



wwPDB EM Validation Summary Report ⓘ

Jul 1, 2026 – 05:14 pm BST

PDB ID : 9RL5 / pdb_00009r15
EMDB ID : EMD-54031
Title : a5b3 GABAAR bound to Topiramate, GABA, and Mb25 in a desensitized state in saposin nanodiscs
Authors : Cowgirl, J.; Lindahl, E.; Howard, R.J.
Deposited on : 2025-06-16
Resolution : 3.10 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:

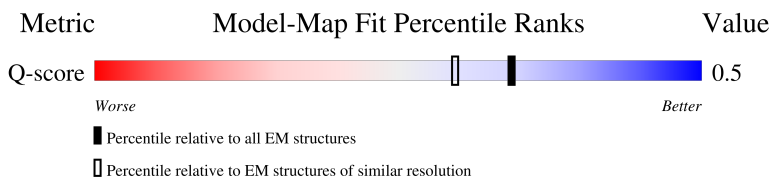
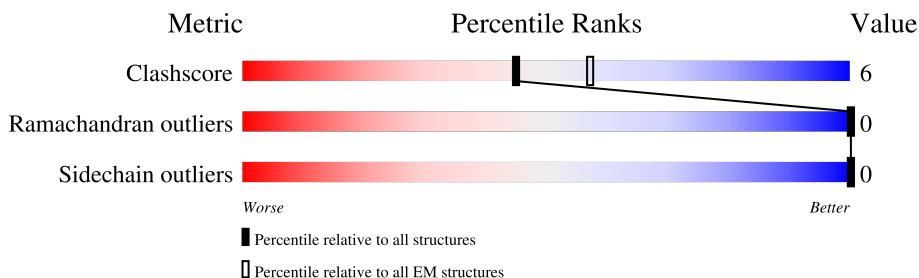
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 3.10 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.



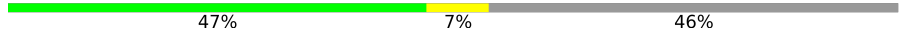



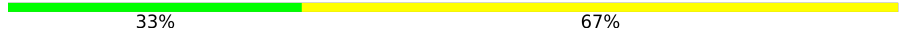
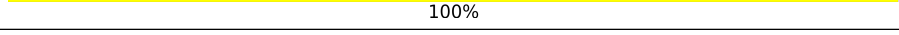
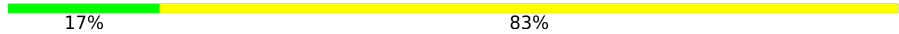
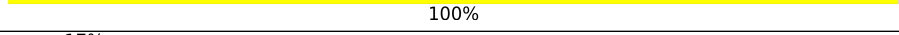
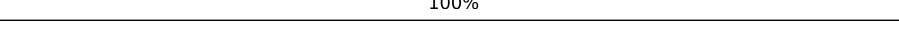
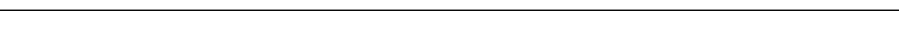

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	679	 44% 6% 50%
1	D	679	 43% 7% 50%
2	B	623	 45% 10% 45%
2	C	623	 46% 8% 46%

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Mol	Chain	Length	Quality of chain
2	E	623	 47% 7% 46%
3	P	541	 19% 78%
4	F	2	 50% 50%
5	G	3	 33% 67% 100%
5	H	3	 33% 67%
5	M	3	 100%
6	I	6	 17% 83%
6	N	6	 17% 100%
7	J	6	 17% 100%
8	K	3	 33% 67%
9	L	2	 50% 50%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 15218 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 Green fluorescent protein,Gamma-aminobutyric acid receptor subunit alpha-5,Gamma-aminobutyric acid receptor subunit alpha-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	342	Total	C	N	O	S	0	0
			2745	1769	454	506	16		
1	D	339	Total	C	N	O	S	0	0
			2719	1754	451	498	16		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	SER	-	linker	UNP P31644
A	316	GLN	-	linker	UNP P31644
A	317	PRO	-	linker	UNP P31644
A	318	ALA	-	linker	UNP P31644
A	319	ARG	-	linker	UNP P31644
A	320	ALA	-	linker	UNP P31644
A	321	ALA	-	linker	UNP P31644
D	315	SER	-	linker	UNP P31644
D	316	GLN	-	linker	UNP P31644
D	317	PRO	-	linker	UNP P31644
D	318	ALA	-	linker	UNP P31644
D	319	ARG	-	linker	UNP P31644
D	320	ALA	-	linker	UNP P31644
D	321	ALA	-	linker	UNP P31644

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	340	Total	C	N	O	S	0	0
			2785	1822	455	492	16		
2	C	339	Total	C	N	O	S	0	0
			2776	1817	453	490	16		
2	E	336	Total	C	N	O	S	0	0
			2747	1797	450	484	16		

There are 153 discrepancies between the modelled and reference sequences:

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	GLY	-	linker	UNP P28472
B	312	ARG	-	linker	UNP P28472
B	313	ALA	-	linker	UNP P28472
B	314	MET	-	linker	UNP P28472
B	315	VAL	-	linker	UNP P28472
B	332	MET	LEU	conflict	UNP P42212
B	339	ARG	HIS	conflict	UNP P42212
B	344	ARG	SER	conflict	UNP P42212
B	346	VAL	GLU	conflict	UNP P42212
B	353	HIS	TYR	conflict	UNP P42212
B	364	SER	THR	conflict	UNP P42212
B	378	LEU	PHE	conflict	UNP P42212
B	419	SER	ASN	conflict	UNP P42212
B	438	VAL	GLU	conflict	UNP P42212
B	442	THR	ILE	conflict	UNP P42212
B	459	MET	TYR	conflict	UNP P42212
B	461	VAL	SER	conflict	UNP P42212
B	462	GLY	HIS	conflict	UNP P42212
B	467	THR	MET	conflict	UNP P42212
B	477	ALA	VAL	conflict	UNP P42212
B	480	GLU	LYS	conflict	UNP P42212
B	485	VAL	ILE	conflict	UNP P42212
B	489	GLY	SER	conflict	UNP P42212
B	506	SER	PRO	conflict	UNP P42212
B	517	VAL	THR	conflict	UNP P42212
B	519	VAL	SER	conflict	UNP P42212
B	520	LYS	ALA	conflict	UNP P42212
B	538	ARG	VAL	conflict	UNP P42212
B	545	PRO	HIS	conflict	UNP P42212
B	553	GLY	-	linker	UNP P42212
B	554	ARG	-	linker	UNP P42212
B	555	ALA	-	linker	UNP P42212
B	556	ALA	-	linker	UNP P42212
B	584	SER	-	expression tag	UNP P28472
B	585	ARG	-	expression tag	UNP P28472
B	586	GLU	-	expression tag	UNP P28472
B	587	ASN	-	expression tag	UNP P28472
B	588	LEU	-	expression tag	UNP P28472
B	589	TYR	-	expression tag	UNP P28472

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Chain	Residue	Modelled	Actual	Comment	Reference
B	590	PHE	-	expression tag	UNP P28472
B	591	GLN	-	expression tag	UNP P28472
B	592	ALA	-	expression tag	UNP P28472
B	593	HIS	-	expression tag	UNP P28472
B	594	HIS	-	expression tag	UNP P28472
B	595	HIS	-	expression tag	UNP P28472
B	596	HIS	-	expression tag	UNP P28472
B	597	HIS	-	expression tag	UNP P28472
B	598	HIS	-	expression tag	UNP P28472
C	308	SER	-	linker	UNP P28472
C	309	GLN	-	linker	UNP P28472
C	310	PRO	-	linker	UNP P28472
C	311	GLY	-	linker	UNP P28472
C	312	ARG	-	linker	UNP P28472
C	313	ALA	-	linker	UNP P28472
C	314	MET	-	linker	UNP P28472
C	315	VAL	-	linker	UNP P28472
C	332	MET	LEU	conflict	UNP P42212
C	339	ARG	HIS	conflict	UNP P42212
C	344	ARG	SER	conflict	UNP P42212
C	346	VAL	GLU	conflict	UNP P42212
C	353	HIS	TYR	conflict	UNP P42212
C	364	SER	THR	conflict	UNP P42212
C	378	LEU	PHE	conflict	UNP P42212
C	419	SER	ASN	conflict	UNP P42212
C	438	VAL	GLU	conflict	UNP P42212
C	442	THR	ILE	conflict	UNP P42212
C	459	MET	TYR	conflict	UNP P42212
C	461	VAL	SER	conflict	UNP P42212
C	462	GLY	HIS	conflict	UNP P42212
C	467	THR	MET	conflict	UNP P42212
C	477	ALA	VAL	conflict	UNP P42212
C	480	GLU	LYS	conflict	UNP P42212
C	485	VAL	ILE	conflict	UNP P42212
C	489	GLY	SER	conflict	UNP P42212
C	506	SER	PRO	conflict	UNP P42212
C	517	VAL	THR	conflict	UNP P42212
C	519	VAL	SER	conflict	UNP P42212
C	520	LYS	ALA	conflict	UNP P42212
C	538	ARG	VAL	conflict	UNP P42212
C	545	PRO	HIS	conflict	UNP P42212
C	553	GLY	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	554	ARG	-	linker	UNP P42212
C	555	ALA	-	linker	UNP P42212
C	556	ALA	-	linker	UNP P42212
C	584	SER	-	expression tag	UNP P28472
C	585	ARG	-	expression tag	UNP P28472
C	586	GLU	-	expression tag	UNP P28472
C	587	ASN	-	expression tag	UNP P28472
C	588	LEU	-	expression tag	UNP P28472
C	589	TYR	-	expression tag	UNP P28472
C	590	PHE	-	expression tag	UNP P28472
C	591	GLN	-	expression tag	UNP P28472
C	592	ALA	-	expression tag	UNP P28472
C	593	HIS	-	expression tag	UNP P28472
C	594	HIS	-	expression tag	UNP P28472
C	595	HIS	-	expression tag	UNP P28472
C	596	HIS	-	expression tag	UNP P28472
C	597	HIS	-	expression tag	UNP P28472
C	598	HIS	-	expression tag	UNP P28472
E	308	SER	-	linker	UNP P28472
E	309	GLN	-	linker	UNP P28472
E	310	PRO	-	linker	UNP P28472
E	311	GLY	-	linker	UNP P28472
E	312	ARG	-	linker	UNP P28472
E	313	ALA	-	linker	UNP P28472
E	314	MET	-	linker	UNP P28472
E	315	VAL	-	linker	UNP P28472
E	332	MET	LEU	conflict	UNP P42212
E	339	ARG	HIS	conflict	UNP P42212
E	344	ARG	SER	conflict	UNP P42212
E	346	VAL	GLU	conflict	UNP P42212
E	353	HIS	TYR	conflict	UNP P42212
E	364	SER	THR	conflict	UNP P42212
E	378	LEU	PHE	conflict	UNP P42212
E	419	SER	ASN	conflict	UNP P42212
E	438	VAL	GLU	conflict	UNP P42212
E	442	THR	ILE	conflict	UNP P42212
E	459	MET	TYR	conflict	UNP P42212
E	461	VAL	SER	conflict	UNP P42212
E	462	GLY	HIS	conflict	UNP P42212
E	467	THR	MET	conflict	UNP P42212
E	477	ALA	VAL	conflict	UNP P42212
E	480	GLU	LYS	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
E	485	VAL	ILE	conflict	UNP P42212
E	489	GLY	SER	conflict	UNP P42212
E	506	SER	PRO	conflict	UNP P42212
E	517	VAL	THR	conflict	UNP P42212
E	519	VAL	SER	conflict	UNP P42212
E	520	LYS	ALA	conflict	UNP P42212
E	538	ARG	VAL	conflict	UNP P42212
E	545	PRO	HIS	conflict	UNP P42212
E	553	GLY	-	linker	UNP P42212
E	554	ARG	-	linker	UNP P42212
E	555	ALA	-	linker	UNP P42212
E	556	ALA	-	linker	UNP P42212
E	584	SER	-	expression tag	UNP P28472
E	585	ARG	-	expression tag	UNP P28472
E	586	GLU	-	expression tag	UNP P28472
E	587	ASN	-	expression tag	UNP P28472
E	588	LEU	-	expression tag	UNP P28472
E	589	TYR	-	expression tag	UNP P28472
E	590	PHE	-	expression tag	UNP P28472
E	591	GLN	-	expression tag	UNP P28472
E	592	ALA	-	expression tag	UNP P28472
E	593	HIS	-	expression tag	UNP P28472
E	594	HIS	-	expression tag	UNP P28472
E	595	HIS	-	expression tag	UNP P28472
E	596	HIS	-	expression tag	UNP P28472
E	597	HIS	-	expression tag	UNP P28472
E	598	HIS	-	expression tag	UNP P28472

- Molecule 3 is a protein called Megabody 25.

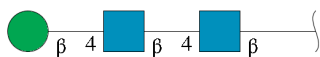
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	P	120	931	588	159	180	4	0	0

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



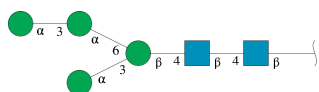
Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
4	F	2	28	16	2	10	0	0

- Molecule 5 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.



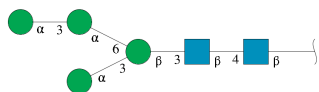
Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
5	G	3	39	22	2	15	0	0
5	H	3	39	22	2	15	0	0
5	M	3	39	22	2	15	0	0

- Molecule 6 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.



