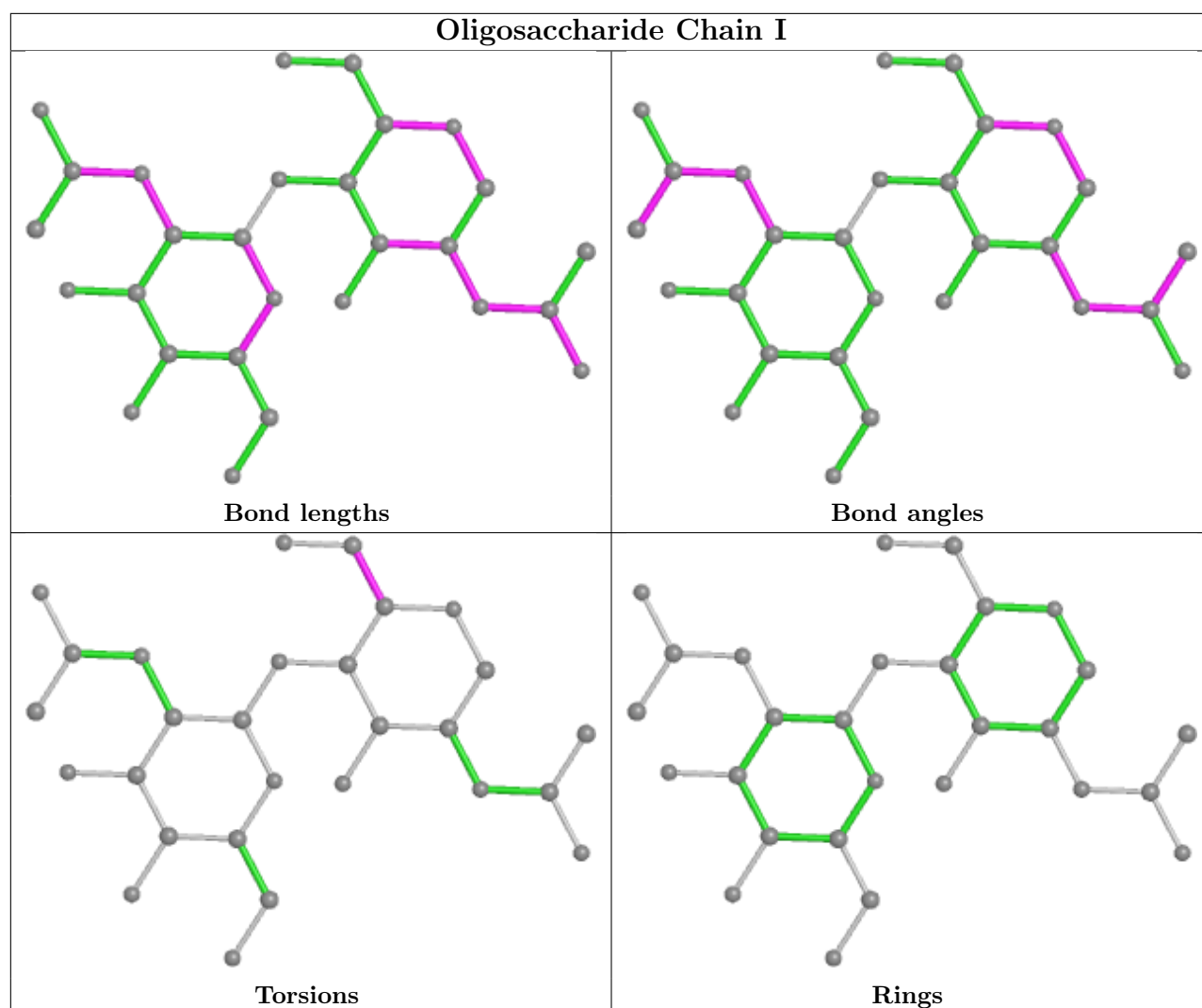
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	3	0

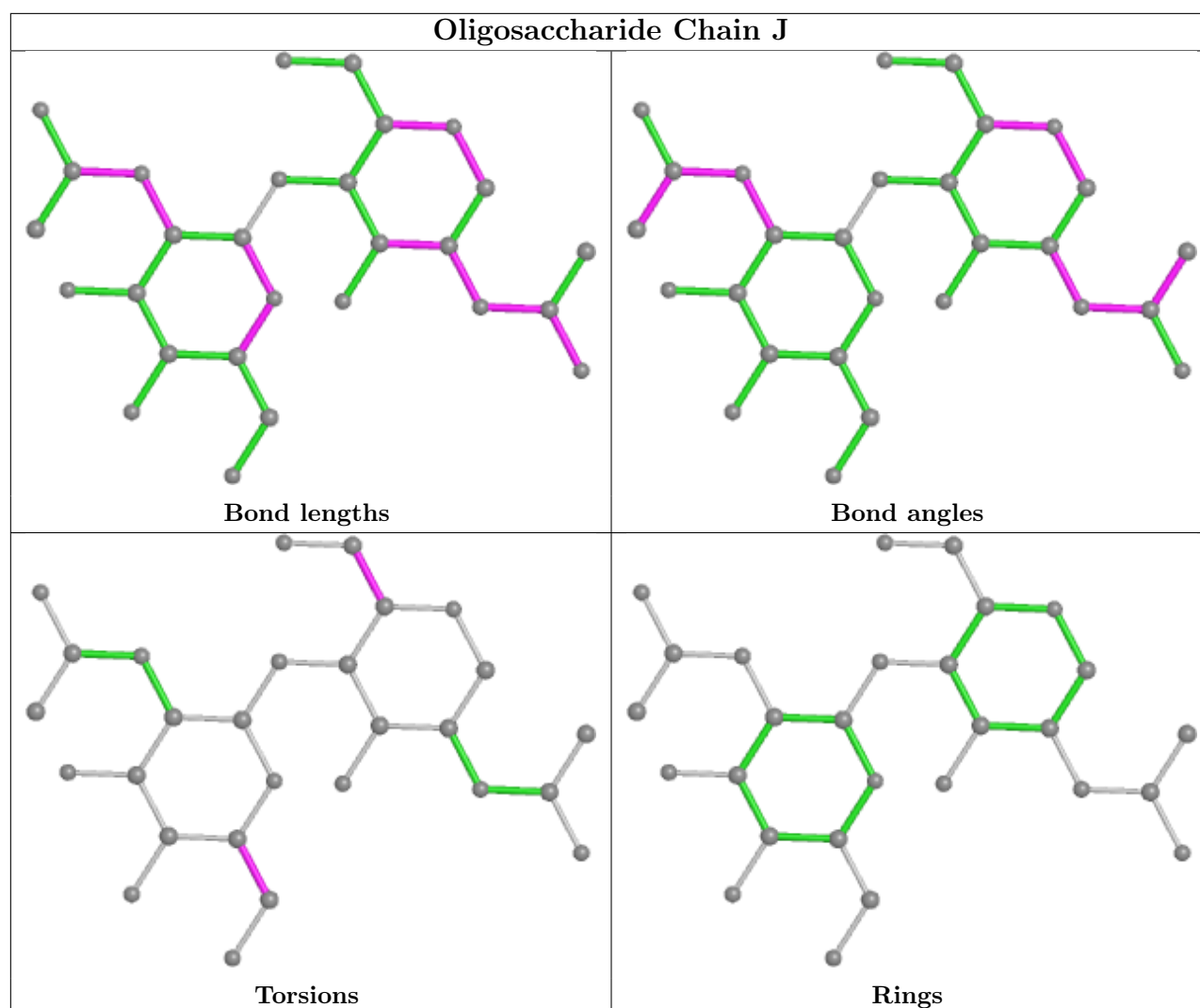
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	601	1	14,14,15	2.02	4 (28%)	17,19,21	1.22	3 (17%)
4	NAG	C	601	1	14,14,15	2.00	4 (28%)	17,19,21	1.20	3 (17%)
4	NAG	D	601	1	14,14,15	2.03	4 (28%)	17,19,21	1.21	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	E	601	1	14,14,15	2.02	3 (21%)	17,19,21	1.11	2 (11%)
4	NAG	A	602	1	14,14,15	1.97	3 (21%)	17,19,21	1.19	2 (11%)
3	NCT	A	601	-	13,13,13	2.93	4 (30%)	17,17,17	1.43	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	601	1	-	1/6/23/26	0/1/1/1
4	NAG	C	601	1	-	2/6/23/26	0/1/1/1
4	NAG	D	601	1	-	0/6/23/26	0/1/1/1
4	NAG	E	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NCT	A	601	-	-	0/4/14/14	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NCT	C7-C6	-6.54	1.37	1.54
3	A	601	NCT	C9-N2	-5.72	1.30	1.46
4	E	601	NAG	O5-C1	4.88	1.51	1.43
4	D	601	NAG	O5-C1	4.84	1.51	1.43
4	B	601	NAG	O5-C1	4.77	1.51	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NCT	C3-C2-C1	2.81	119.87	116.88
4	A	602	NAG	C2-N2-C7	-2.67	119.09	122.90
4	B	601	NAG	C2-N2-C7	-2.67	119.11	122.90
3	A	601	NCT	C2-C1-N1	-2.66	119.97	124.14
4	C	601	NAG	C2-N2-C7	-2.65	119.13	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	601	NAG	O5-C5-C6-O6

