



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 08:08 PM UTC

PDB ID : 8JXA / pdb_00008jxa
EMDB ID : EMD-36694
Title : cryo-EM structure of rat megalin bodyB
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on : 2023-06-30
Resolution : 3.80 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

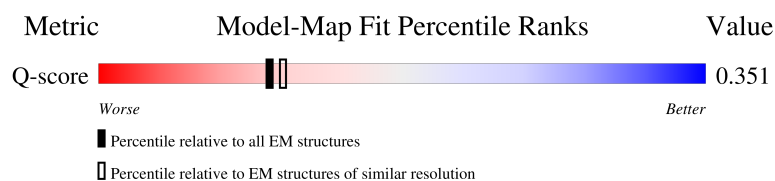
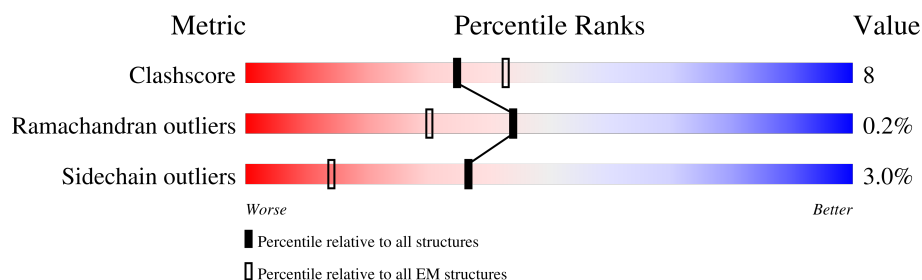
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	4660	
1	B	4660	
2	M	5	
3	C	3	

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Mol	Chain	Length	Quality of chain
3	D	3	33% 33% 67%
4	E	5	40% 80% 20%
4	H	5	60% 80% 20%
4	I	5	20% 80% 20%
5	F	2	50% 100%
5	G	2	100%
5	J	2	100%
6	K	3	100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 11889 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.

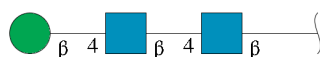
- Molecule 1 is a protein called LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1077	Total	C	N	O	S	0	0
			8455	5100	1537	1687	131		
1	B	361	Total	C	N	O	S	0	0
			2904	1844	493	549	18		

- Molecule 2 is a protein called unclear peptide.

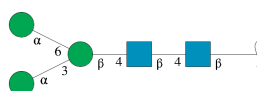
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 3 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
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 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.



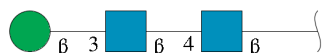
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	5	Total	C	N	O	0	0
			61	34	2	25		
4	H	5	Total	C	N	O	0	0
			61	34	2	25		
4	I	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 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
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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.



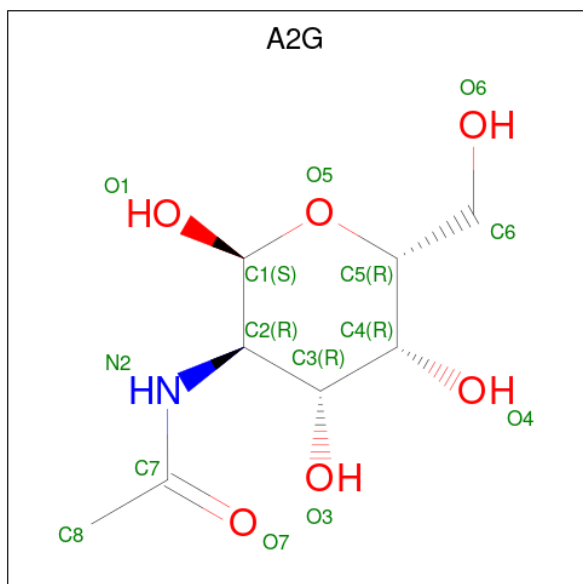
Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
9	A	20	Total	Ca	0
			20	20	







[illegible]





H4387	G4388	G4389	M4390	C4391	Y4392	F4393	D4394	A4395	E4396	E4397	L4398	F4399	K4400	C4401	K4402	C4403	S4404	S4405	G4406	Y4407	S4408	G4409	E4410	Y4411	C4412	E4413	V4414	G4415	LEU			
R4327	Y4328	M4329	Q4330	S4331	F4332	S4333	N4334	P4335	C4336	K4337	Q4338	F4339	V4339	C4340	L4341	L4342	L4343	L4344	L4345	L4346	R4347	G4348	G4349	G4350	Y4351	C4352	C4353	A4354	C4355	LEU		
R4267	L4268	I4269	T4270	M4271	E4272	M4273	M4274	K4275	P4276	F4277	S4278	L4279	D4280	I4281	F4282	E4283	D4284	K4285	L4286	F4287	W4288	W4289	A4290	K4291	E4292	K4293	G4294	E4295	P4296	ARG		
G4207	K4208	Q4209	P4210	K4211	I4212	E4213	S4214	A4215	W4216	M4217	M4218	G4219	E4220	H4221	R4222	S4223	V4224	L4225	V4226	S4227	E4228	M4229	L4230	G4231	W4232	P4233	M4234	G4235	L4236	ARG		
P4146	G4148	L4149	A4150	V4151	D4152	W4153	V4154	G4155	R4156	T4158	Y4159	W4160	S4161	A4162	A4163	S4165	G4166	R4167	T4168	A4171	T4172	L4173	D4174	G4175	R4176	Y4177	R4178	K4179	W4180	LEU		
E4081	E4082	E4083	E4084	H4085	I4086	Q4087	T4088	I4089	D4090	Y4091	D4092	W4093	D4094	P4095	E4096	H4097	I4098	G4099	L4100	S4101	W4102	V4103	Y4105	T4106	V4107	Q4110	G4111	S4112	L4117	LEU		
GLN	SER	CYS	ARG	ASN	SER	LYS	GLY	SER	TYR	GLU	CYS	PHE	GLN	LYS	ASN	GLY	GLU	GLY	GLU	GLY	ARG	CYS	ALA	ALA	ASP	SER	P4055	P4056	L4057	L4058	L4059	L4060
THR	GLY	PRO	ASN	ASN	GLY	ASP	VAL	ASN	THR	CYS	ALA	GLU	GLN	ASN	GLU	THR	GLY	SER	SER	GLY	THR	GLY	ILE	CYS	THR	CYS	THR	THR	PRO	GLY	PHE	LYS
THR	TYR	CYS	ASN	CYS	GLY	VAL	ASP	ASP	THR	GLY	GLY	SER	VAL	ASN	VAL	ASP	GLY	GLU	GLY	THR	GLY	GLY	VAL	GLY	THR	THR	THR	TYR	ARG	ALA	GLN	
GLY	THR	TYR	PRO	ALA	ALA	MET	PHE	GLU	THR	CYS	GLY	ASN	HIS	VAL	CYS	GLU	GLY	GLN	SER	PHE	THR	GLY	THR	ASN	GLY	ALA	ALA	LEU	GLY	THR	GLN	
THR	GLY	PRO	ASN	GLY	ASP	ASP	THR	GLY	GLY	ASN	HIS	VAL	CYS	VAL	GLY	ILE	GLN	GLY	GLY	THR	GLY	GLY	THR	ASN	GLY	THR	THR	TYR	ARG	ALA	GLN	
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THR	GLN	CYS	ALA	LYS	ARG	CYS	ASP	ASP	PRO	ILE	THR	ASN	VAL	ASP	ASP	GLY	THR	VAL	ASP	GLY	GLY	THR	THR	ASN	GLY	ALA	ALA	LEU	GLY	THR	GLN	
ASP	CYS	HIS	PRO	GLY	PHE	ARG	ASP	ASP	PRO	ILE	THR	ASN	VAL	ASP	ASP	GLY	THR	VAL	ASP	GLY	GLY	THR	THR	ASN	GLY	ALA	ALA	LEU	GLY	THR	GLN	
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ASP	CYS	HIS	PRO	GLY	PHE	ARG	ASP	ASP	PRO	ILE	THR	ASN	VAL	ASP	ASP	GLY	THR	VAL														

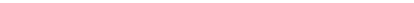
[illegible]

- Molecule 2: unclear peptide

Chain M: 100%

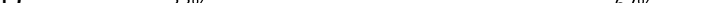
There are no outlier residues recorded for this chain.

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

Chain C:  67% 100%

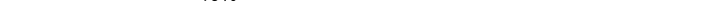


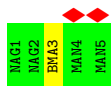
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  33% 33% 67%

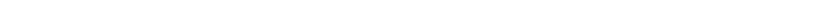


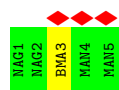
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  40% 80% 20%

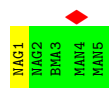
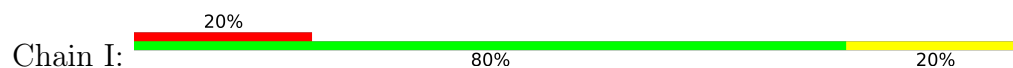


- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain H:  60% 80% 20%



- Molecule 4: 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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0434	Depositor
Map size ($\text{\AA}$)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.411, 1.411, 1.411	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: CA, BMA, NAG, MAN, A2G

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	0.21	0/8659	0.46	0/11737
1	B	0.12	0/2981	0.34	0/4047
2	M	0.13	0/7	0.27	0/8
All	All	0.19	0/11647	0.43	0/15792

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	8455	0	7527	137	0
1	B	2904	0	2797	45	0
2	M	28	0	12	0	0
3	C	39	0	34	0	0
3	D	39	0	34	1	0
4	E	61	0	52	0	0
4	H	61	0	52	0	0
4	I	61	0	52	0	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	28	0	25	0	0
6	K	39	0	34	0	0
7	A	28	0	26	0	0
8	A	70	0	60	0	0
9	A	20	0	0	0	0
All	All	11889	0	10755	181	0

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

The worst 5 of 181 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4179:LYS:HA	1:B:4357:GLN:HB2	1.66	0.76
1:A:3225:LEU:HD13	1:A:3256:MET:HE1	1.71	0.71
1:B:4086:ILE:HG22	1:B:4107:VAL:HG12	1.74	0.70
1:A:3238:ARG:NH1	1:A:3464:GLN:O	2.26	0.69
1:A:3092:MET:SD	1:A:3092:MET:N	2.67	0.66

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	1073/4660 (23%)	984 (92%)	87 (8%)	2 (0%)	43	73
1	B	359/4660 (8%)	332 (92%)	26 (7%)	1 (0%)	36	67
2	M	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1433/9325 (15%)	1317 (92%)	113 (8%)	3 (0%)	44	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3315	ASP
1	B	4414	VAL
1	A	3305	HIS

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	965/4089 (24%)	944 (98%)	21 (2%)	45	63
1	B	320/4089 (8%)	302 (94%)	18 (6%)	19	45
2	M	1/1 (100%)	1 (100%)	0	100	100
All	All	1286/8179 (16%)	1247 (97%)	39 (3%)	37	57

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4236	LEU
1	B	4313	VAL
1	B	4246	VAL
1	B	4279	LEU
1	B	4387	HIS

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

Mol	Chain	Res	Type
1	A	3599	ASN
1	A	3714	GLN
1	B	4195	ASN
1	B	4130	ASN
1	B	4145	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

