



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:23 AM UTC

PDB ID : 9FFV / pdb_00009ffv
EMDB ID : EMD-50375
Title : Cryo-EM structure of the alpha1beta3gamma2 GABA(A) receptor in complex with Nb38 in the long-lived symmetric resting state
Authors : Mihaylov, D.B.; Malinauskas, T.; Aricescu, A.R.
Deposited on : 2024-05-23
Resolution : 2.80 Å(reported)
Based on initial model : 6HUK

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

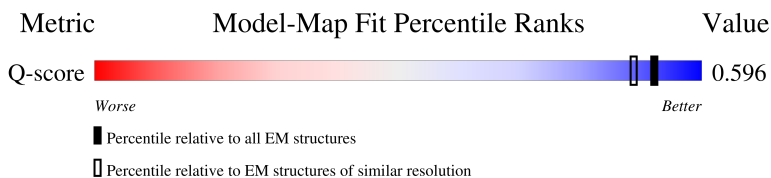
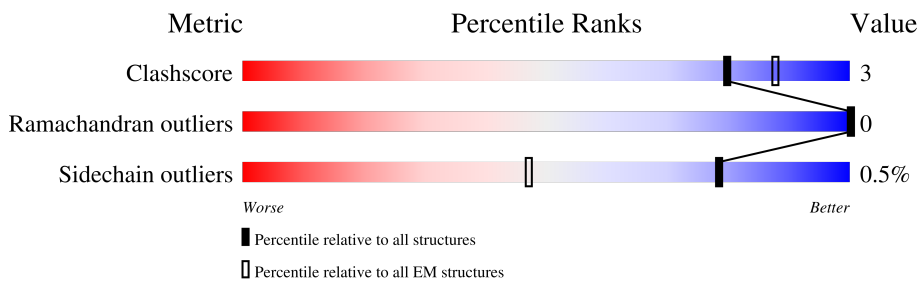
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.






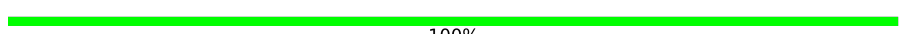


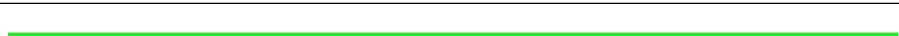
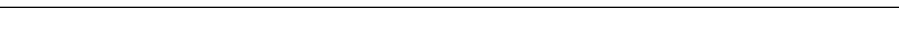
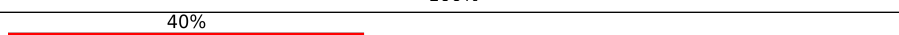
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	411	76% (green), 6% (yellow), 18% (grey)
1	D	411	75% (green), 7% (yellow), 18% (grey)
2	B	395	78% (green), 6% (yellow), 16% (grey)
2	E	395	78% (green), 6% (yellow), 16% (grey)

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Mol	Chain	Length	Quality of chain
3	C	373	 82% 7% 10%
4	F	133	 86% 7% 8%
5	a	10	 70% 30%
6	b	2	 100%
6	c	2	 50% 50%
6	e	2	 100%
7	G	6	 100%
7	H	6	 100%
8	d	5	 40% 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	a	5	X	-	-	-
5	MAN	a	6	X	-	-	-

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 15371 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 Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	338	2763	1784	469	494	16	5	0
1	D	338	2736	1767	461	492	16	1	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-52	MET	-	initiating methionine	UNP P14867
A	-51	ASP	-	expression tag	UNP P14867
A	-50	GLU	-	expression tag	UNP P14867
A	-49	LYS	-	expression tag	UNP P14867
A	-48	THR	-	expression tag	UNP P14867
A	-47	THR	-	expression tag	UNP P14867
A	-46	GLY	-	expression tag	UNP P14867
A	-45	TRP	-	expression tag	UNP P14867
A	-44	ARG	-	expression tag	UNP P14867
A	-43	GLY	-	expression tag	UNP P14867
A	-42	GLY	-	expression tag	UNP P14867
A	-41	HIS	-	expression tag	UNP P14867
A	-40	VAL	-	expression tag	UNP P14867
A	-39	VAL	-	expression tag	UNP P14867
A	-38	GLU	-	expression tag	UNP P14867
A	-37	GLY	-	expression tag	UNP P14867
A	-36	LEU	-	expression tag	UNP P14867
A	-35	ALA	-	expression tag	UNP P14867
A	-34	GLY	-	expression tag	UNP P14867
A	-33	GLU	-	expression tag	UNP P14867
A	-32	LEU	-	expression tag	UNP P14867
A	-31	GLU	-	expression tag	UNP P14867
A	-30	GLN	-	expression tag	UNP P14867
A	-29	LEU	-	expression tag	UNP P14867
A	-28	ARG	-	expression tag	UNP P14867
A	-27	ALA	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	ARG	-	expression tag	UNP P14867
A	-25	LEU	-	expression tag	UNP P14867
A	-24	GLU	-	expression tag	UNP P14867
A	-23	HIS	-	expression tag	UNP P14867
A	-22	HIS	-	expression tag	UNP P14867
A	-21	PRO	-	expression tag	UNP P14867
A	-20	GLN	-	expression tag	UNP P14867
A	-19	GLY	-	expression tag	UNP P14867
A	-18	GLN	-	expression tag	UNP P14867
A	-17	ARG	-	expression tag	UNP P14867
A	-16	GLU	-	expression tag	UNP P14867
A	-15	PRO	-	expression tag	UNP P14867
A	-14	ASP	-	expression tag	UNP P14867
A	-13	TYR	-	expression tag	UNP P14867
A	-12	ASP	-	expression tag	UNP P14867
A	-11	ILE	-	expression tag	UNP P14867
A	-10	PRO	-	expression tag	UNP P14867
A	-9	THR	-	expression tag	UNP P14867
A	-8	THR	-	expression tag	UNP P14867
A	-7	GLU	-	expression tag	UNP P14867
A	-6	ASN	-	expression tag	UNP P14867
A	-5	LEU	-	expression tag	UNP P14867
A	-4	TYR	-	expression tag	UNP P14867
A	-3	PHE	-	expression tag	UNP P14867
A	-2	GLN	-	expression tag	UNP P14867
A	-1	GLY	-	expression tag	UNP P14867
A	0	THR	-	expression tag	UNP P14867
A	1	GLY	-	expression tag	UNP P14867
A	2	GLN	-	expression tag	UNP P14867
A	3	PRO	-	expression tag	UNP P14867
A	4	SER	-	expression tag	UNP P14867
A	313	SER	-	linker	UNP P14867
A	314	GLN	-	linker	UNP P14867
A	315	PRO	-	linker	UNP P14867
A	316	ALA	-	linker	UNP P14867
A	317	ARG	-	linker	UNP P14867
A	318	ALA	-	linker	UNP P14867
A	319	ALA	-	linker	UNP P14867
D	-52	MET	-	initiating methionine	UNP P14867
D	-51	ASP	-	expression tag	UNP P14867
D	-50	GLU	-	expression tag	UNP P14867
D	-49	LYS	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-48	THR	-	expression tag	UNP P14867
D	-47	THR	-	expression tag	UNP P14867
D	-46	GLY	-	expression tag	UNP P14867
D	-45	TRP	-	expression tag	UNP P14867
D	-44	ARG	-	expression tag	UNP P14867
D	-43	GLY	-	expression tag	UNP P14867
D	-42	GLY	-	expression tag	UNP P14867
D	-41	HIS	-	expression tag	UNP P14867
D	-40	VAL	-	expression tag	UNP P14867
D	-39	VAL	-	expression tag	UNP P14867
D	-38	GLU	-	expression tag	UNP P14867
D	-37	GLY	-	expression tag	UNP P14867
D	-36	LEU	-	expression tag	UNP P14867
D	-35	ALA	-	expression tag	UNP P14867
D	-34	GLY	-	expression tag	UNP P14867
D	-33	GLU	-	expression tag	UNP P14867
D	-32	LEU	-	expression tag	UNP P14867
D	-31	GLU	-	expression tag	UNP P14867
D	-30	GLN	-	expression tag	UNP P14867
D	-29	LEU	-	expression tag	UNP P14867
D	-28	ARG	-	expression tag	UNP P14867
D	-27	ALA	-	expression tag	UNP P14867
D	-26	ARG	-	expression tag	UNP P14867
D	-25	LEU	-	expression tag	UNP P14867
D	-24	GLU	-	expression tag	UNP P14867
D	-23	HIS	-	expression tag	UNP P14867
D	-22	HIS	-	expression tag	UNP P14867
D	-21	PRO	-	expression tag	UNP P14867
D	-20	GLN	-	expression tag	UNP P14867
D	-19	GLY	-	expression tag	UNP P14867
D	-18	GLN	-	expression tag	UNP P14867
D	-17	ARG	-	expression tag	UNP P14867
D	-16	GLU	-	expression tag	UNP P14867
D	-15	PRO	-	expression tag	UNP P14867
D	-14	ASP	-	expression tag	UNP P14867
D	-13	TYR	-	expression tag	UNP P14867
D	-12	ASP	-	expression tag	UNP P14867
D	-11	ILE	-	expression tag	UNP P14867
D	-10	PRO	-	expression tag	UNP P14867
D	-9	THR	-	expression tag	UNP P14867
D	-8	THR	-	expression tag	UNP P14867
D	-7	GLU	-	expression tag	UNP P14867

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	ASN	-	expression tag	UNP P14867
D	-5	LEU	-	expression tag	UNP P14867
D	-4	TYR	-	expression tag	UNP P14867
D	-3	PHE	-	expression tag	UNP P14867
D	-2	GLN	-	expression tag	UNP P14867
D	-1	GLY	-	expression tag	UNP P14867
D	0	THR	-	expression tag	UNP P14867
D	1	GLY	-	expression tag	UNP P14867
D	2	GLN	-	expression tag	UNP P14867
D	3	PRO	-	expression tag	UNP P14867
D	4	SER	-	expression tag	UNP P14867
D	313	SER	-	linker	UNP P14867
D	314	GLN	-	linker	UNP P14867
D	315	PRO	-	linker	UNP P14867
D	316	ALA	-	linker	UNP P14867
D	317	ARG	-	linker	UNP P14867
D	318	ALA	-	linker	UNP P14867
D	319	ALA	-	linker	UNP P14867

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	333	Total	C	N	O	S	1	0
			2736	1792	447	481	16		
2	E	333	Total	C	N	O	S	2	0
			2741	1796	447	481	17		

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-53	MET	-	initiating methionine	UNP P28472
B	-52	ASP	-	expression tag	UNP P28472
B	-51	GLU	-	expression tag	UNP P28472
B	-50	LYS	-	expression tag	UNP P28472
B	-49	THR	-	expression tag	UNP P28472
B	-48	THR	-	expression tag	UNP P28472
B	-47	GLY	-	expression tag	UNP P28472
B	-46	TRP	-	expression tag	UNP P28472
B	-45	ARG	-	expression tag	UNP P28472
B	-44	GLY	-	expression tag	UNP P28472
B	-43	GLY	-	expression tag	UNP P28472
B	-42	HIS	-	expression tag	UNP P28472

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-41	VAL	-	expression tag	UNP P28472
B	-40	VAL	-	expression tag	UNP P28472
B	-39	GLU	-	expression tag	UNP P28472
B	-38	GLY	-	expression tag	UNP P28472
B	-37	LEU	-	expression tag	UNP P28472
B	-36	ALA	-	expression tag	UNP P28472
B	-35	GLY	-	expression tag	UNP P28472
B	-34	GLU	-	expression tag	UNP P28472
B	-33	LEU	-	expression tag	UNP P28472
B	-32	GLU	-	expression tag	UNP P28472
B	-31	GLN	-	expression tag	UNP P28472
B	-30	LEU	-	expression tag	UNP P28472
B	-29	ARG	-	expression tag	UNP P28472
B	-28	ALA	-	expression tag	UNP P28472
B	-27	ARG	-	expression tag	UNP P28472
B	-26	LEU	-	expression tag	UNP P28472
B	-25	GLU	-	expression tag	UNP P28472
B	-24	HIS	-	expression tag	UNP P28472
B	-23	HIS	-	expression tag	UNP P28472
B	-22	PRO	-	expression tag	UNP P28472
B	-21	GLN	-	expression tag	UNP P28472
B	-20	GLY	-	expression tag	UNP P28472
B	-19	GLN	-	expression tag	UNP P28472
B	-18	ARG	-	expression tag	UNP P28472
B	-17	GLU	-	expression tag	UNP P28472
B	-16	PRO	-	expression tag	UNP P28472
B	-15	ASP	-	expression tag	UNP P28472
B	-14	TYR	-	expression tag	UNP P28472
B	-13	ASP	-	expression tag	UNP P28472
B	-12	ILE	-	expression tag	UNP P28472
B	-11	PRO	-	expression tag	UNP P28472
B	-10	THR	-	expression tag	UNP P28472
B	-9	THR	-	expression tag	UNP P28472
B	-8	GLU	-	expression tag	UNP P28472
B	-7	ASN	-	expression tag	UNP P28472
B	-6	LEU	-	expression tag	UNP P28472
B	-5	TYR	-	expression tag	UNP P28472
B	-4	PHE	-	expression tag	UNP P28472
B	-3	GLN	-	expression tag	UNP P28472
B	-2	GLY	-	expression tag	UNP P28472
B	-1	THR	-	expression tag	UNP P28472
B	0	GLY	-	expression tag	UNP P28472