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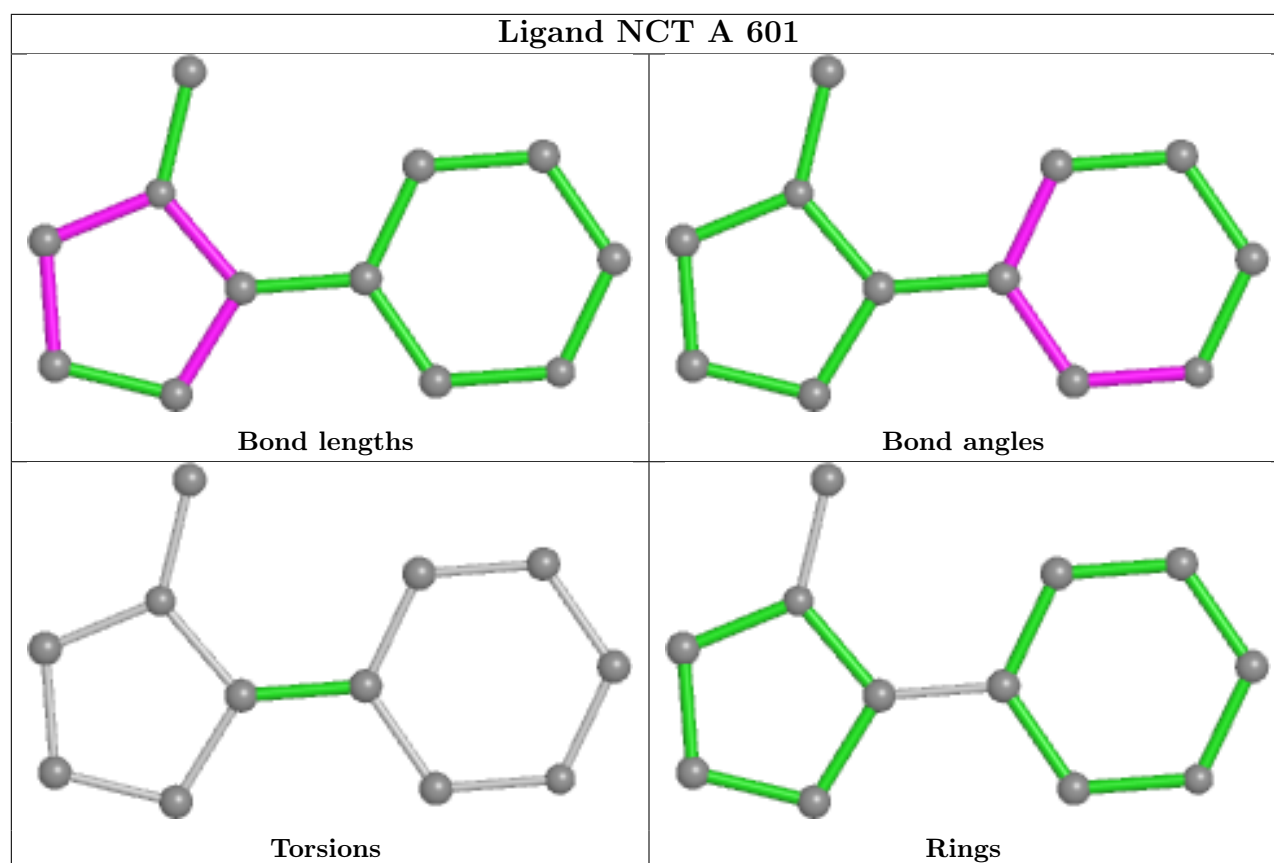
Mol	Chain	Res	Type	Atoms
4	C	601	NAG	O5-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6
4	E	601	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	601	NAG	1	0
4	E	601	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.



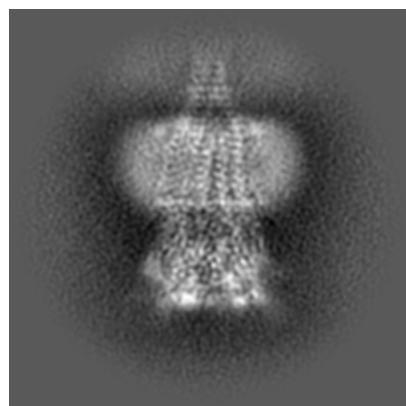
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63094. These allow visual inspection of the internal detail of the map and identification of artifacts.