30 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	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	0.33	0	17,19,21	0.49	0
3	NAG	C	2	3	14,14,15	0.30	0	17,19,21	0.64	0
3	BMA	C	3	3	11,11,12	0.25	0	15,15,17	0.64	0
3	NAG	D	1	3,1	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
3	BMA	D	3	3	11,11,12	0.23	0	15,15,17	0.49	0
4	NAG	E	1	1,4	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	E	2	4	14,14,15	0.31	0	17,19,21	0.69	0
4	BMA	E	3	4	11,11,12	0.27	0	15,15,17	0.91	1 (6%)
4	MAN	E	4	4	11,11,12	0.25	0	15,15,17	0.60	0
4	MAN	E	5	4	11,11,12	0.21	0	15,15,17	0.59	0
5	NAG	F	1	1,5	14,14,15	0.27	0	17,19,21	0.70	0
5	NAG	F	2	5	14,14,15	0.31	0	17,19,21	0.55	0
5	NAG	G	1	1,5	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	H	1	1,4	14,14,15	0.32	0	17,19,21	0.89	0
4	NAG	H	2	4	14,14,15	0.32	0	17,19,21	0.59	0
4	BMA	H	3	4	11,11,12	0.24	0	15,15,17	0.85	1 (6%)
4	MAN	H	4	4	11,11,12	0.22	0	15,15,17	0.54	0
4	MAN	H	5	4	11,11,12	0.22	0	15,15,17	0.60	0
4	NAG	I	1	1,4	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	0.70	0
4	BMA	I	3	4	11,11,12	0.23	0	15,15,17	0.74	0
4	MAN	I	4	4	11,11,12	0.23	0	15,15,17	0.55	0
4	MAN	I	5	4	11,11,12	0.22	0	15,15,17	0.53	0
5	NAG	J	1	5	14,14,15	0.28	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	2	5	14,14,15	0.32	0	17,19,21	0.69	0
6	NAG	K	1	6	14,14,15	0.27	0	17,19,21	0.53	0
6	NAG	K	2	6	14,14,15	0.32	0	17,19,21	0.60	0
6	BMA	K	3	6	11,11,12	0.23	0	15,15,17	0.66	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
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
4	MAN	I	5	4	-	1/2/19/22	0/1/1/1
5	NAG	J	1	5	-	1/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
6	NAG	K	1	6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C1-O5-C5	2.50	115.54	112.19
4	H	3	BMA	C1-O5-C5	2.36	115.34	112.19
3	D	1	NAG	C2-N2-C7	-2.25	119.88	122.90
4	E	3	BMA	C1-C2-C3	2.12	112.72	109.64
3	D	2	NAG	C2-N2-C7	-2.04	120.16	122.90

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

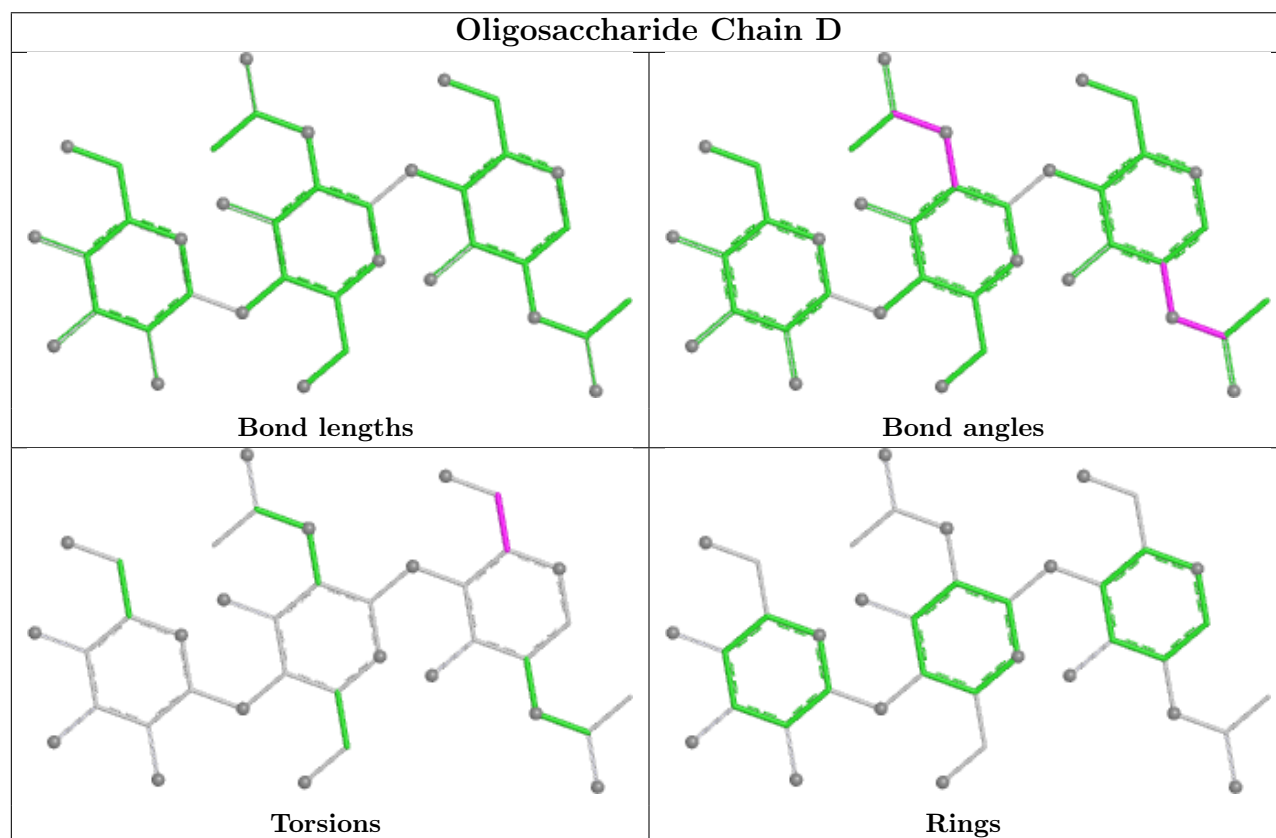
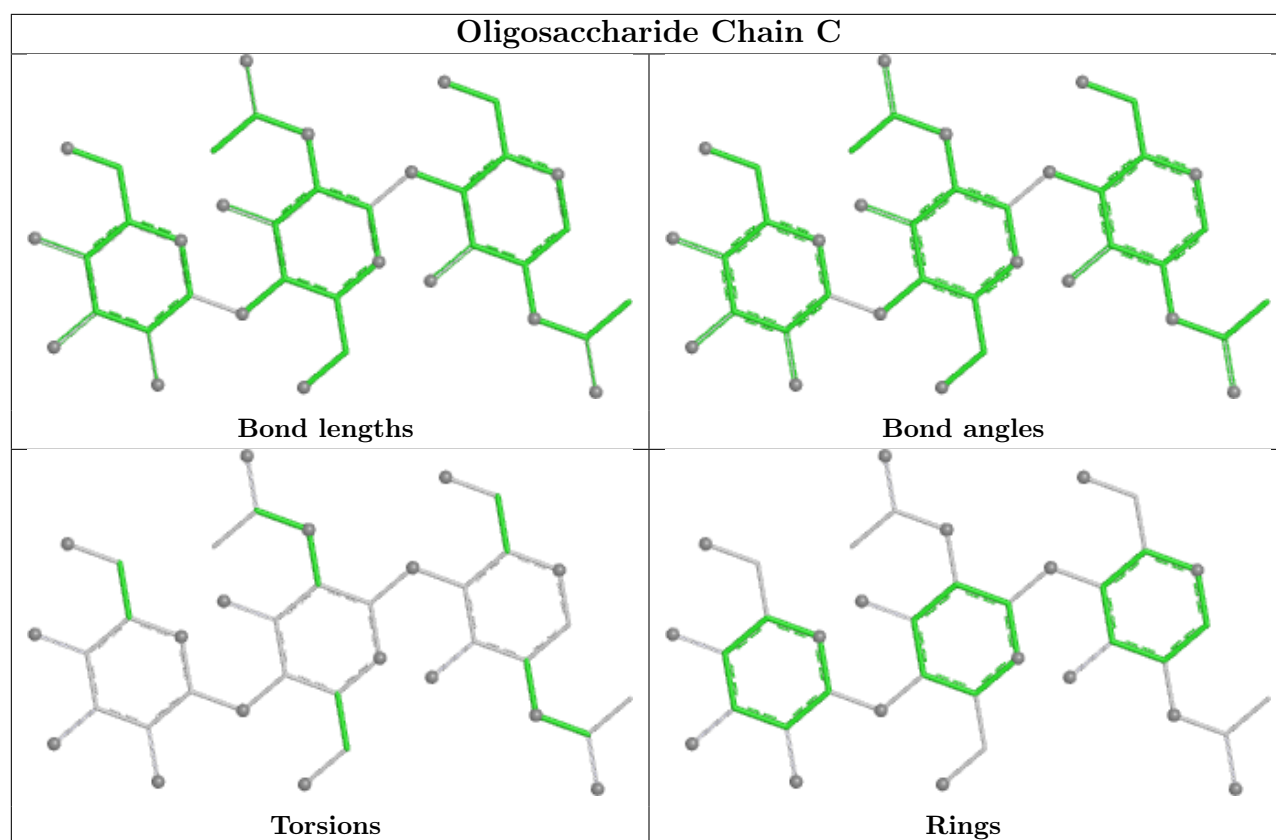
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
6	K	3	BMA	O5-C5-C6-O6

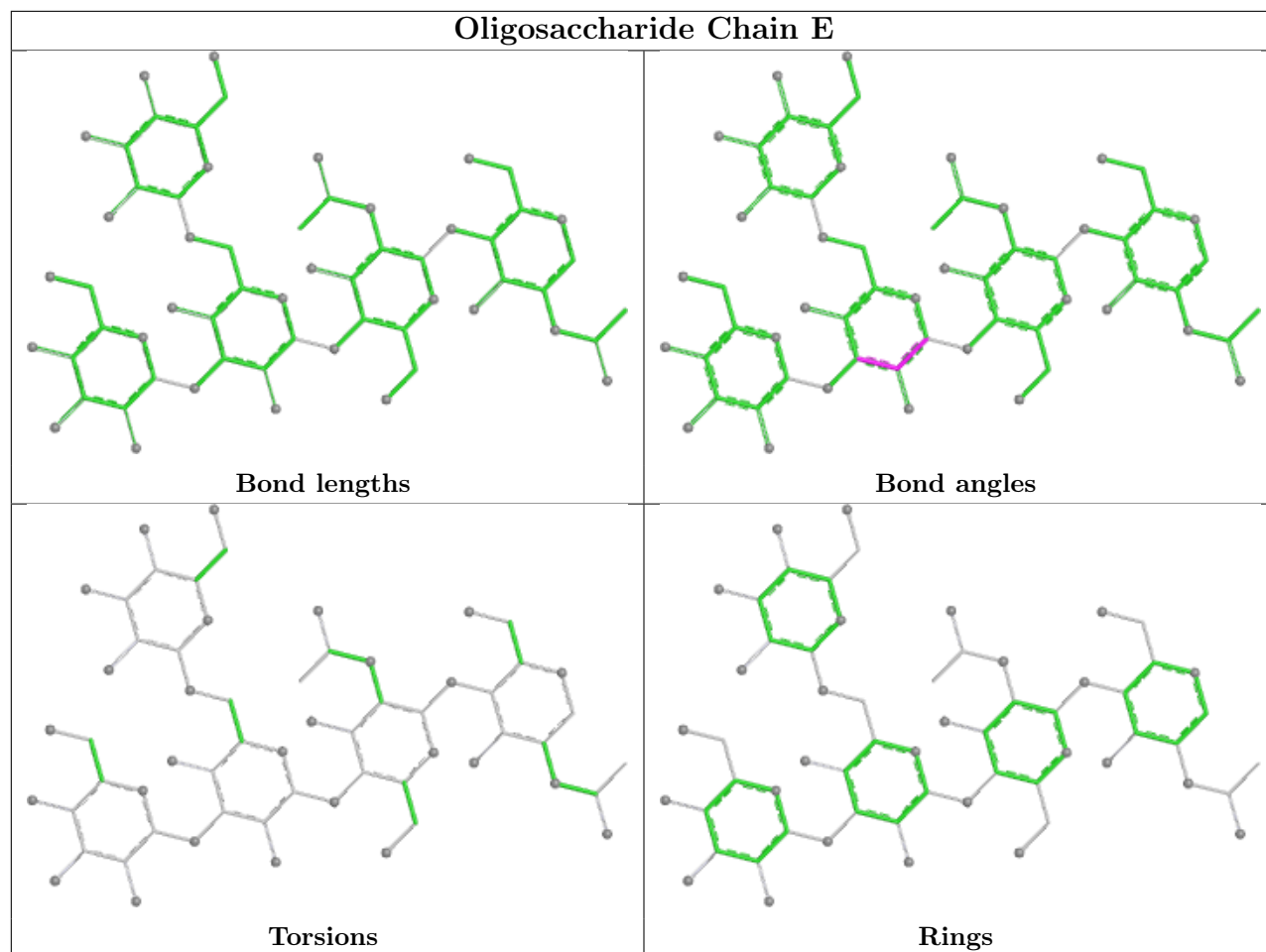
There are no ring outliers.