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Chain	Residue	Modelled	Actual	Comment	Reference
B	308	SER	-	linker	UNP P28472
B	309	GLN	-	linker	UNP P28472
B	310	PRO	-	linker	UNP P28472
B	311	ALA	-	linker	UNP P28472
B	312	ARG	-	linker	UNP P28472
B	313	ALA	-	linker	UNP P28472
B	314	ALA	-	linker	UNP P28472
E	-53	MET	-	initiating methionine	UNP P28472
E	-52	ASP	-	expression tag	UNP P28472
E	-51	GLU	-	expression tag	UNP P28472
E	-50	LYS	-	expression tag	UNP P28472
E	-49	THR	-	expression tag	UNP P28472
E	-48	THR	-	expression tag	UNP P28472
E	-47	GLY	-	expression tag	UNP P28472
E	-46	TRP	-	expression tag	UNP P28472
E	-45	ARG	-	expression tag	UNP P28472
E	-44	GLY	-	expression tag	UNP P28472
E	-43	GLY	-	expression tag	UNP P28472
E	-42	HIS	-	expression tag	UNP P28472
E	-41	VAL	-	expression tag	UNP P28472
E	-40	VAL	-	expression tag	UNP P28472
E	-39	GLU	-	expression tag	UNP P28472
E	-38	GLY	-	expression tag	UNP P28472
E	-37	LEU	-	expression tag	UNP P28472
E	-36	ALA	-	expression tag	UNP P28472
E	-35	GLY	-	expression tag	UNP P28472
E	-34	GLU	-	expression tag	UNP P28472
E	-33	LEU	-	expression tag	UNP P28472
E	-32	GLU	-	expression tag	UNP P28472
E	-31	GLN	-	expression tag	UNP P28472
E	-30	LEU	-	expression tag	UNP P28472
E	-29	ARG	-	expression tag	UNP P28472
E	-28	ALA	-	expression tag	UNP P28472
E	-27	ARG	-	expression tag	UNP P28472
E	-26	LEU	-	expression tag	UNP P28472
E	-25	GLU	-	expression tag	UNP P28472
E	-24	HIS	-	expression tag	UNP P28472
E	-23	HIS	-	expression tag	UNP P28472
E	-22	PRO	-	expression tag	UNP P28472
E	-21	GLN	-	expression tag	UNP P28472
E	-20	GLY	-	expression tag	UNP P28472
E	-19	GLN	-	expression tag	UNP P28472

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	ARG	-	expression tag	UNP P28472
E	-17	GLU	-	expression tag	UNP P28472
E	-16	PRO	-	expression tag	UNP P28472
E	-15	ASP	-	expression tag	UNP P28472
E	-14	TYR	-	expression tag	UNP P28472
E	-13	ASP	-	expression tag	UNP P28472
E	-12	ILE	-	expression tag	UNP P28472
E	-11	PRO	-	expression tag	UNP P28472
E	-10	THR	-	expression tag	UNP P28472
E	-9	THR	-	expression tag	UNP P28472
E	-8	GLU	-	expression tag	UNP P28472
E	-7	ASN	-	expression tag	UNP P28472
E	-6	LEU	-	expression tag	UNP P28472
E	-5	TYR	-	expression tag	UNP P28472
E	-4	PHE	-	expression tag	UNP P28472
E	-3	GLN	-	expression tag	UNP P28472
E	-2	GLY	-	expression tag	UNP P28472
E	-1	THR	-	expression tag	UNP P28472
E	0	GLY	-	expression tag	UNP P28472
E	308	SER	-	linker	UNP P28472
E	309	GLN	-	linker	UNP P28472
E	310	PRO	-	linker	UNP P28472
E	311	ALA	-	linker	UNP P28472
E	312	ARG	-	linker	UNP P28472
E	313	ALA	-	linker	UNP P28472
E	314	ALA	-	linker	UNP P28472

- Molecule 3 is a protein called Isoform 1 of Gamma-aminobutyric acid receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	334	2765	1808	452	488	17	6	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	THR	-	expression tag	UNP P18507
C	0	GLY	-	expression tag	UNP P18507
C	11	THR	ALA	conflict	UNP P18507
C	323	SER	-	linker	UNP P18507
C	324	GLN	-	linker	UNP P18507

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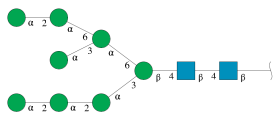
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Chain	Residue	Modelled	Actual	Comment	Reference
C	325	PRO	-	linker	UNP P18507
C	326	ALA	-	linker	UNP P18507
C	327	ARG	-	linker	UNP P18507
C	328	ALA	-	linker	UNP P18507
C	429	GLY	-	expression tag	UNP P18507
C	430	THR	-	expression tag	UNP P18507
C	431	GLY	-	expression tag	UNP P18507
C	432	GLY	-	expression tag	UNP P18507
C	433	THR	-	expression tag	UNP P18507
C	434	THR	-	expression tag	UNP P18507
C	435	GLU	-	expression tag	UNP P18507
C	436	THR	-	expression tag	UNP P18507
C	437	SER	-	expression tag	UNP P18507
C	438	GLN	-	expression tag	UNP P18507
C	439	VAL	-	expression tag	UNP P18507
C	440	ALA	-	expression tag	UNP P18507
C	441	PRO	-	expression tag	UNP P18507
C	442	ALA	-	expression tag	UNP P18507

- Molecule 4 is a protein called Nanobody38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	123	950	594	171	181	4	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



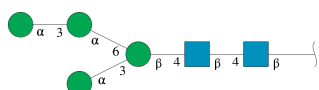
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	a	10	116	64	2	50	0	0

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



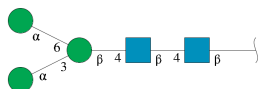
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	b	2	28	16	2	10	0	0
6	c	2	28	16	2	10	0	0
6	e	2	28	16	2	10	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.



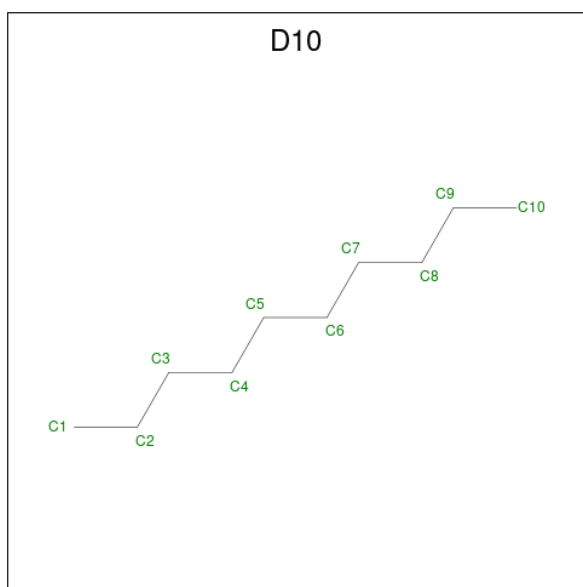
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	6	72	40	2	30	0	0
7	H	6	72	40	2	30	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	d	5	61	34	2	25	0	0

- Molecule 9 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C 10 10	0
9	B	1	Total C 10 10	0
9	C	1	Total C 10 10	0
9	D	1	Total C 10 10	0
9	E	1	Total C 10 10	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
10	C	1	Total Cl 1 1	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	AltConf
11	A	45	Total O 45 45	0
11	B	58	Total O 58 58	0
11	C	39	Total O 39 39	0

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Mol	Chain	Residues	Atoms		AltConf
11	D	33	Total 33	O 33	0
11	E	44	Total 44	O 44	0
11	F	5	Total 5	O 5	0

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

Chain e:  100%

MAG1
MAG2

- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 G:  100%



MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 H:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  40%  100%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.601	Depositor
Minimum map value	-0.284	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	327.98, 327.98, 327.98	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.713, 0.713, 0.713	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: MAN, D10, NAG, BMA, CL

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	0.10	0/2847	0.24	0/3868
1	D	0.09	0/2808	0.24	0/3817
2	B	0.10	0/2813	0.25	0/3829
2	E	0.10	0/2821	0.24	0/3840
3	C	0.10	0/2859	0.24	0/3892
4	F	0.09	0/971	0.23	0/1312
All	All	0.10	0/15119	0.24	0/20558

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	2763	0	2770	17	0
1	D	2736	0	2730	22	0
2	B	2736	0	2733	18	0
2	E	2741	0	2742	18	0
3	C	2765	0	2773	15	0
4	F	950	0	900	5	0
5	a	116	0	97	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	b	28	0	25	0	0
6	c	28	0	25	1	0
6	e	28	0	25	0	0
7	G	72	0	61	0	0
7	H	72	0	61	0	0
8	d	61	0	52	0	0
9	A	10	0	22	0	0
9	B	10	0	22	1	0
9	C	10	0	22	0	0
9	D	10	0	22	0	0
9	E	10	0	22	0	0
10	C	1	0	0	0	0
11	A	45	0	0	0	0
11	B	58	0	0	2	0
11	C	39	0	0	0	0
11	D	33	0	0	0	0
11	E	44	0	0	1	0
11	F	5	0	0	0	0
All	All	15371	0	15104	83	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 3.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:THR:HG21	2:B:281:ILE:HD11	1.61	0.81
2:E:225:THR:HG21	2:E:281:ILE:HD11	1.72	0.72
2:B:102:LYS:HD2	2:B:135:ALA:HB2	1.75	0.68
3:C:100:SER:HB3	3:C:129:ARG:HB2	1.80	0.64
2:E:64:GLN:NE2	11:E:605:HOH:O	2.33	0.61
1:D:59:GLU:OE1	1:D:105:LYS:NZ	2.33	0.61
1:D:112:MET:HE1	2:E:106:VAL:HG23	1.84	0.60
2:B:180:ARG:NH2	11:B:607:HOH:O	2.35	0.60
2:E:102:LYS:HD2	2:E:135:ALA:HB2	1.84	0.60
1:A:112:MET:HE1	2:B:106:VAL:HG23	1.84	0.59
3:C:199:TYR:HB3	1:D:280:VAL:HG12	1.82	0.59
3:C:282:ILE:HD12	1:D:271:ILE:HG23	1.84	0.59
4:F:39:ARG:HB2	4:F:49:LEU:HD11	1.84	0.58
1:A:67[A]:ARG:HG2	1:A:130:THR:HG22	1.86	0.57
2:B:140:LEU:HD13	2:B:275:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:MET:HG2	2:E:95:ASP:HA	1.89	0.55
4:F:83:LEU:HD23	4:F:86:LEU:HD21	1.88	0.55
1:D:114:MET:HE3	2:E:95:ASP:HB2	1.89	0.55
3:C:186:SER:OG	3:C:189:GLU:OE2	2.23	0.54
1:A:236:MET:HE1	2:B:290:VAL:HG22	1.91	0.52
1:D:121:ILE:HG12	1:D:127:LEU:HD22	1.90	0.52
3:C:183:TRP:HB2	6:c:1:NAG:H62	1.90	0.52
1:A:156:LYS:HG2	1:A:214:THR:HG23	1.92	0.52
2:B:36:VAL:HG13	2:B:164:ILE:HG13	1.91	0.51
1:D:73:GLU:O	1:D:76:LYS:NZ	2.43	0.51
1:D:149:ASP:OD2	1:D:151:HIS:NE2	2.41	0.51
1:D:236:MET:HE1	2:E:290:VAL:HG22	1.92	0.51
2:E:66:TYR:CZ	2:E:125:LEU:HD13	2.47	0.50
1:D:115:PRO:HB3	5:a:9:MAN:H4	1.94	0.49
1:D:156:LYS:HG2	1:D:214:THR:HG23	1.95	0.49
2:B:41:ASN:ND2	2:B:169:ARG:O	2.45	0.48
1:D:110:HIS:HE2	1:D:134:THR:HG1	1.56	0.48
2:E:12:VAL:HG22	2:E:77:ILE:HD13	1.96	0.48
1:A:114:MET:HE3	2:B:95:ASP:HB2	1.95	0.48
2:E:302:VAL:HG13	2:E:313:ALA:HB1	1.95	0.48
3:C:320:PHE:HD2	3:C:402:MET:HE1	1.81	0.46
5:a:2:NAG:O7	5:a:10:MAN:O2	2.31	0.46
3:C:317:LEU:HD12	3:C:328:ALA:HB1	1.98	0.45
1:A:121:ILE:HG12	1:A:127:LEU:HD22	1.99	0.45
2:E:62:TYR:HB3	2:E:64:GLN:HE22	1.81	0.45
2:B:238:VAL:HG22	9:B:501:D10:H41	1.99	0.44
4:F:13:VAL:HG21	4:F:86:LEU:HD12	1.99	0.44
1:D:149:ASP:OD1	1:D:149:ASP:N	2.48	0.44
1:A:301:LEU:HD23	2:E:235:LEU:HD22	2.00	0.44
1:D:404:PHE:O	1:D:408:ASN:ND2	2.41	0.44
1:A:149:ASP:OD1	1:A:149:ASP:N	2.49	0.43
3:C:254:SER:HB2	3:C:268:LEU:HD23	2.01	0.43
3:C:158:PHE:CD2	3:C:287:LEU:HD11	2.54	0.43
1:A:122:THR:OG1	1:A:124:ASP:OD1	2.28	0.43
1:A:225:TYR:HB2	2:B:277:TYR:HA	2.01	0.43
2:B:233:THR:O	2:B:236:SER:OG	2.37	0.42
3:C:166:PRO:HB3	3:C:226:TYR:CE2	2.55	0.42
1:D:274:ARG:HH22	1:D:280:VAL:HG23	1.83	0.42
3:C:295:ALA:O	3:C:421:TYR:OH	2.35	0.42
1:A:112:MET:HA	1:A:113:THR:HA	1.78	0.42
2:B:48:ASP:OD1	2:B:48:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:TYR:CE1	3:C:239[A]:GLN:HG3	2.54	0.42
4:F:2:GLN:HG2	4:F:3:VAL:H	1.85	0.42
1:D:117:LYS:HE2	1:D:131:MET:HE2	2.00	0.42
1:D:190:GLN:N	1:D:190:GLN:OE1	2.53	0.42
1:A:409:LEU:HD13	1:A:409:LEU:HA	1.95	0.42
1:A:70:TRP:NE1	1:A:127:LEU:HD12	2.36	0.41
2:E:146:ASP:OD2	2:E:148:GLN:NE2	2.47	0.41
1:D:112:MET:HA	1:D:113:THR:HA	1.74	0.41
1:D:122:THR:OG1	1:D:124:ASP:OD1	2.25	0.41
2:B:235:LEU:HD22	3:C:311:LEU:HD23	2.02	0.41
1:A:85[A]:ARG:NH1	2:B:158:GLY:O	2.54	0.41
2:E:281:ILE:HD12	2:E:281:ILE:HA	1.87	0.41
1:A:204[B]:GLN:HG2	1:A:209:GLU:HG2	2.02	0.41
2:B:37:CYS:SG	11:B:645:HOH:O	2.63	0.41
3:C:124:ILE:HA	3:C:125:THR:HA	1.75	0.41
4:F:62:ASP:OD1	4:F:65:ARG:NH2	2.54	0.41
3:C:59:VAL:HB	3:C:190:VAL:HG12	2.02	0.40
1:D:15:PHE:HE1	1:D:80:PRO:HG2	1.85	0.40
2:E:233:THR:O	2:E:236:SER:OG	2.37	0.40
1:A:86:LEU:HD11	1:A:121:ILE:HD11	2.03	0.40
2:E:40:MET:HG3	2:E:208:LEU:HD12	2.02	0.40
2:E:40:MET:SD	2:E:65:GLN:HG2	2.60	0.40
2:B:146:ASP:OD1	2:B:146:ASP:N	2.53	0.40
2:E:48:ASP:N	2:E:48:ASP:OD1	2.54	0.40
1:A:87:ASN:ND2	1:A:89:LEU:H	2.19	0.40
1:D:184:ASP:OD1	1:D:184:ASP:N	2.45	0.40
2:B:99:LEU:HB3	2:B:153:GLU:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/411 (83%)	337 (99%)	4 (1%)	0	100	100
1	D	337/411 (82%)	332 (98%)	5 (2%)	0	100	100
2	B	332/395 (84%)	330 (99%)	2 (1%)	0	100	100
2	E	333/395 (84%)	332 (100%)	1 (0%)	0	100	100
3	C	338/373 (91%)	330 (98%)	8 (2%)	0	100	100
4	F	121/133 (91%)	116 (96%)	5 (4%)	0	100	100
All	All	1802/2118 (85%)	1777 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/362 (84%)	301 (99%)	4 (1%)	61	86
1	D	301/362 (83%)	299 (99%)	2 (1%)	76	91
2	B	299/349 (86%)	299 (100%)	0	100	100
2	E	300/349 (86%)	300 (100%)	0	100	100
3	C	311/339 (92%)	308 (99%)	3 (1%)	68	88
4	F	94/103 (91%)	94 (100%)	0	100	100
All	All	1610/1864 (86%)	1601 (99%)	9 (1%)	78	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	MET
1	A	240	LEU
1	A	393	ASP
1	A	409	LEU
3	C	130[A]	MET
3	C	130[B]	MET
3	C	199	TYR