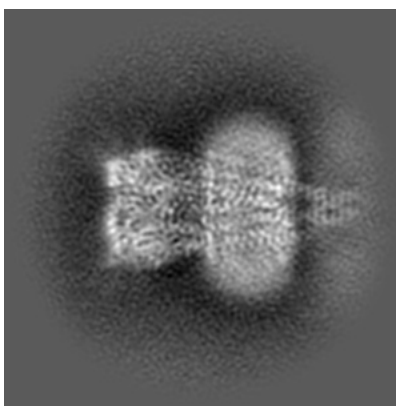
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

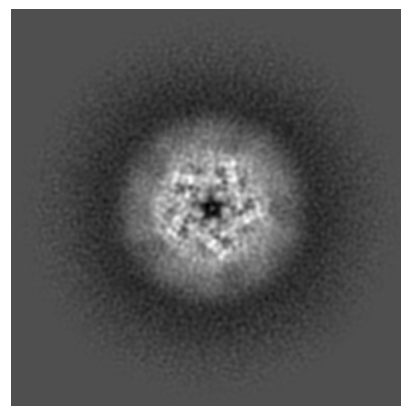
#### 6.1.1 Primary map



X

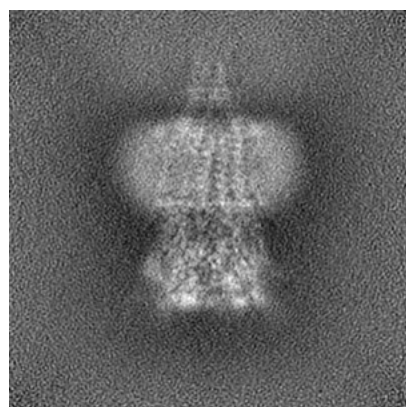


Y

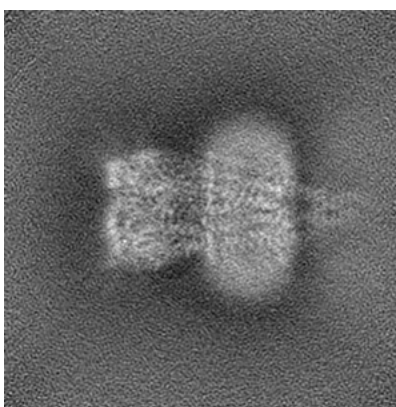


Z

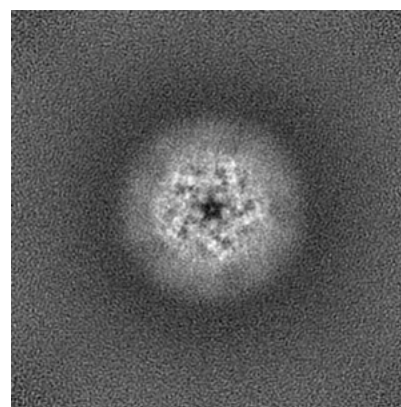
#### 6.1.2 Raw map



X



Y

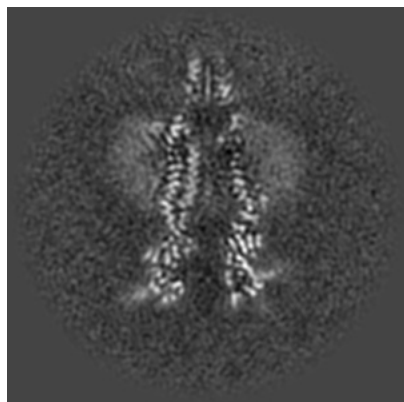


Z

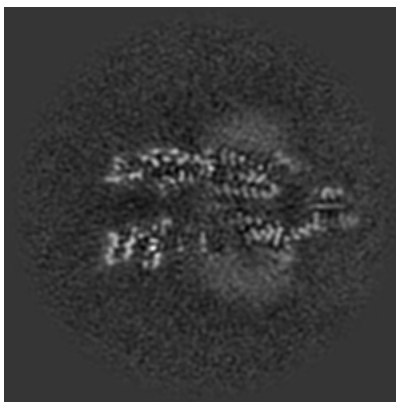
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

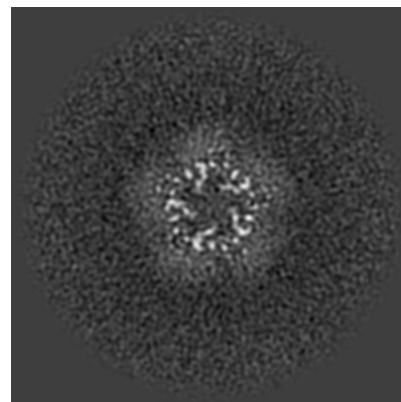
### 6.2.1 Primary map



X Index: 120

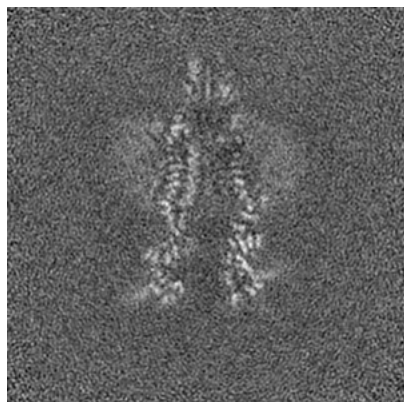


Y Index: 120

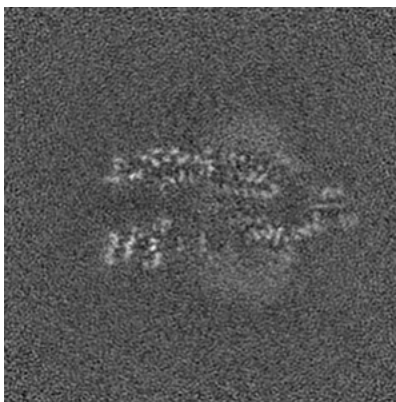


Z Index: 120

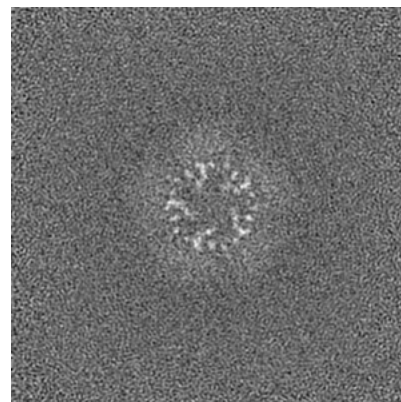
### 6.2.2 Raw map



X Index: 120



Y Index: 120

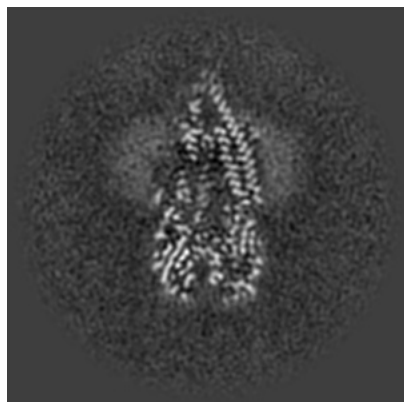


Z Index: 120

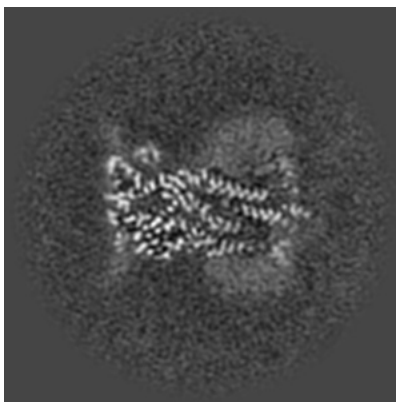
The images above show central slices of the map in three orthogonal directions.