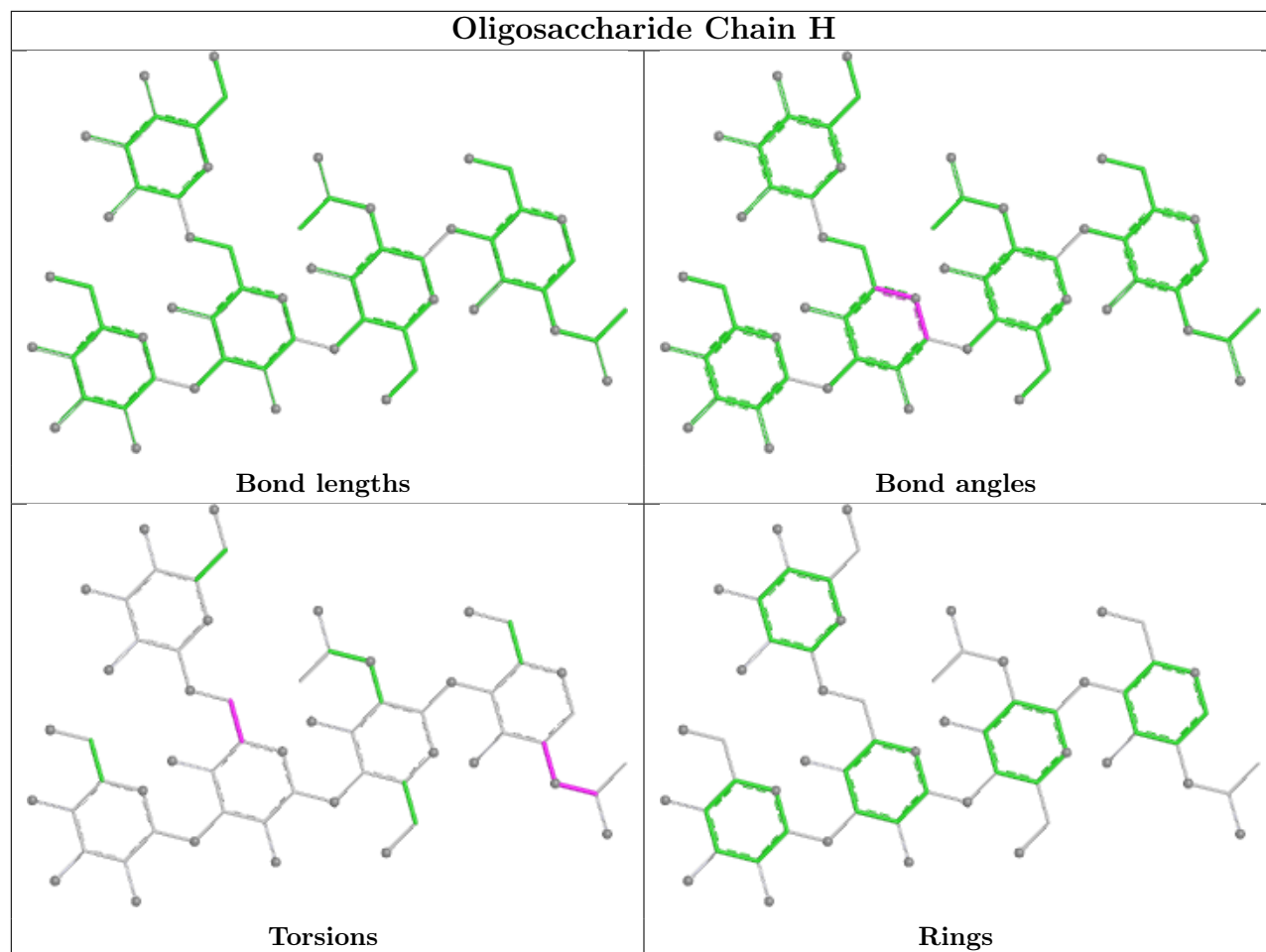
2 monomers are involved in 1 short contact:

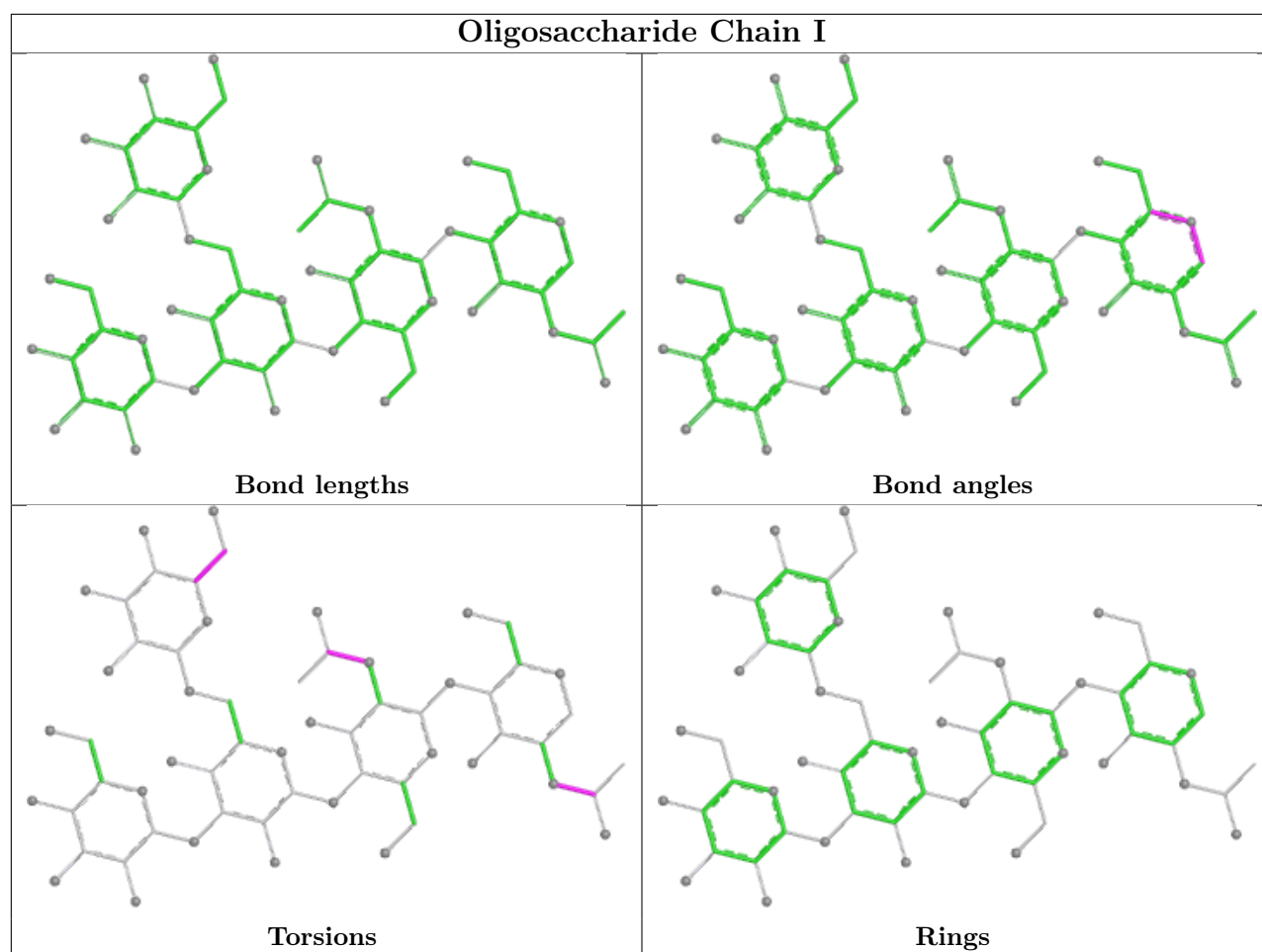
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	D	1	NAG	1	0

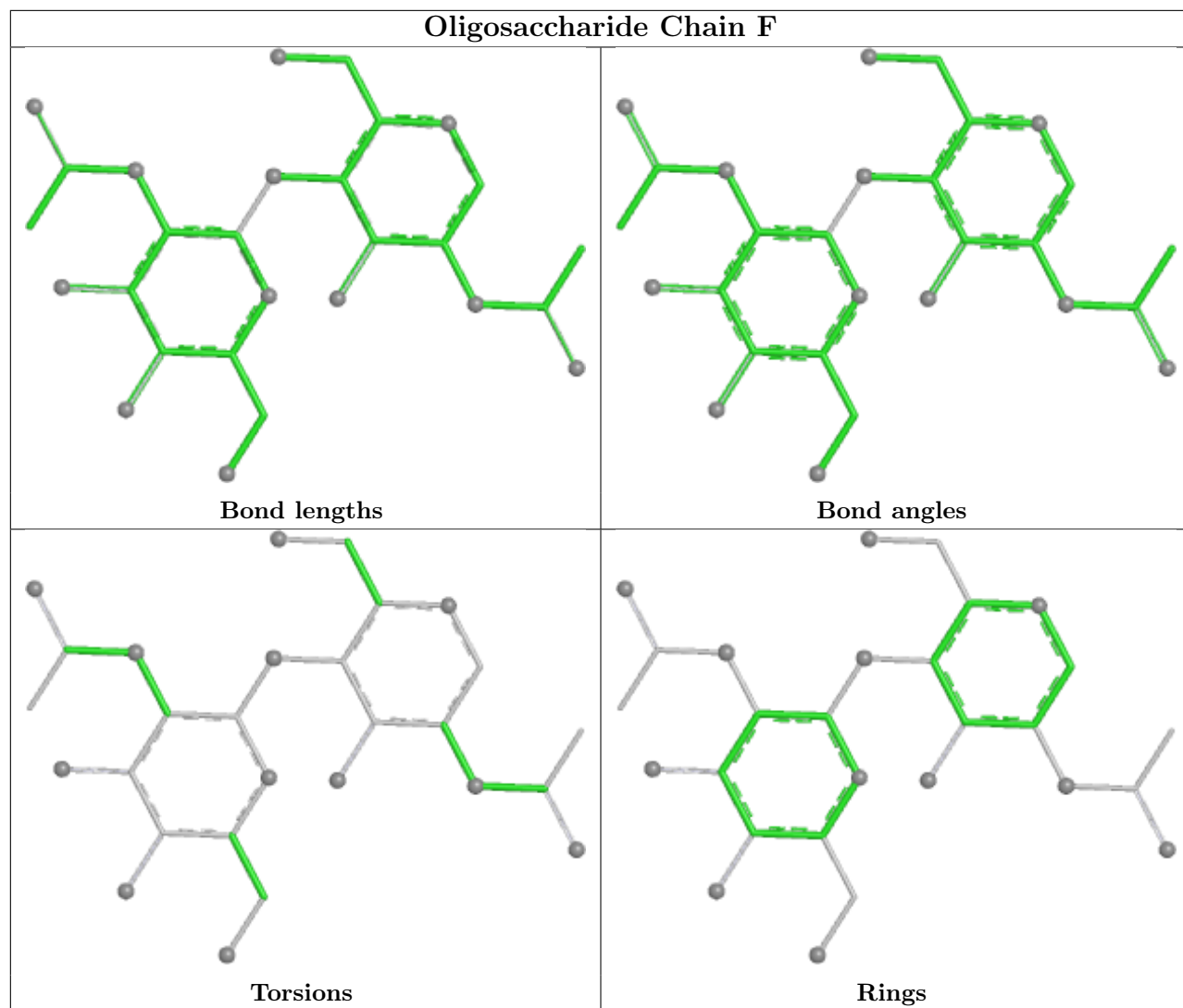
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