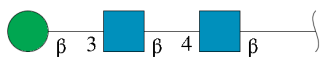
Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
6	I	6	72	40	2	30	0	0
6	N	6	72	40	2	30	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



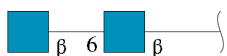
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	J	6	72	40	2	30	0	0

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



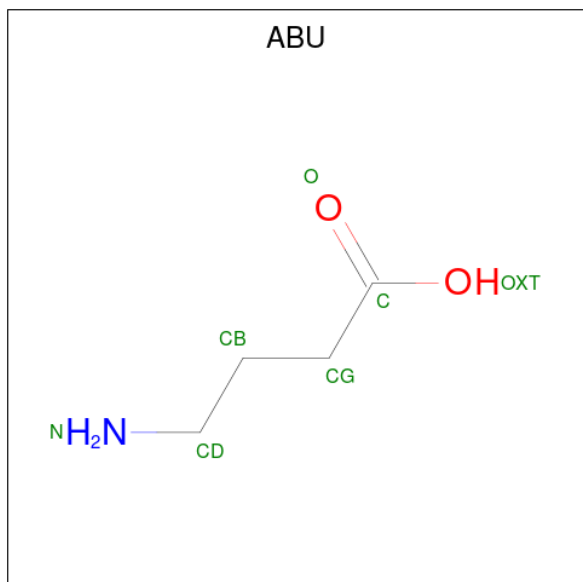
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	K	3	39	22	2	15	0	0

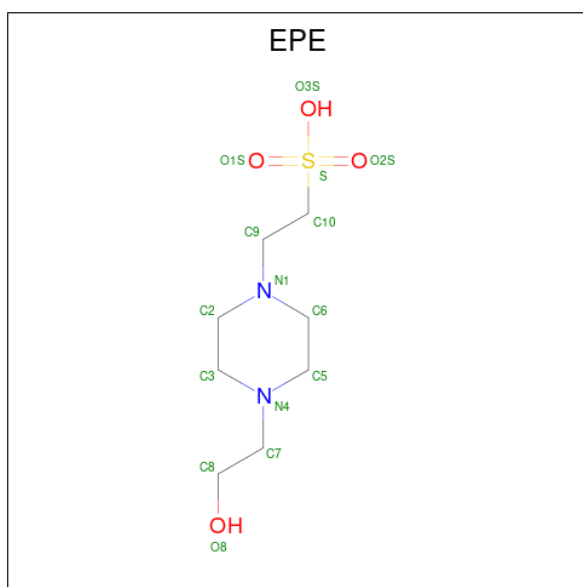
- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

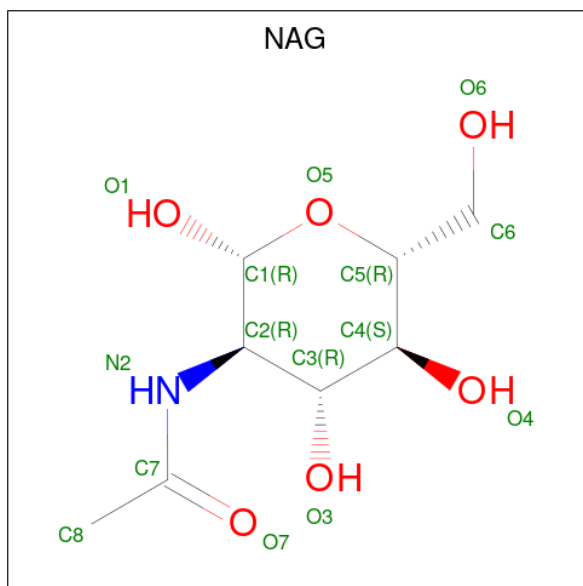
- Molecule 10 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: C₄H₉NO₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
12	C	1	15	8	2	4	1	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6: 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 I:  17% 83%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 6: 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 N:  17% 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-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  17% 100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

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

Chain K:  33% 67%

MAG1
MAG2
BMA3

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90532	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)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	35.069	Depositor
Minimum map value	-22.916	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size (Å)	286.0, 286.0, 286.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	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: NAG, TOR, MAN, BMA, ABU, EPE

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	0.15	0/2813	0.46	0/3826
1	D	0.14	0/2786	0.44	0/3788
2	B	0.14	0/2859	0.44	0/3887
2	C	0.16	0/2850	0.48	0/3875
2	E	0.15	0/2820	0.46	0/3834
3	P	0.23	0/954	0.47	0/1292
All	All	0.15	0/15082	0.46	0/20502

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	2745	0	2719	34	0
1	D	2719	0	2700	43	0
2	B	2785	0	2776	45	0
2	C	2776	0	2768	41	0
2	E	2747	0	2742	38	0
3	P	931	0	879	13	0
4	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	39	0	34	0	0
5	H	39	0	34	0	0
5	M	39	0	34	0	0
6	I	72	0	61	0	0
6	N	72	0	61	0	0
7	J	72	0	61	0	0
8	K	39	0	34	0	0
9	L	28	0	25	0	0
10	B	7	0	0	0	0
10	D	7	0	0	0	0
11	B	22	0	21	4	0
11	E	22	0	21	2	0
12	C	15	0	18	0	0
13	D	14	0	13	0	0
All	All	15218	0	15026	189	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 189 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:88:ALA:HB2	2:B:116:ILE:HD11	1.62	0.80
1:D:115:THR:O	1:D:116:THR:HG23	1.82	0.79
3:P:469:GLU:OE1	3:P:469:GLU:N	2.17	0.78
1:A:115:THR:O	1:A:116:THR:OG1	2.02	0.76
2:B:185:GLN:OE1	2:B:185:GLN:N	2.21	0.73

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	338/679 (50%)	324 (96%)	14 (4%)	0	100	100
1	D	335/679 (49%)	322 (96%)	13 (4%)	0	100	100
2	B	336/623 (54%)	328 (98%)	8 (2%)	0	100	100
2	C	335/623 (54%)	328 (98%)	7 (2%)	0	100	100
2	E	332/623 (53%)	321 (97%)	11 (3%)	0	100	100
3	P	116/541 (21%)	112 (97%)	4 (3%)	0	100	100
All	All	1792/3768 (48%)	1735 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/589 (52%)	306 (100%)	0	100	100
1	D	302/589 (51%)	302 (100%)	0	100	100
2	B	304/544 (56%)	304 (100%)	0	100	100
2	C	303/544 (56%)	303 (100%)	0	100	100
2	E	300/544 (55%)	300 (100%)	0	100	100
3	P	96/443 (22%)	96 (100%)	0	100	100
All	All	1611/3253 (50%)	1611 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	303	ASN
1	D	166	ASN
3	P	3	GLN
2	E	191	HIS
2	E	243	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

34 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
4	NAG	F	1	4,1	14,14,15	0.74	0	17,19,21	1.37	2 (11%)
4	NAG	F	2	4	14,14,15	0.69	0	17,19,21	0.91	0
5	NAG	G	1	5,1	14,14,15	0.63	0	17,19,21	1.33	2 (11%)
5	NAG	G	2	5	14,14,15	0.73	0	17,19,21	0.81	0
5	BMA	G	3	5	11,11,12	0.80	0	15,15,17	2.03	1 (6%)
5	NAG	H	1	2,5	14,14,15	0.75	0	17,19,21	1.18	2 (11%)
5	NAG	H	2	5	14,14,15	0.71	0	17,19,21	0.97	0
5	BMA	H	3	5	11,11,12	0.82	0	15,15,17	1.84	1 (6%)
6	NAG	I	1	6,2	14,14,15	0.82	0	17,19,21	1.20	2 (11%)
6	NAG	I	2	6	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
6	BMA	I	3	6	11,11,12	0.84	0	15,15,17	1.72	3 (20%)
6	MAN	I	4	6	11,11,12	0.70	0	15,15,17	1.17	1 (6%)
6	MAN	I	5	6	11,11,12	0.69	0	15,15,17	1.16	1 (6%)
6	MAN	I	6	6	11,11,12	0.79	0	15,15,17	0.88	0
7	NAG	J	1	2,7	14,14,15	0.61	0	17,19,21	2.66	5 (29%)
7	NAG	J	2	7	14,14,15	0.76	0	17,19,21	1.07	1 (5%)
7	BMA	J	3	7	11,11,12	0.79	0	15,15,17	2.02	2 (13%)
7	MAN	J	4	7	11,11,12	0.65	0	15,15,17	1.47	2 (13%)
7	MAN	J	5	7	11,11,12	0.69	0	15,15,17	1.12	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	J	6	7	11,11,12	0.68	0	15,15,17	1.25	1 (6%)
8	NAG	K	1	2,8	14,14,15	0.71	0	17,19,21	1.09	2 (11%)
8	NAG	K	2	8	14,14,15	0.73	0	17,19,21	0.91	0
8	BMA	K	3	8	11,11,12	0.82	0	15,15,17	1.83	1 (6%)
9	NAG	L	1	9,1	14,14,15	0.63	0	17,19,21	1.14	1 (5%)
9	NAG	L	2	9	14,14,15	0.69	0	17,19,21	0.94	0
5	NAG	M	1	2,5	14,14,15	0.74	0	17,19,21	1.08	2 (11%)
5	NAG	M	2	5	14,14,15	0.73	0	17,19,21	1.19	1 (5%)
5	BMA	M	3	5	11,11,12	0.82	0	15,15,17	1.95	1 (6%)
6	NAG	N	1	6,2	14,14,15	0.76	0	17,19,21	1.19	2 (11%)
6	NAG	N	2	6	14,14,15	0.69	0	17,19,21	1.03	1 (5%)
6	BMA	N	3	6	11,11,12	0.83	0	15,15,17	1.80	3 (20%)
6	MAN	N	4	6	11,11,12	0.66	0	15,15,17	1.34	1 (6%)
6	MAN	N	5	6	11,11,12	0.72	0	15,15,17	1.06	1 (6%)
6	MAN	N	6	6	11,11,12	0.65	0	15,15,17	1.43	1 (6%)

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	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	NAG	G	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	NAG	H	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	MAN	I	5	6	-	1/2/19/22	0/1/1/1
6	MAN	I	6	6	-	1/2/19/22	0/1/1/1
7	NAG	J	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	J	4	7	-	1/2/19/22	0/1/1/1
7	MAN	J	5	7	-	0/2/19/22	0/1/1/1
7	MAN	J	6	7	-	0/2/19/22	0/1/1/1
8	NAG	K	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	0/6/23/26	0/1/1/1
8	BMA	K	3	8	-	1/2/19/22	0/1/1/1
9	NAG	L	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	L	2	9	-	0/6/23/26	0/1/1/1
5	NAG	M	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
6	MAN	N	6	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	1	NAG	C1-O5-C5	9.04	124.44	112.19
5	G	3	BMA	C1-O5-C5	6.75	121.34	112.19
5	M	3	BMA	C1-O5-C5	6.30	120.72	112.19
7	J	3	BMA	C1-O5-C5	6.25	120.66	112.19
5	H	3	BMA	C1-O5-C5	5.79	120.04	112.19

There are no chirality outliers.

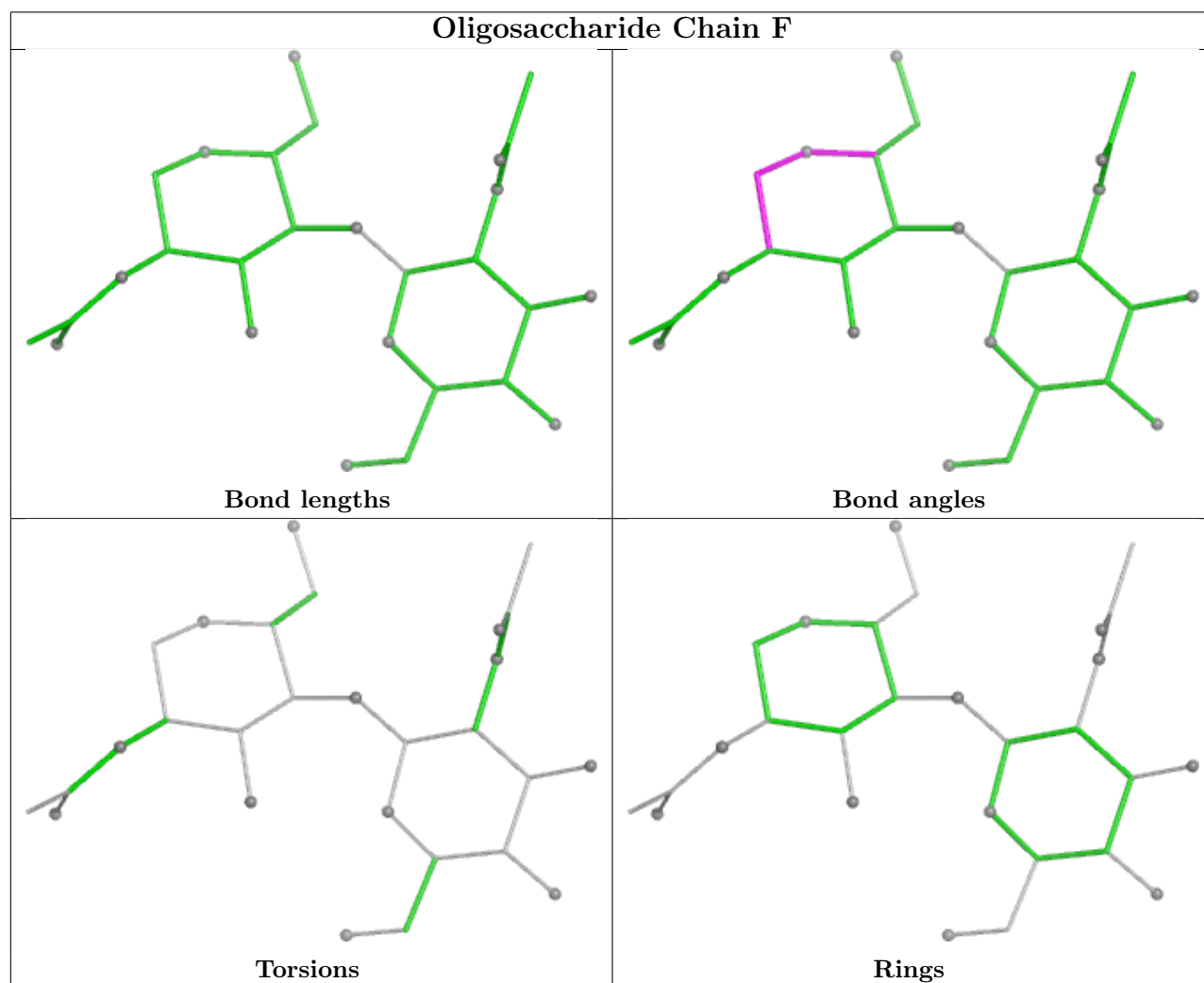
5 of 12 torsion outliers are listed below:

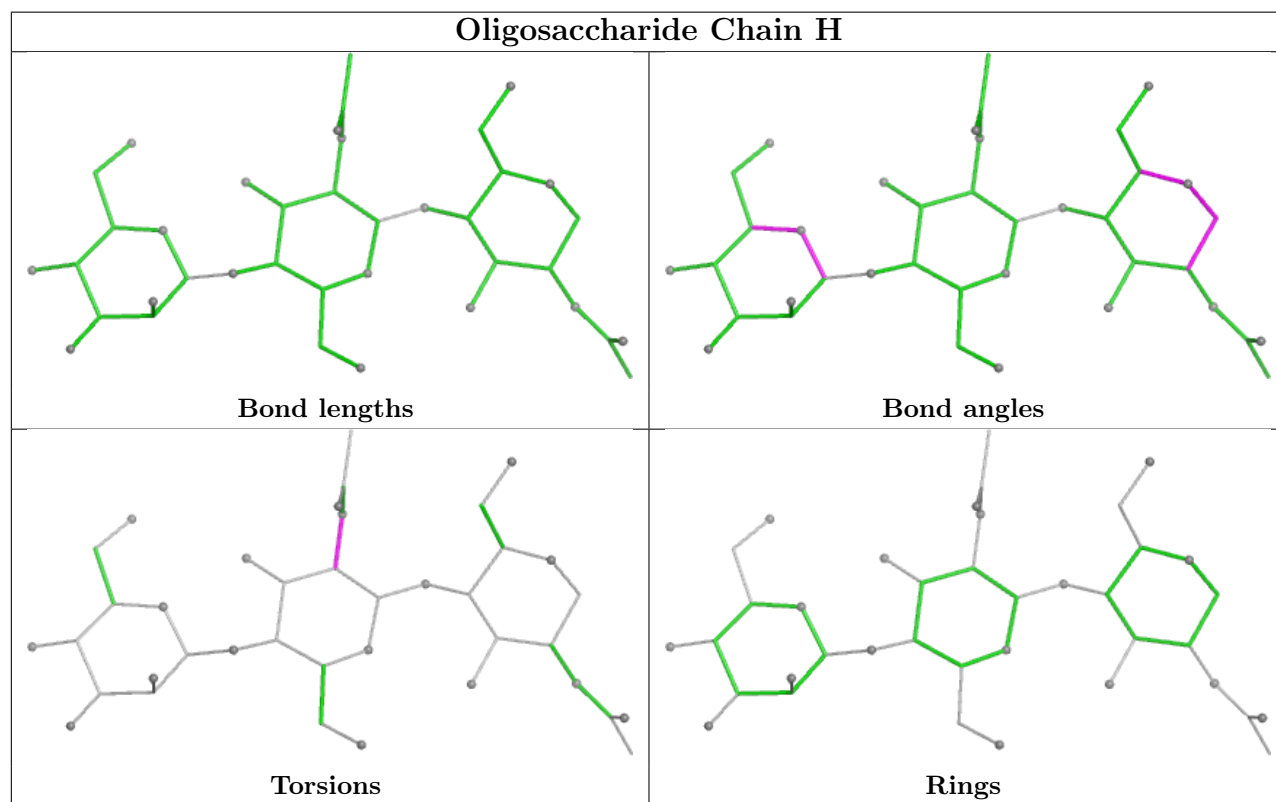
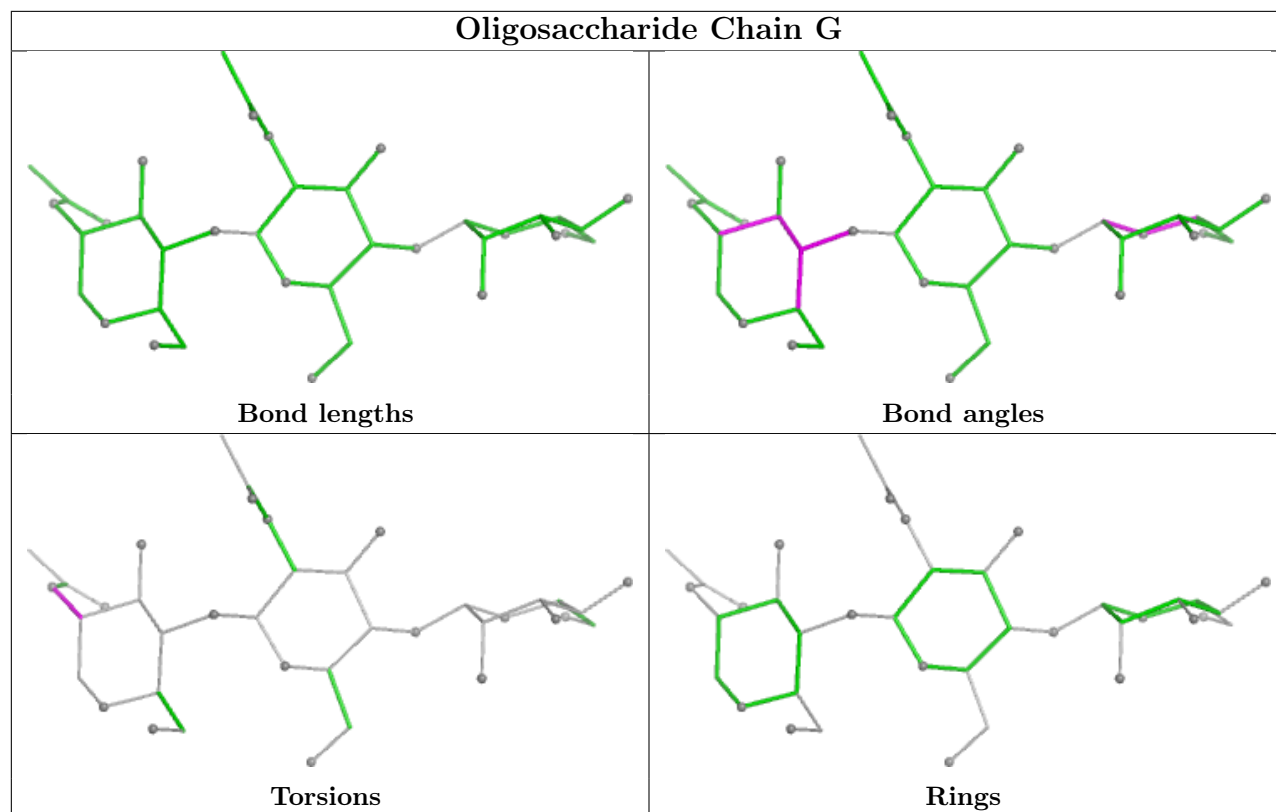
Mol	Chain	Res	Type	Atoms
9	L	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
6	I	5	MAN	O5-C5-C6-O6
7	J	4	MAN	O5-C5-C6-O6
6	I	6	MAN	O5-C5-C6-O6

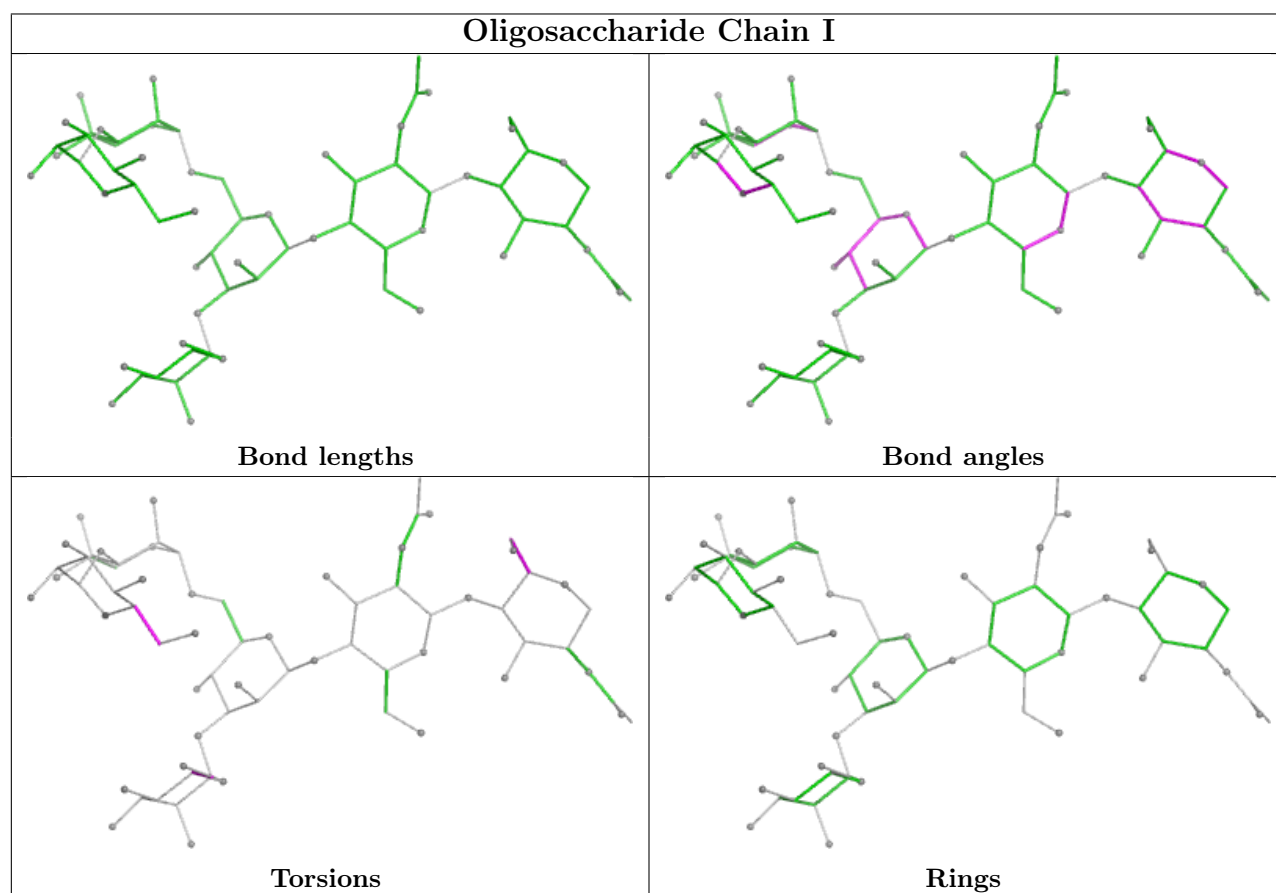
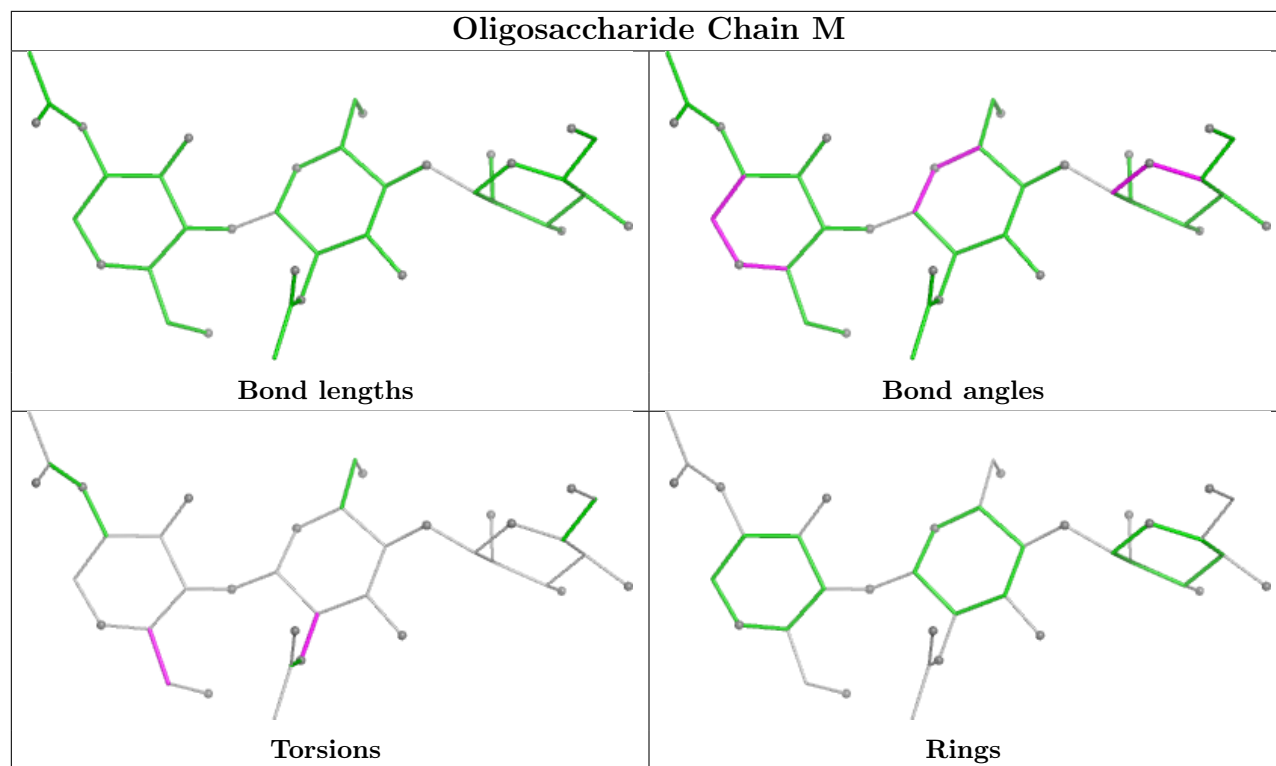
There are no ring outliers.

