



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 05:58 PM UTC

PDB ID : 8JXF / pdb_00008jxf
EMDB ID : EMD-36699
Title : rat megalin RAP complex bodyA
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 : 3.60 Å(reported)
Based on initial model : .

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:

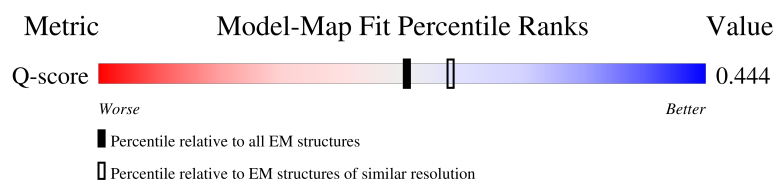
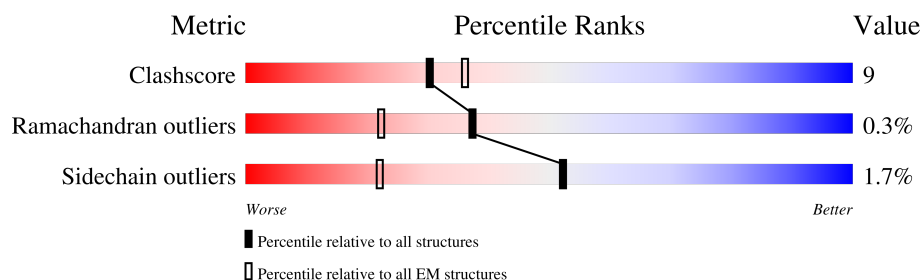
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.60 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.



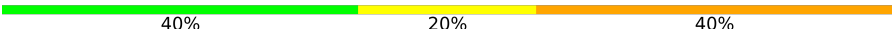
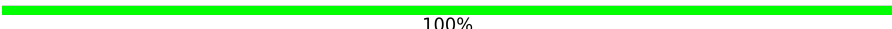
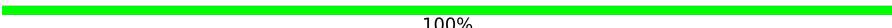
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	C	360	
2	B	4660	
3	O	5	
4	A	3	

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Mol	Chain	Length	Quality of chain
5	D	3	 33% 67%
6	E	5	 60% 40%
6	H	5	 40% 20% 40%
6	I	5	 100%
7	F	3	 33% 67% 67%
7	G	3	 100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9618 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 Alpha-2-macroglobulin receptor-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	72	Total	C	N	O	S	0	0
			599	381	110	107	1		

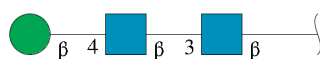
- Molecule 2 is a protein called LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1089	Total	C	N	O	S	0	0
			8548	5154	1550	1711	133		

- Molecule 3 is a protein called unclear peptide.

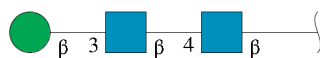
Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	5	Total	C	N	O	0	0
			28	16	6	6		

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



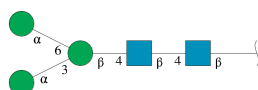
Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 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.



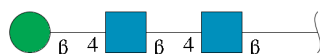
Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 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.



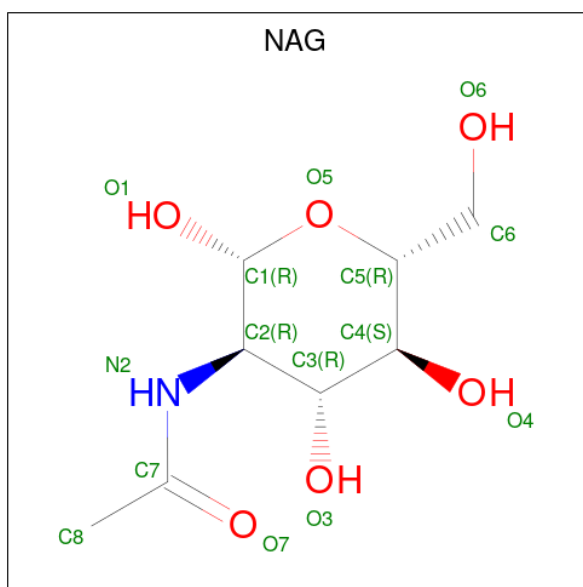
Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	5	Total	C	N	O	0	0
			61	34	2	25		
6	H	5	Total	C	N	O	0	0
			61	34	2	25		
6	I	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 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.



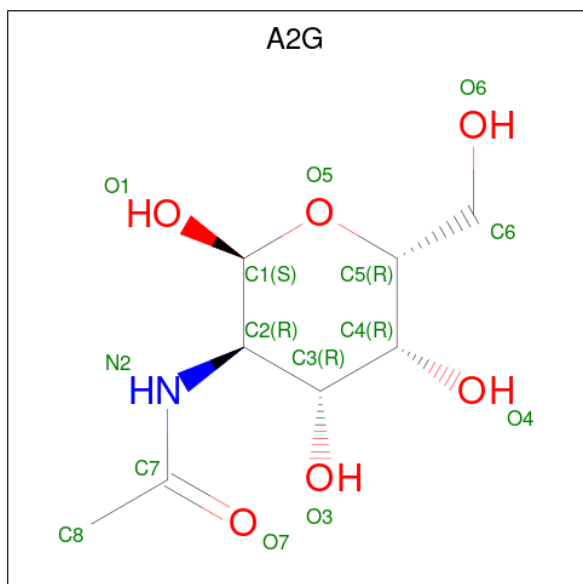
Mol	Chain	Residues	Atoms				AltConf	Trace
7	F	3	Total	C	N	O	0	0
			39	22	2	15		
7	G	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



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

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

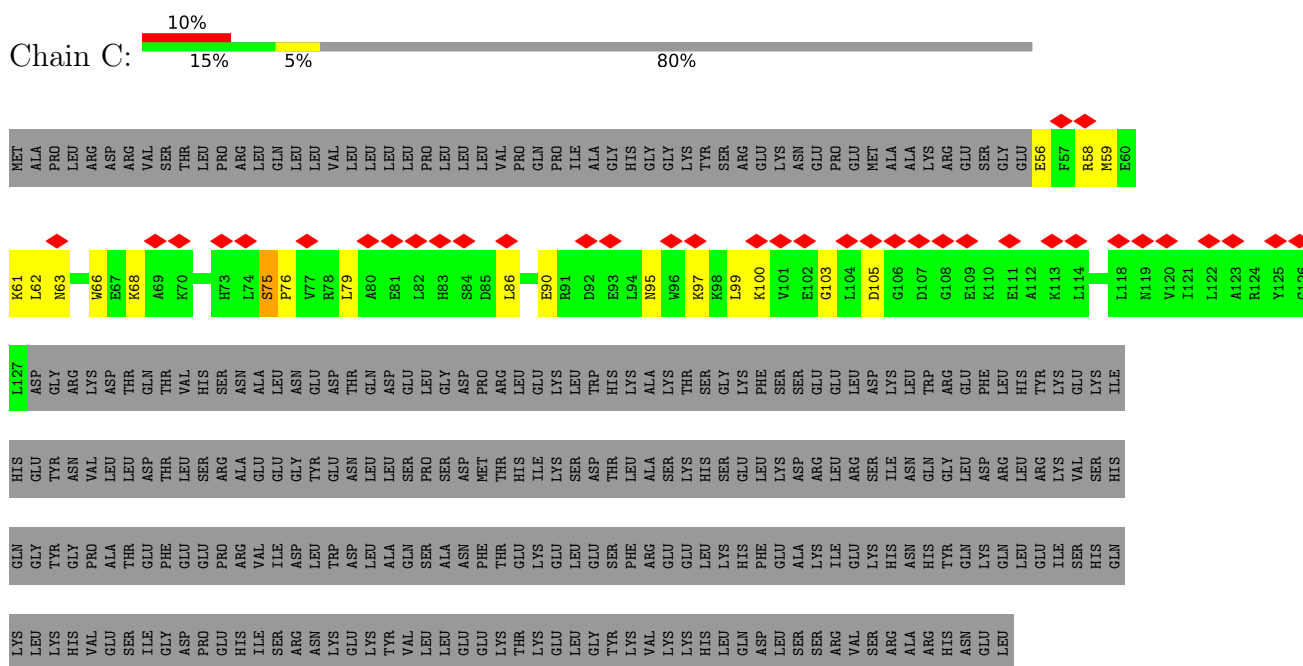
- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	B	20	Total	Ca	0
			20	20	