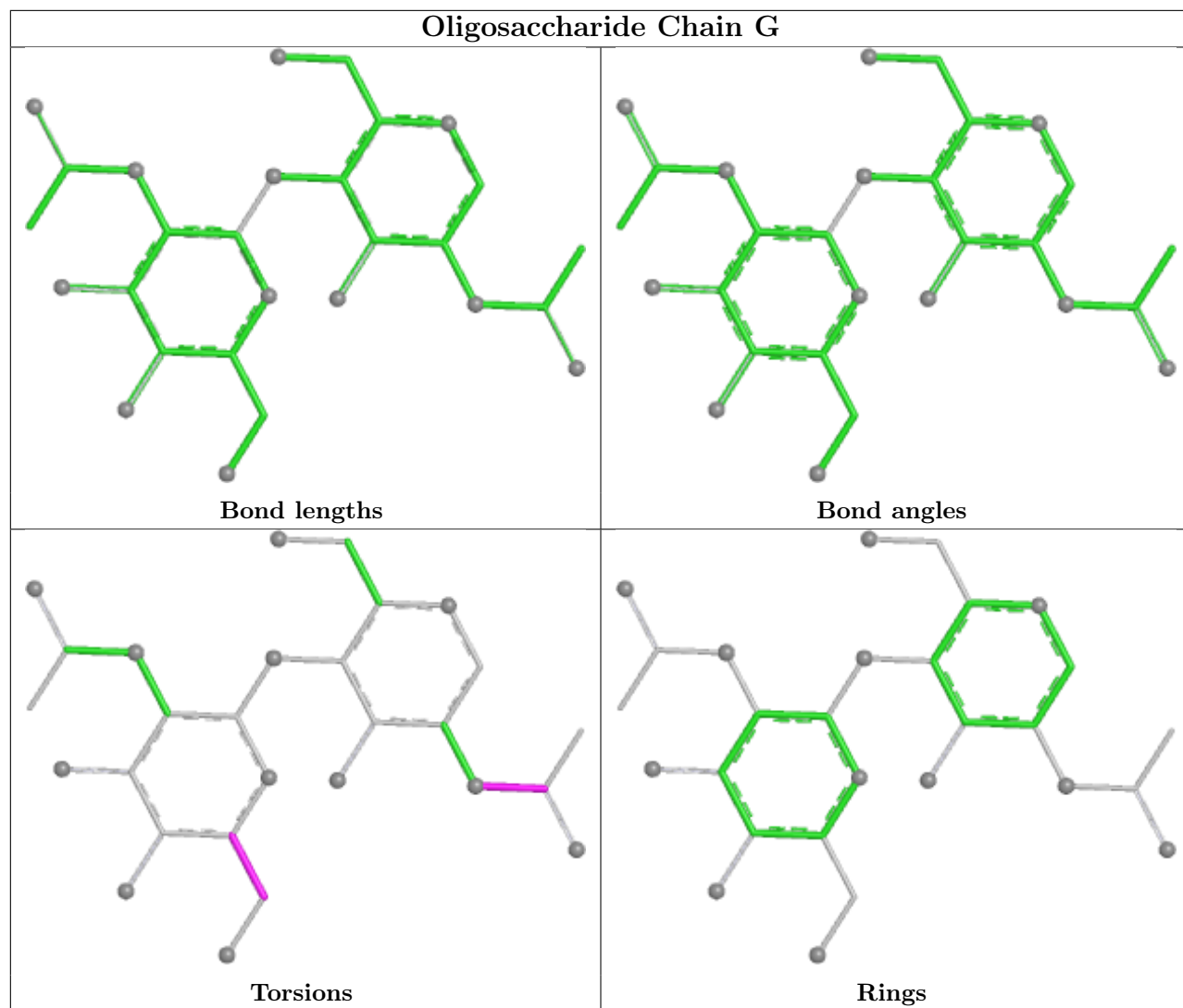


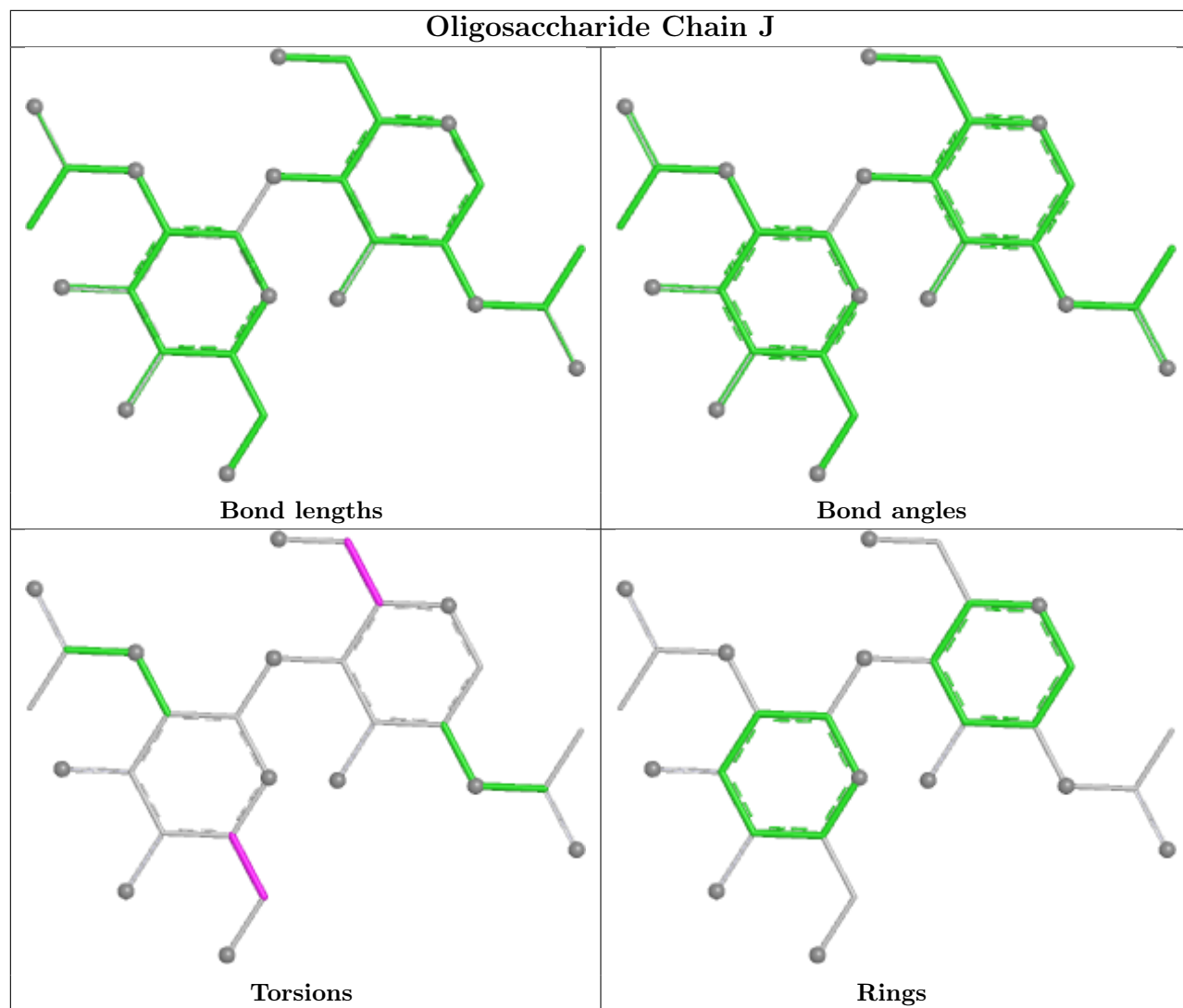


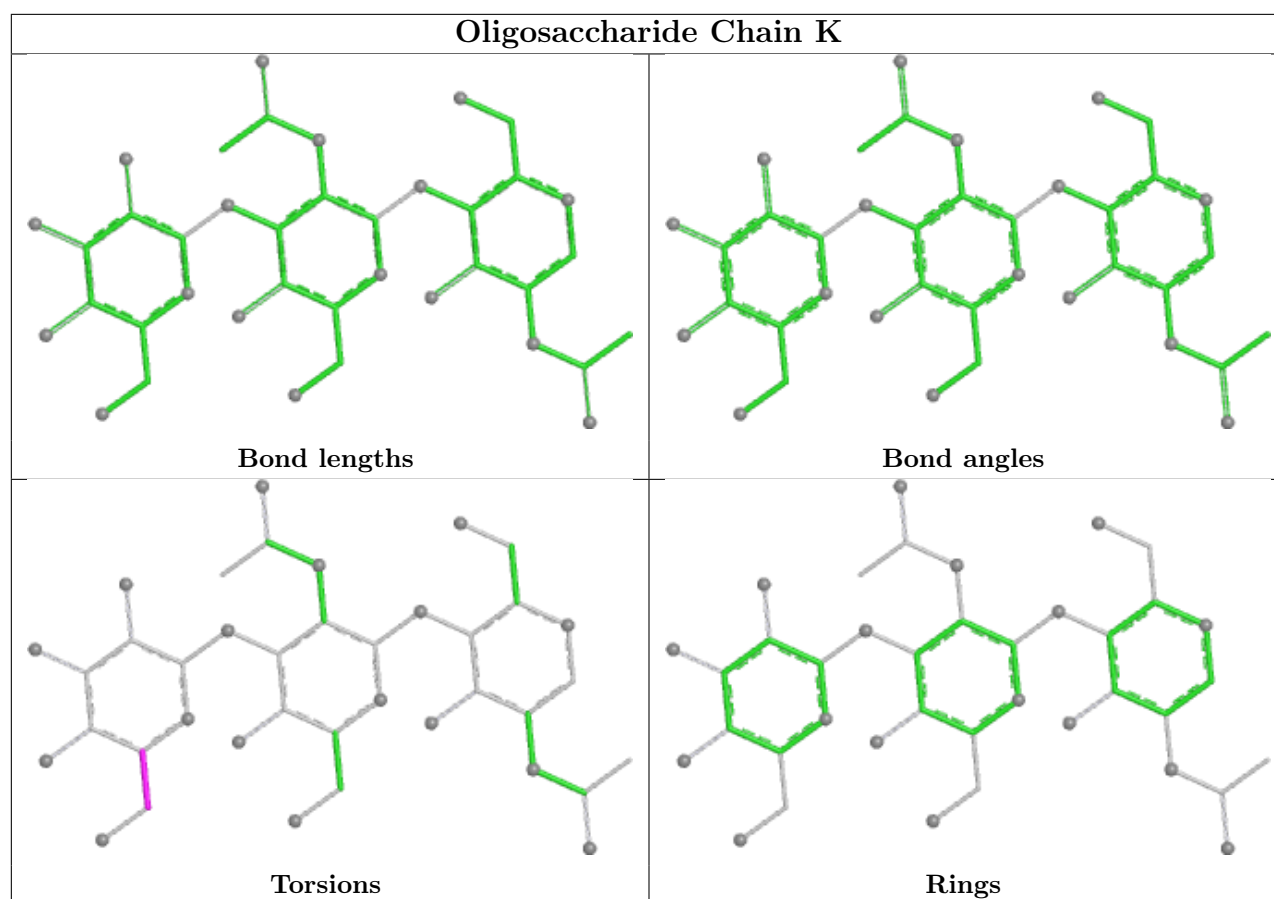












5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 20 are monoatomic - leaving 7 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	$\# Z > 2$
8	A2G	A	4705	1	14,14,15	0.42	0	17,19,21	0.55	0
7	NAG	A	4701	1	14,14,15	0.31	0	17,19,21	0.57	0
7	NAG	A	4702	1	14,14,15	0.26	0	17,19,21	0.64	0
8	A2G	A	4706	1	14,14,15	0.39	0	17,19,21	0.63	0
8	A2G	A	4707	1	14,14,15	0.39	0	17,19,21	0.61	0
8	A2G	A	4703	1	14,14,15	0.40	0	17,19,21	0.72	0
8	A2G	A	4704	1	14,14,15	0.40	0	17,19,21	0.71	1 (5%)

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
8	A2G	A	4705	1	-	1/6/23/26	0/1/1/1
7	NAG	A	4701	1	-	0/6/23/26	0/1/1/1
7	NAG	A	4702	1	-	3/6/23/26	0/1/1/1
8	A2G	A	4706	1	-	0/6/23/26	0/1/1/1
8	A2G	A	4707	1	-	1/6/23/26	0/1/1/1
8	A2G	A	4703	1	-	0/6/23/26	0/1/1/1
8	A2G	A	4704	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	4704	A2G	C1-C2-N2	2.03	113.63	110.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4702	NAG	C1-C2-N2-C7
7	A	4702	NAG	C8-C7-N2-C2
7	A	4702	NAG	O7-C7-N2-C2
8	A	4707	A2G	O5-C5-C6-O6