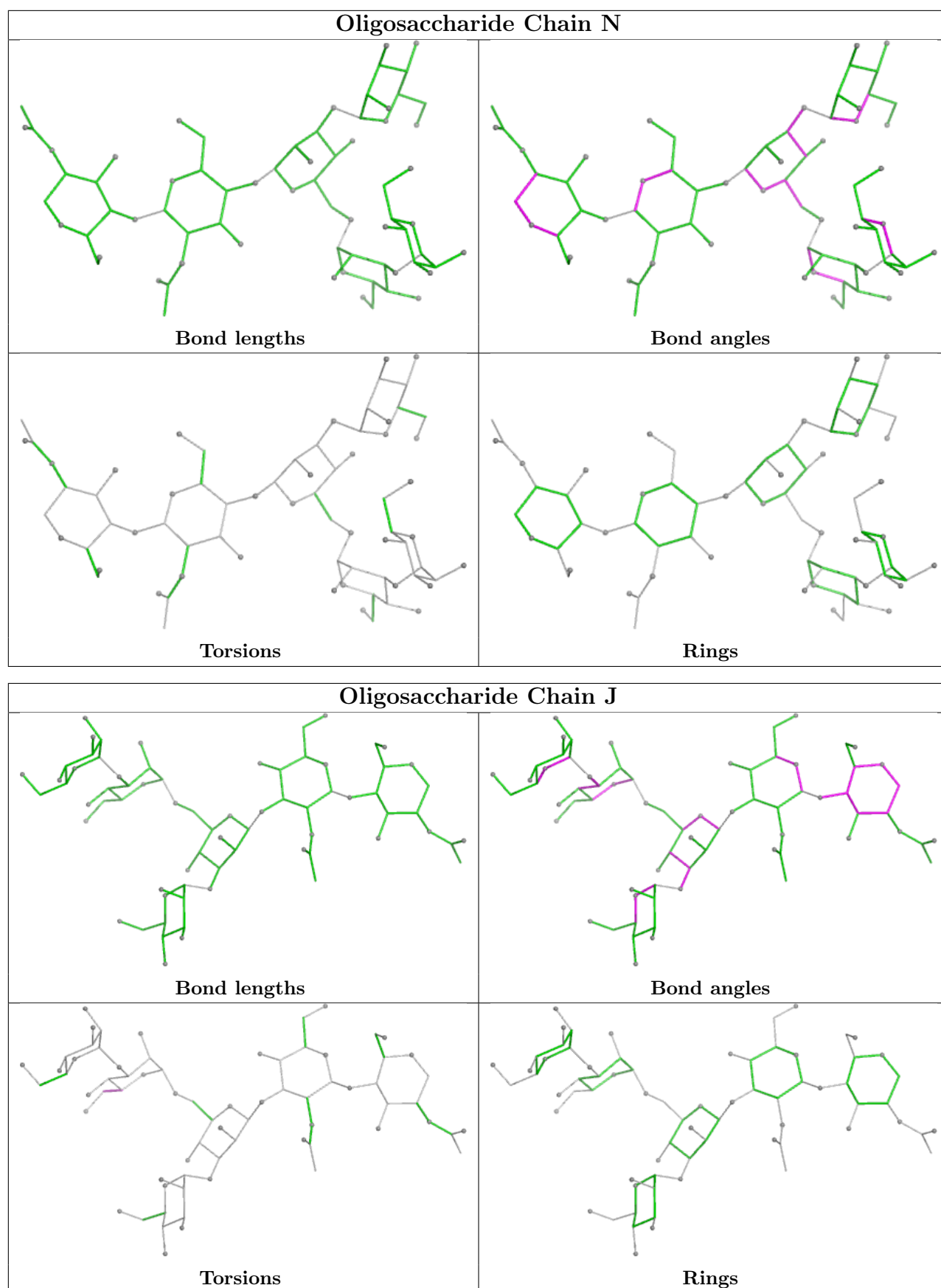
No monomer is involved in short contacts.

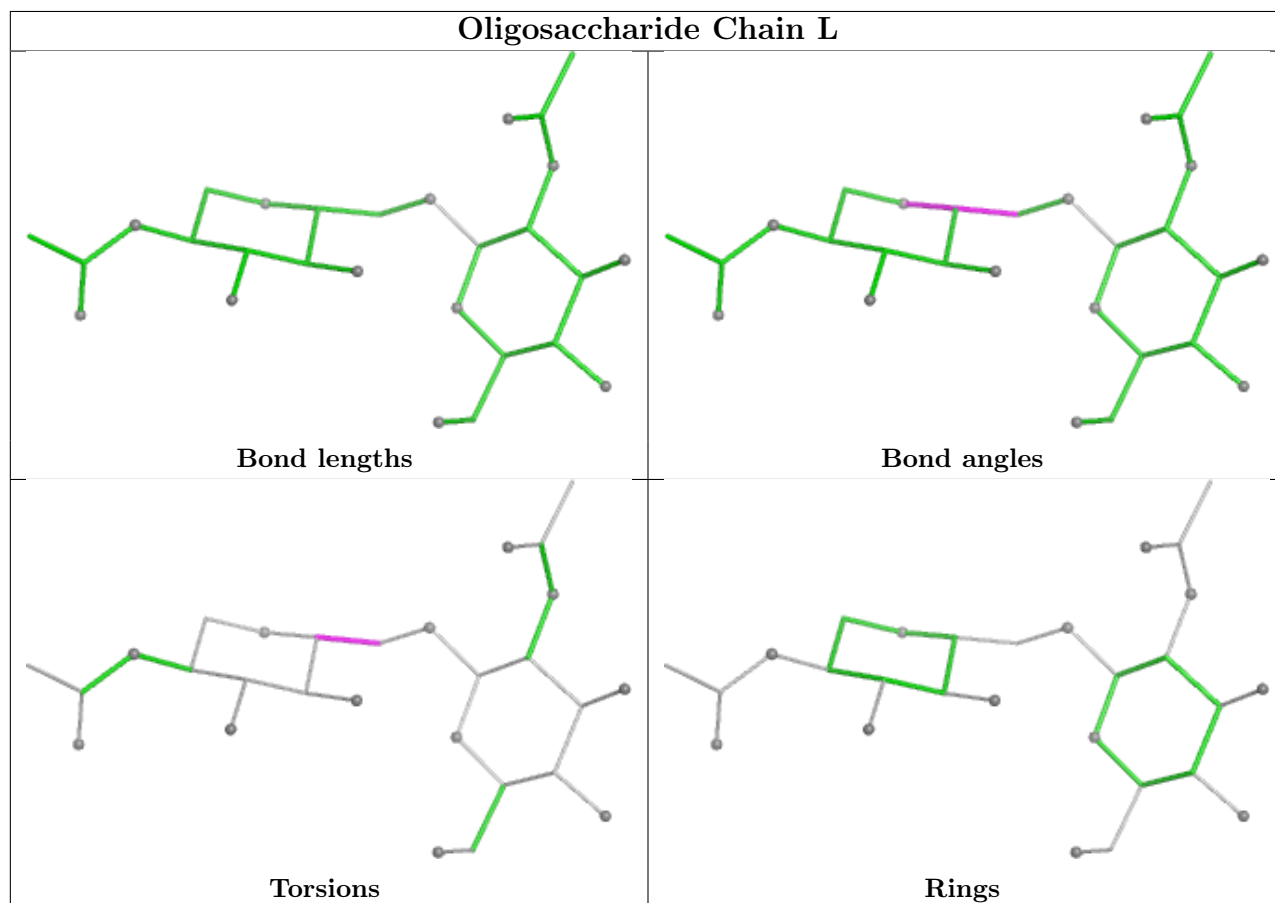
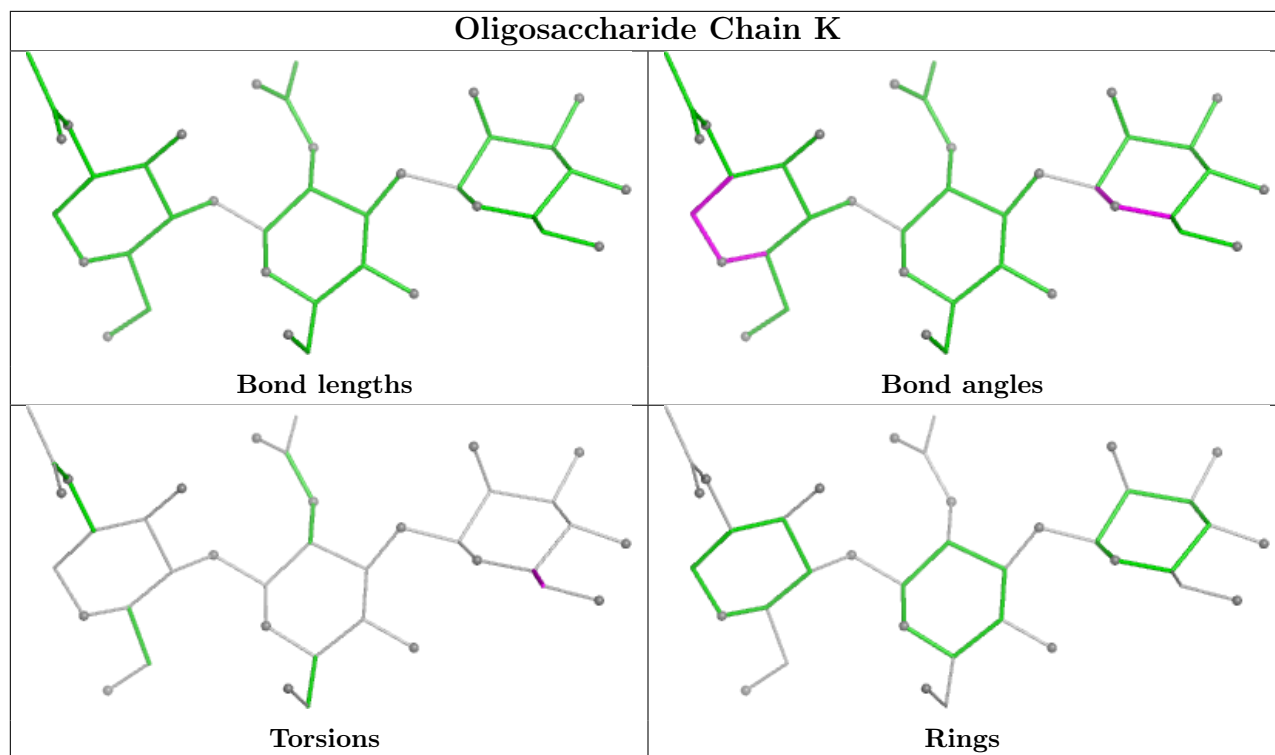
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry

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
10	ABU	B	601	-	6,6,6	1.04	0	6,6,6	1.17	1 (16%)
11	TOR	B	602	-	24,24,24	0.24	0	37,41,41	0.62	0
10	ABU	D	402	-	6,6,6	1.04	0	6,6,6	1.17	1 (16%)
13	NAG	D	401	1	14,14,15	0.68	0	17,19,21	0.96	1 (5%)
12	EPE	C	601	-	15,15,15	0.82	1 (6%)	18,20,20	0.86	0
11	TOR	E	601	-	24,24,24	0.15	0	37,41,41	0.36	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	ABU	B	601	-	-	2/4/4/4	-
11	TOR	B	602	-	-	7/7/48/48	0/3/3/3
10	ABU	D	402	-	-	0/4/4/4	-
13	NAG	D	401	1	-	1/6/23/26	0/1/1/1
12	EPE	C	601	-	-	1/9/19/19	0/1/1/1
11	TOR	E	601	-	-	5/7/48/48	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	601	EPE	C10-S	2.28	1.80	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	402	ABU	O-C-CG	-2.25	115.85	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	601	ABU	O-C-CG	-2.23	115.91	123.08
13	D	401	NAG	O5-C1-C2	-2.10	107.98	111.29