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

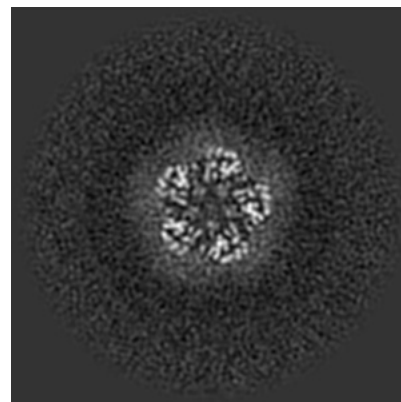
### 6.3.1 Primary map



X Index: 132

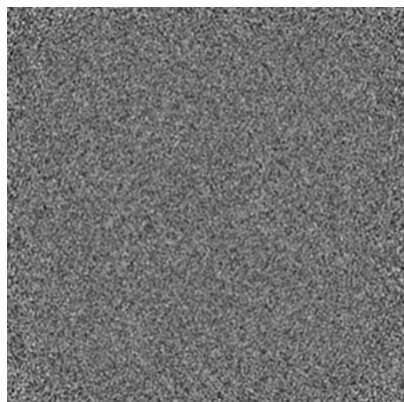


Y Index: 104

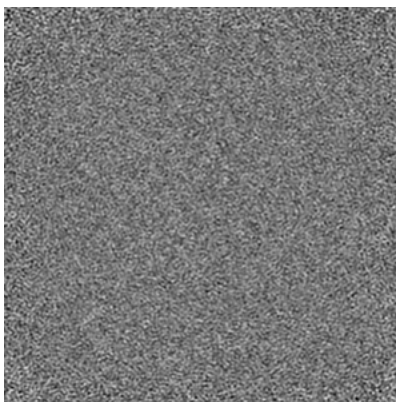


Z Index: 123

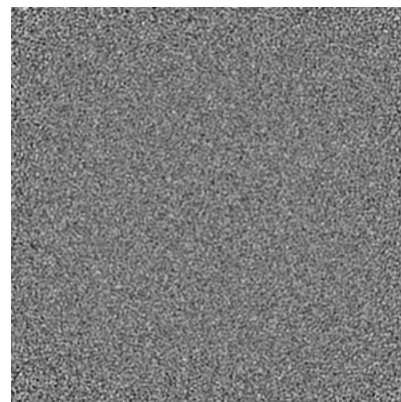
### 6.3.2 Raw map



X Index: 0



Y Index: 0



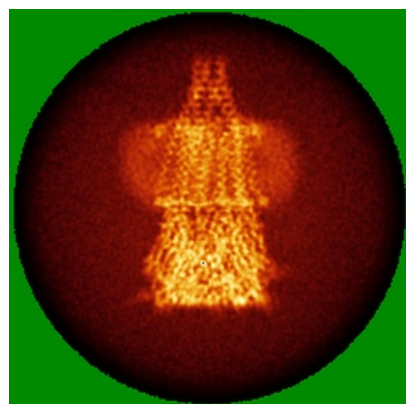
Z Index: 0

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

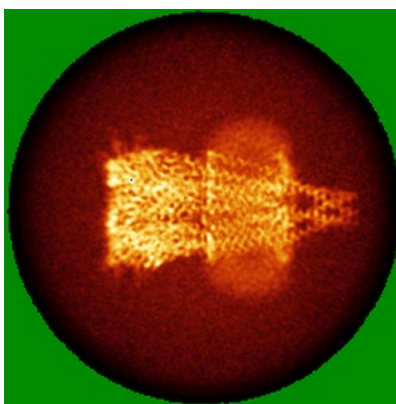


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

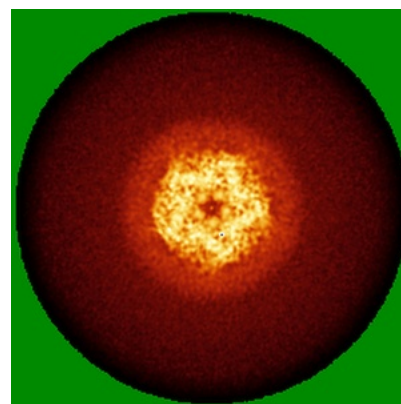
### 6.4.1 Primary map



X

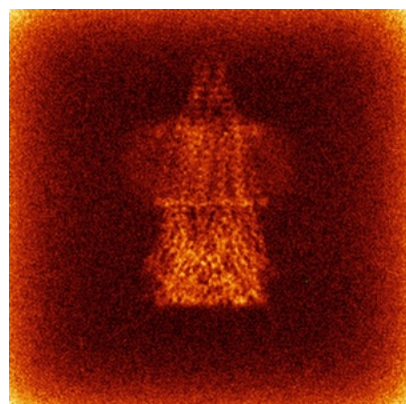


Y

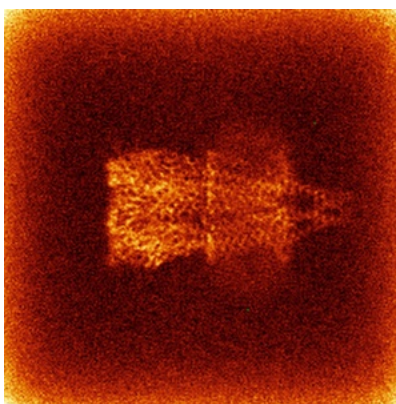


Z

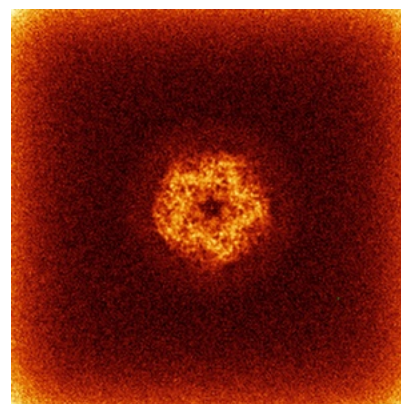
### 6.4.2 Raw map



X



Y

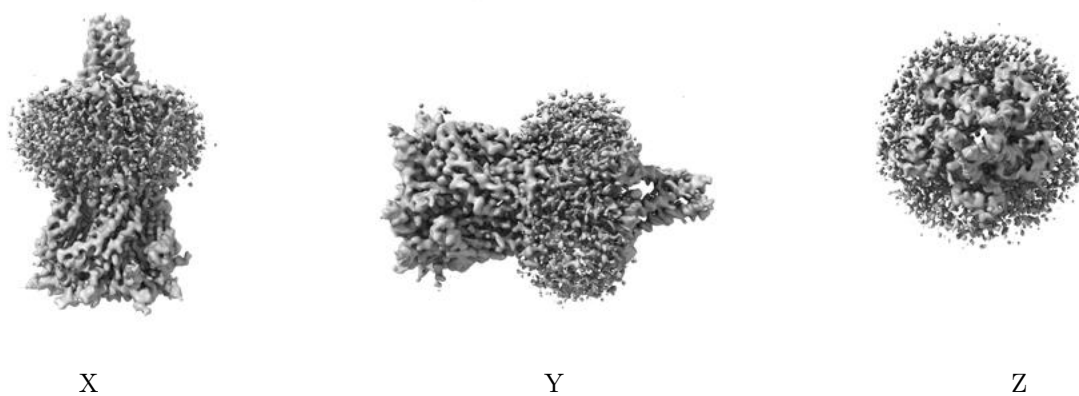


Z

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.