8	A	4705	A2G	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

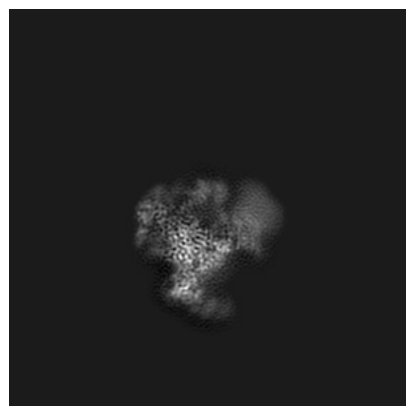
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36694. These allow visual inspection of the internal detail of the map and identification of artifacts.

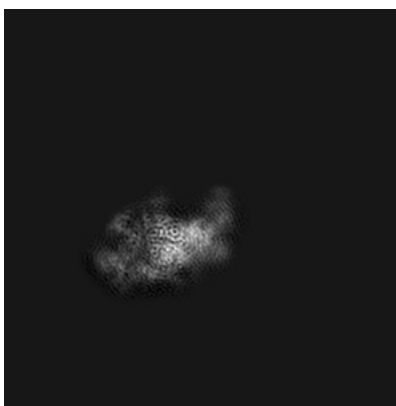
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

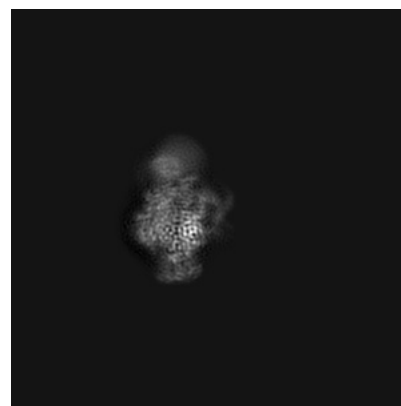
6.1.1 Primary map



X

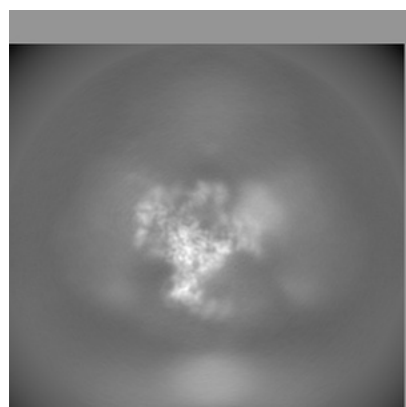


Y

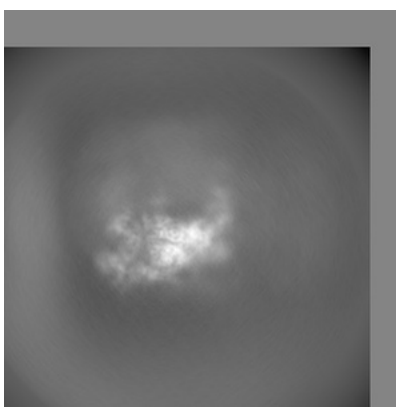


Z

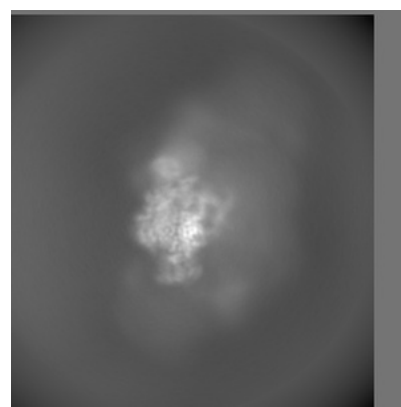
6.1.2 Raw map



X



Y

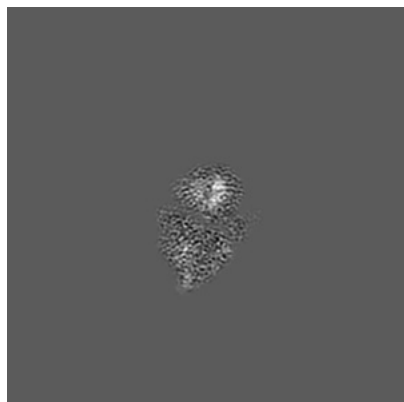


Z

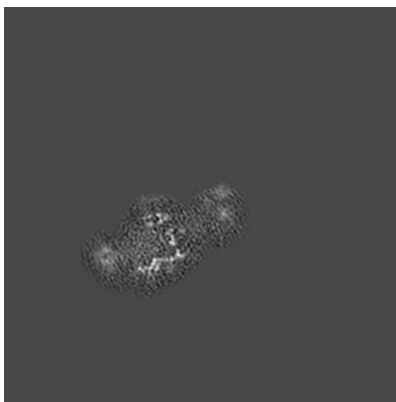
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

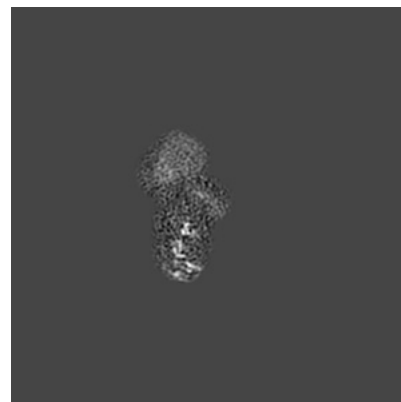
6.2.1 Primary map



X Index: 130

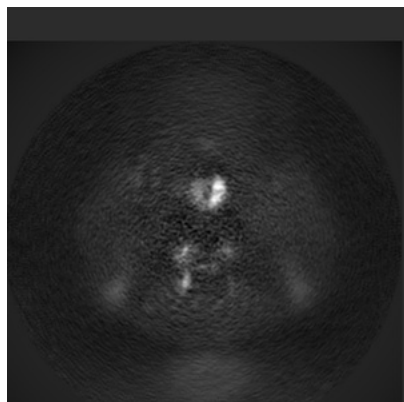


Y Index: 130

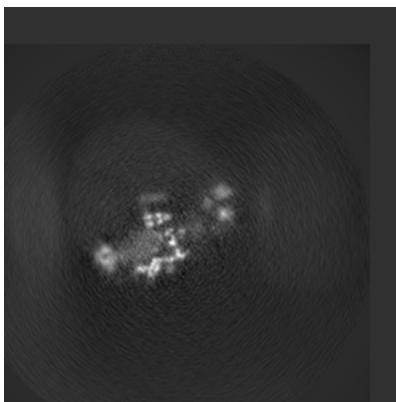


Z Index: 130

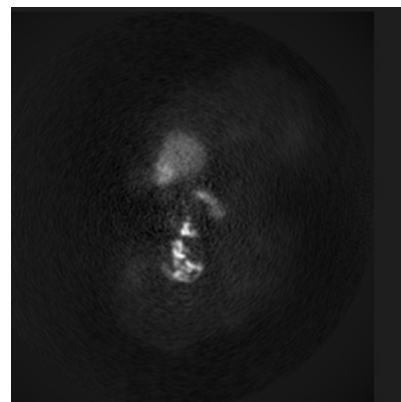
6.2.2 Raw map



X Index: 130



Y Index: 130

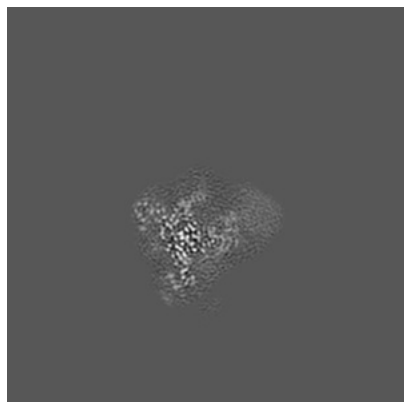


Z Index: 130

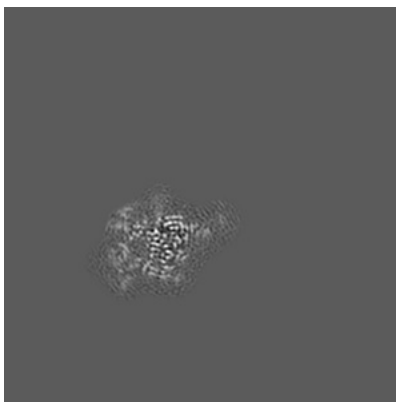
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