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

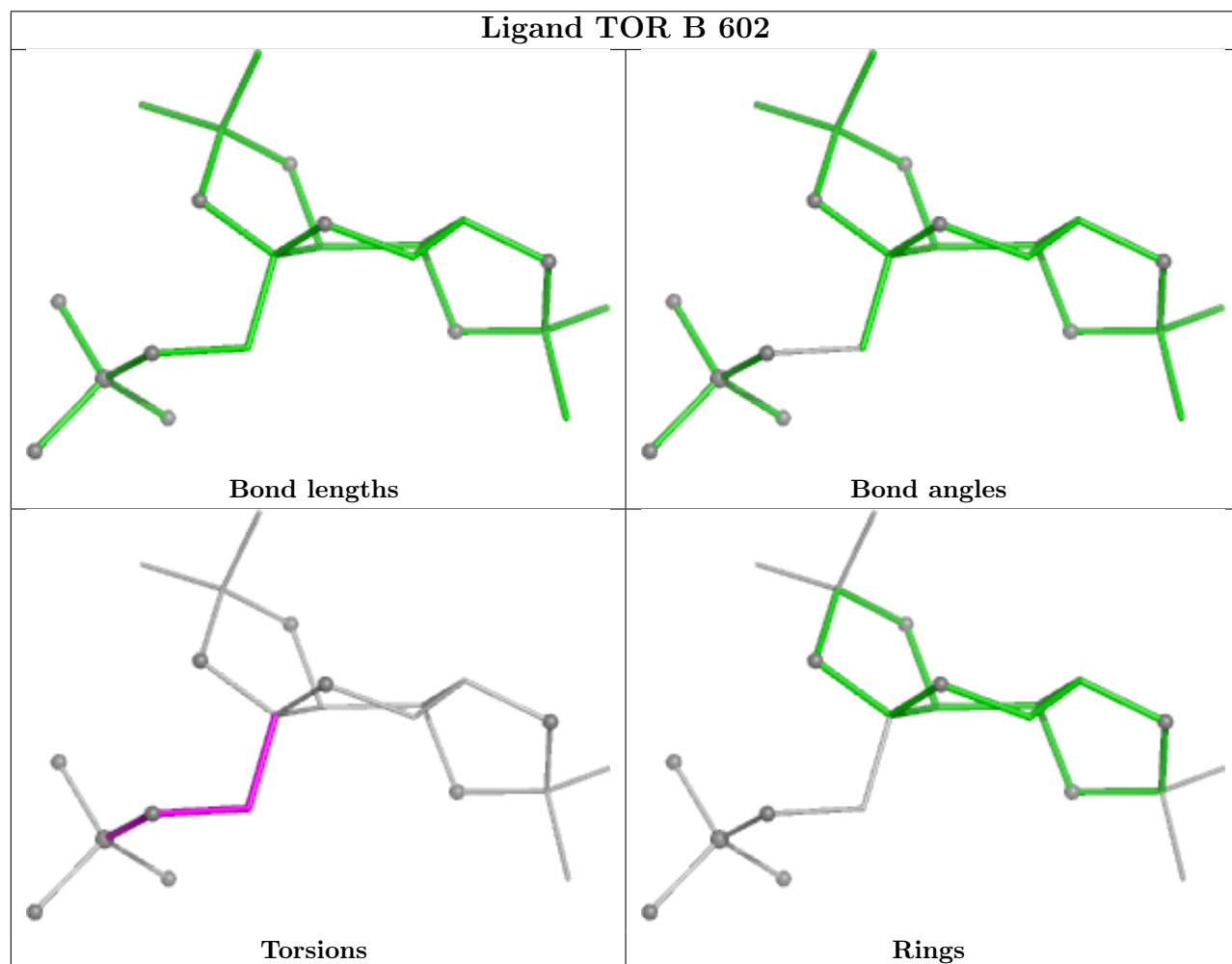
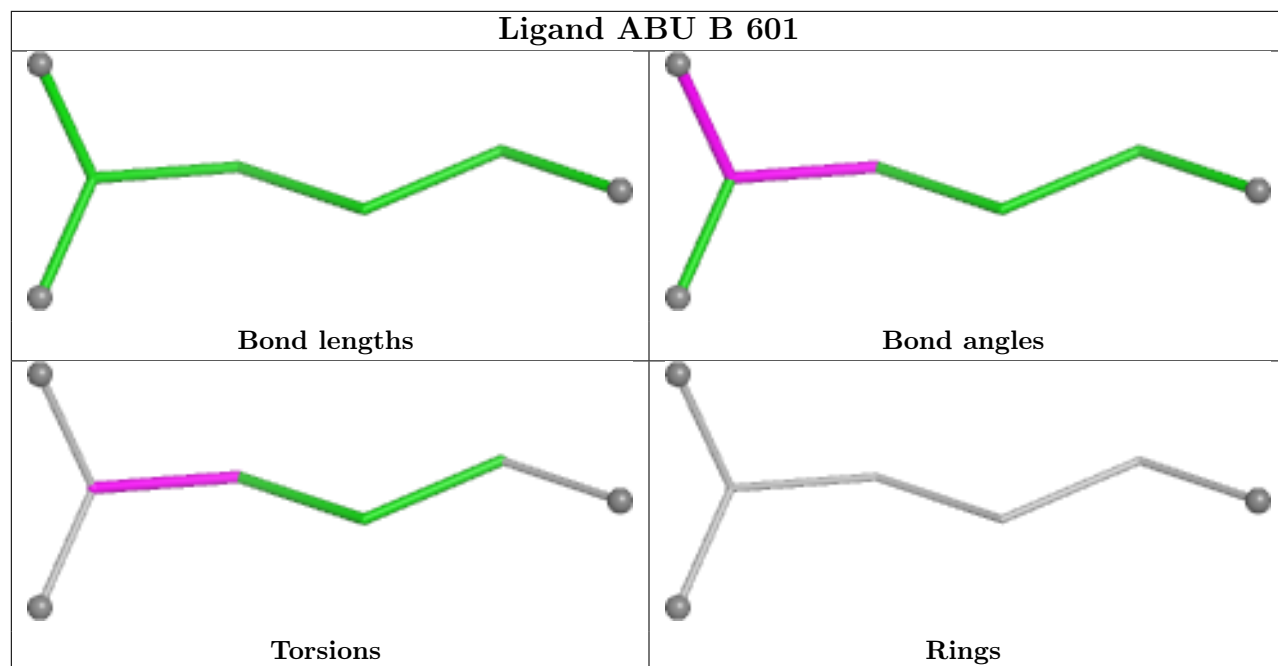
Mol	Chain	Res	Type	Atoms
11	B	602	TOR	OAR-CAL-CAM-OAN
11	B	602	TOR	CAK-CAL-CAM-OAN
11	B	602	TOR	OAH-CAL-CAM-OAN
11	B	602	TOR	CAL-CAM-OAN-SAO
11	B	602	TOR	CAM-OAN-SAO-OAS

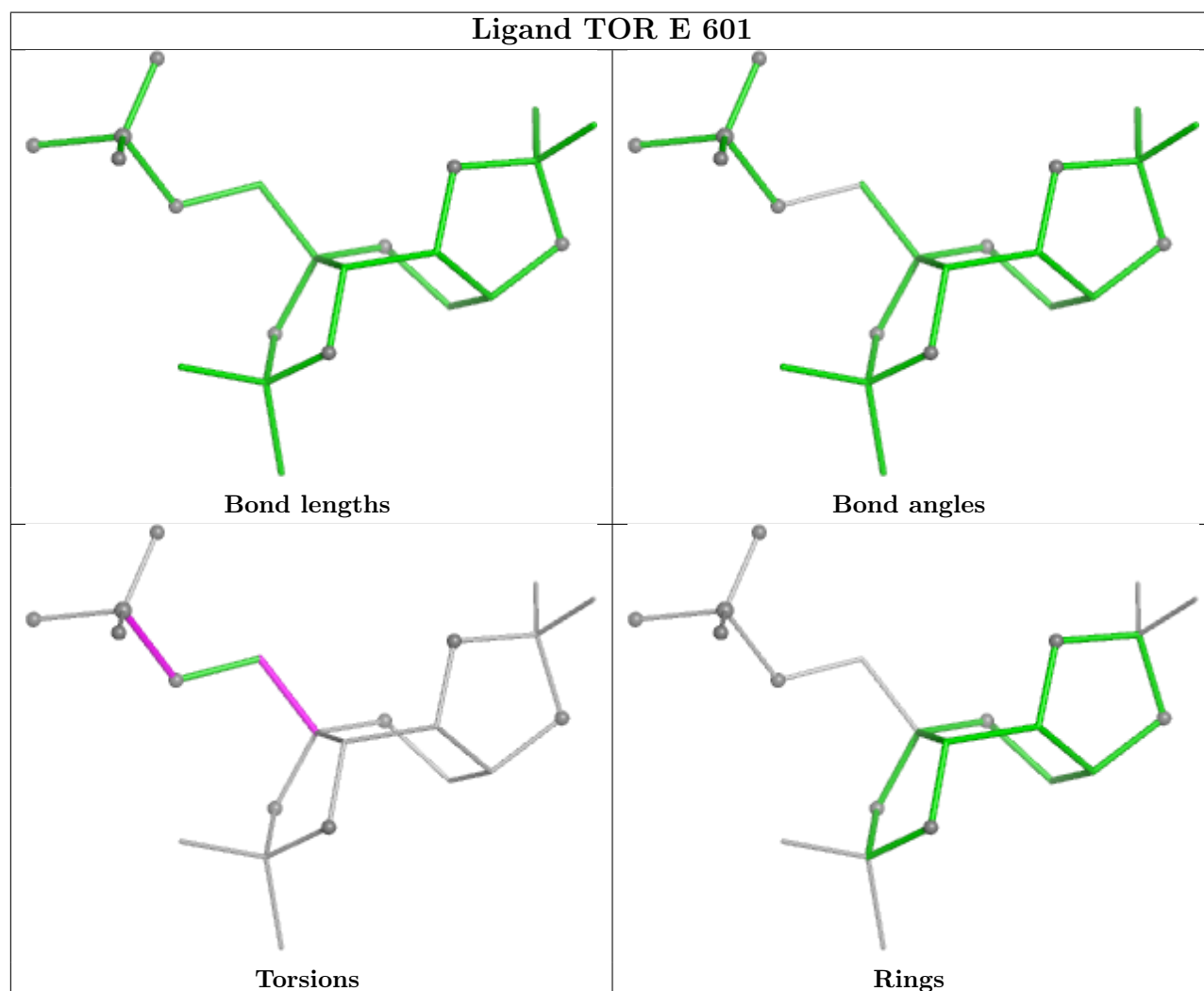
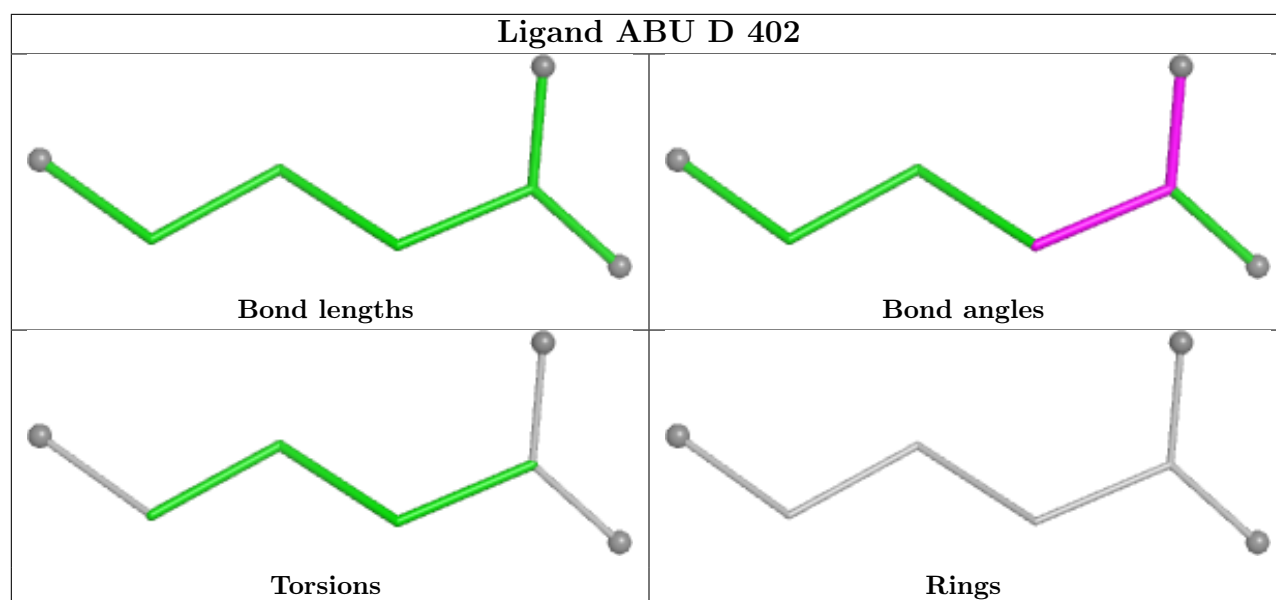
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	602	TOR	4	0
11	E	601	TOR	2	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.

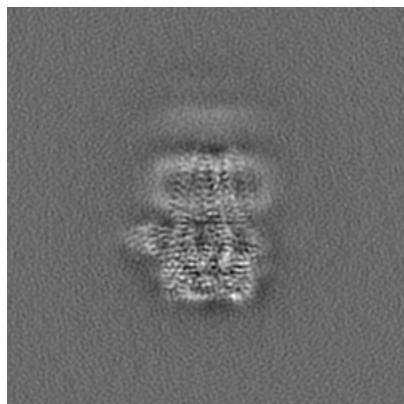
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54031. These allow visual inspection of the internal detail of the map and identification of artifacts.