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Mol	Chain	Res	Type
1	D	114	MET
1	D	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	88	ASN
1	A	142	HIS
1	A	248	ASN
2	B	85	ASN
2	B	265	ASN
2	B	303	ASN
2	B	309	GLN
3	C	80	GLN
3	C	128	ASN
3	C	324	GLN
1	D	68	GLN
1	D	87	ASN
1	D	218	HIS
1	D	229	GLN
2	E	41	ASN
2	E	64	GLN
2	E	65	GLN
2	E	85	ASN
4	F	6	GLN
4	F	14	GLN

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](#)

33 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	G	1	7,2	14,14,15	0.24	0	17,19,21	0.50	0
7	NAG	G	2	7	14,14,15	0.23	0	17,19,21	0.47	0
7	BMA	G	3	7	11,11,12	0.18	0	15,15,17	0.42	0
7	MAN	G	4	7	11,11,12	0.17	0	15,15,17	0.49	0
7	MAN	G	5	7	11,11,12	0.20	0	15,15,17	0.33	0
7	MAN	G	6	7	11,11,12	0.18	0	15,15,17	0.39	0
7	NAG	H	1	7,2	14,14,15	0.23	0	17,19,21	0.44	0
7	NAG	H	2	7	14,14,15	0.23	0	17,19,21	0.48	0
7	BMA	H	3	7	11,11,12	0.18	0	15,15,17	0.34	0
7	MAN	H	4	7	11,11,12	0.18	0	15,15,17	0.38	0
7	MAN	H	5	7	11,11,12	0.19	0	15,15,17	0.49	0
7	MAN	H	6	7	11,11,12	0.18	0	15,15,17	0.39	0
5	NAG	a	1	5,1	14,14,15	0.23	0	17,19,21	0.53	0
5	MAN	a	10	5	11,11,12	0.21	0	15,15,17	0.48	0
5	NAG	a	2	5	14,14,15	0.23	0	17,19,21	0.43	0
5	BMA	a	3	5	11,11,12	0.19	0	15,15,17	0.48	0
5	MAN	a	4	5	11,11,12	0.19	0	15,15,17	0.50	0
5	MAN	a	5	5	11,11,12	0.19	0	15,15,17	0.42	0
5	MAN	a	6	5	11,11,12	0.18	0	15,15,17	0.32	0
5	MAN	a	7	5	11,11,12	0.18	0	15,15,17	0.45	0
5	MAN	a	8	5	11,11,12	0.17	0	15,15,17	0.45	0
5	MAN	a	9	5	11,11,12	0.19	0	15,15,17	0.33	0
6	NAG	b	1	6,2	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	b	2	6	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	c	1	3,6	14,14,15	0.25	0	17,19,21	0.48	0
6	NAG	c	2	6	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	d	1	8,1	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	d	2	8	14,14,15	0.23	0	17,19,21	0.50	0
8	BMA	d	3	8	11,11,12	0.19	0	15,15,17	0.30	0
8	MAN	d	4	8	11,11,12	0.18	0	15,15,17	0.39	0
8	MAN	d	5	8	11,11,12	0.19	0	15,15,17	0.36	0
6	NAG	e	1	6,2	14,14,15	0.22	0	17,19,21	0.46	0
6	NAG	e	2	6	14,14,15	0.23	0	17,19,21	0.45	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	G	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	1/2/19/22	0/1/1/1
7	MAN	G	5	7	-	0/2/19/22	0/1/1/1
7	MAN	G	6	7	-	1/2/19/22	0/1/1/1
7	NAG	H	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	H	2	7	-	0/6/23/26	0/1/1/1
7	BMA	H	3	7	-	0/2/19/22	0/1/1/1
7	MAN	H	4	7	-	0/2/19/22	0/1/1/1
7	MAN	H	5	7	-	1/2/19/22	0/1/1/1
7	MAN	H	6	7	-	0/2/19/22	0/1/1/1
5	NAG	a	1	5,1	-	0/6/23/26	0/1/1/1
5	MAN	a	10	5	-	0/2/19/22	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
5	MAN	a	4	5	-	0/2/19/22	0/1/1/1
5	MAN	a	5	5	1/1/4/5	1/2/19/22	0/1/1/1
5	MAN	a	6	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	a	7	5	-	0/2/19/22	0/1/1/1
5	MAN	a	8	5	-	0/2/19/22	0/1/1/1
5	MAN	a	9	5	-	0/2/19/22	0/1/1/1
6	NAG	b	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1
6	NAG	c	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	c	2	6	-	2/6/23/26	0/1/1/1
8	NAG	d	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	d	2	8	-	0/6/23/26	0/1/1/1
8	BMA	d	3	8	-	0/2/19/22	0/1/1/1
8	MAN	d	4	8	-	0/2/19/22	0/1/1/1
8	MAN	d	5	8	-	0/2/19/22	0/1/1/1
6	NAG	e	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	a	5	MAN	C1
5	a	6	MAN	C1

All (8) torsion outliers are listed below:

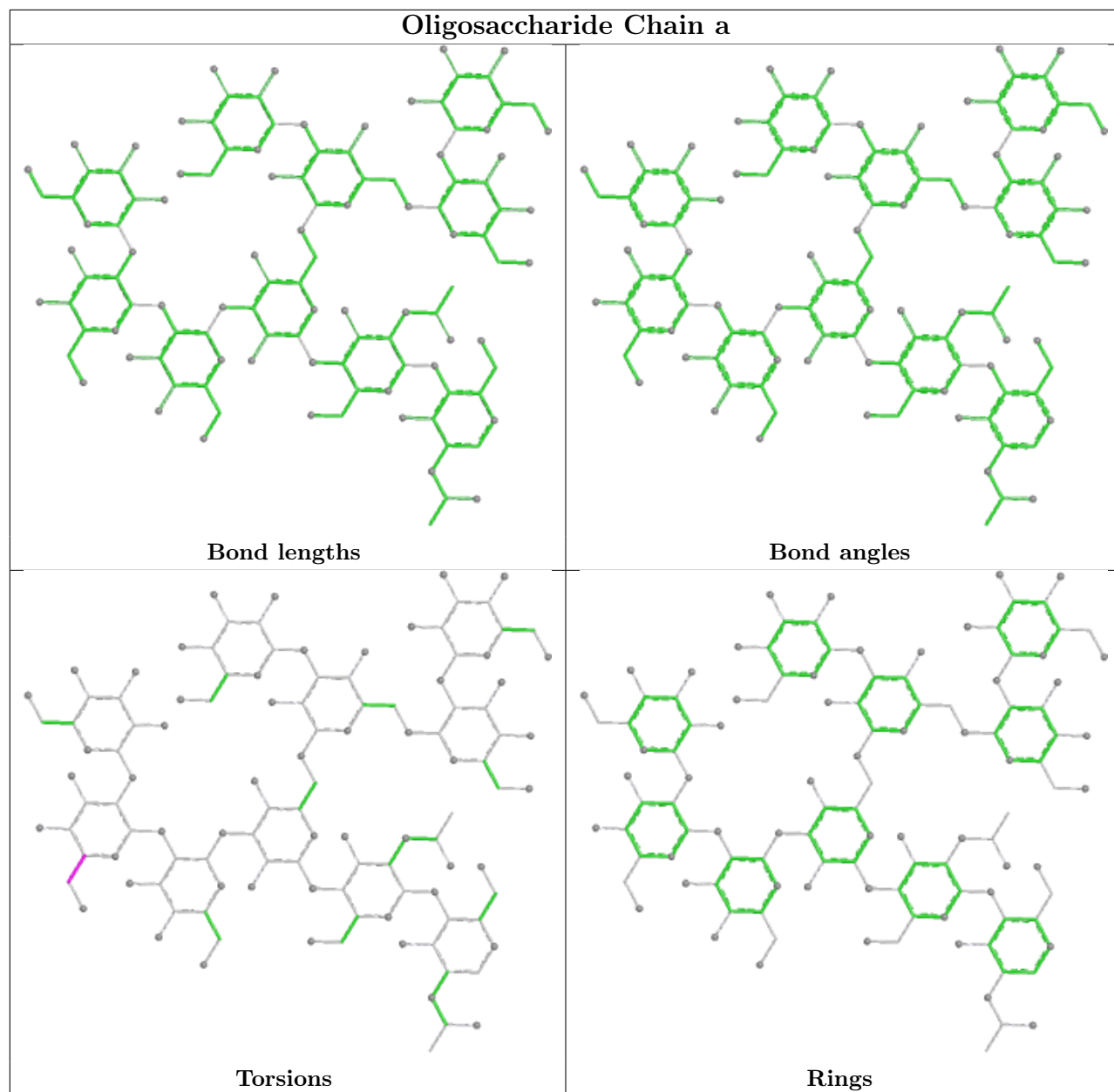
Mol	Chain	Res	Type	Atoms
6	c	1	NAG	C8-C7-N2-C2
6	c	1	NAG	O7-C7-N2-C2
6	c	2	NAG	C8-C7-N2-C2
6	c	2	NAG	O7-C7-N2-C2
7	G	4	MAN	O5-C5-C6-O6
7	G	6	MAN	O5-C5-C6-O6
7	H	5	MAN	O5-C5-C6-O6
5	a	5	MAN	O5-C5-C6-O6