3 Residue-property plots

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

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



- Molecule 2: LDL receptor related protein 2



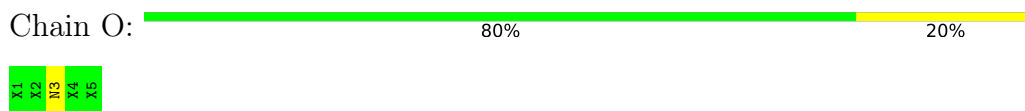




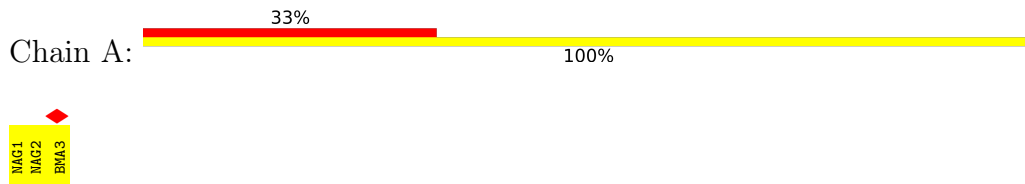
ALA	TRP	MET	ASN	GLY	TRP	GLY	PRO	VAL	ASN	S3915	C3716	V3458	Q3333	H3146	D3064	Q2954	C2891	GLN	SER	GLY
TRP	MET	ASN	GLY	HIS	GLY	HIS	GLU	ASP	ILE	D3916	L3737	Q3464	R3334	R3150	C3070	T2955	A2892	THR	ASP	HIS
ASN	ILE	GLY	ILE	TRP	ASN	E3917	GLY	PHE	CYS	E3918	N3755	Q3464	G3335	C3165	G3070	T2956	D2893	THR	GLU	CYS
GLY	TRP	GLY	LEU	TRP	ASN	K3918	GLY	GLY	ASN	K3919	S3762	K3467	H3336	C3165	C3070	C2957	S2894	ILE	GLY	ASN
HIS	ARG	HIS	SER	SER	CYS	E3920	THR	MET	CYS	E3921	S3762	K3485	R3350	V3173	C3077	V2958	D2896	VAL	LEU	GLN
VAL	VAL	VAL	VAL	THR	THR	H3922	THR	SER	THR	H3923	D3788	K3485	I3351	C3178	L3079	N2959	P2897	PRO	PHE	TRP
VAL	VAL	VAL	THR	THR	THR	C3921	THR	THR	THR	C3922	D3791	D3497	D3354	P3201	H3080	P2962	D2898	ALA	ARG	LYS
VAL	VAL	VAL	THR	THR	THR	K3924	THR	THR	THR	K3925	D3791	D3497	G3355	F3202	F3082	P2963	C2900	ALA	CYS	ASP
SER	SER	SER	VAL	GLY	GLY	K3925	THR	ARG	GLY	D3506	E3796	D3506	T3356	L3203	C3084	N2964	C2901	ASP	ASN	ASN
ASN	GLU	GLU	ALA	GLY	GLY	THR	THR	CYS	PHE	R3553	H3797	R3553	I3361	N3207	D3085	P2969	G2902	GLY	THR	ASN
LEU	LEU	LEU	GLN	VAL	ILE	HIS	LYS	CYS	ILE	F3554	C3807	F3554	I3362	N3213	N3086	V2972	H2903	ASP	GLU	CYS
GLY	TRP	TRP	GLY	ALA	ALA	E3917	PRO	ASP	CYS	C3555	G3821	C3555	I3366	L3214	G3087	W2972	S2904	THR	PHE	GLY
PRO	PRO	PRO	GLN	GLY	GLY	G3821	ASP	GLY	ASP	R3556	R3822	R3556	I3366	L3215	H3088	D2975	V2905	THR	THR	ASP
ASN	ASN	ASN	PHE	LEU	GLY	S3829	ARG	SER	ARG	F3560	S3829	F3560	P3389	T3216	C3089	D2976	N2906	CYS	SER	GLY
GLY	GLY	GLY	ALA	GLY	GLY	D3830	PRO	PRO	THR	L3573	D3830	L3573	N3370	T3217	I3090	D2977	T2907	GLY	ASN	SER
LEU	LEU	LEU	ILE	ILE	ILE	E3831	GLY	GLY	PHE	L3573	E3831	L3573	A3371	D3217	M3092	D2977	C2908	GLY	GLY	GLY
ILE	ILE	ILE	LYS	LYS	LYS	S3832	LYS	LEU	LYS	R3588	S3832	R3588	N3378	T3218	G3093	D2982	R2909	ASP	PRO	ILE
ASP	ASP	ASP	ARG	ARG	ARG	T3836	PRO	LEU	PRO	V3589	T3836	V3589	N3378	T3218	G3093	D2982	C2910	GLY	VAL	THR
TRP	TRP	TRP	ALA	ALA	ALA	R3837	THR	LEU	SER	L3590	R3837	L3590	L3381	I3224	C3096	D2982	S2911	PRO	LEU	VAL
LEU	LEU	LEU	TRP	TRP	TRP	F3838	THR	GLY	THR	C3591	F3838	C3591	L3381	I3224	C3096	D2982	Q2912	PRO	LEU	CYS
ASN	ASN	ASN	ASN	ASN	ASN	E3592	ASN	ASN	ASN	E3592	E3592	E3592	L3381	I3224	C3096	D2982	F2913	SER	LEU	ALA
ASP	ASP	ASP	ASN	ASN	ASN	E3592	ASN	ASN	ASN	E3592	E3592	E3592	L3381	I3224	C3096	D2982	Q2913	THR	TYR	PHE
ARG	ARG	ARG	ASN	ASN	ASN	K3606	LYS	VAL	LYS	K3606	K3606	K3606	L3381	I3224	C3096	D2982	Q2914	VAL	VAL	HIS
GLU	GLU	GLU	PHE	PHE	PHE	G3841	LYS	ARG	ASN	G3841	G3841	G3841	L3381	I3224	C3096	D2982	C2915	CYS	THR	THR
ILE	ILE	ILE	GLU	GLU	GLU	T3842	ILE	ILE	ILE	T3842	T3842	T3842	L3381	I3224	C3096	D2982	C2916	ASN	ASN	CYS
SER	SER	SER	GLY	GLY	GLY	Y3843	SER	ARG	CYS	Q3610	Y3843	Q3610	L3381	I3224	C3096	D2982	D2916	GLY	ARG	ARG
GLN	GLN	GLN	GLY	GLY	GLY	Y3843	GLN	ARG	GLN	Q3611	Y3843	Q3611	L3381	I3224	C3096	D2982	N2917	ILE	ILE	SER
ASP	ASP	ASP	THR	THR	THR	K3852	THR	LYS	THR	S3612	K3852	S3612	L3381	I3224	C3096	D2982	C2918	ASN	ASN	THR
ASN	ASN	ASN	ASN	ASN	ASN	H3853	ASN	ASN	ASN	S3613	H3853	S3613	L3381	I3224	C3096	D2982	C2919	ASN	ASN	ALA