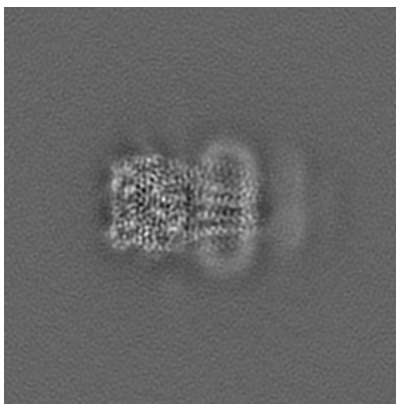
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

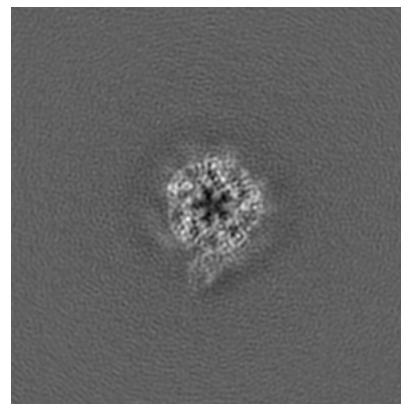
6.1.1 Primary map



X

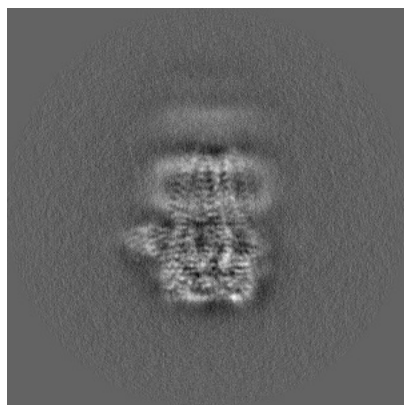


Y

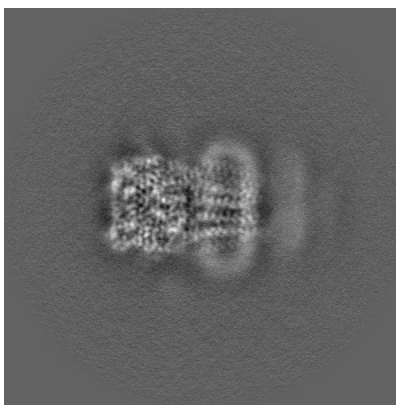


Z

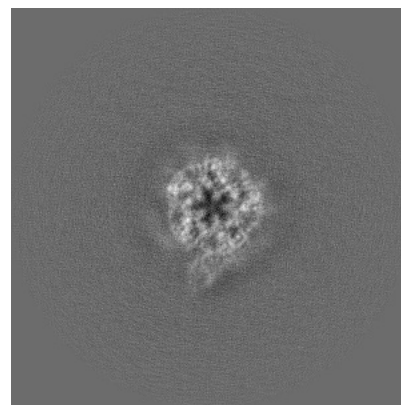
6.1.2 Raw map



X



Y

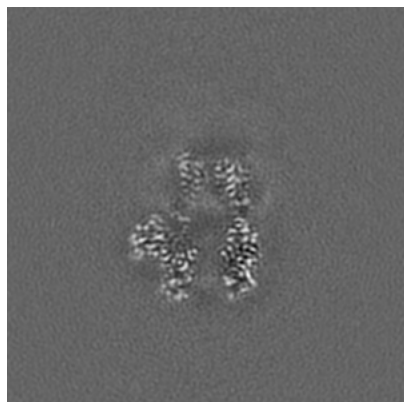


Z

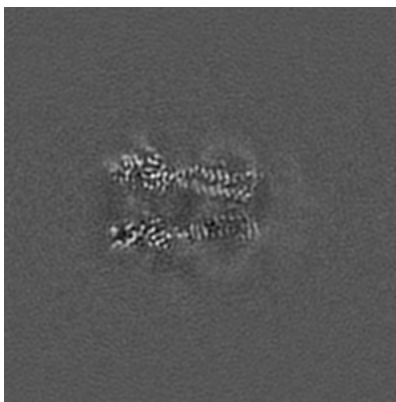
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

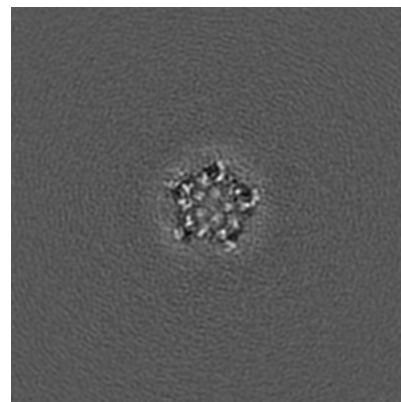
6.2.1 Primary map



X Index: 220

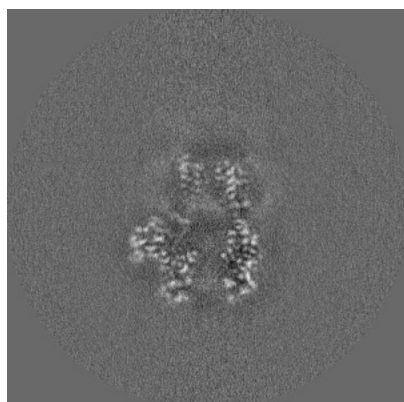


Y Index: 220

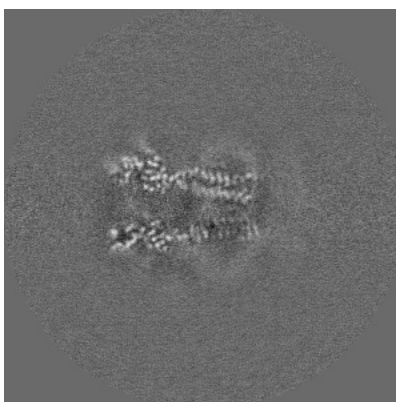


Z Index: 220

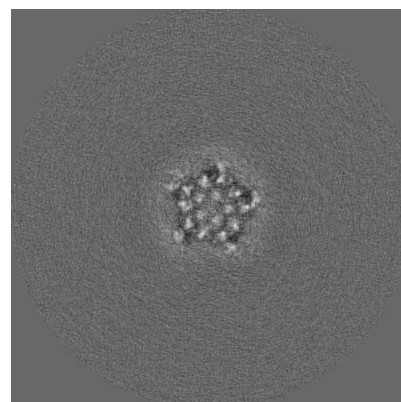
6.2.2 Raw map



X Index: 220



Y Index: 220

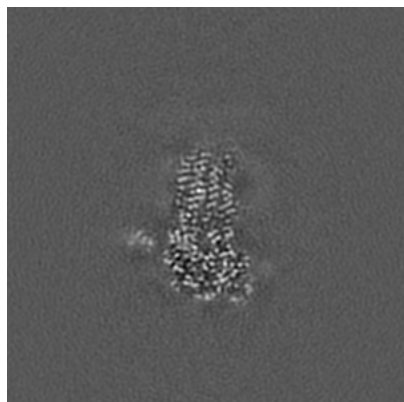


Z Index: 220

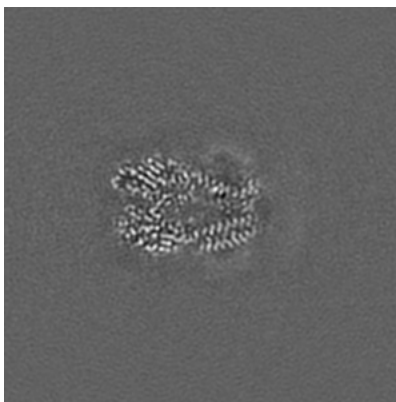
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

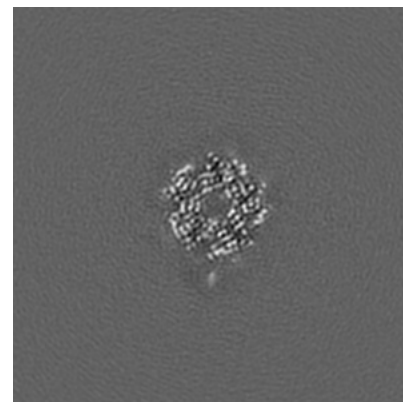
6.3.1 Primary map



X Index: 195

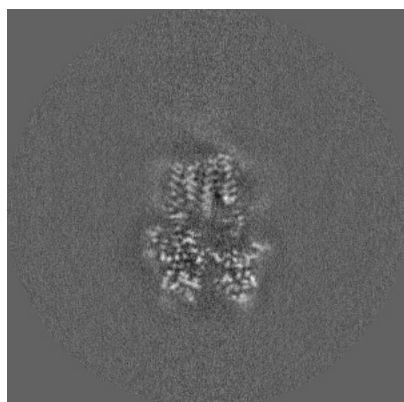


Y Index: 240

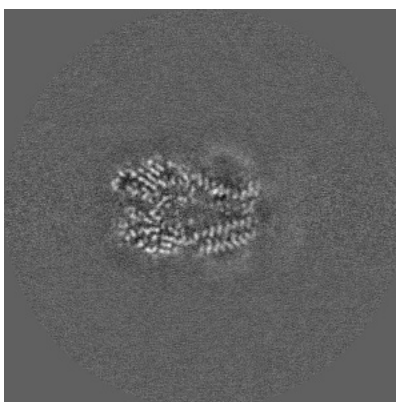


Z Index: 164

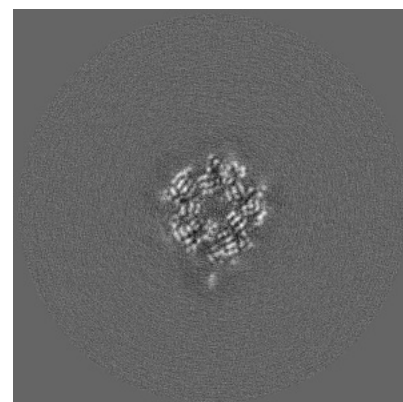
6.3.2 Raw map



X Index: 238



Y Index: 240

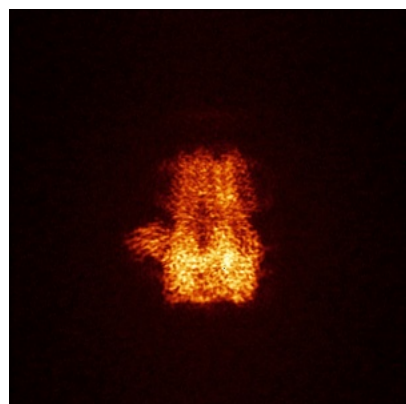


Z Index: 165

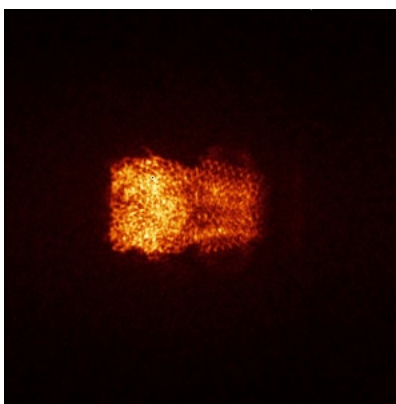
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

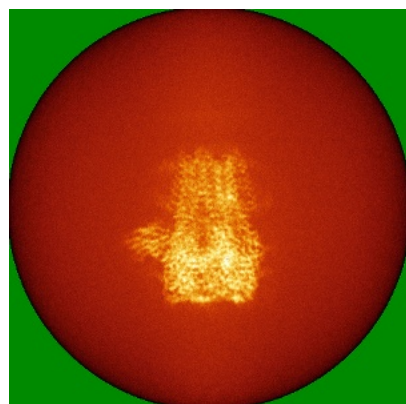


Y

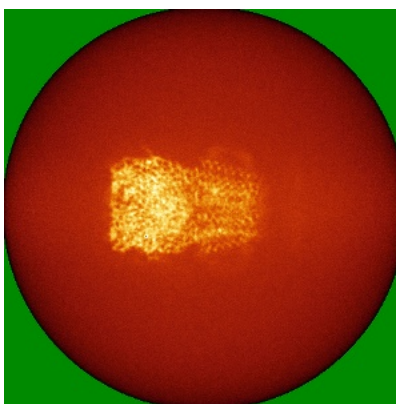


Z

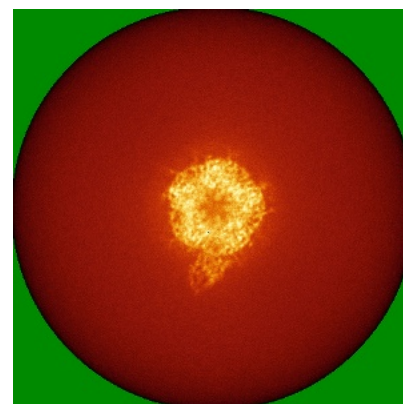
6.4.2 Raw map



X



Y

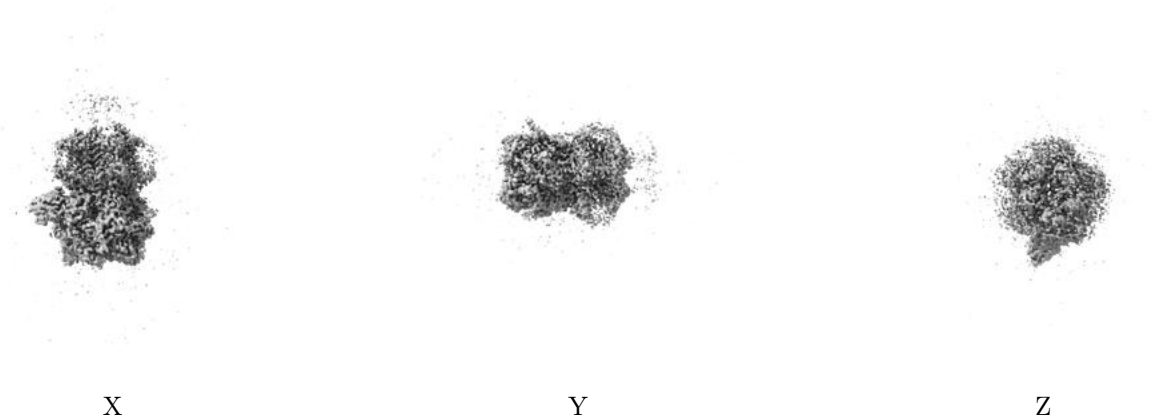


Z

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.