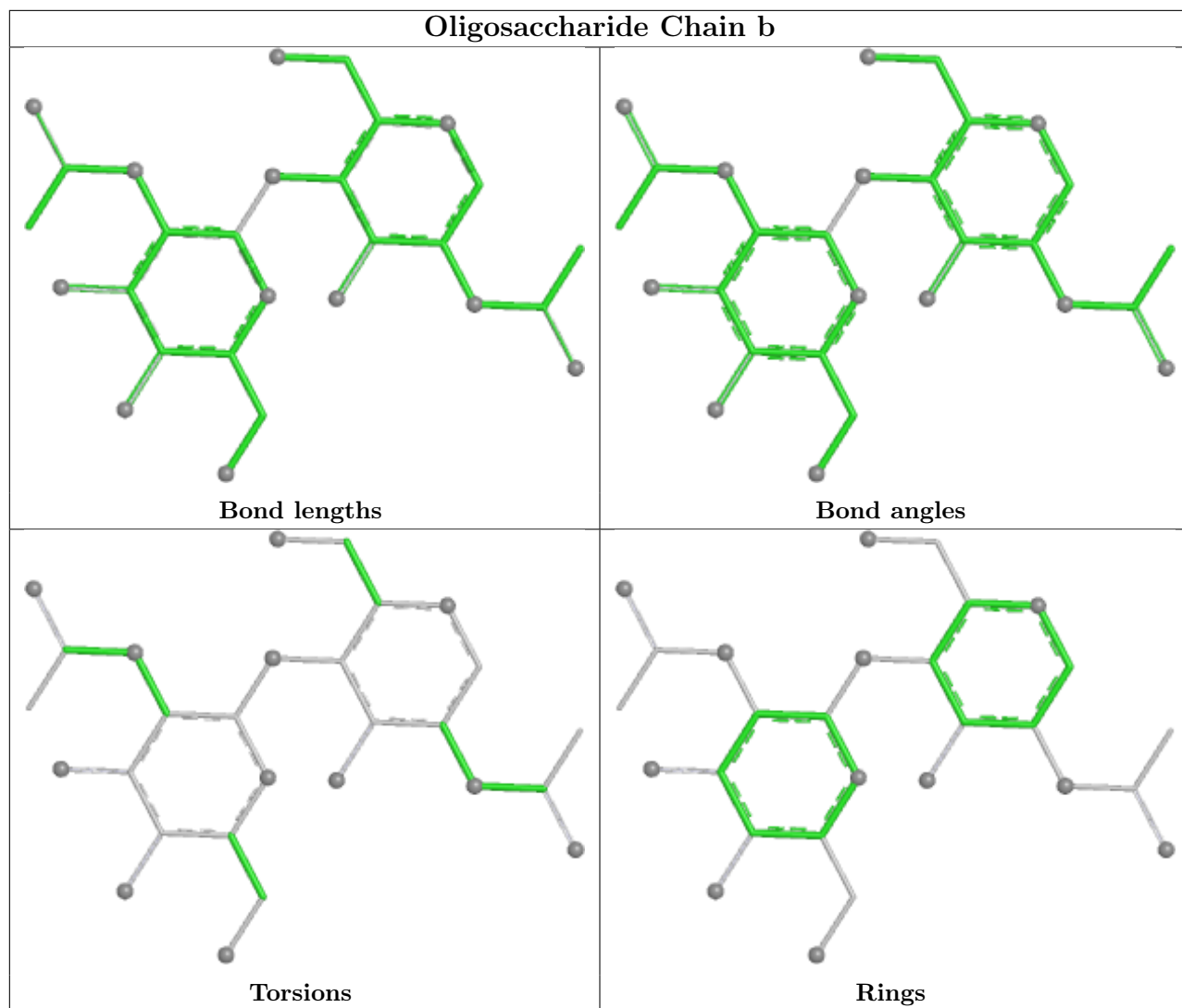
There are no ring outliers.

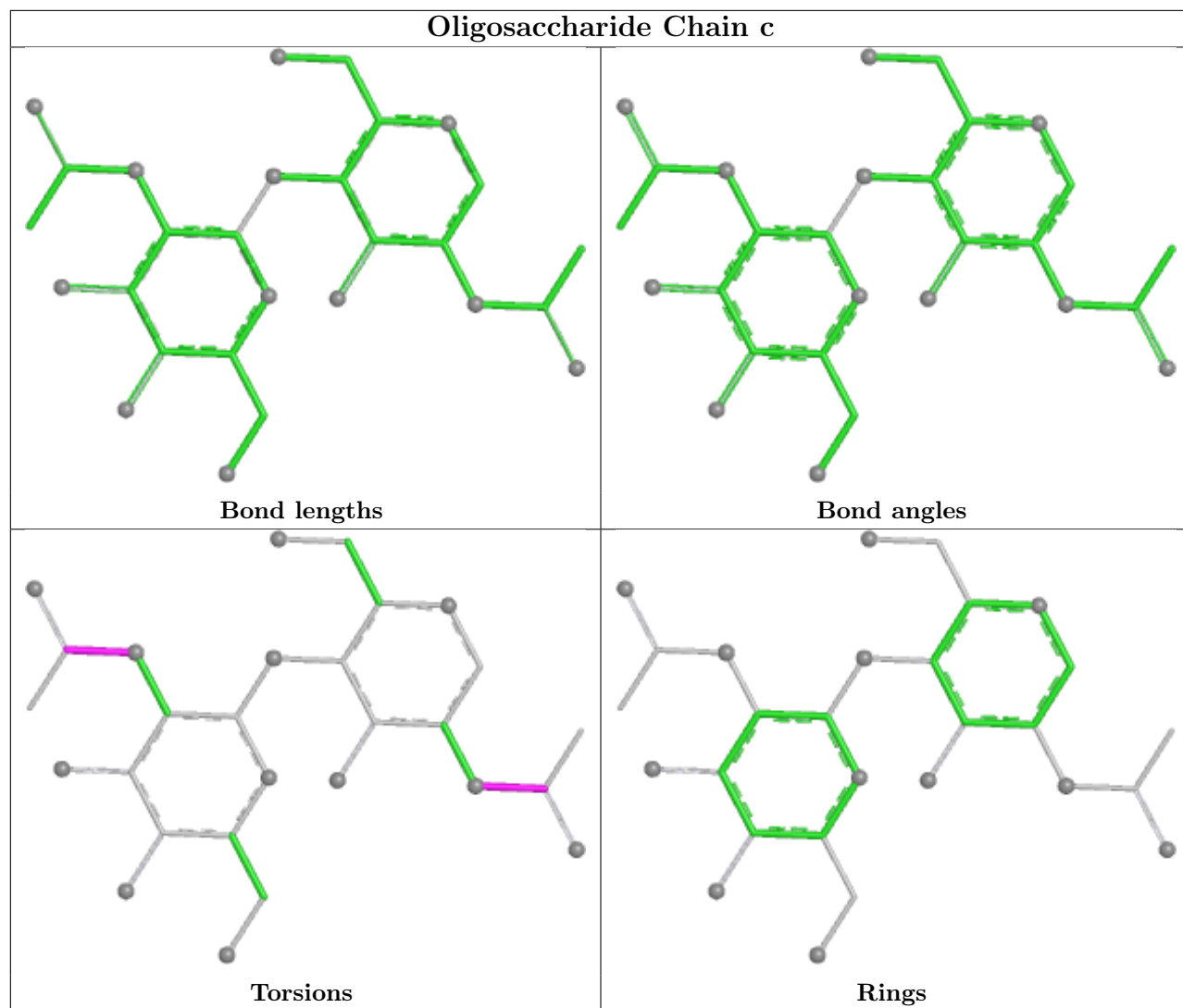
4 monomers are involved in 3 short contacts:

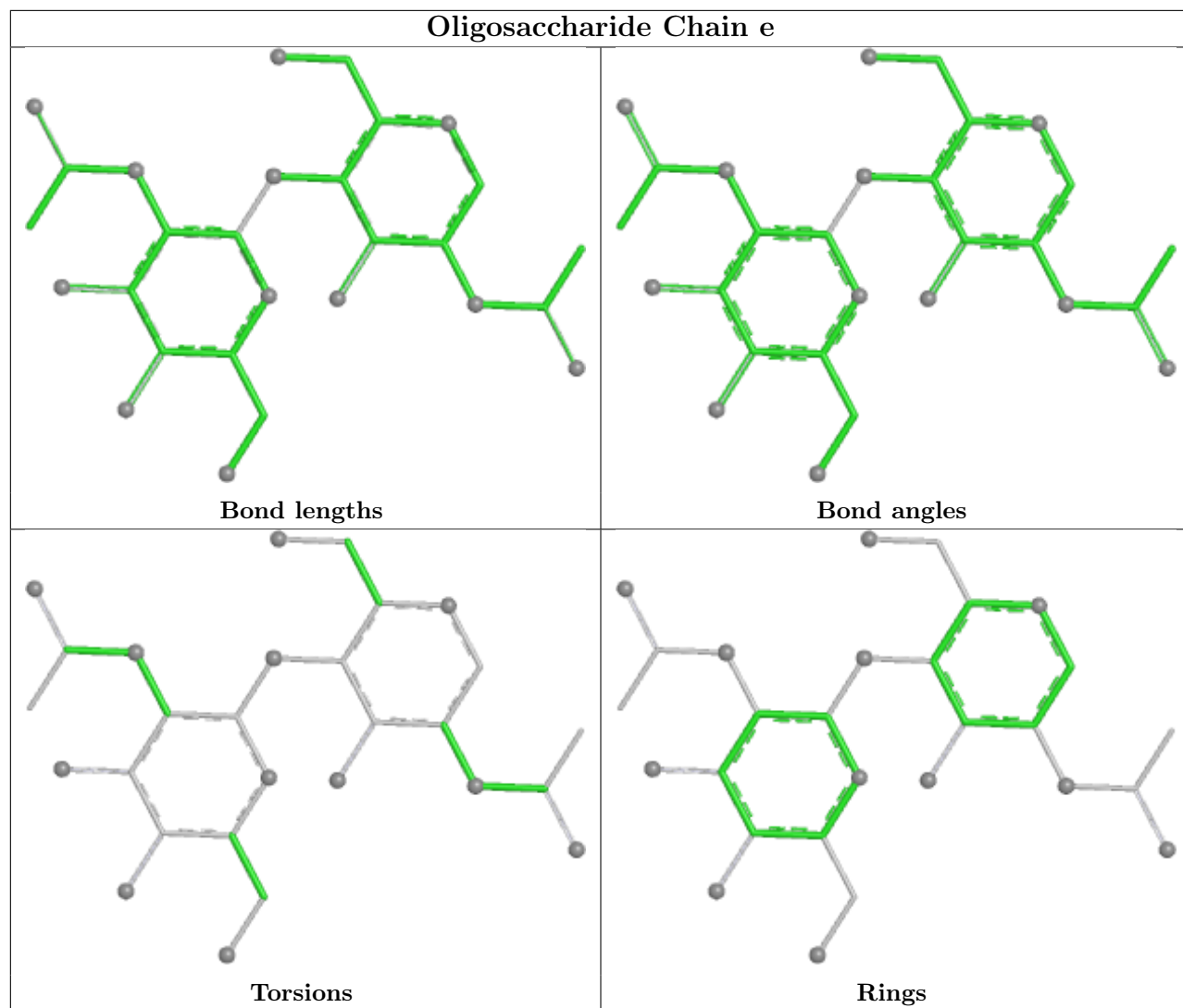
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	a	10	MAN	1	0
6	c	1	NAG	1	0
5	a	2	NAG	1	0
5	a	9	MAN	1	0

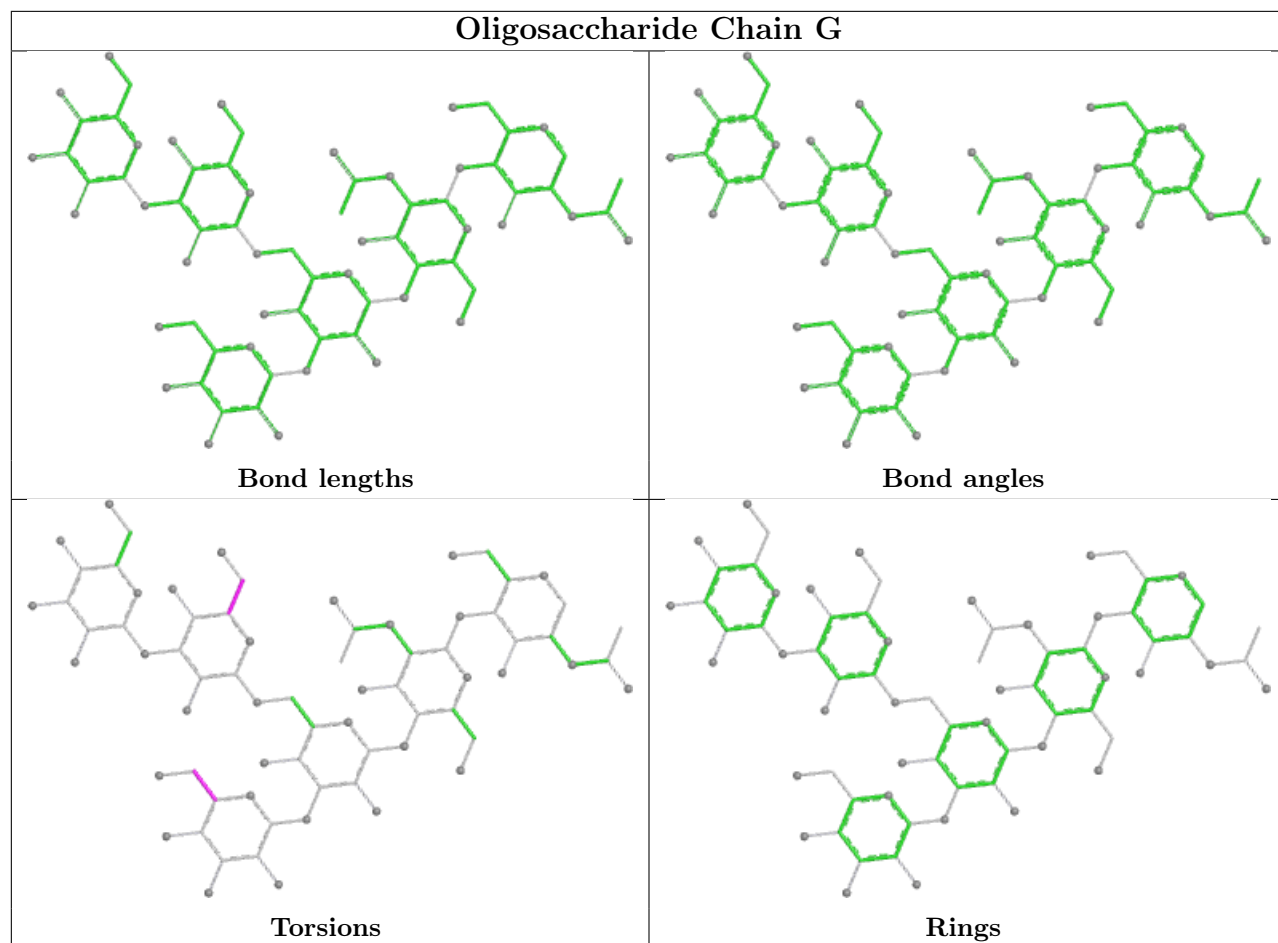
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