THR	THR	THR	THR	THR	THR	H3854	THR	THR	THR	S3613	H3854	S3613	L3381	I3224	C3096	D2982	C2920	CYS	PHE	THR
GLY	GLY	GLY	GLY	GLY	GLY	V3855	CYS	SER	GLY	R3635	V3855	R3635	L3381	I3224	C3096	D2982	C2921	HIS	THR	THR
ILE	ILE	ILE	ILE	ILE	ILE	V3855	ILE	SER	GLY	T3636	V3855	T3636	L3381	I3224	C3096	D2982	C2922	ASP	CYS	THR
ALA	ALA	ALA	ALA	ALA	ALA	C3837	CYS	SER	CYS	C3837	C3837	C3837	L3381	I3224	C3096	D2982	C2923	ASN	ASN	GLY
ASP	ASP	ASP	VAL	VAL	VAL	C3838	VAL	GLY	VAL	R3638	C3838	R3638	L3381	I3224	C3096	D2982	C2924	THR	THR	GLY
VAL	VAL	VAL	VAL	VAL	VAL	C3838	VAL	GLY	VAL	F3418	C3838	F3418	L3381	I3224	C3096	D2982	C2925	ARG	SER	ARG
GLY	GLY	GLY	GLY	GLY	GLY	V3870	GLY	PHE	ASP	E3264	V3870	E3264	L3381	I3224	C3096	D2982	C2926	ASP	ASP	CYS
ILE	ILE	ILE	ILE	ILE	ILE	S3873	CYS	GLY	ASP	E3264	S3873	E3264	L3381	I3224	C3096	D2982	C2927	GLY	GLY	GLY
LYS	LYS	LYS	LYS	LYS	LYS	E3886	ASP	THR	ASP	T3425	E3886	T3425	L3381	I3224	C3096	D2982	C2928	THR	THR	THR
THR	THR	THR	THR	THR	THR	E3886	THR	THR	THR	D3426	E3886	D3426	L3381	I3224	C3096	D2982	C2929	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	E3886	ASP	THR	THR	T3429	E3886	T3429	L3381	I3224	C3096	D2982	C2930	VAL	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	E3886	GLY	THR	THR	R3430	E3886	R3430	L3381	I3224	C3096	D2982	C2931	THR	THR	THR
THR	THR	THR	THR	THR	THR	E3886	THR	THR	THR	T3431	E3886	T3431	L3381	I3224	C3096	D2982	C2932	ASN	ASN	THR
GLY	GLY	GLY	GLY	GLY	GLY	E3886	GLY	THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2933	PRO	PRO	PRO
ASN	ASN	ASN	ASN	ASN	ASN	E3886	ASN	THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2934	THR	THR	THR
GLY	GLY	GLY	GLY	GLY	GLY	E3886	GLY	THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2935	ASN	ASN	ASN
THR	THR	THR	THR	THR	THR	E3886	THR	THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2936	PHE	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	E3886	GLY	THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2937	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	E3886	ASP	THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2938	LYS	LYS	LYS
THR	THR	THR	THR	THR	THR	E3886	THR	THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2939	CYS	CYS	CYS
ALA	ALA	ALA	ALA	ALA	ALA	E3886	ALA	THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2940	THR	THR	THR
MET	MET	MET	MET	MET	MET	E3886	MET	THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2941	THR	THR	THR
						E3886		THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2942	THR	THR	THR
						E3886		THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2943	THR	THR	THR
						E3886		THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2944	THR	THR	THR
						E3886		THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2945	THR	THR	THR
						E3886		THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2946	THR	THR	THR
						E3886		THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2947	THR	THR	THR
						E3886		THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2948	THR	THR	THR
						E3886		THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2949	THR	THR	THR
						E3886		THR	THR	V3282	E3886	V3282	L3381	I3224	C3096	D2982	C2950	THR	THR	THR