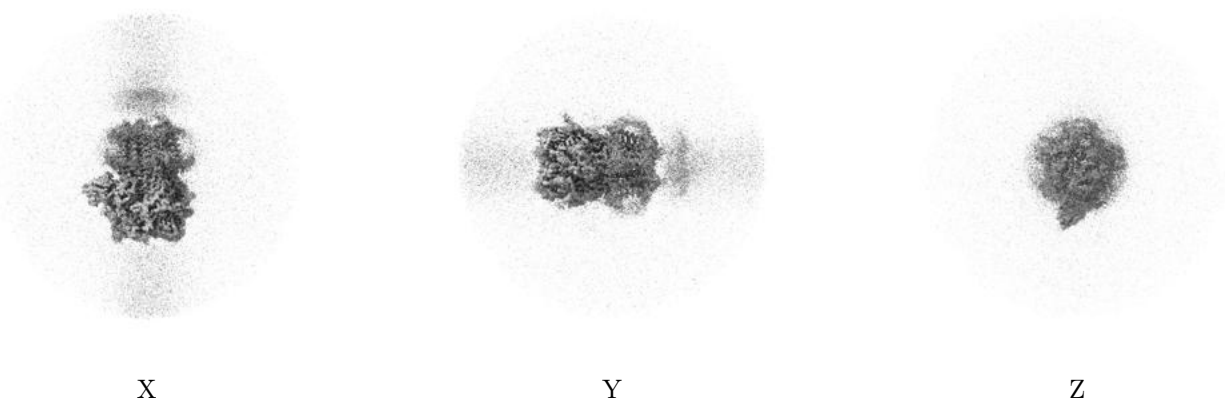
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

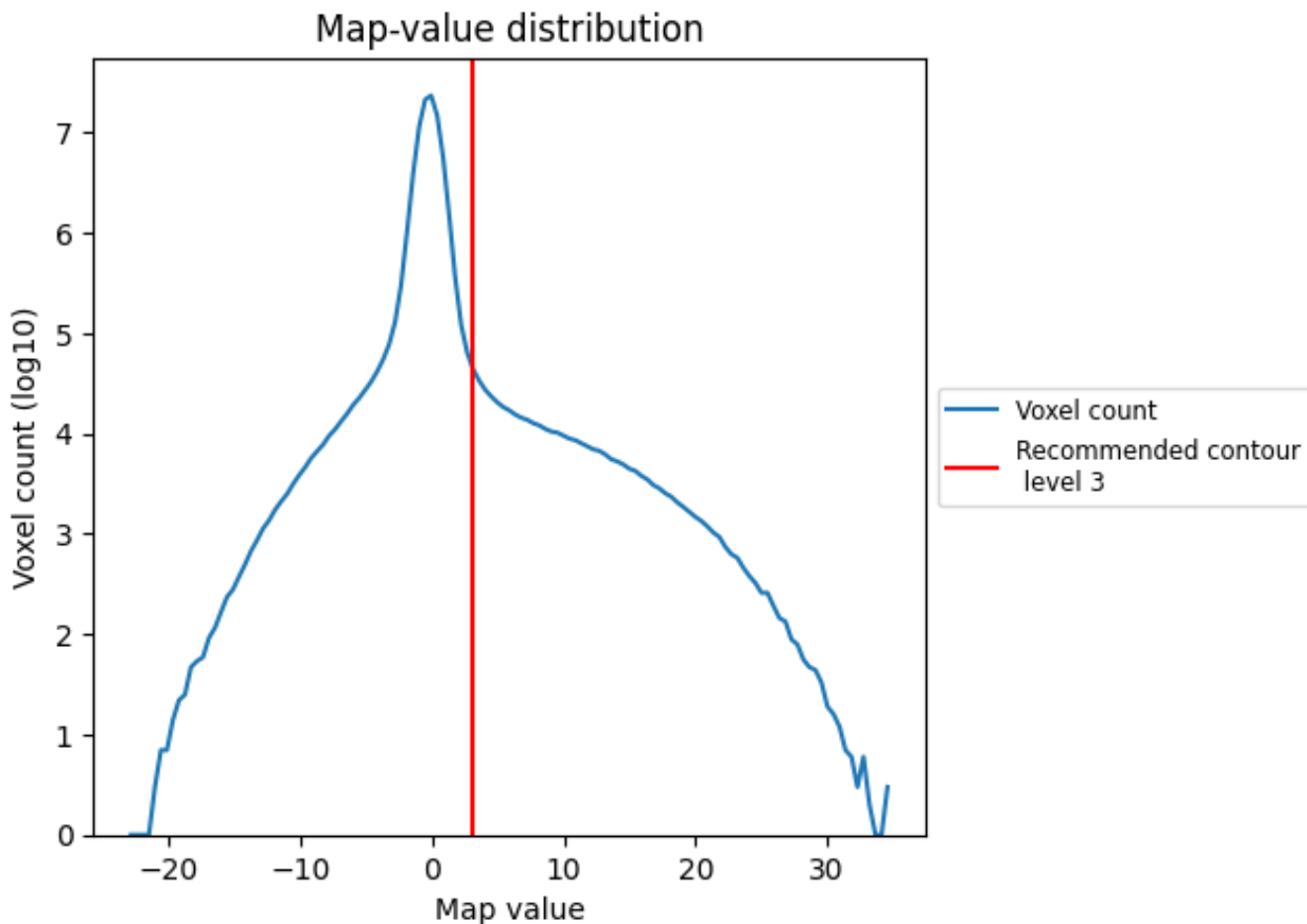
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

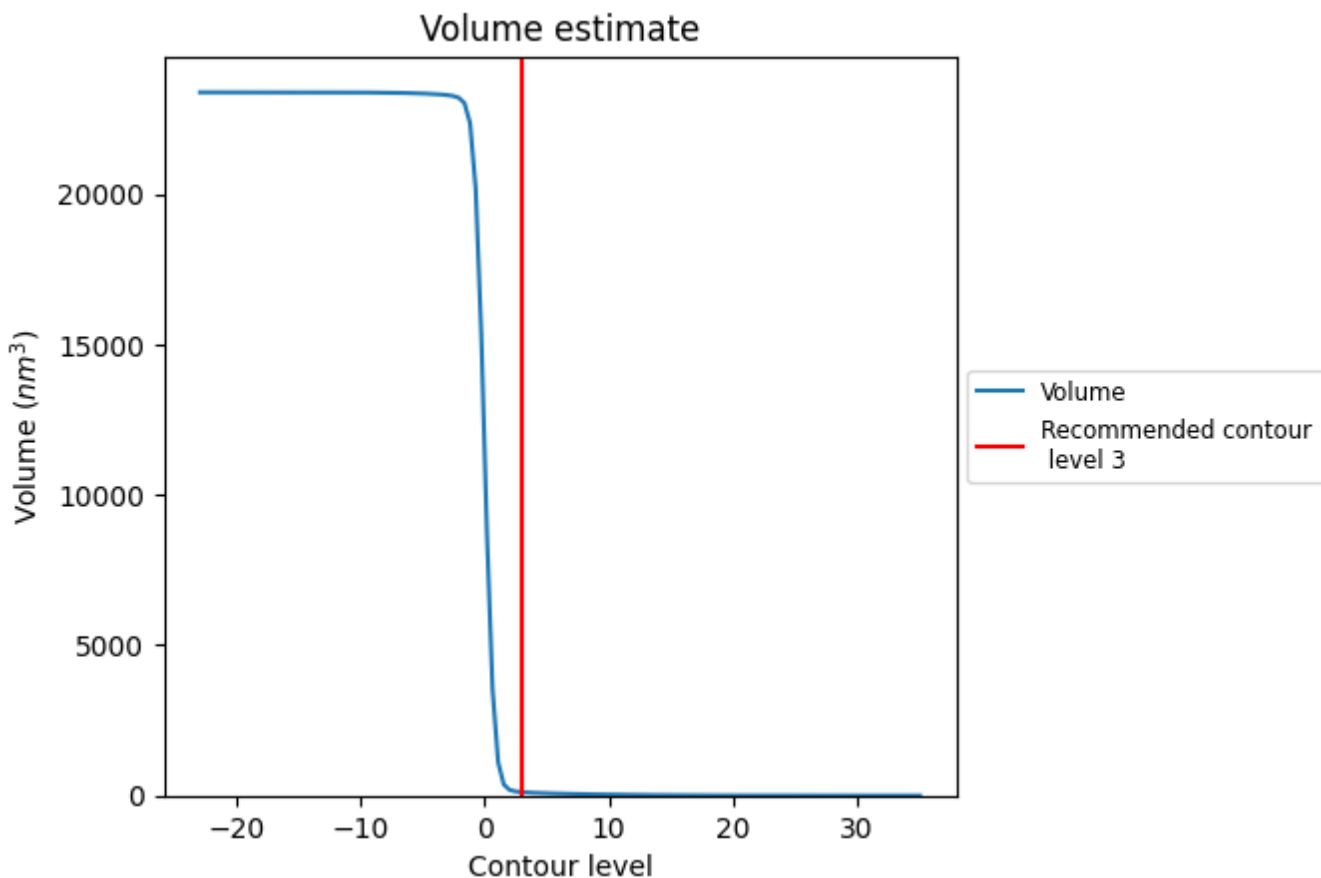
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

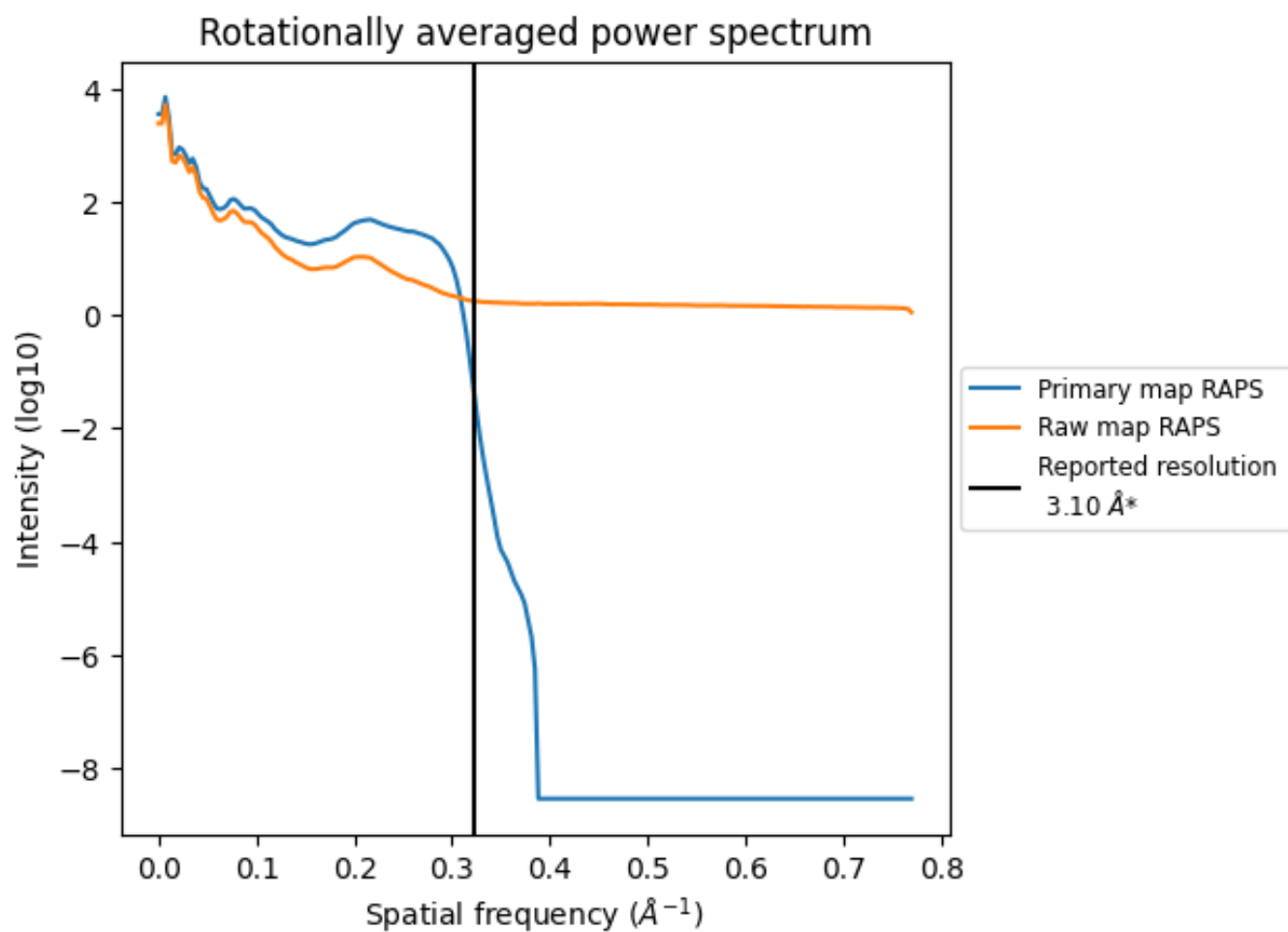
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm^3 ; this corresponds to an approximate mass of 104 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](#)