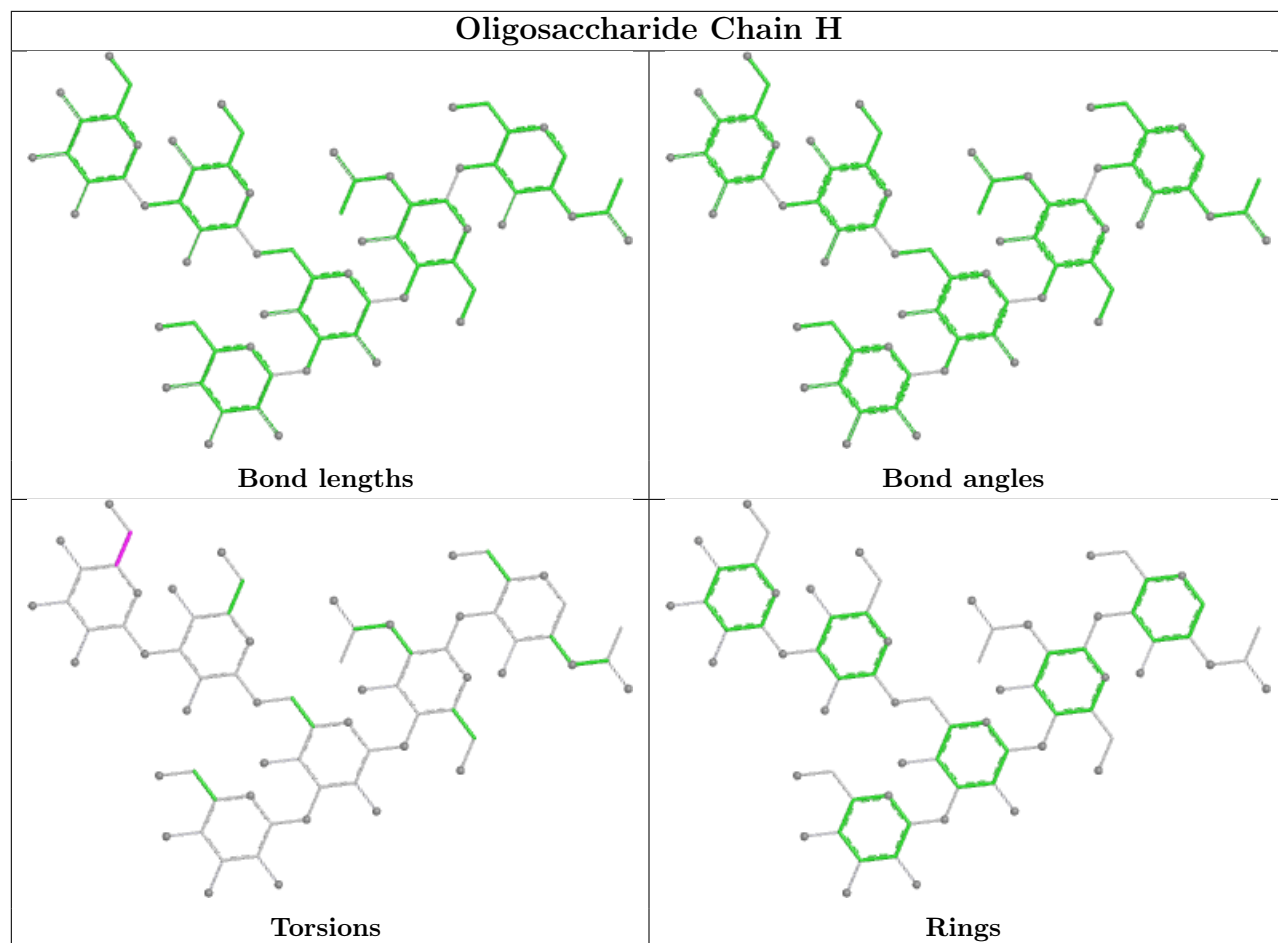


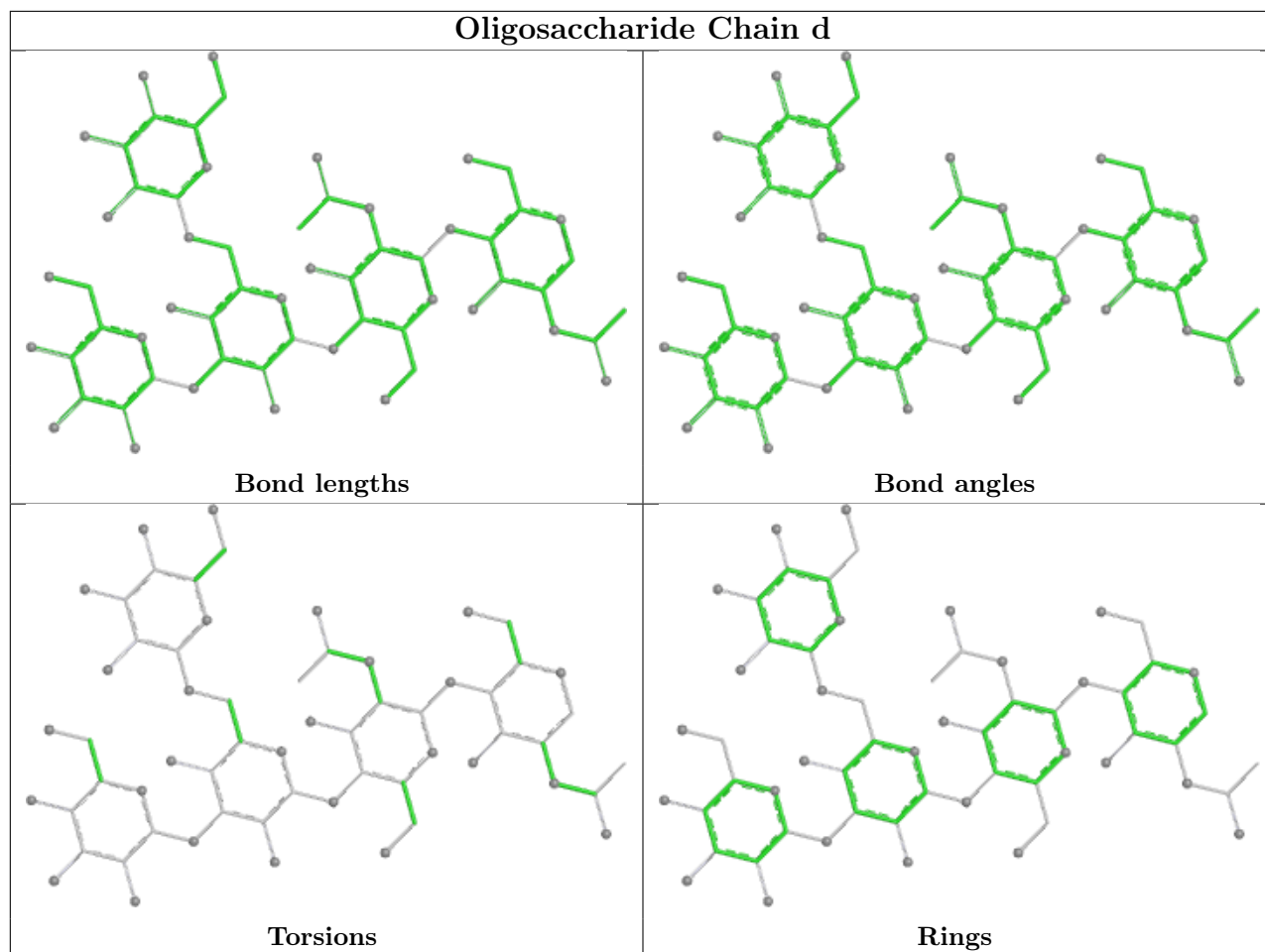












5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	D10	A	501	-	9,9,9	0.13	0	8,8,8	0.11	0
9	D10	D	501	-	9,9,9	0.13	0	8,8,8	0.11	0
9	D10	E	501	-	9,9,9	0.13	0	8,8,8	0.11	0
9	D10	C	502	-	9,9,9	0.12	0	8,8,8	0.11	0
9	D10	B	501	-	9,9,9	0.12	0	8,8,8	0.14	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
9	D10	A	501	-	-	0/7/7/7	-
9	D10	D	501	-	-	0/7/7/7	-
9	D10	E	501	-	-	0/7/7/7	-
9	D10	C	502	-	-	0/7/7/7	-
9	D10	B	501	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	501	D10	C3-C4-C5-C6
9	B	501	D10	C6-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	D10	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.

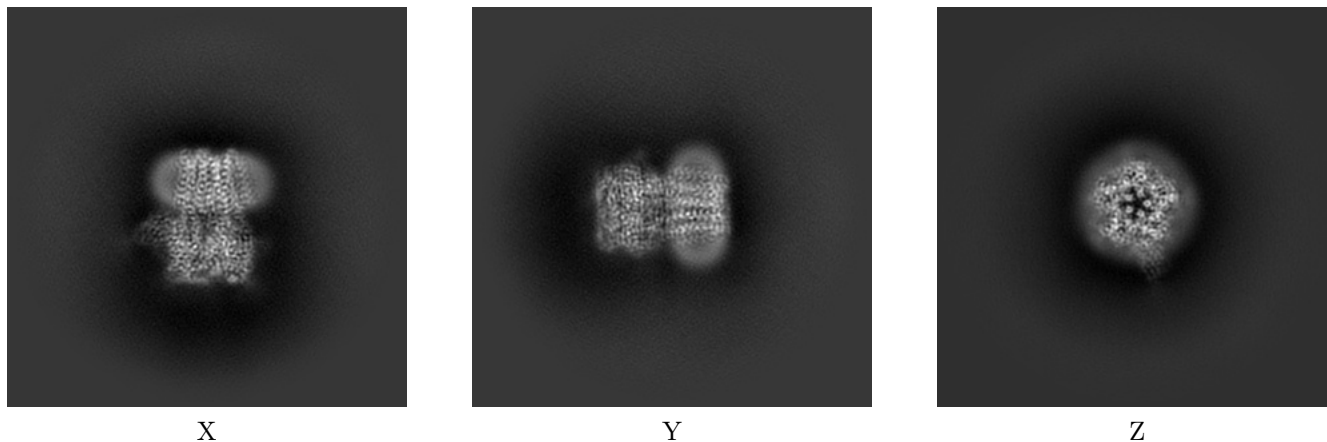
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50375. These allow visual inspection of the internal detail of the map and identification of artifacts.

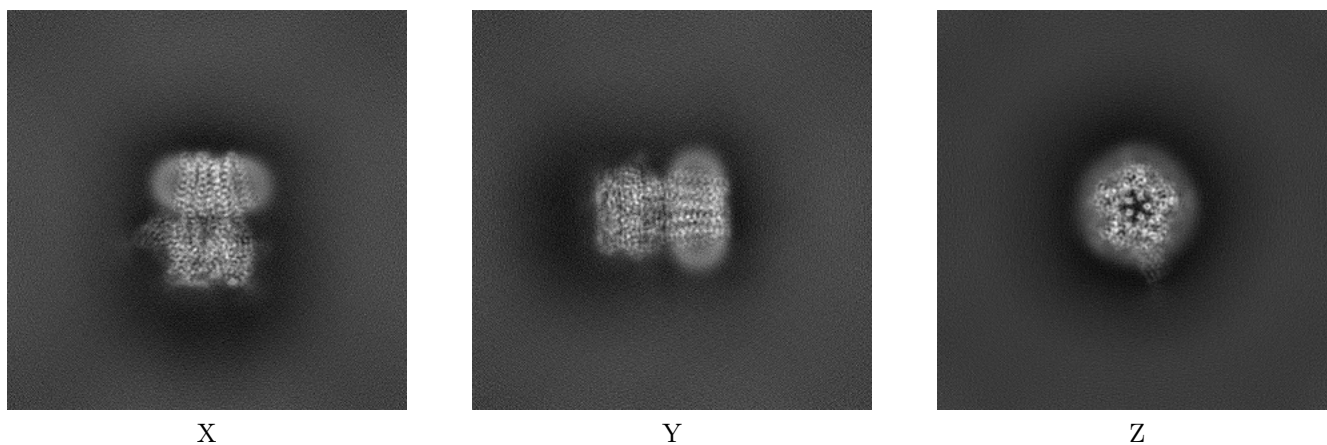
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