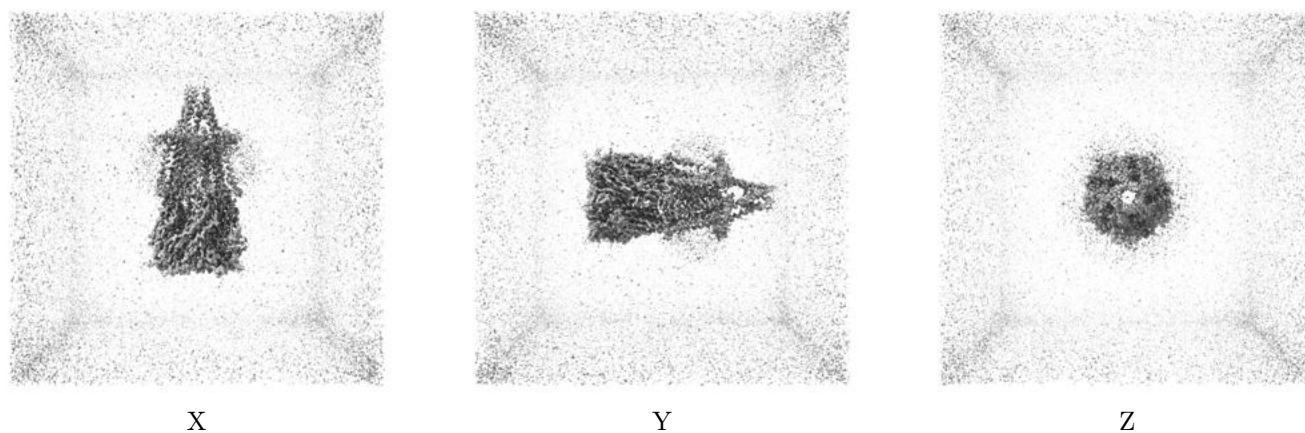
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.27. 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.

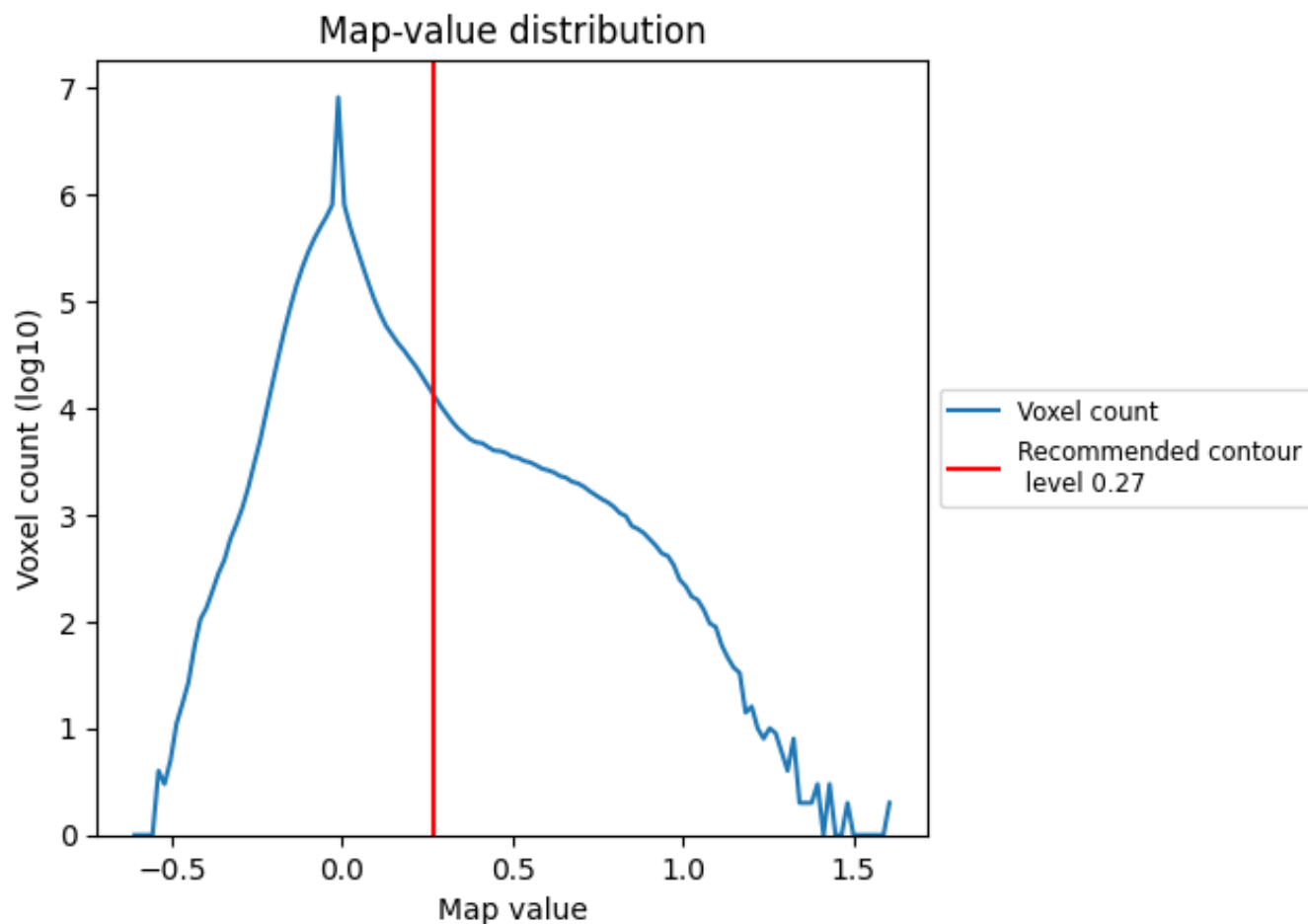
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