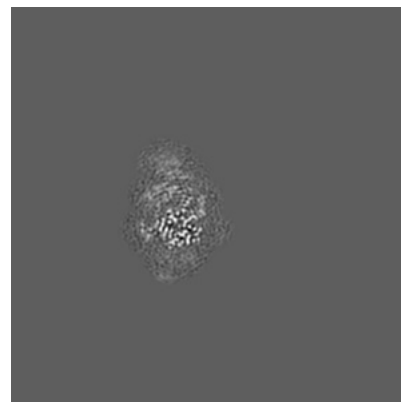
6.3.1 Primary map



X Index: 113

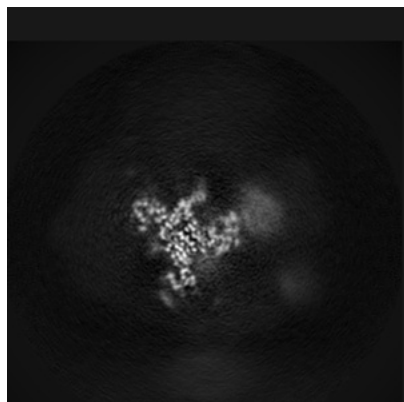


Y Index: 115

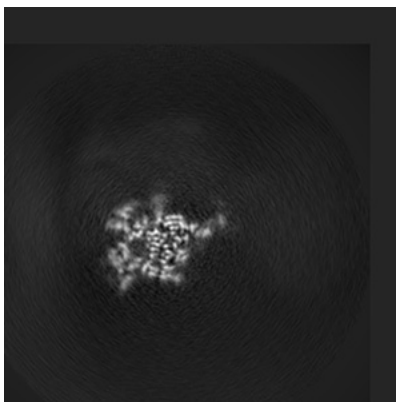


Z Index: 106

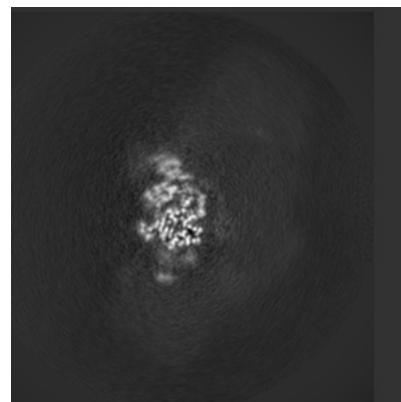
6.3.2 Raw map



X Index: 113



Y Index: 115

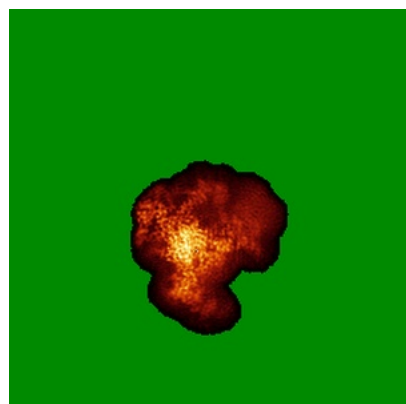


Z Index: 106

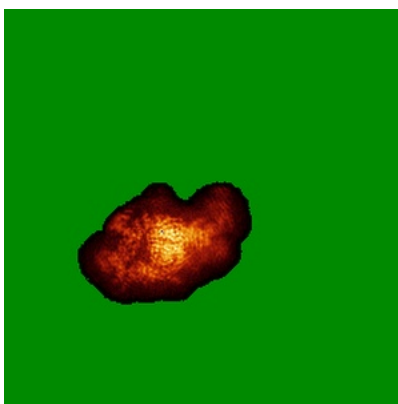
The images above show the largest variance slices of the map in three orthogonal directions.

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

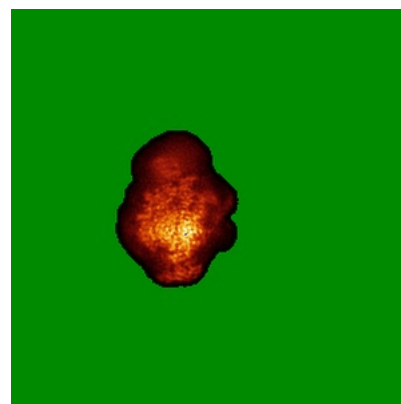
6.4.1 Primary map



X

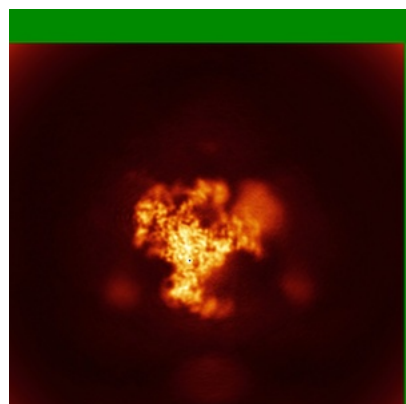


Y

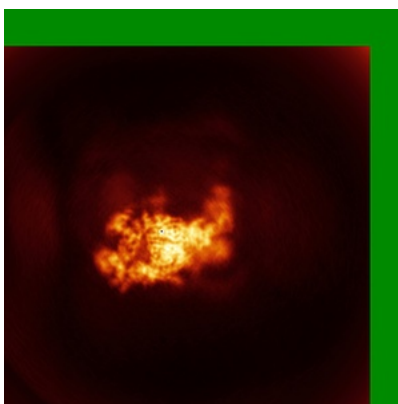


Z

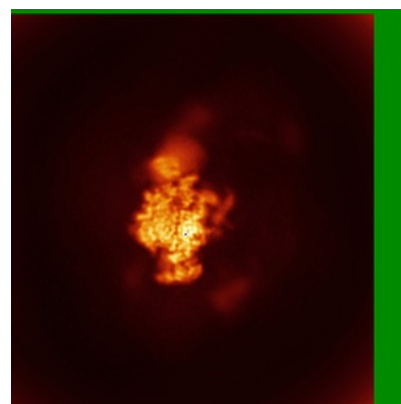
6.4.2 Raw map



X



Y



Z

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

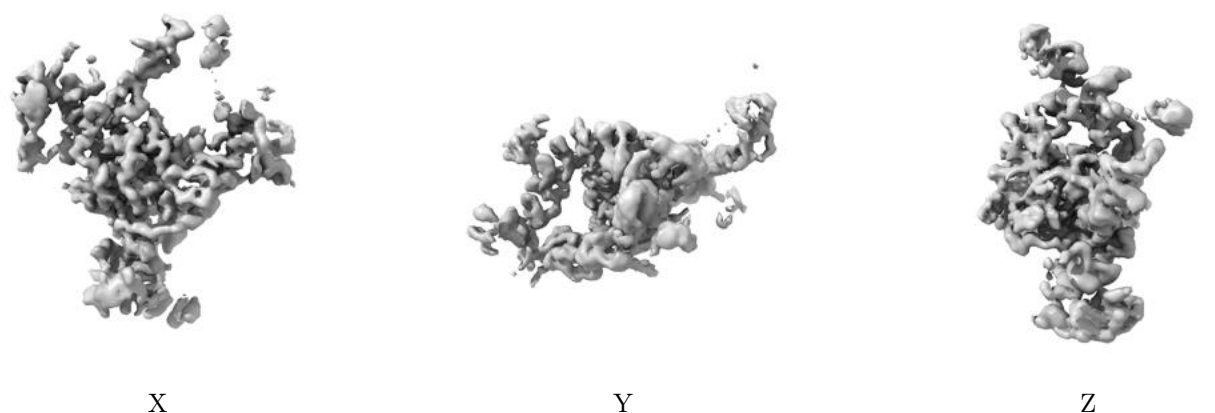
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0434. 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.

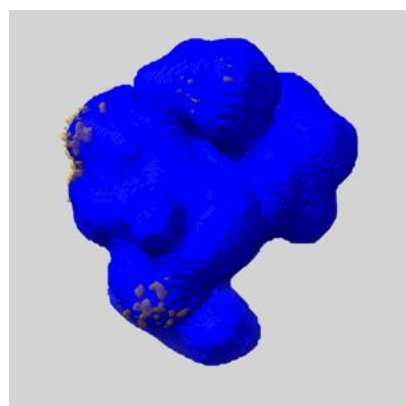
6.6 Mask visualisation [i](#)

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

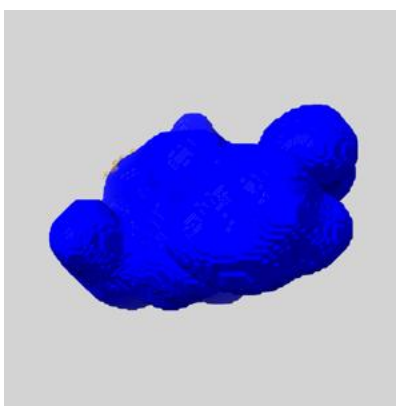
A mask typically either:

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

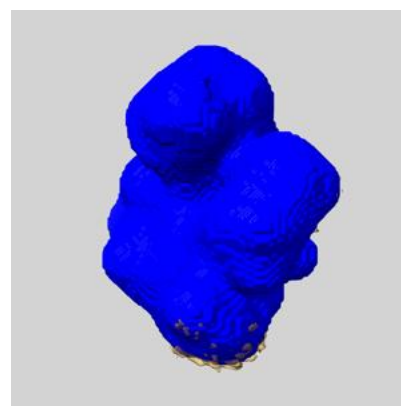
6.6.1 emd_36694_msk_1.map [i](#)