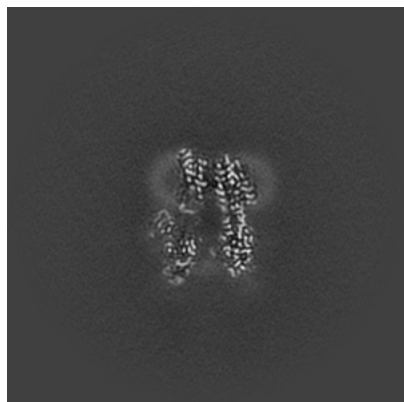
6.1.2 Raw map



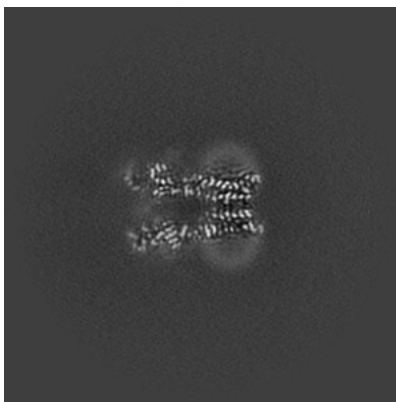
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

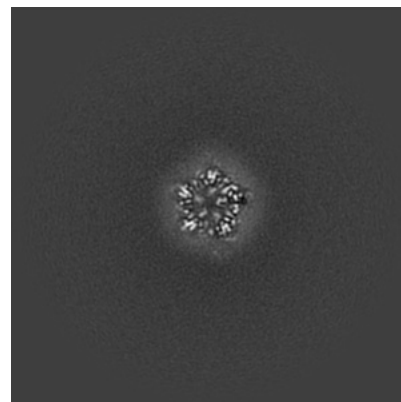
6.2.1 Primary map



X Index: 230

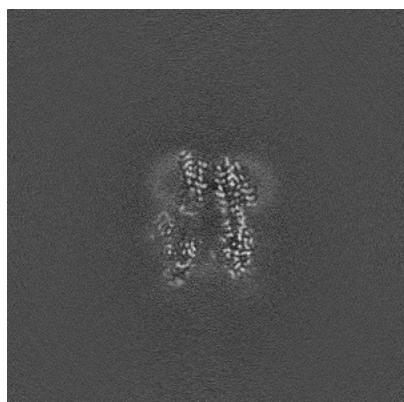


Y Index: 230

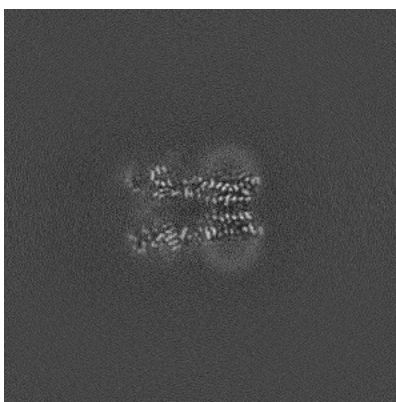


Z Index: 230

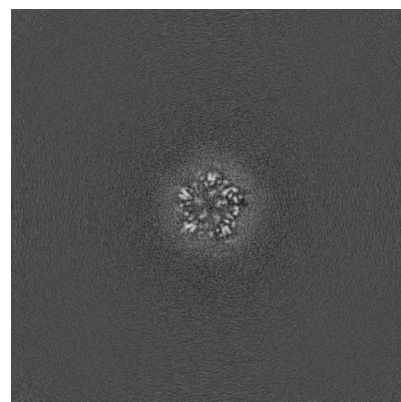
6.2.2 Raw map



X Index: 230



Y Index: 230

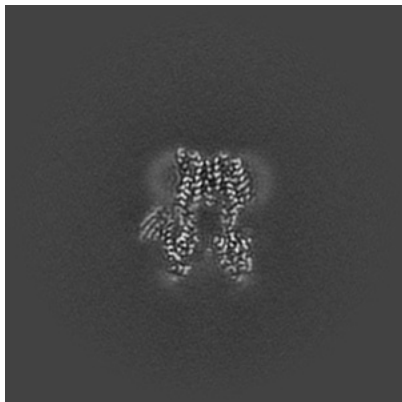


Z Index: 230

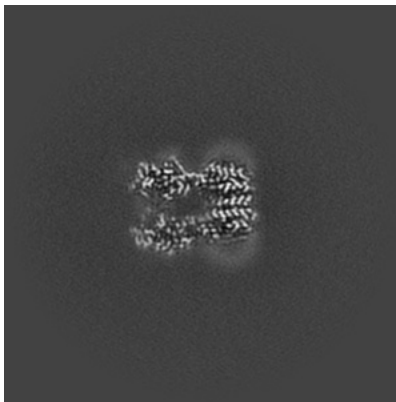
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

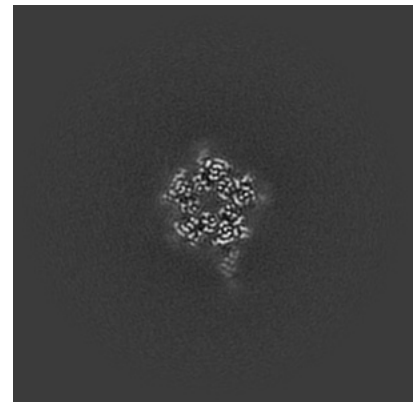
6.3.1 Primary map



X Index: 237

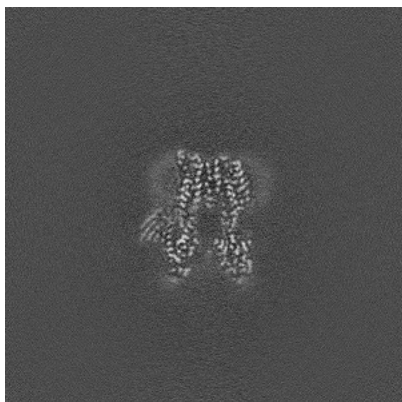


Y Index: 242

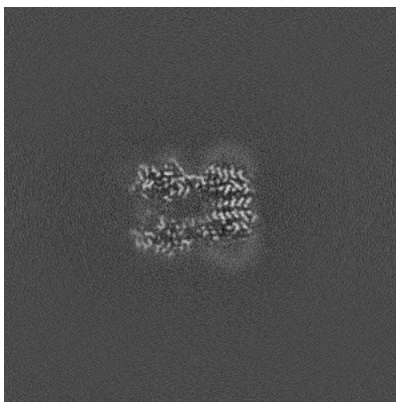


Z Index: 188

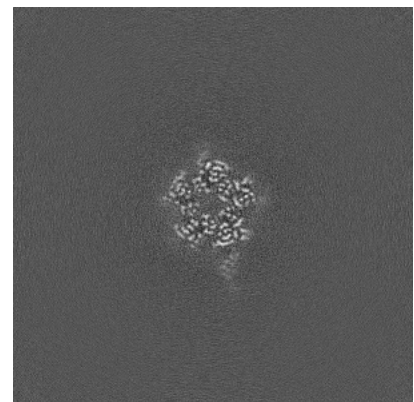
6.3.2 Raw map



X Index: 237



Y Index: 242

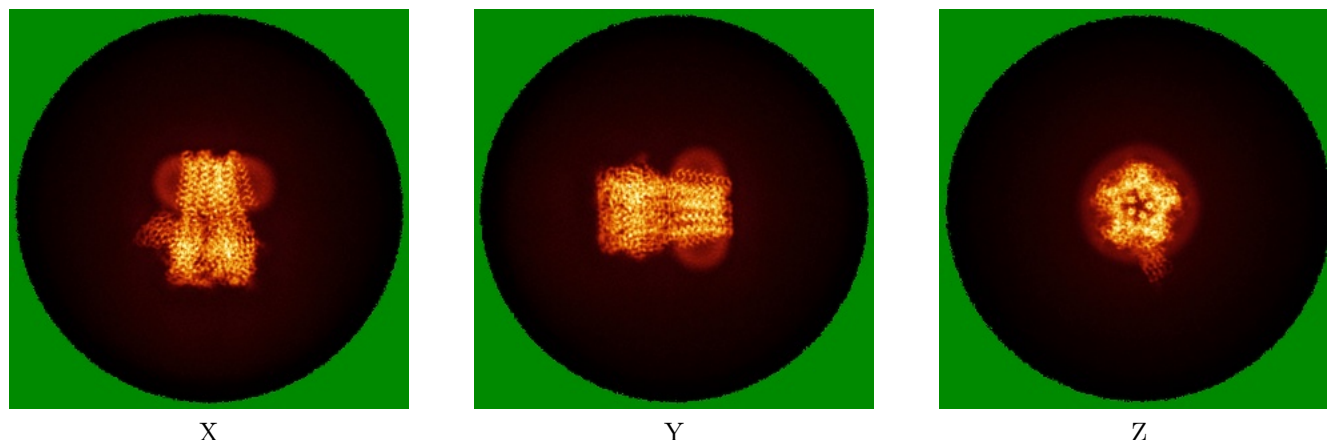


Z Index: 188

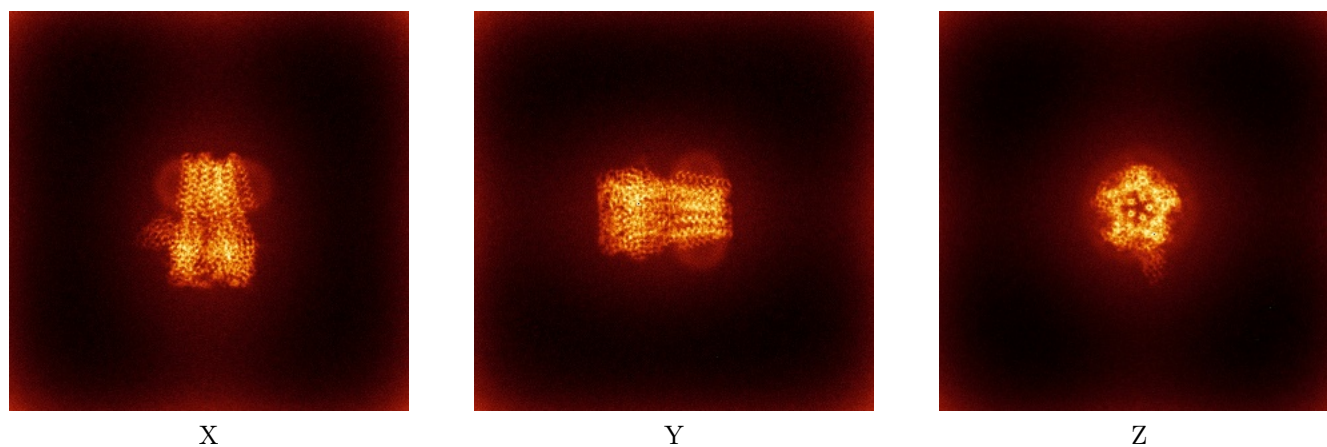
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



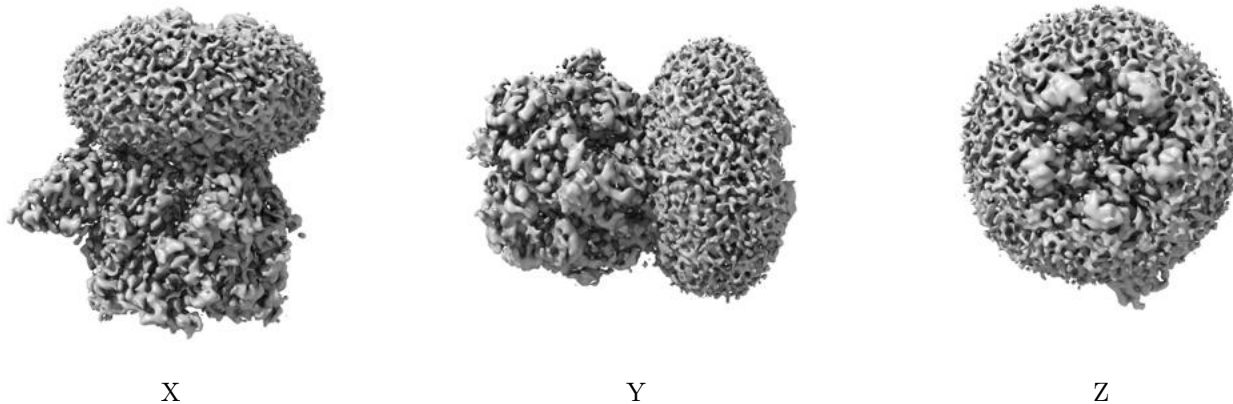
6.4.2 Raw map



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.