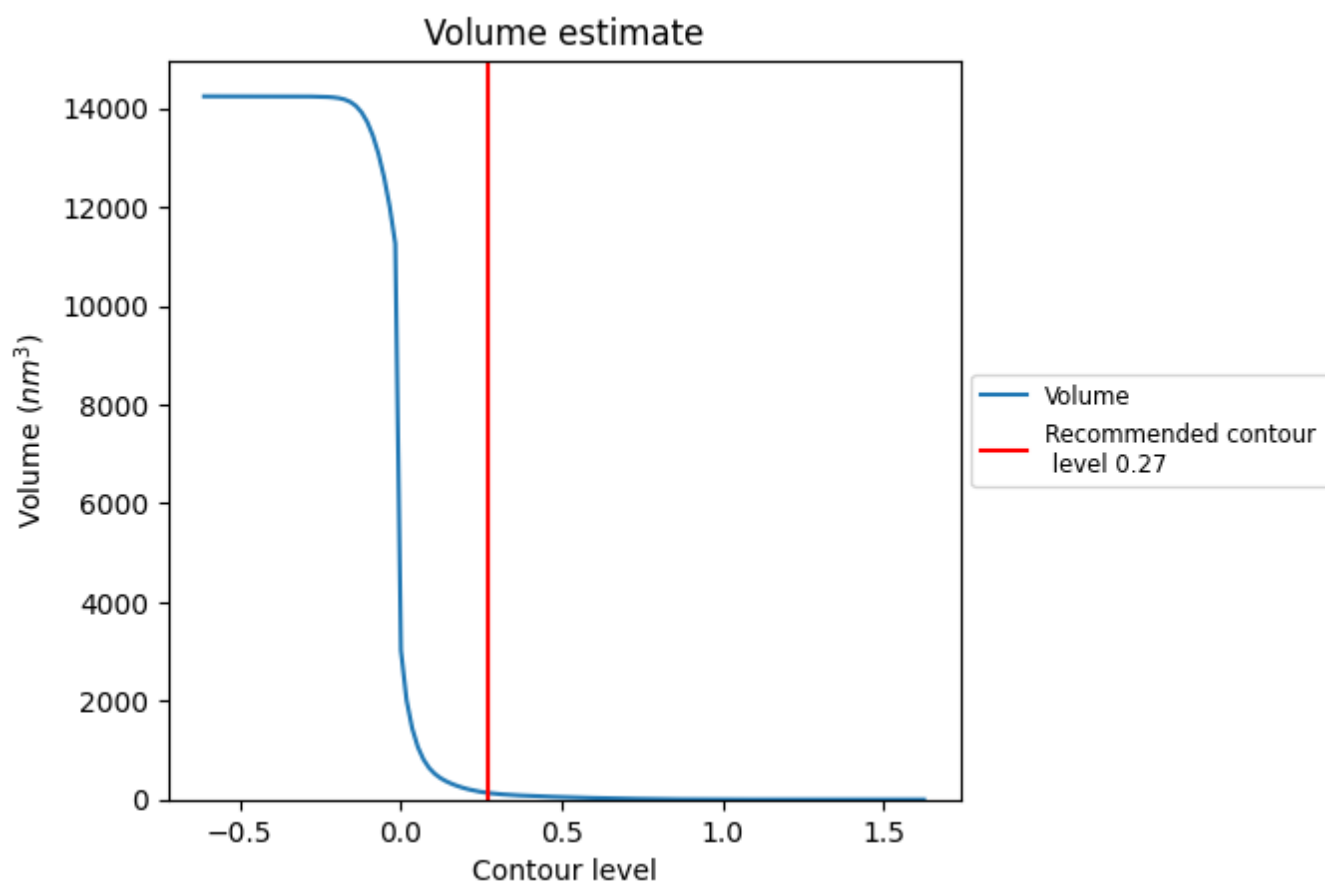
This section contains the results of statistical analysis of the map.

### 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.

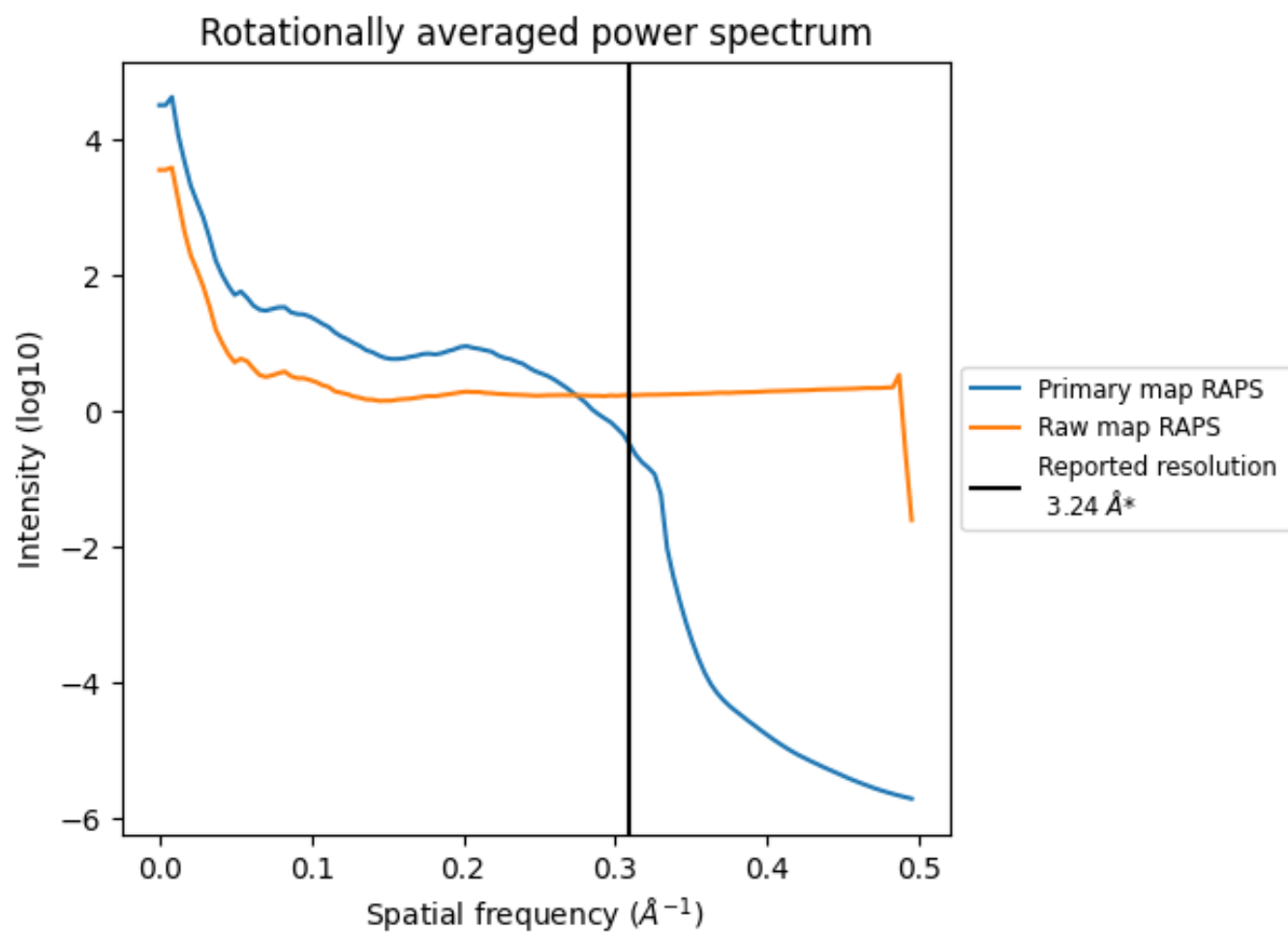
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm<sup>3</sup>; this corresponds to an approximate mass of 123 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