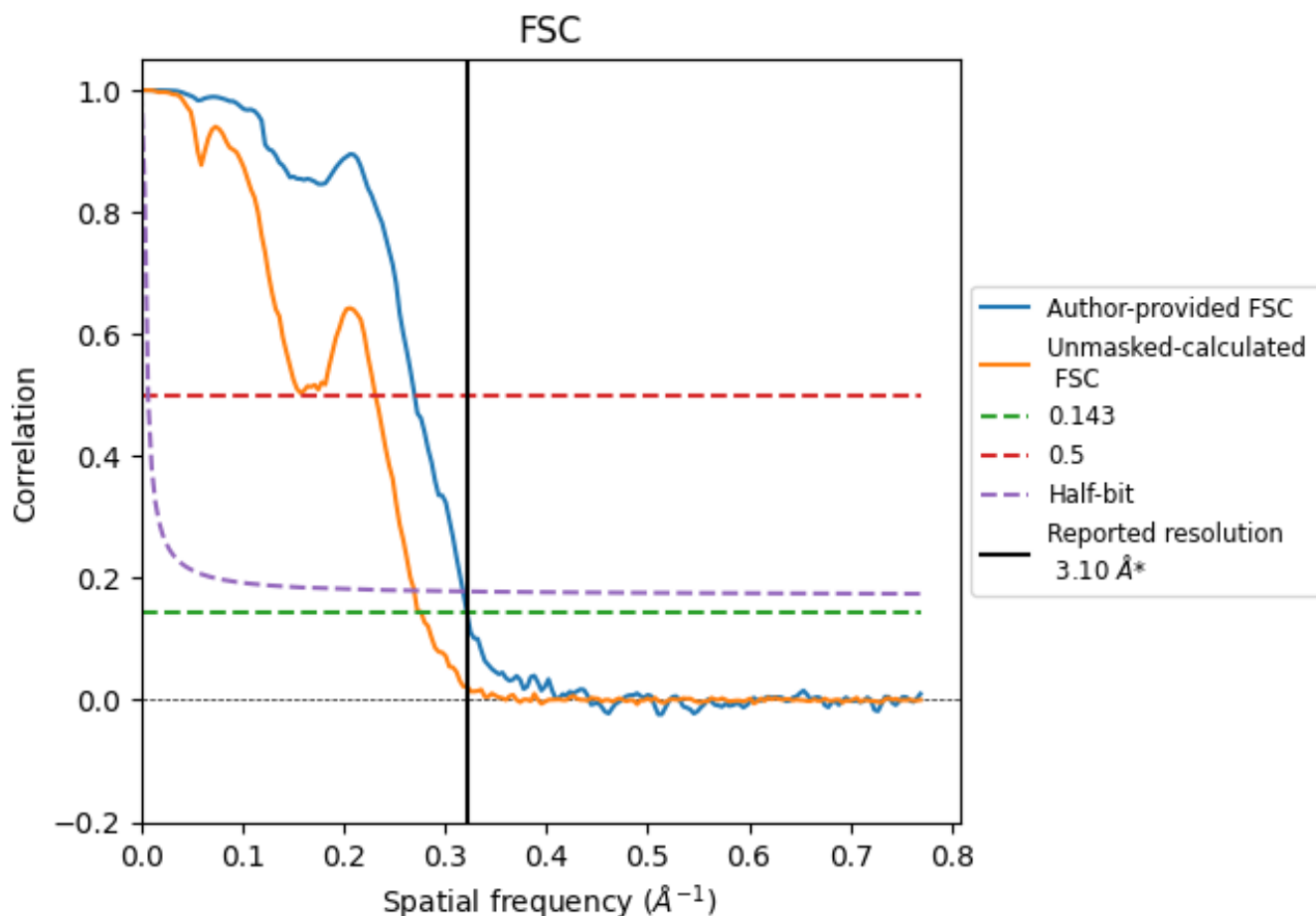


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

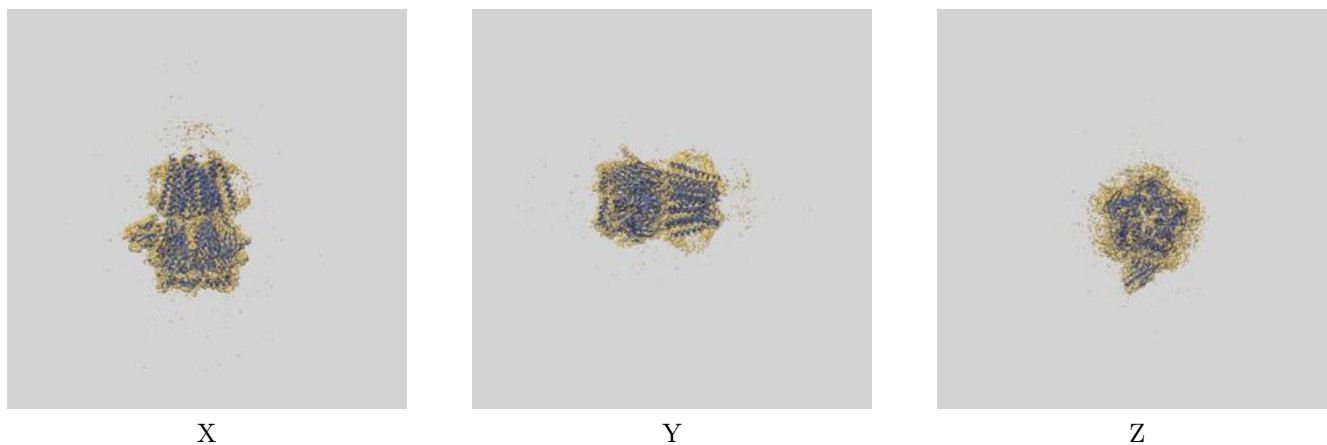
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.71	3.15
Unmasked-calculated*	3.62	4.33	3.71

*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 3.62 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

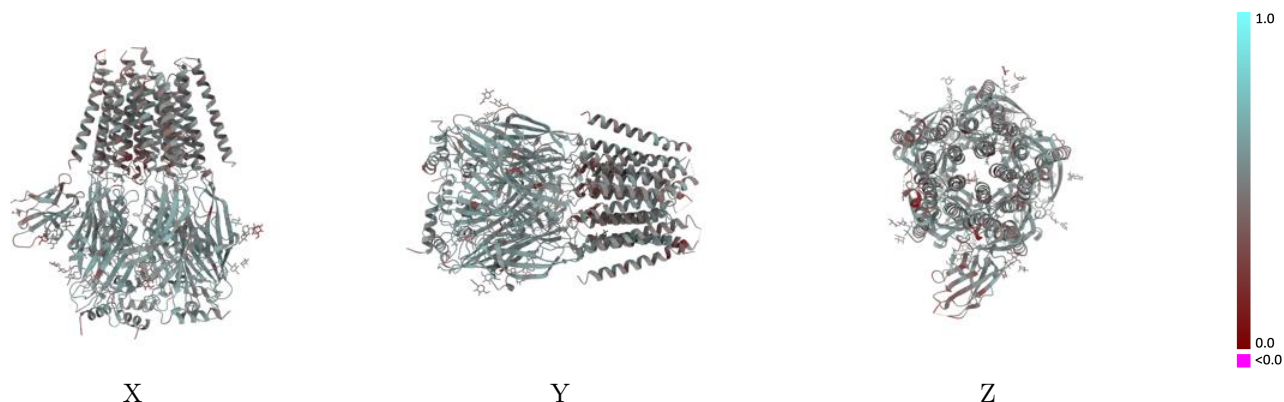
This section contains information regarding the fit between EMDB map EMD-54031 and PDB model 9RL5. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



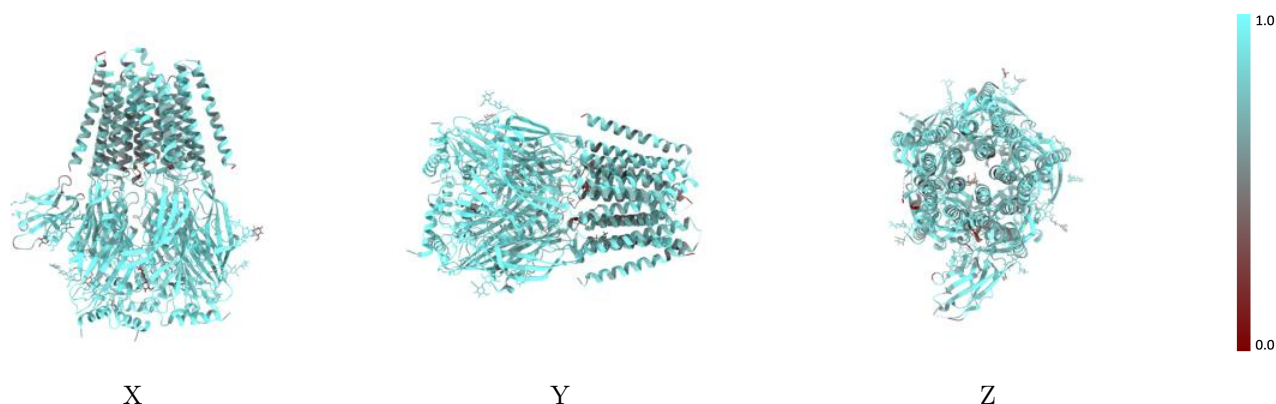
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



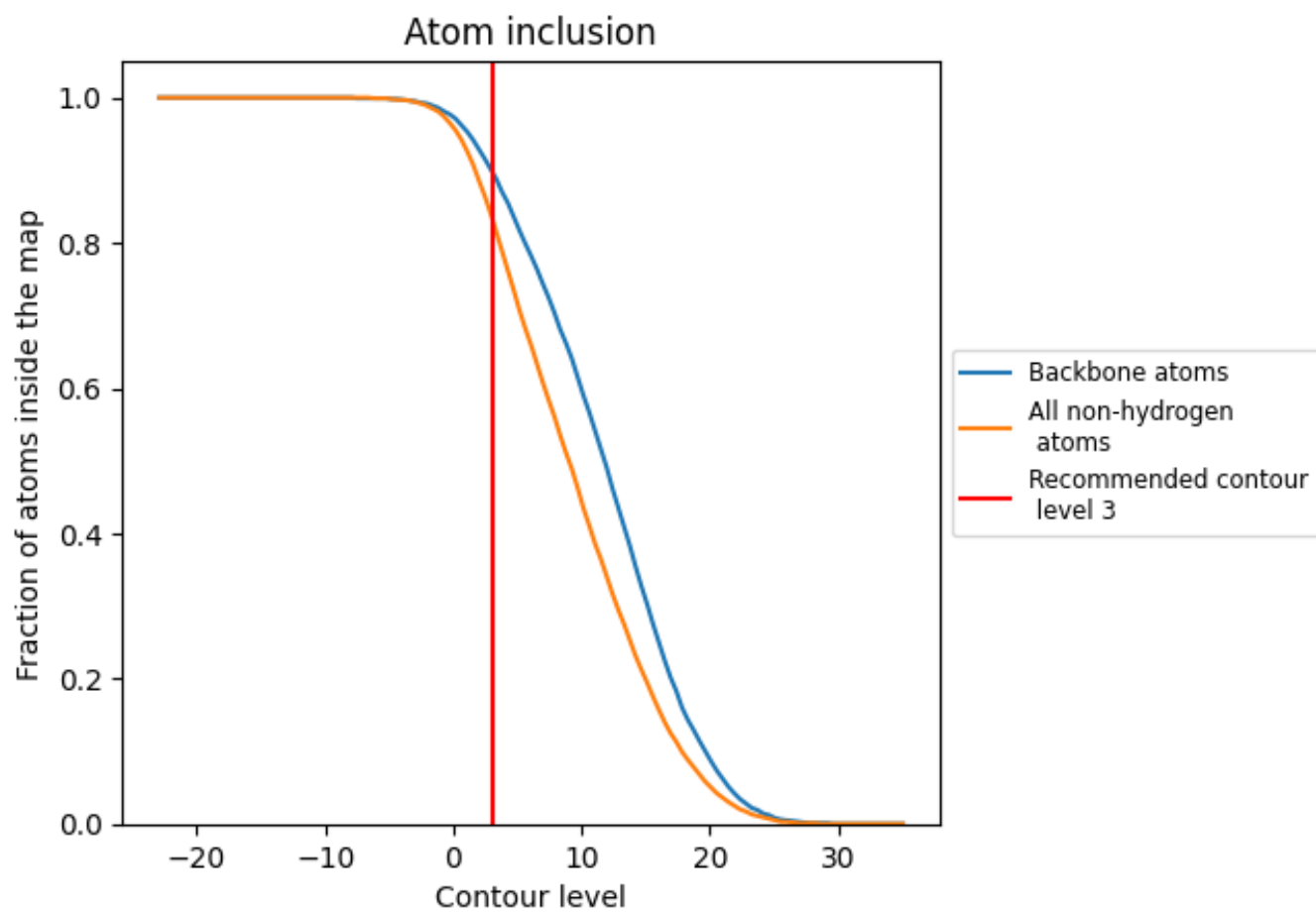
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.5000
A	 0.8350	 0.5050
B	 0.8350	 0.5040
C	 0.8240	 0.5090
D	 0.8450	 0.5030
E	 0.8610	 0.5110
F	 0.7860	 0.4490
G	 0.1540	 0.1960
H	 0.7950	 0.3990
I	 0.8470	 0.4670
J	 0.7920	 0.4180
K	 0.6150	 0.4040
L	 0.7860	 0.4350
M	 0.8970	 0.4300
N	 0.7920	 0.4320
P	 0.8170	 0.4530