X



Y

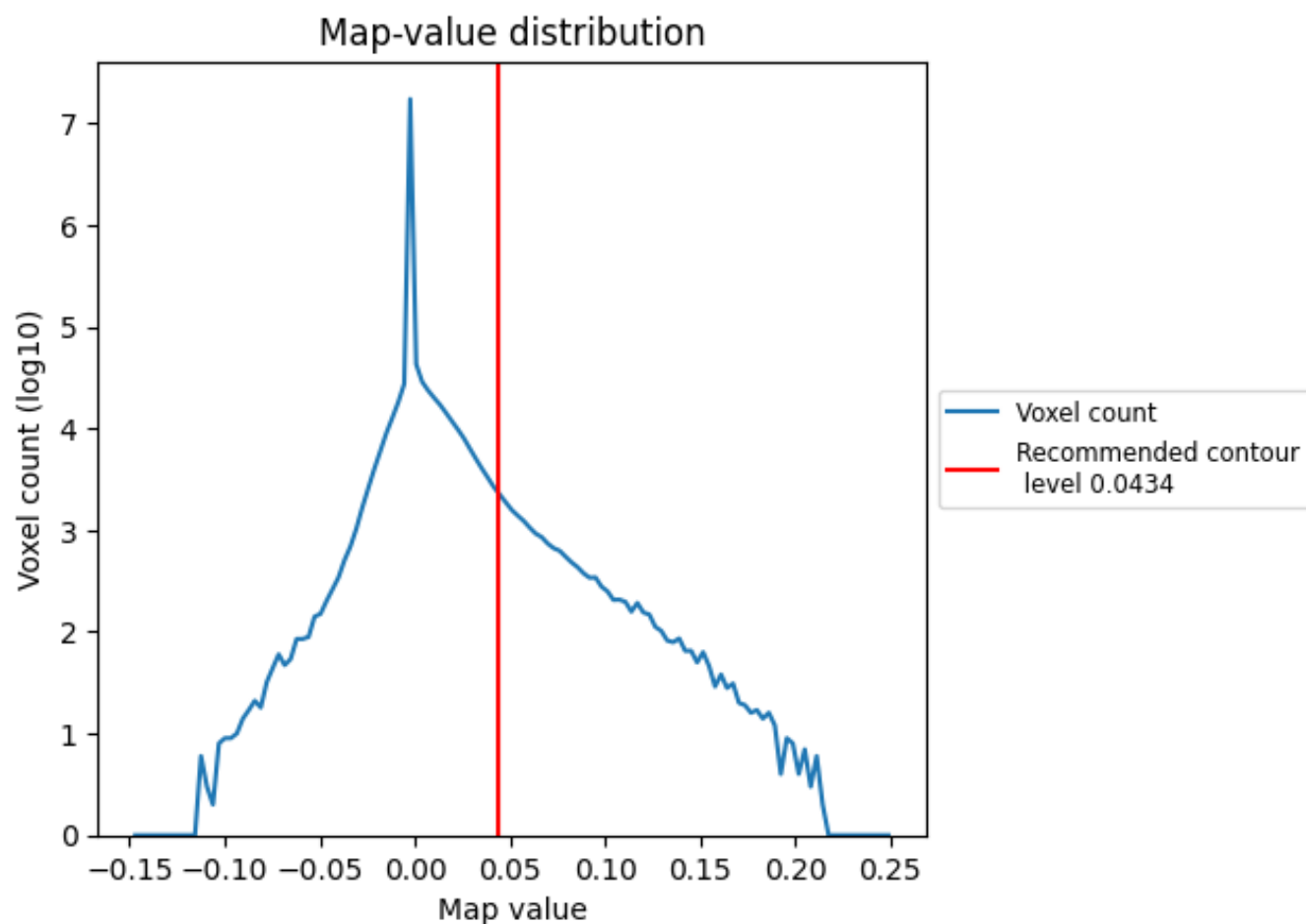


Z

7 Map analysis [i](#)

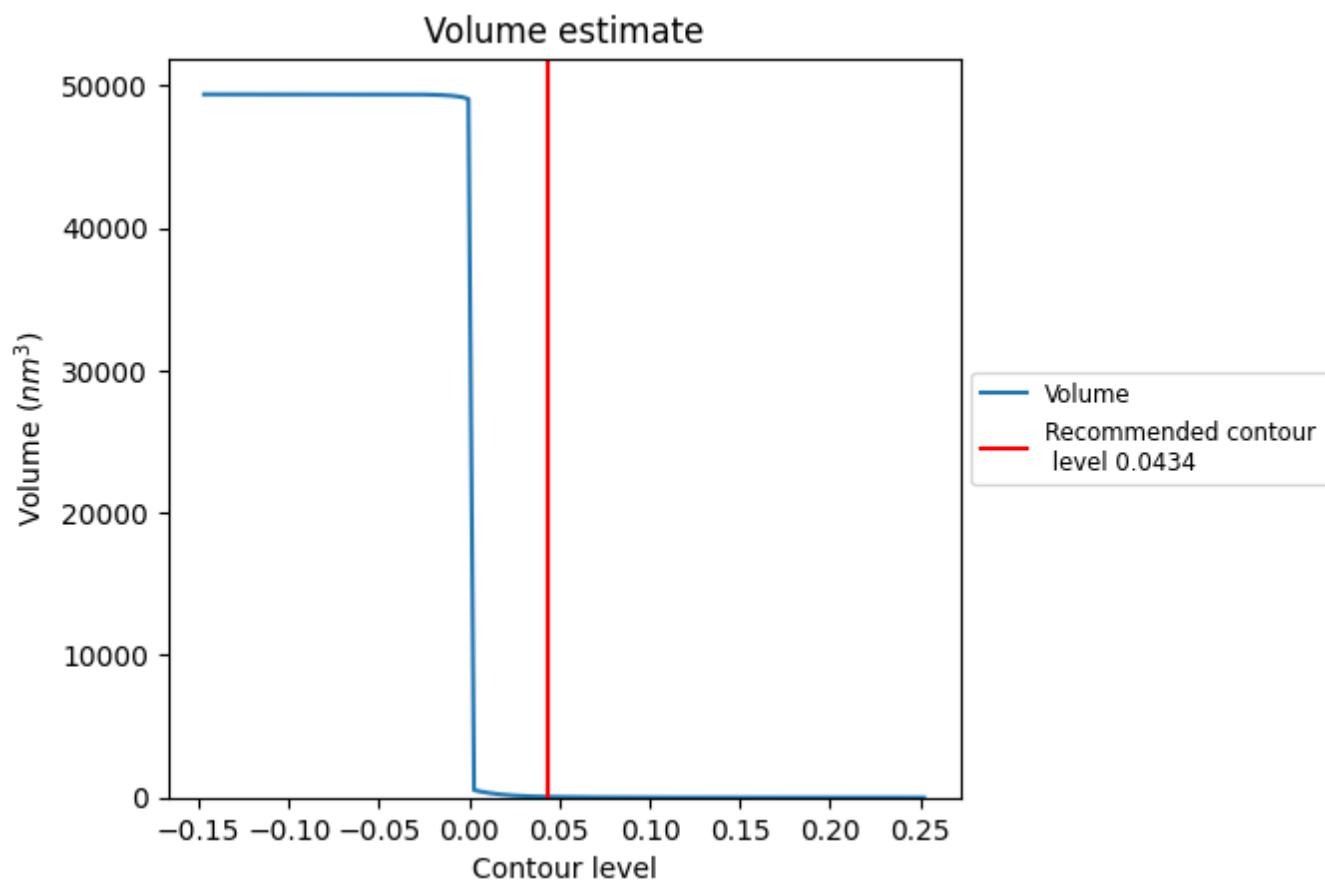
This section contains the results of statistical analysis of the map.

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.

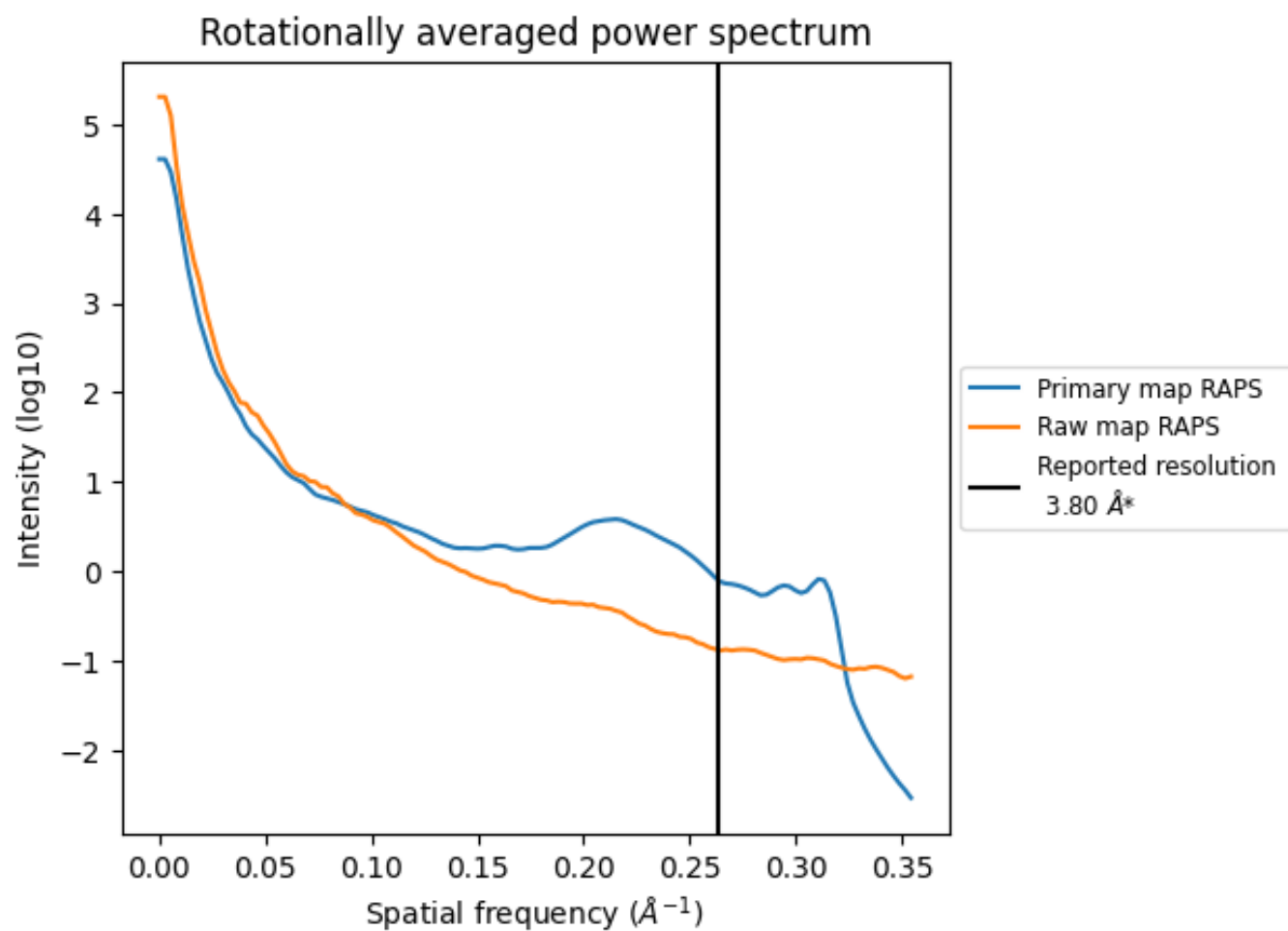
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 55 nm^3 ; this corresponds to an approximate mass of 49 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