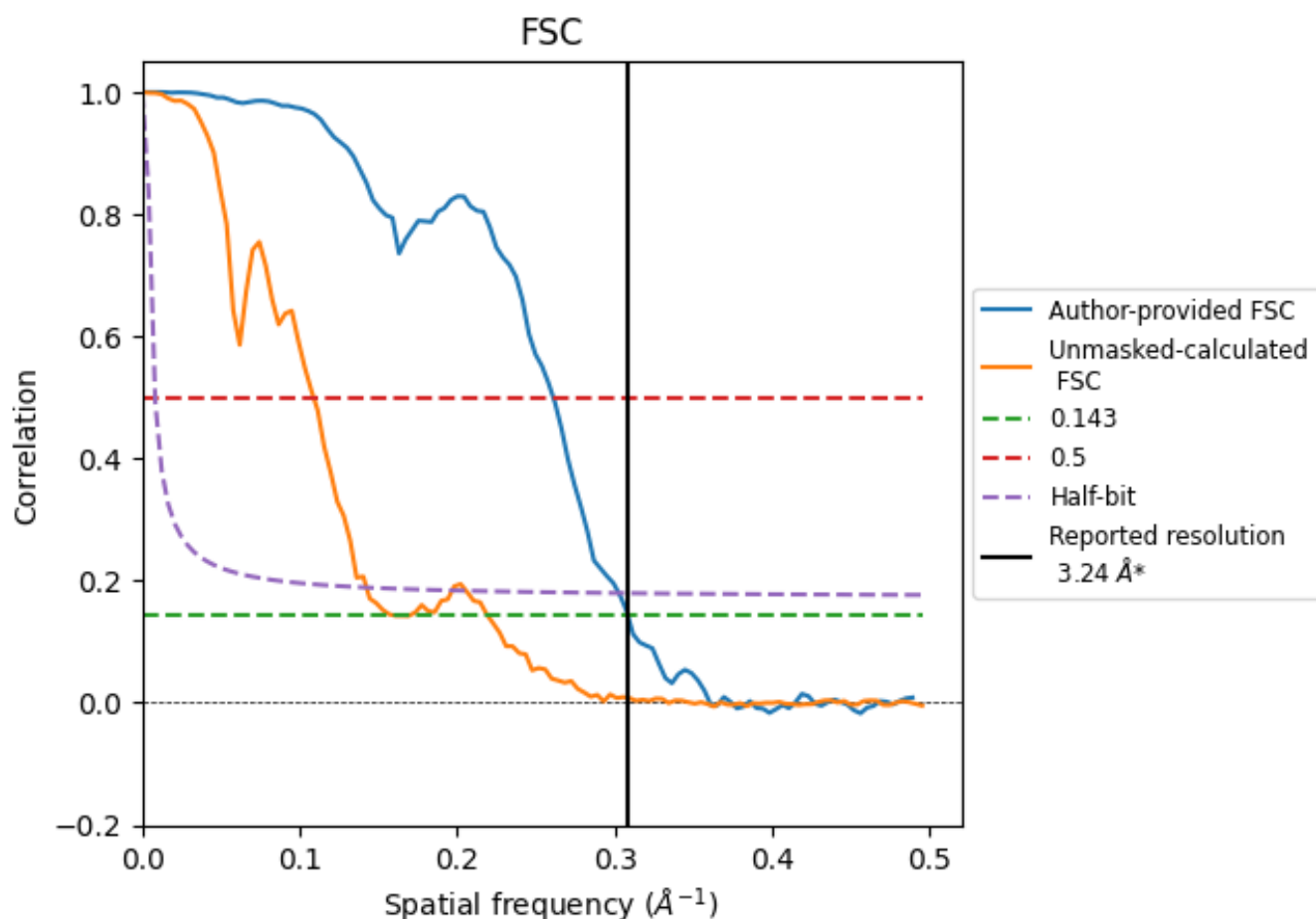
\*Reported resolution corresponds to spatial frequency of 0.309 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.309 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

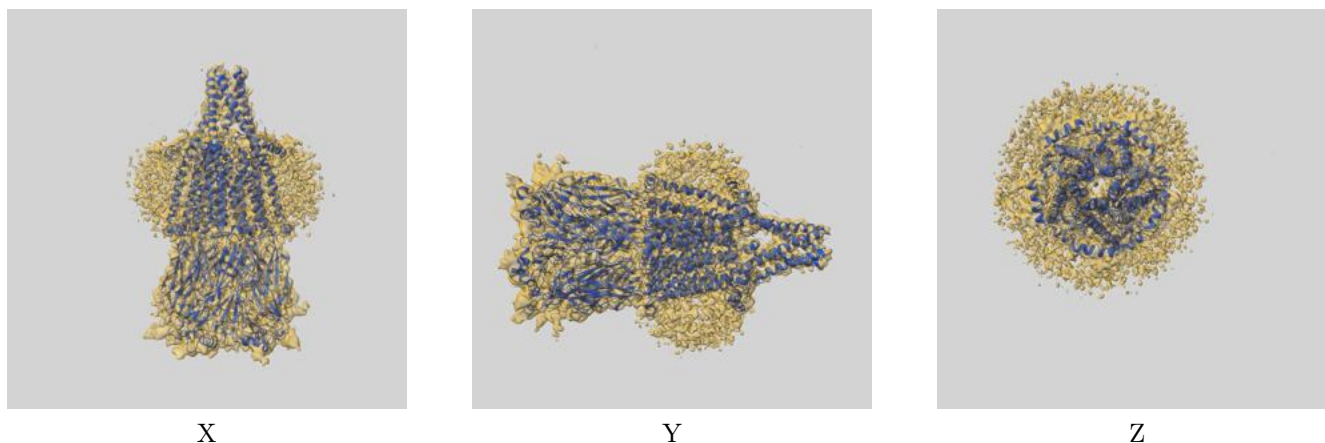
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.24	3.83	3.31
Unmasked-calculated*	6.25	9.20	7.03

\*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 6.25 differs from the reported value 3.24 by more than 10 %

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

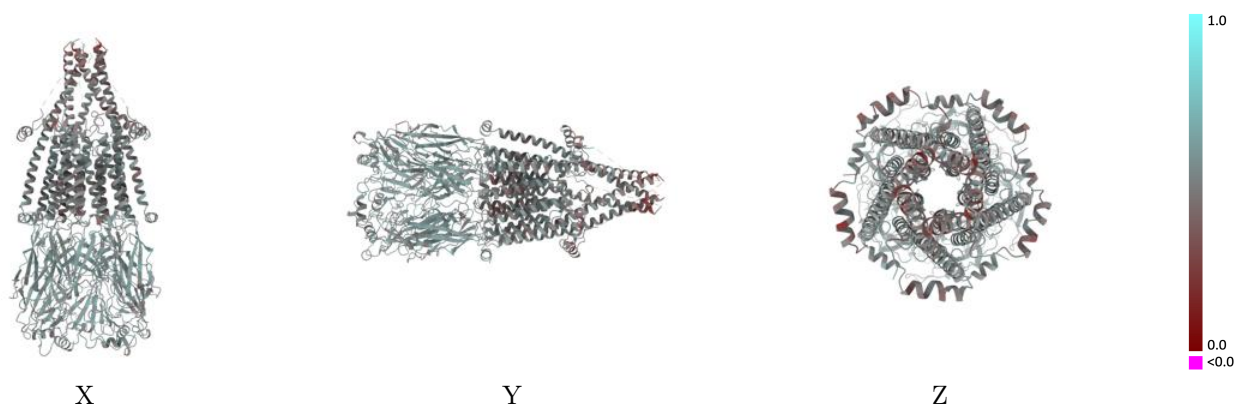
This section contains information regarding the fit between EMDB map EMD-63094 and PDB model 9LHD. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