[illegible]

- Molecule 3: unclear peptide



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



- Molecule 5: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

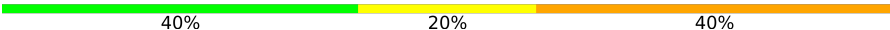


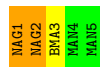
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 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

nose

Chain H: 



• Molecule 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

Chain I: 



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

Chain F: 



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

Chain G: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	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	0.173	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0271	Depositor
Map size (Å)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: A2G, MAN, BMA, CA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.12	0/608	0.32	0/813
2	B	0.22	0/8752	0.46	0/11862
3	O	0.18	0/7	0.51	0/8
All	All	0.21	0/9367	0.45	0/12683

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	C	599	0	620	16	0
2	B	8548	0	7601	150	0
3	O	28	0	12	1	0
4	A	39	0	34	0	0
5	D	39	0	34	0	0
6	E	61	0	52	0	0
6	H	61	0	52	1	0
6	I	61	0	52	0	0
7	F	39	0	34	0	0
7	G	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	28	0	26	0	0
9	B	56	0	48	6	0
10	B	20	0	0	0	0
All	All	9618	0	8599	163	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 9.

All (163) 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:1225:THR:OG1	9:B:4703:A2G:C1	1.82	1.27
2:B:1225:THR:CB	9:B:4703:A2G:C1	2.26	1.14
2:B:1225:THR:HB	9:B:4703:A2G:C1	1.92	0.96
2:B:3505:ARG:HD3	2:B:3505:ARG:H	1.37	0.88
2:B:1225:THR:HB	9:B:4703:A2G:O5	1.78	0.84
2:B:3115:GLU:HA	2:B:3118:ASP:HB3	1.65	0.77
2:B:3689:LYS:HE2	2:B:3711:SER:HB2	1.65	0.76
1:C:68:LYS:NZ	2:B:2975:ASP:OD2	2.22	0.71
2:B:3356:THR:O	2:B:3357:ASN:HB2	1.91	0.70
2:B:2959:ASN:ND2	2:B:2982:ASP:OD2	2.28	0.67
2:B:3611:GLN:OE1	2:B:3638:ARG:HD3	1.95	0.67
1:C:97:LYS:HA	1:C:100:LYS:HG2	1.77	0.66
2:B:2872:CYS:SG	2:B:2879:ILE:HG12	2.36	0.66
2:B:2939:GLU:HG2	2:B:2941:GLN:H	1.61	0.64
2:B:3083:ARG:NE	2:B:3084:CYS:O	2.31	0.63
2:B:3016:ARG:HD3	2:B:3045:ARG:HD2	1.80	0.63
1:C:97:LYS:HE3	2:B:2925:TRP:CZ3	2.33	0.63
2:B:2870:PHE:O	2:B:2879:ILE:N	2.31	0.63
2:B:3425:THR:HG22	2:B:3432:VAL:HG22	1.81	0.63
1:C:56:GLU:OE2	1:C:66:TRP:NE1	2.32	0.62
2:B:2880:PRO:HB2	2:B:2883:TRP:HD1	1.62	0.62
2:B:3378:ASN:ND2	2:B:3438:TYR:OH	2.33	0.61
2:B:3118:ASP:CG	2:B:3121:ILE:H	2.09	0.61
2:B:3395:ASP:OD1	2:B:3399:HIS:N	2.34	0.60
2:B:3079:LEU:O	2:B:3081:GLN:N	2.33	0.60
2:B:3048:PRO:HD2	2:B:3051:PHE:HE1	1.65	0.60
2:B:3282:VAL:HG21	2:B:3467:MET:HE2	1.84	0.59
2:B:3915:SER:HA	2:B:3918:LYS:HG3	1.84	0.59
2:B:3843:TYR:CD2	2:B:3854:HIS:HB3	2.38	0.58
2:B:1225:THR:HB	9:B:4703:A2G:C5	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:HE3	2:B:2925:TRP:CH2	2.38	0.58
2:B:3333:GLN:HG3	2:B:3467:MET:SD	2.44	0.57
2:B:3039:PHE:N	2:B:3047:ILE:O	2.37	0.57
1:C:99:LEU:O	1:C:103:GLY:N	2.37	0.57
2:B:2999:GLU:HA	2:B:3009:ARG:HA	1.87	0.56
2:B:3831:GLU:O	2:B:3854:HIS:HB2	2.05	0.56
1:C:59:MET:HB3	1:C:62:LEU:HB2	1.87	0.56
2:B:3145:LEU:HD22	2:B:3146:MET:H	1.71	0.56
2:B:3366:ILE:HD11	2:B:3369:PRO:HB3	1.88	0.55
2:B:2933:CYS:HB2	2:B:2938:ASP:HB3	1.87	0.55
2:B:2950:CYS:HB3	2:B:2956:THR:HB	1.88	0.55
2:B:3838:PHE:HB3	2:B:3839:PRO:HD2	1.87	0.55
1:C:62:LEU:HG	1:C:86:LEU:HD22	1.89	0.55
2:B:3797:MET:HA	2:B:3797:MET:HE3	1.88	0.55
2:B:2959:ASN:O	2:B:2961:ARG:NH2	2.40	0.54
2:B:3425:THR:HB	2:B:3453:PRO:HG2	1.90	0.54
2:B:3238:ARG:NH1	2:B:3464:GLN:O	2.41	0.54
2:B:3843:TYR:HD2	2:B:3854:HIS:HB3	1.73	0.54
2:B:3016:ARG:NE	2:B:3044:GLY:O	2.41	0.54
2:B:3125:ASP:N	2:B:3125:ASP:OD1	2.41	0.54
2:B:3225:LEU:HD13	2:B:3256:MET:HE1	1.89	0.53
2:B:3215:THR:OG1	2:B:3217:ASP:OD1	2.25	0.53
1:C:59:MET:O	1:C:63:ASN:ND2	2.29	0.52
2:B:2886:ASP:OD1	2:B:2919:ARG:NH2	2.41	0.52
2:B:3839:PRO:C	2:B:3841:GLY:H	2.16	0.52
2:B:2870:PHE:N	2:B:2879:ILE:O	2.26	0.52
2:B:3246:ILE:HG12	2:B:3253:ILE:HG12	1.91	0.52
2:B:2969:PRO:HD2	2:B:2972:TRP:CD2	2.45	0.51
2:B:3106:SER:HA	2:B:3109:LYS:HE3	1.92	0.51
2:B:3635:ARG:NH1	2:B:3649:CYS:SG	2.83	0.51
2:B:3333:GLN:OE1	2:B:3333:GLN:N	2.28	0.51
2:B:3392:GLU:HG3	2:B:3403:THR:HA	1.91	0.51
1:C:68:LYS:HZ1	2:B:2972:TRP:CG	2.28	0.51
2:B:3048:PRO:HD2	2:B:3051:PHE:CE1	2.46	0.51
2:B:3126:HIS:HD1	2:B:3139:CYS:HA	1.75	0.51
6:H:1:NAG:H83	6:H:2:NAG:H83	1.93	0.51
2:B:3354:ASP:OD2	2:B:3485:LYS:HA	2.11	0.50
2:B:3356:THR:O	2:B:3357:ASN:CB	2.58	0.50
2:B:2932:ASP:HB2	2:B:2938:ASP:CG	2.36	0.49
1:C:58:ARG:N	1:C:90:GLU:OE1	2.45	0.49
2:B:3788:ASP:OD1	2:B:3788:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3836:THR:HG22	2:B:3843:TYR:CE1	2.47	0.49
2:B:3086:ASN:ND2	2:B:3102:CYS:O	2.44	0.49
2:B:1226:ARG:HD3	2:B:1231:CYS:HA	1.95	0.49
2:B:3372:ILE:HD11	2:B:3381:LEU:HD11	1.94	0.49
2:B:3681:ASP:OD2	2:B:3684:THR:HG22	2.12	0.48