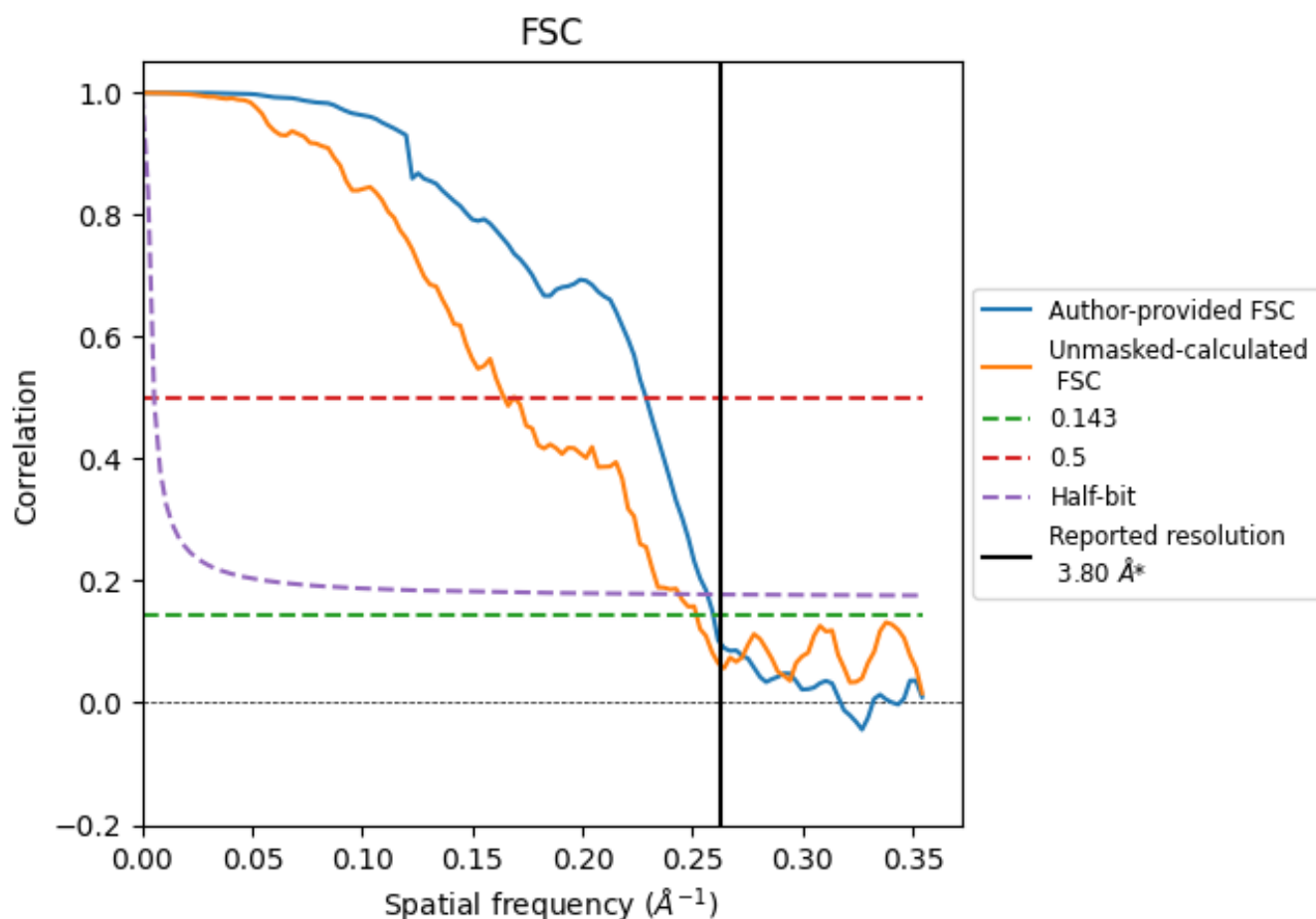


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

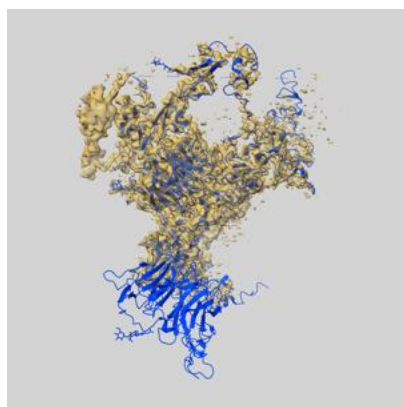
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.86	4.37	3.89
Unmasked-calculated*	3.97	6.08	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

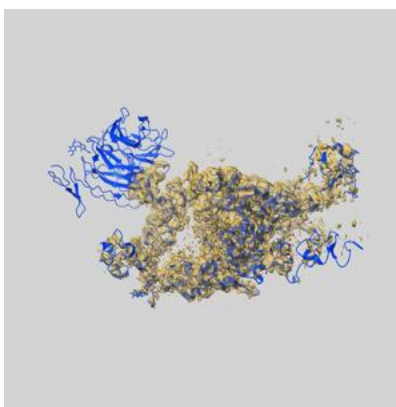
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36694 and PDB model 8JXA. Per-residue inclusion information can be found in section [3](#) on page [8](#).

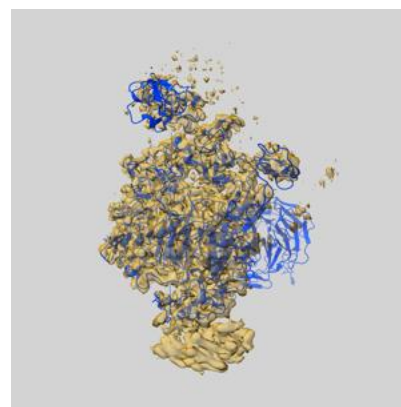
9.1 Map-model overlay [i](#)



X



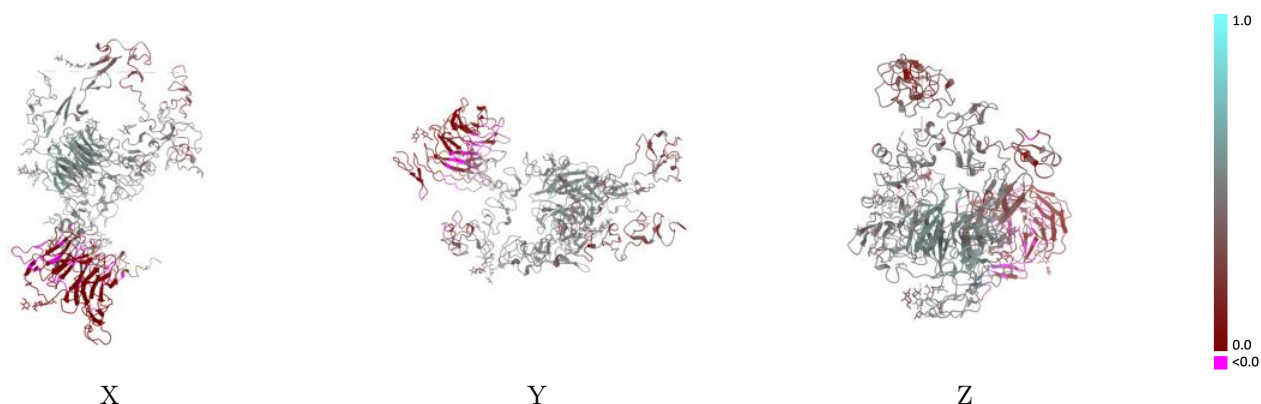
Y



Z

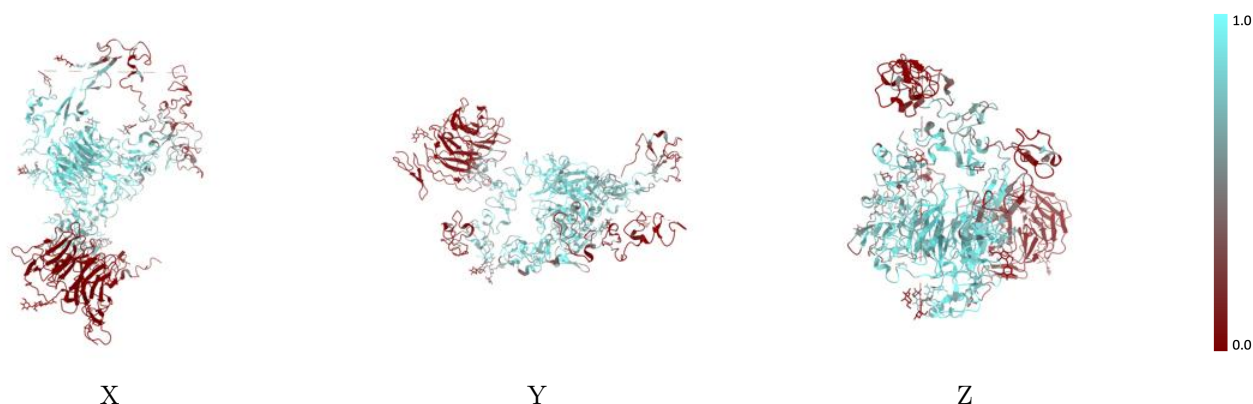
The images above show the 3D surface view of the map at the recommended contour level 0.0434 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



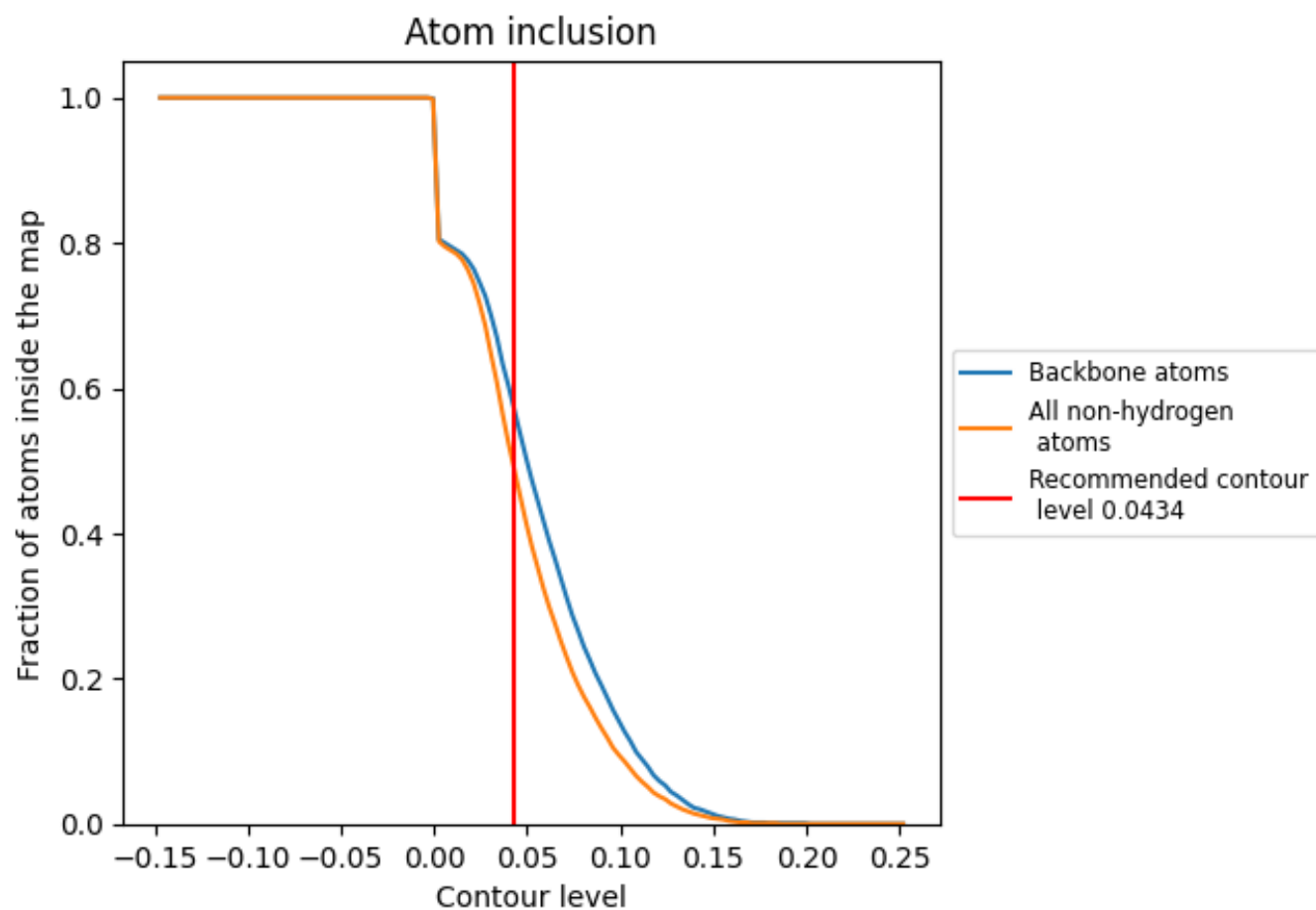
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0434).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 48% 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 (0.0434) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4850	0.3510
A	0.6310	0.4470
B	0.0620	0.0650
C	0.2560	0.3670
D	0.6150	0.4640
E	0.5250	0.4390
F	0.3210	0.4710
G	0.6430	0.5270
H	0.3930	0.3770
I	0.5570	0.4580
J	0.0000	0.0000
K	0.0000	0.0000
M	0.8930	0.5560

1.0

0.0

<0.0