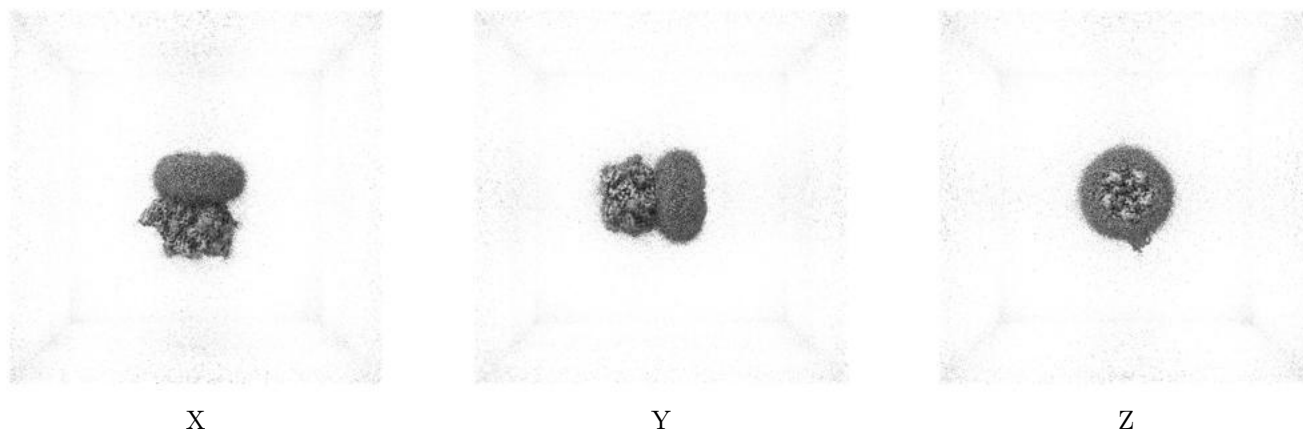
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

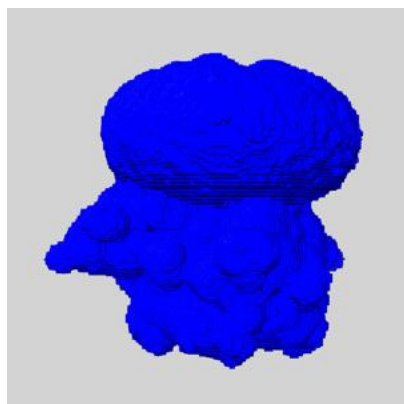
6.6 Mask visualisation [i](#)

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

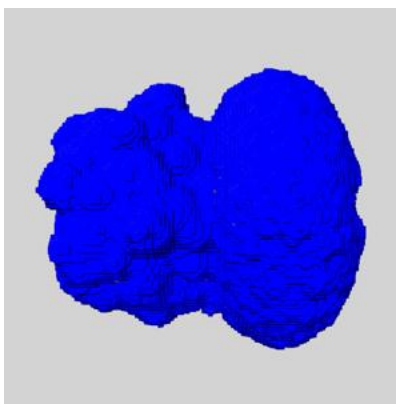
A mask typically either:

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

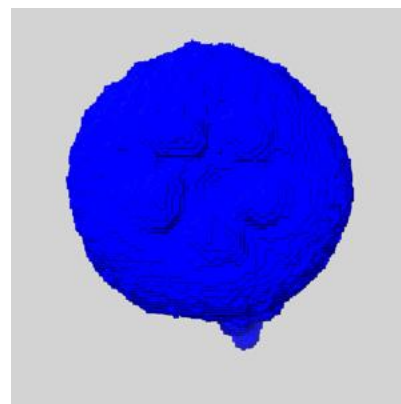
6.6.1 emd_50375_msk_1.map [i](#)



X



Y

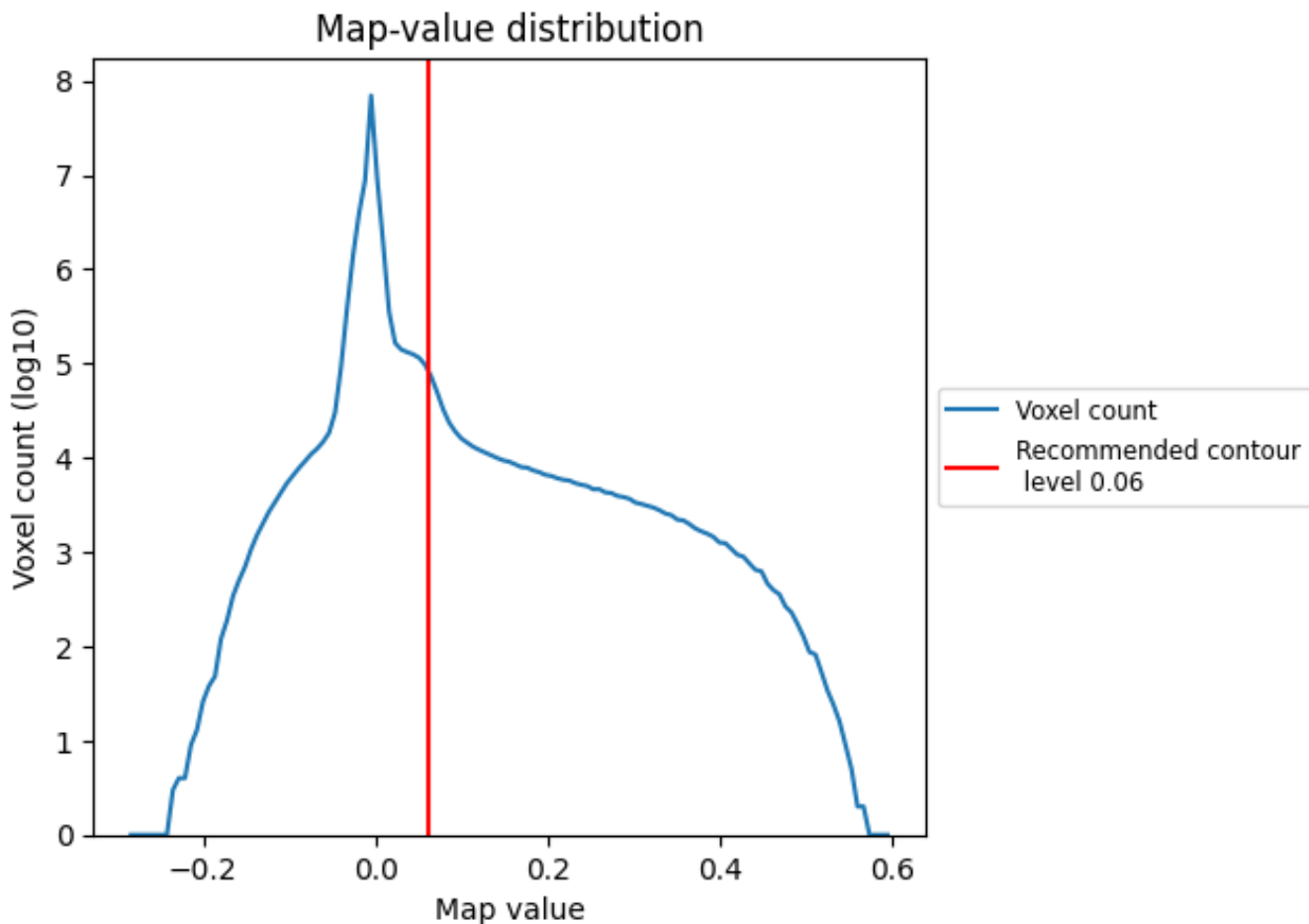


Z

7 Map analysis [i](#)

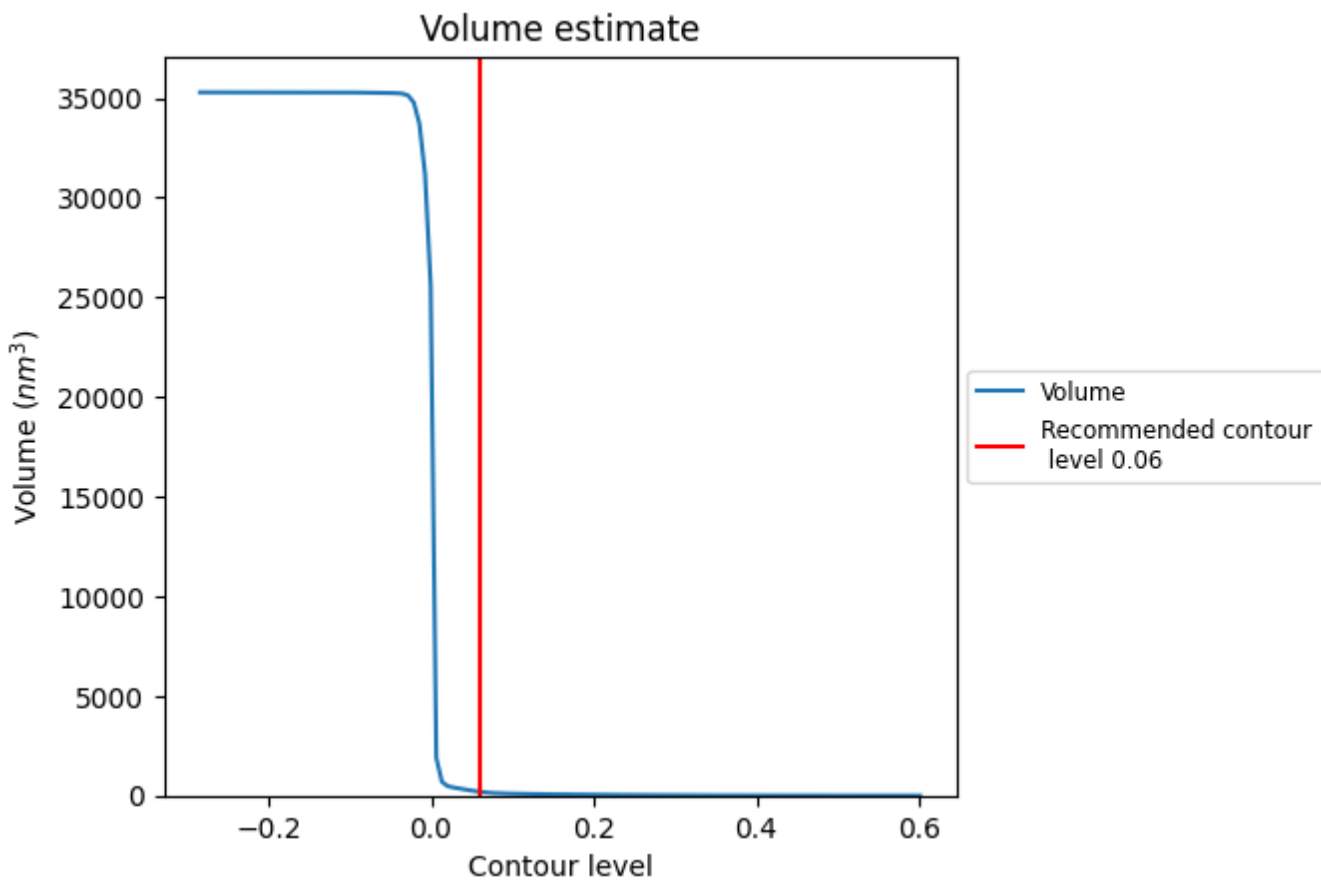
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

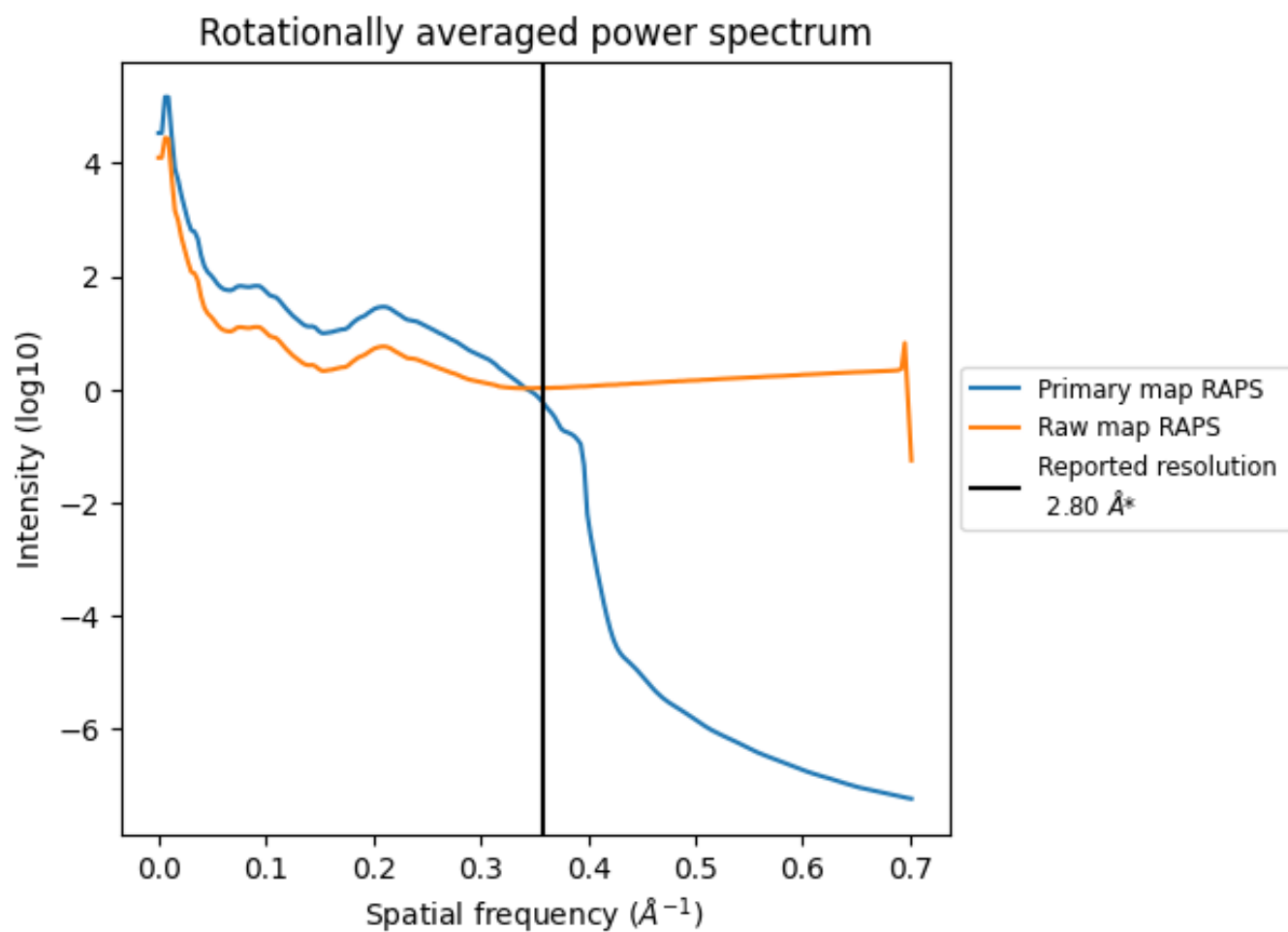
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 189 nm^3 ; this corresponds to an approximate mass of 171 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