2:B:2898:PRO:HD2	2:B:2900:THR:HG22	1.95	0.48
2:B:3123:ARG:HB2	2:B:3150:ARG:HG3	1.94	0.48
2:B:2984:LEU:O	2:B:2988:GLN:HG2	2.13	0.48
2:B:3334:ARG:HB3	2:B:3336:HIS:CD2	2.48	0.48
2:B:3225:LEU:HD23	2:B:3228:LEU:HD11	1.96	0.48
2:B:3223:LEU:HD11	2:B:3226:GLN:HB3	1.96	0.47
2:B:3588:ARG:O	2:B:3592:GLU:HB2	2.14	0.47
2:B:3009:ARG:HG2	2:B:3011:SER:H	1.78	0.47
2:B:1225:THR:CB	9:B:4703:A2G:O5	2.48	0.47
2:B:3016:ARG:NH1	2:B:3016:ARG:HB2	2.29	0.47
2:B:3916:ASP:N	2:B:3916:ASP:OD1	2.48	0.47
2:B:2903:HIS:CD2	2:B:2917:ASN:HD22	2.33	0.47
2:B:3246:ILE:HD11	2:B:3277:LEU:HB3	1.97	0.47
2:B:3122:SER:O	2:B:3124:CYS:N	2.48	0.47
2:B:3796:GLU:HG2	2:B:3797:MET:SD	2.55	0.47
2:B:3064:ASP:OD1	2:B:3064:ASP:N	2.33	0.47
2:B:3083:ARG:NE	2:B:3087:GLY:HA2	2.31	0.46
2:B:3043:ASN:OD1	2:B:3043:ASN:N	2.49	0.46
2:B:3308:MET:HE3	2:B:3311:GLN:HB3	1.98	0.46
2:B:3361:ILE:HG22	2:B:3362:ILE:HD13	1.98	0.45
2:B:2921:ILE:HD11	2:B:2938:ASP:HB2	1.98	0.45
2:B:3084:CYS:SG	2:B:3088:HIS:HB2	2.56	0.45
2:B:3115:GLU:H	2:B:3115:GLU:CD	2.24	0.45
2:B:3553:ARG:NH1	2:B:3555:CYS:HB2	2.32	0.45
2:B:3671:ASP:OD1	2:B:3672:GLU:N	2.50	0.45
2:B:2864:THR:HG22	2:B:2864:THR:O	2.17	0.45
2:B:3116:CYS:SG	2:B:3135:PHE:HB2	2.57	0.45
2:B:3122:SER:C	2:B:3124:CYS:N	2.75	0.45
2:B:3699:ALA:HB1	2:B:3706:ASP:CG	2.42	0.45
2:B:2960:SER:HB3	2:B:2964:ASN:HB3	2.00	0.44
1:C:76:PRO:HA	1:C:79:LEU:HB3	2.00	0.44
2:B:3351:ILE:HD11	2:B:3355:GLY:HA2	1.99	0.44
2:B:2957:CYS:HB3	2:B:2984:LEU:HD11	2.00	0.44
2:B:3213:ASN:HB2	2:B:3224:ILE:HG13	1.99	0.44
2:B:3671:ASP:OD1	2:B:3671:ASP:C	2.61	0.44
2:B:3114:ASN:HB3	2:B:3117:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3233:ALA:HA	2:B:3455:ASP:HB2	2.00	0.44
2:B:2962:PRO:N	2:B:2963:PRO:HD2	2.32	0.44
2:B:3077:CYS:HB3	2:B:3081:GLN:HB2	1.98	0.44
2:B:3467:MET:HE3	2:B:3467:MET:HB2	1.70	0.43
2:B:3831:GLU:HB2	2:B:3855:VAL:HG12	1.99	0.43
2:B:3336:HIS:CG	2:B:3350:ARG:HD2	2.53	0.43
2:B:3130:ASP:HA	2:B:3135:PHE:HA	2.00	0.43
2:B:3591:CYS:O	2:B:3606:LYS:HG3	2.18	0.43
2:B:2877:ARG:HB3	2:B:2891:CYS:SG	2.59	0.43
2:B:3051:PHE:HB3	2:B:3058:ASP:OD2	2.19	0.43
2:B:3116:CYS:SG	2:B:3129:THR:C	3.02	0.43
2:B:3560:PHE:CG	2:B:3573:LEU:HD21	2.54	0.43
2:B:3294:ASP:HB3	2:B:3322:PHE:HB3	2.01	0.43
2:B:3863:CYS:O	2:B:3890:ARG:NH2	2.52	0.43
2:B:3116:CYS:SG	2:B:3129:THR:N	2.92	0.43
2:B:3807:CYS:HB3	2:B:3829:SER:HB3	2.01	0.43
2:B:3829:SER:O	2:B:3832:SER:OG	2.25	0.42
2:B:3313:CYS:HA	2:B:3321:CYS:HA	2.01	0.42
2:B:3114:ASN:OD1	2:B:3116:CYS:HB2	2.19	0.42
2:B:3431:THR:OG1	2:B:3433:GLU:OE1	2.37	0.42
2:B:3429:THR:HB	2:B:3431:THR:HG23	2.00	0.42
2:B:3122:SER:C	2:B:3124:CYS:H	2.27	0.42
2:B:3505:ARG:NH1	2:B:3506:ASP:OD1	2.53	0.42
2:B:3165:CYS:HB3	2:B:3178:CYS:HB3	1.90	0.42
2:B:3012:PHE:HB3	2:B:3019:ASP:CG	2.45	0.42
2:B:3280:ASP:OD2	2:B:3283:SER:OG	2.26	0.42
2:B:1225:THR:HG22	2:B:1226:ARG:O	2.20	0.42
1:C:75:SER:O	1:C:79:LEU:N	2.42	0.41
1:C:100:LYS:NZ	1:C:105:ASP:HB3	2.35	0.41
2:B:3203:LEU:HD23	2:B:3458:VAL:HG22	2.01	0.41
2:B:3370:ASN:ND2	3:O:3:ASN:OD1	2.48	0.41
2:B:1230:MET:HE3	2:B:1230:MET:HB3	1.90	0.41
2:B:3791:ASP:OD1	2:B:3791:ASP:N	2.51	0.41
2:B:3371:ALA:HB3	2:B:3384:ALA:HB3	2.02	0.41
2:B:3669:PRO:HG2	2:B:3672:GLU:HB3	2.03	0.41
2:B:3146:MET:SD	2:B:3146:MET:N	2.93	0.41
2:B:3821:GLY:HA2	2:B:3837:ARG:NH2	2.36	0.41
2:B:3392:GLU:OE1	2:B:3401:ARG:NH1	2.54	0.41
2:B:3556:ARG:HD3	2:B:3822:ARG:NH2	2.36	0.41
2:B:1236:PHE:N	2:B:1245:ILE:O	2.46	0.41
2:B:3610:PRO:HG2	2:B:3613:TRP:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:MET:HE2	1:C:61:LYS:HG2	2.03	0.41
2:B:3049:ARG:HE	2:B:3052:VAL:HG21	1.86	0.41
2:B:3207:ASN:HD21	2:B:3449:THR:HG21	1.86	0.41
2:B:3839:PRO:C	2:B:3841:GLY:N	2.78	0.41
1:C:95:ASN:OD1	1:C:95:ASN:C	2.63	0.40
2:B:3201:PRO:HG3	2:B:3418:PHE:CE2	2.56	0.40
2:B:3213:ASN:OD1	2:B:3222:SER:OG	2.39	0.40
2:B:3852:LYS:HG2	2:B:3873:SER:OG	2.21	0.40
2:B:3433:GLU:OE2	2:B:3445:VAL:HG22	2.21	0.40
2:B:3255:ARG:NE	2:B:3264:GLU:OE2	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	C	70/360 (19%)	69 (99%)	1 (1%)	0	100	100
2	B	1085/4660 (23%)	1017 (94%)	64 (6%)	4 (0%)	30	61
3	O	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1156/5025 (23%)	1087 (94%)	65 (6%)	4 (0%)	37	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3357	ASN
2	B	3123	ARG
2	B	3840	ASN
2	B	3839	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	64/326 (20%)	63 (98%)	1 (2%)	55	69
2	B	975/4089 (24%)	958 (98%)	17 (2%)	53	69
3	O	1/1 (100%)	1 (100%)	0	100	100
All	All	1040/4416 (24%)	1022 (98%)	18 (2%)	52	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	75	SER
2	B	2884	PHE
2	B	2993	ARG
2	B	3064	ASP
2	B	3118	ASP
2	B	3145	LEU
2	B	3173	VAL
2	B	3426	ASP
2	B	3449	THR
2	B	3467	MET
2	B	3505	ARG
2	B	3589	VAL
2	B	3636	THR
2	B	3716	CYS
2	B	3737	LEU
2	B	3755	ASN
2	B	3762	SER
2	B	3870	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	73	HIS
1	C	116	HIS
2	B	2903	HIS