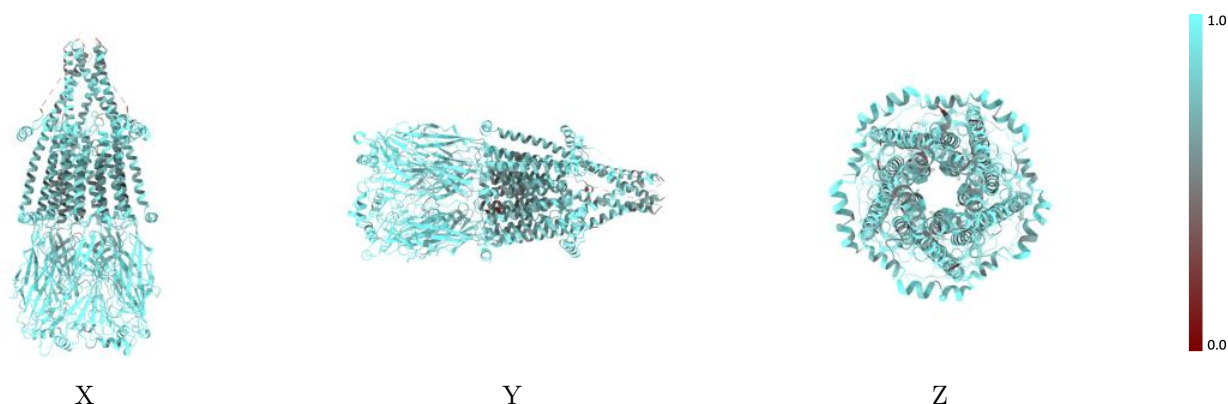
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



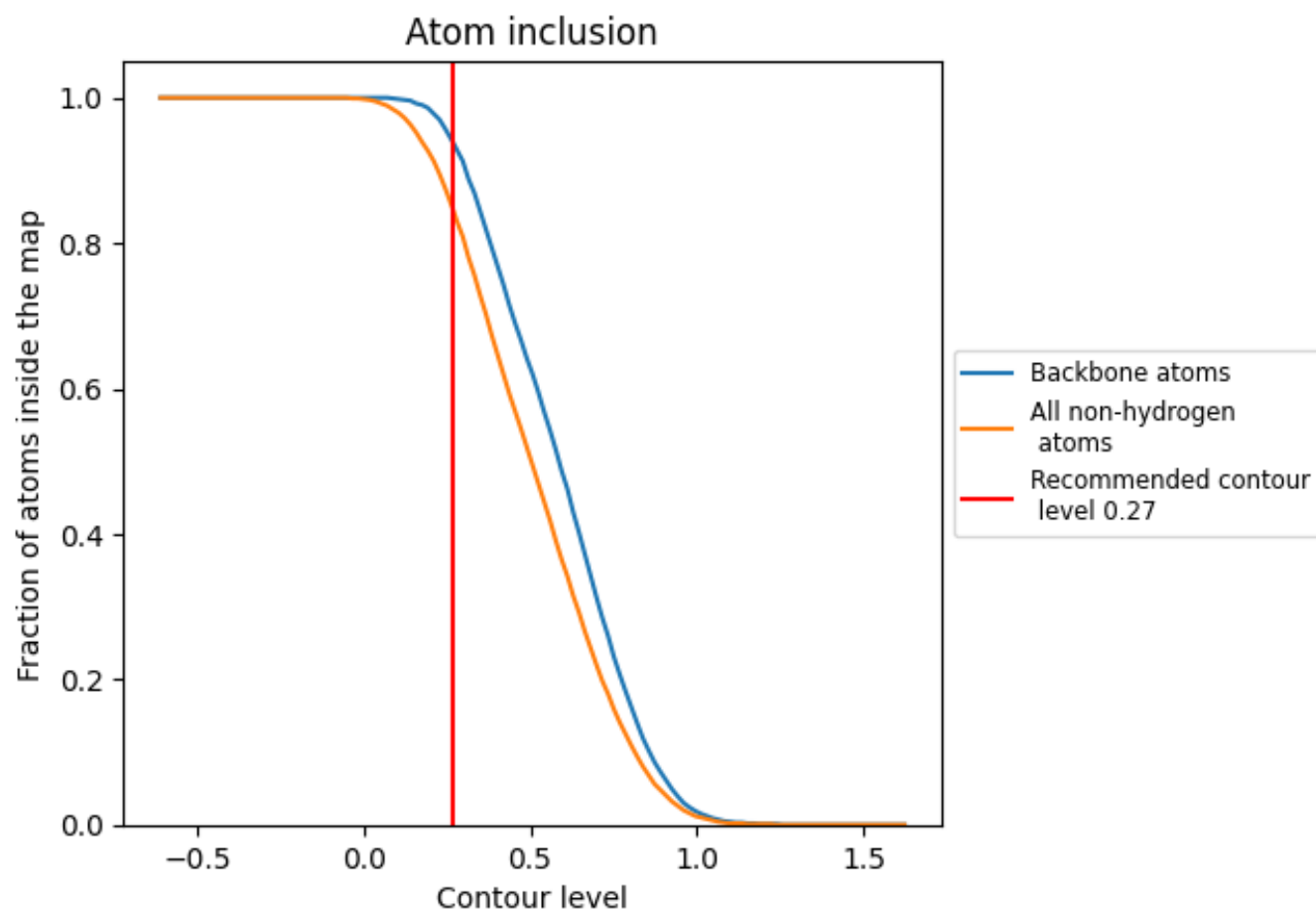
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8440	<div><div></div></div> 0.5140
A	<div><div></div></div> 0.8500	<div><div></div></div> 0.5190
B	<div><div></div></div> 0.8420	<div><div></div></div> 0.5120
C	<div><div></div></div> 0.8480	<div><div></div></div> 0.5110
D	<div><div></div></div> 0.8480	<div><div></div></div> 0.5140
E	<div><div></div></div> 0.8510	<div><div></div></div> 0.5130
F	<div><div></div></div> 0.8210	<div><div></div></div> 0.4890
G	<div><div></div></div> 0.8570	<div><div></div></div> 0.5470
H	<div><div></div></div> 0.8570	<div><div></div></div> 0.5050
I	<div><div></div></div> 0.8930	<div><div></div></div> 0.5140
J	<div><div></div></div> 0.8930	<div><div></div></div> 0.5030

1.0

0.0

<0.0