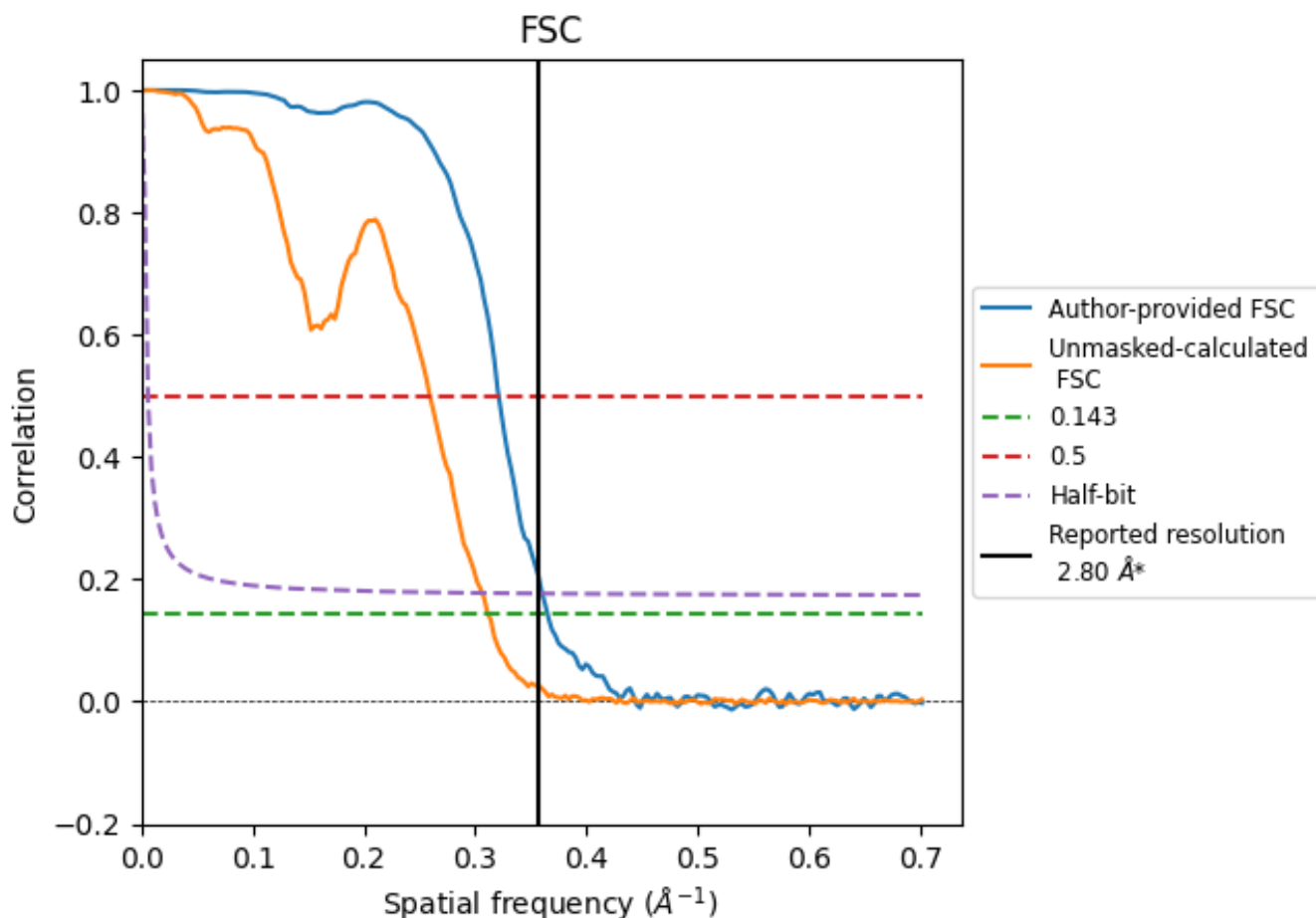


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357\AA^{-1}

8.2 Resolution estimates [i](#)

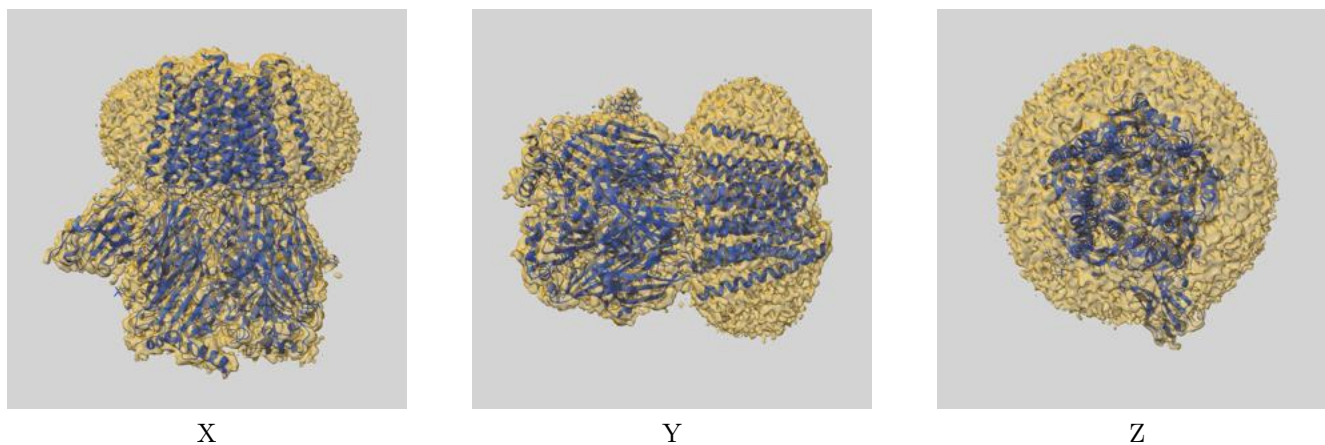
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.74	3.12	2.78
Unmasked-calculated*	3.21	3.86	3.26

*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 3.21 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

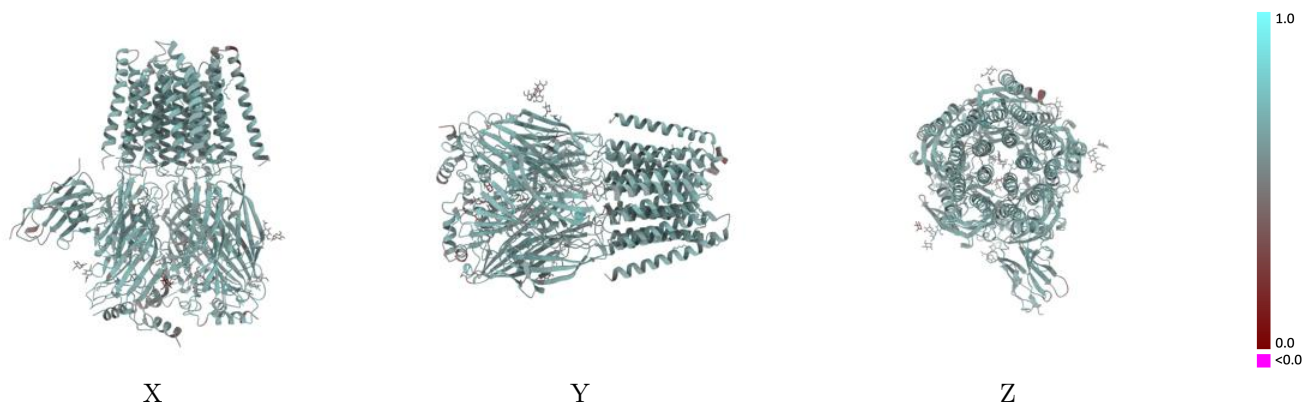
This section contains information regarding the fit between EMDB map EMD-50375 and PDB model 9FFV. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



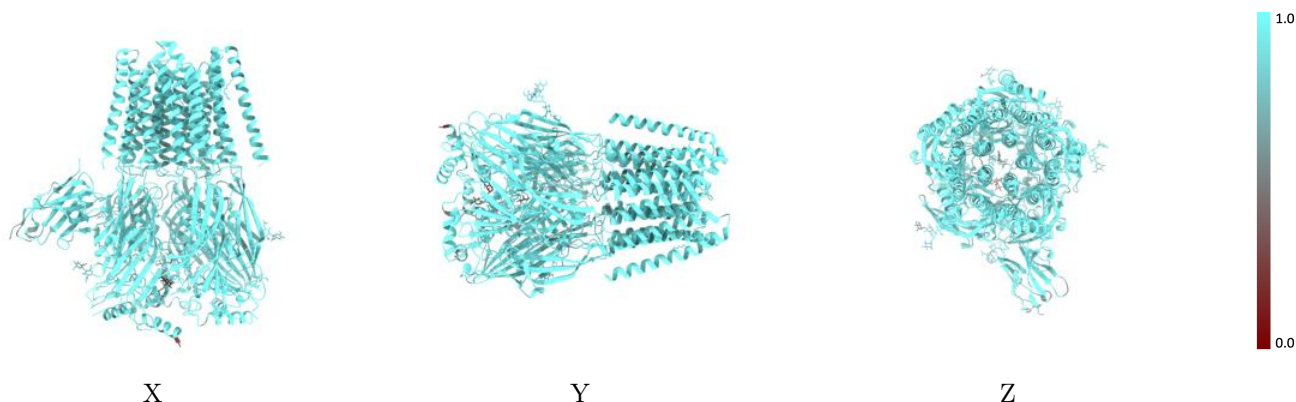
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



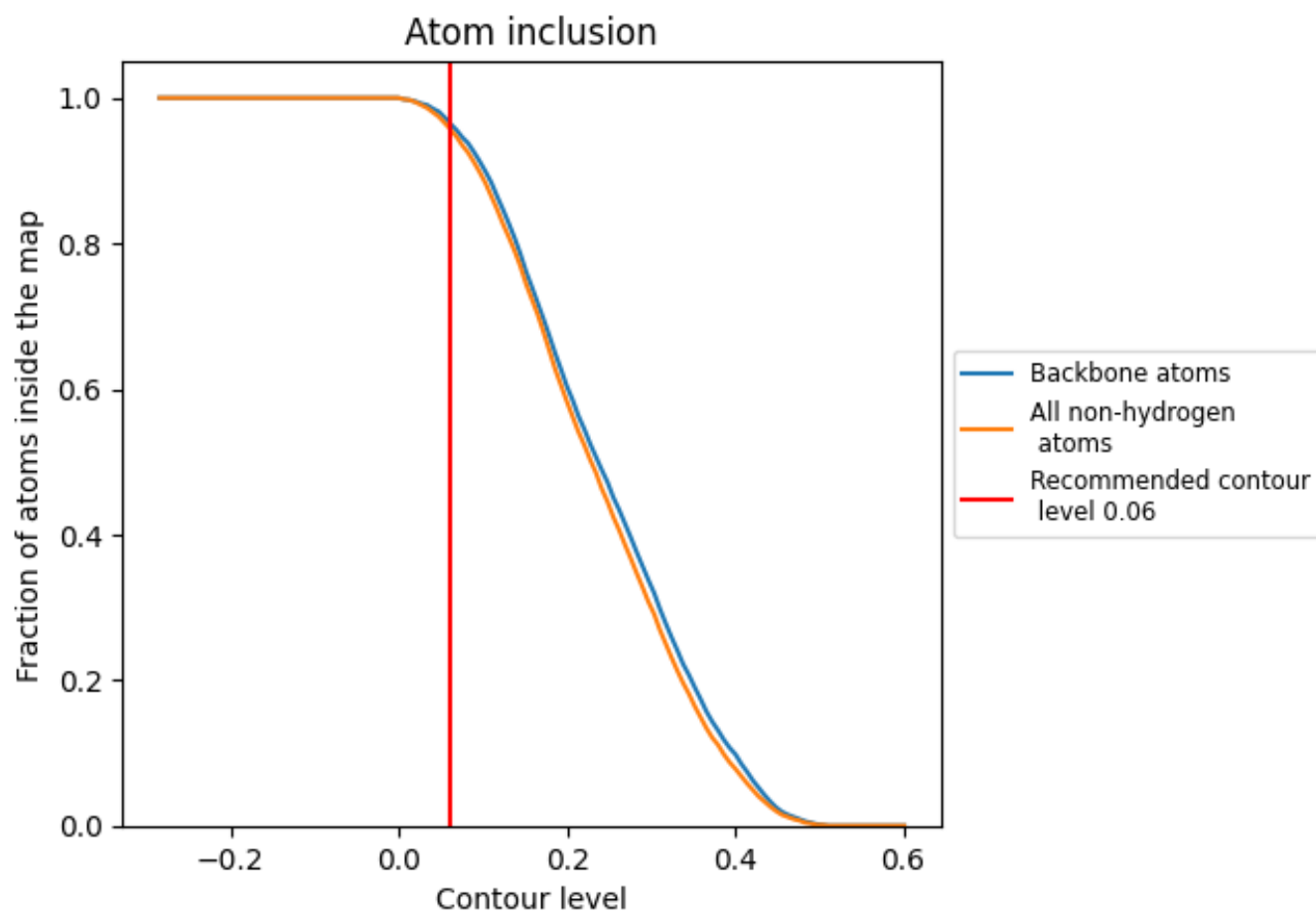
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.5960
A	 0.9650	 0.6030
B	 0.9790	 0.6120
C	 0.9750	 0.6060
D	 0.9540	 0.5850
E	 0.9740	 0.6010
F	 0.9150	 0.5780
G	 0.9170	 0.5080
H	 0.8610	 0.4970
a	 0.7670	 0.4540
b	 0.8930	 0.5090
c	 0.8930	 0.4560
d	 0.4100	 0.3510
e	 0.7860	 0.4930