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Mol	Chain	Res	Type
2	B	2924	ASN
2	B	2989	ASN
2	B	3081	GLN
2	B	3088	HIS
2	B	3105	ASN
2	B	3207	ASN
2	B	3251	GLN
2	B	3324	HIS
2	B	3336	HIS
2	B	3378	ASN
2	B	3387	HIS
2	B	3624	ASN
2	B	3631	HIS
2	B	3641	GLN
2	B	3732	HIS
2	B	3750	ASN
2	B	3755	ASN
2	B	3811	HIS
2	B	3854	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

27 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	A	1	4,2	14,14,15	0.56	0	17,19,21	1.04	2 (11%)
4	NAG	A	2	4	14,14,15	0.33	0	17,19,21	1.19	2 (11%)
4	BMA	A	3	4	11,11,12	0.22	0	15,15,17	0.84	1 (6%)
5	NAG	D	1	5,2	14,14,15	0.34	0	17,19,21	1.13	1 (5%)
5	NAG	D	2	5	14,14,15	0.49	0	17,19,21	0.92	1 (5%)
5	BMA	D	3	5	11,11,12	0.22	0	15,15,17	0.62	0
6	NAG	E	1	2,6	14,14,15	0.33	0	17,19,21	0.86	0
6	NAG	E	2	6	14,14,15	0.30	0	17,19,21	0.80	0
6	BMA	E	3	6	11,11,12	0.25	0	15,15,17	1.12	1 (6%)
6	MAN	E	4	6	11,11,12	0.24	0	15,15,17	0.75	1 (6%)
6	MAN	E	5	6	11,11,12	0.24	0	15,15,17	0.59	0
7	NAG	F	1	7,2	14,14,15	0.34	0	17,19,21	1.04	1 (5%)
7	NAG	F	2	7	14,14,15	0.42	0	17,19,21	1.34	1 (5%)
7	BMA	F	3	7	11,11,12	0.23	0	15,15,17	0.57	0
7	NAG	G	1	7,2	14,14,15	0.43	0	17,19,21	0.70	0
7	NAG	G	2	7	14,14,15	0.33	0	17,19,21	0.75	0
7	BMA	G	3	7	11,11,12	0.19	0	15,15,17	0.51	0
6	NAG	H	1	2,6	14,14,15	0.40	0	17,19,21	1.09	2 (11%)
6	NAG	H	2	6	14,14,15	0.40	0	17,19,21	1.33	1 (5%)
6	BMA	H	3	6	11,11,12	0.25	0	15,15,17	1.31	2 (13%)
6	MAN	H	4	6	11,11,12	0.22	0	15,15,17	0.46	0
6	MAN	H	5	6	11,11,12	0.22	0	15,15,17	0.44	0
6	NAG	I	1	2,6	14,14,15	0.27	0	17,19,21	0.72	0
6	NAG	I	2	6	14,14,15	0.29	0	17,19,21	0.62	0
6	BMA	I	3	6	11,11,12	0.22	0	15,15,17	0.70	0
6	MAN	I	4	6	11,11,12	0.26	0	15,15,17	0.60	0
6	MAN	I	5	6	11,11,12	0.26	0	15,15,17	0.59	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
4	NAG	A	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1
5	NAG	D	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	D	3	5	-	0/2/19/22	0/1/1/1
6	NAG	E	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
6	BMA	E	3	6	-	2/2/19/22	0/1/1/1
6	MAN	E	4	6	-	0/2/19/22	0/1/1/1
6	MAN	E	5	6	-	0/2/19/22	0/1/1/1
7	NAG	F	1	7,2	-	3/6/23/26	0/1/1/1
7	NAG	F	2	7	-	3/6/23/26	0/1/1/1
7	BMA	F	3	7	-	0/2/19/22	0/1/1/1
7	NAG	G	1	7,2	-	4/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
6	NAG	H	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	H	2	6	-	3/6/23/26	0/1/1/1
6	BMA	H	3	6	-	2/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
6	MAN	H	5	6	-	0/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	3/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	MAN	I	5	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	2	NAG	C1-O5-C5	3.94	117.47	112.19
7	F	2	NAG	C1-O5-C5	3.88	117.38	112.19
6	H	3	BMA	C1-O5-C5	3.80	117.27	112.19
5	D	1	NAG	C1-O5-C5	3.19	116.47	112.19
6	H	1	NAG	C1-O5-C5	3.17	116.44	112.19
4	A	2	NAG	O5-C1-C2	-3.13	106.45	111.29
6	E	3	BMA	C1-C2-C3	2.87	113.82	109.64
6	H	3	BMA	C1-C2-C3	2.43	113.19	109.64
4	A	3	BMA	C1-O5-C5	2.39	115.39	112.19
6	H	1	NAG	O4-C4-C5	2.32	115.03	109.32
7	F	1	NAG	O5-C1-C2	-2.26	107.80	111.29
6	E	4	MAN	C1-O5-C5	2.26	115.21	112.19
5	D	2	NAG	O3-C3-C2	-2.18	104.87	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	O4-C4-C5	-2.11	104.13	109.32
4	A	1	NAG	C1-O5-C5	-2.05	109.44	112.19
4	A	2	NAG	C2-N2-C7	2.03	125.62	122.90

There are no chirality outliers.

All (32) torsion outliers are listed below:

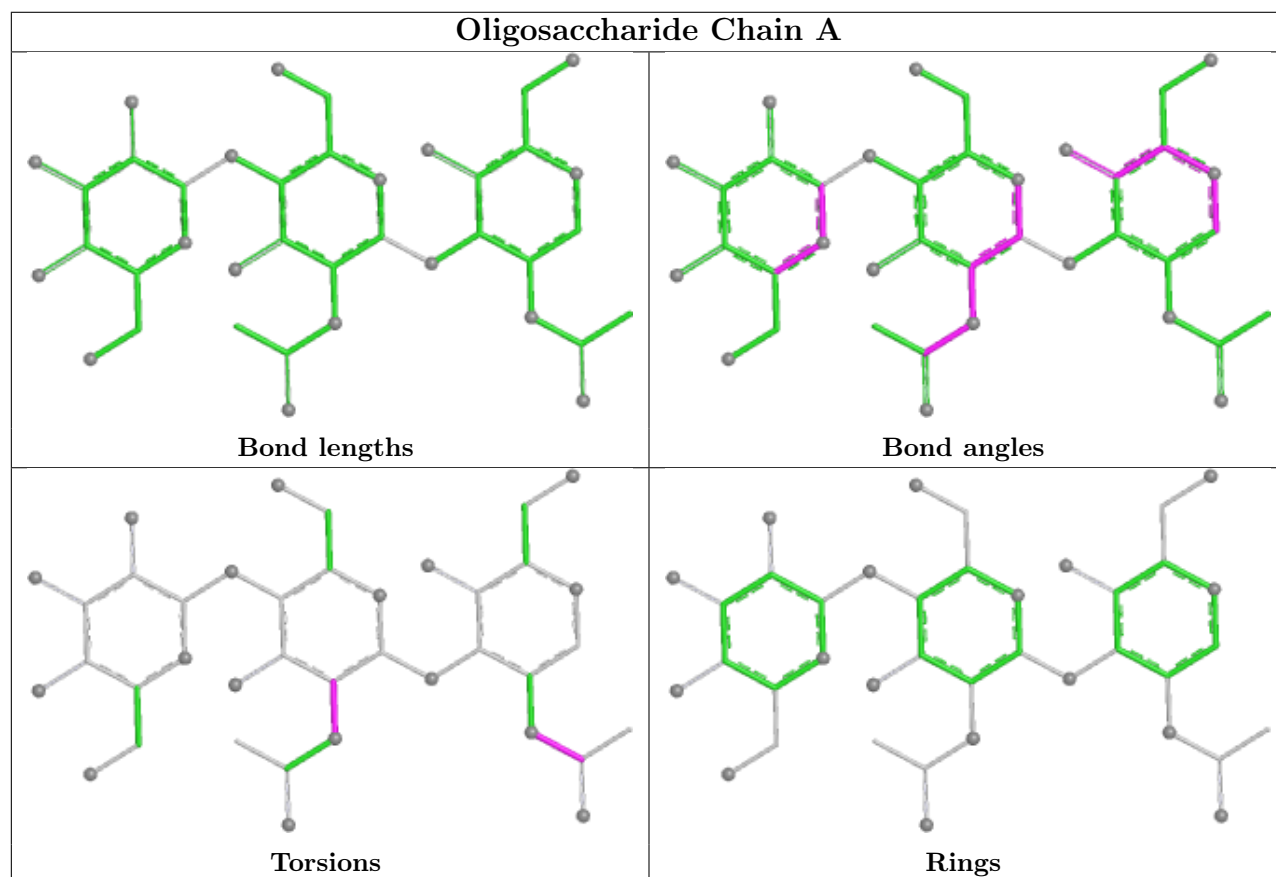
Mol	Chain	Res	Type	Atoms
6	I	1	NAG	C1-C2-N2-C7
7	F	1	NAG	C3-C2-N2-C7
7	F	2	NAG	C1-C2-N2-C7
6	H	1	NAG	C8-C7-N2-C2
6	H	1	NAG	O7-C7-N2-C2
6	I	1	NAG	C8-C7-N2-C2
7	F	1	NAG	C8-C7-N2-C2
7	F	1	NAG	O7-C7-N2-C2
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2
6	H	3	BMA	O5-C5-C6-O6
6	H	3	BMA	C4-C5-C6-O6
7	G	1	NAG	C8-C7-N2-C2
6	E	3	BMA	C4-C5-C6-O6
6	I	3	BMA	C4-C5-C6-O6
6	E	3	BMA	O5-C5-C6-O6
7	G	1	NAG	O7-C7-N2-C2
6	I	3	BMA	O5-C5-C6-O6
4	A	2	NAG	C3-C2-N2-C7
6	H	1	NAG	C3-C2-N2-C7
6	H	2	NAG	C3-C2-N2-C7
7	F	2	NAG	C8-C7-N2-C2
4	A	2	NAG	C1-C2-N2-C7
6	H	1	NAG	C1-C2-N2-C7
7	G	1	NAG	C1-C2-N2-C7
7	F	2	NAG	O7-C7-N2-C2
7	G	2	NAG	C8-C7-N2-C2
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
7	G	1	NAG	C4-C5-C6-O6
7	G	2	NAG	O7-C7-N2-C2

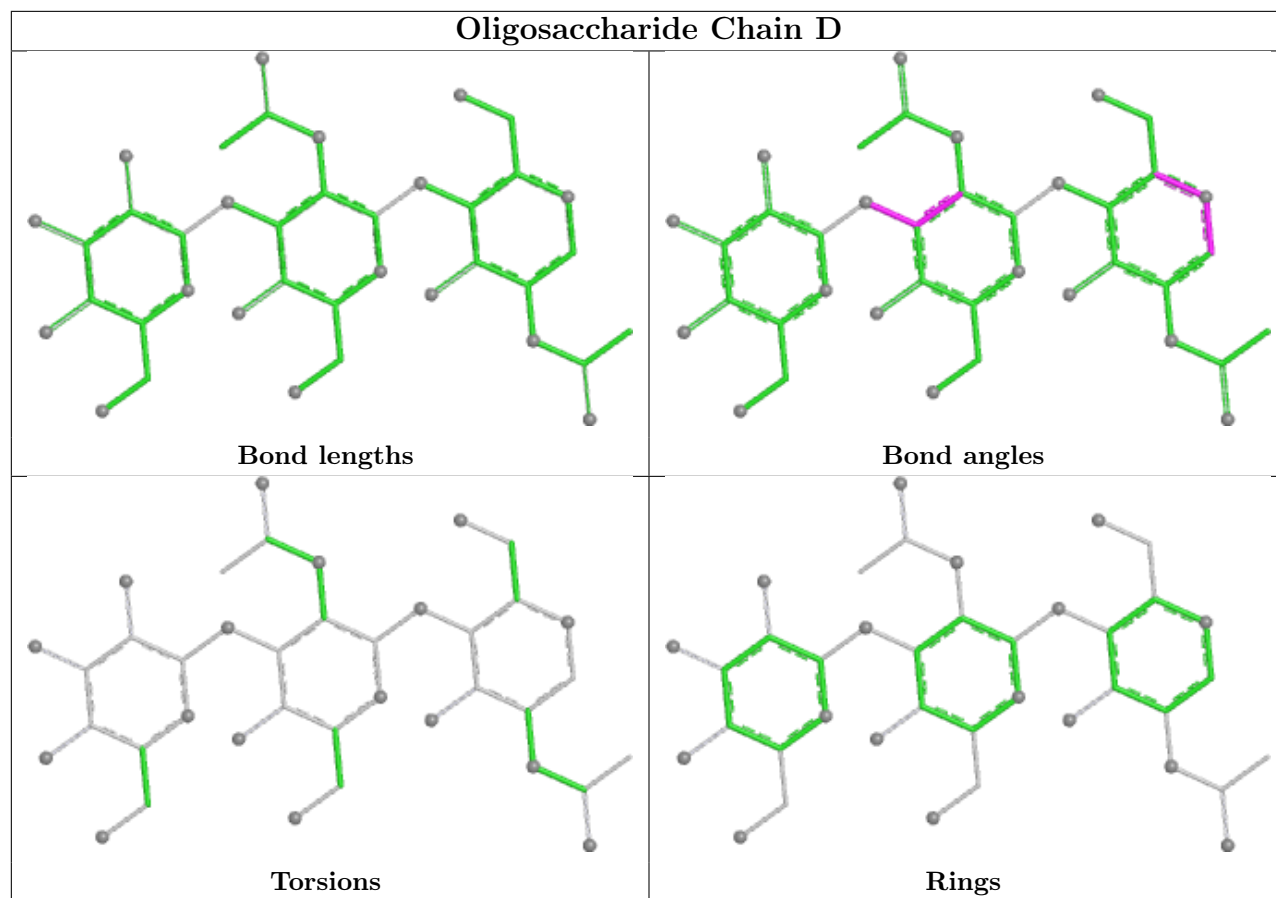
There are no ring outliers.

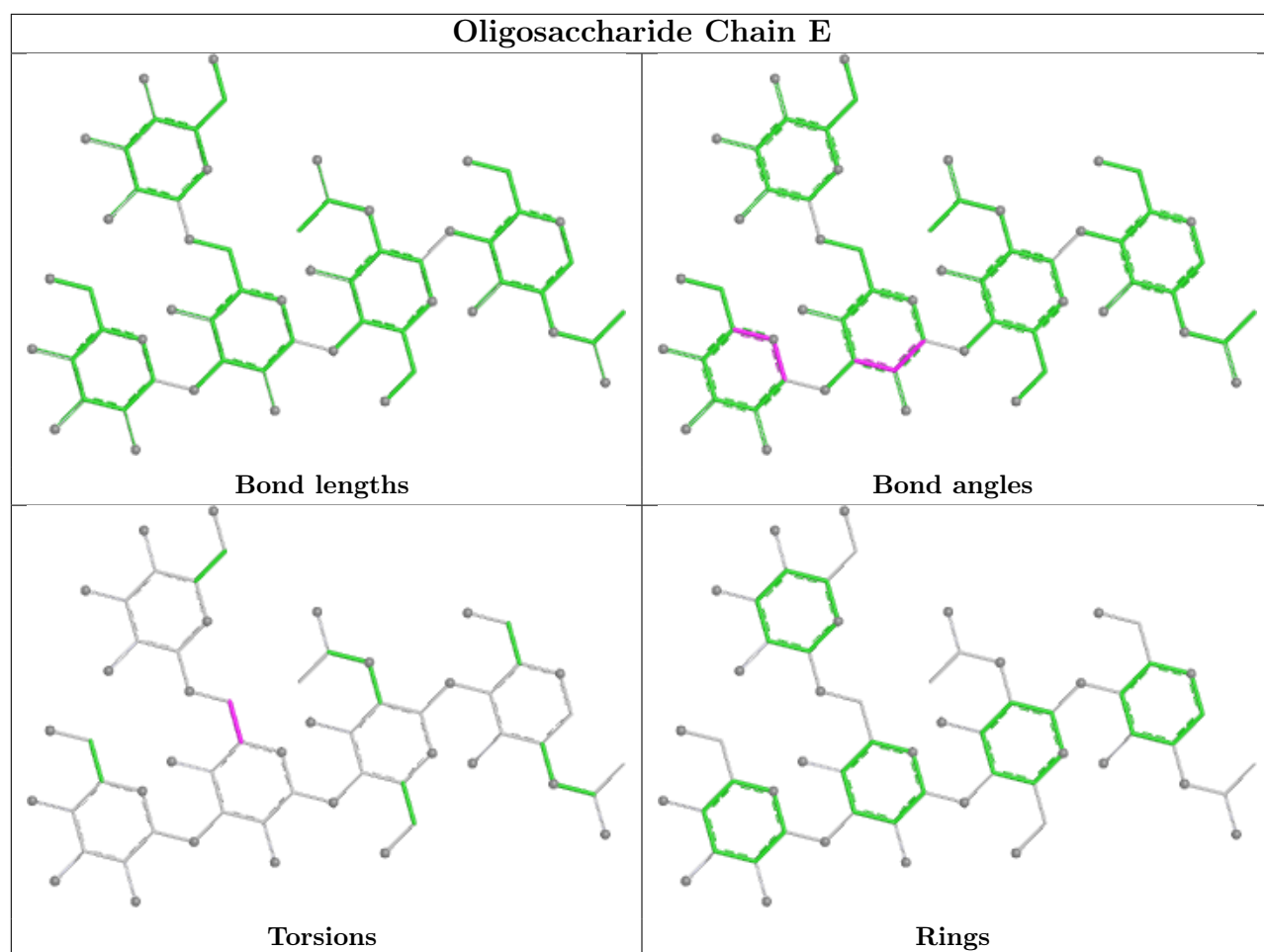
2 monomers are involved in 1 short contact:

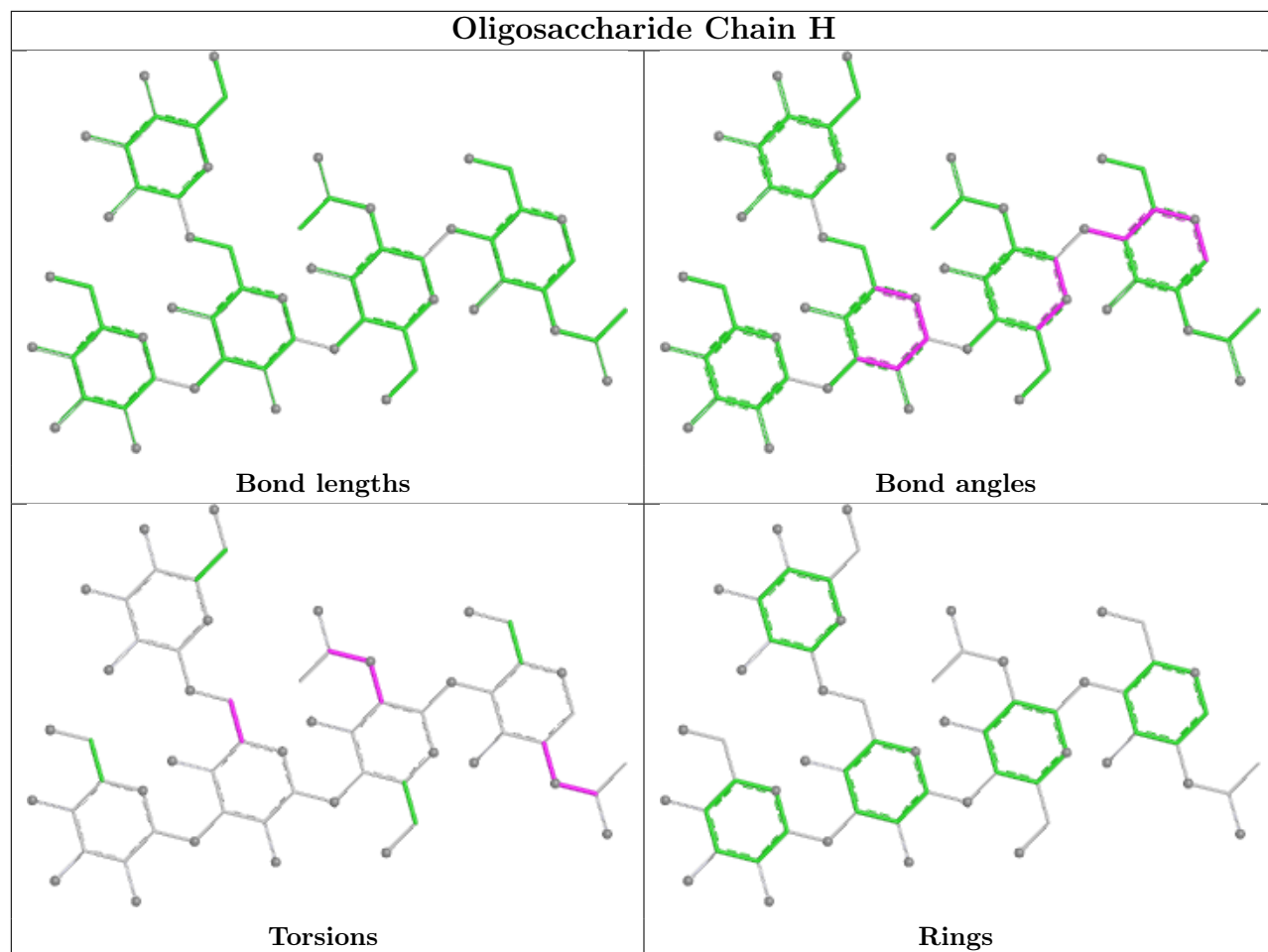
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1	NAG	1	0
6	H	2	NAG	1	0

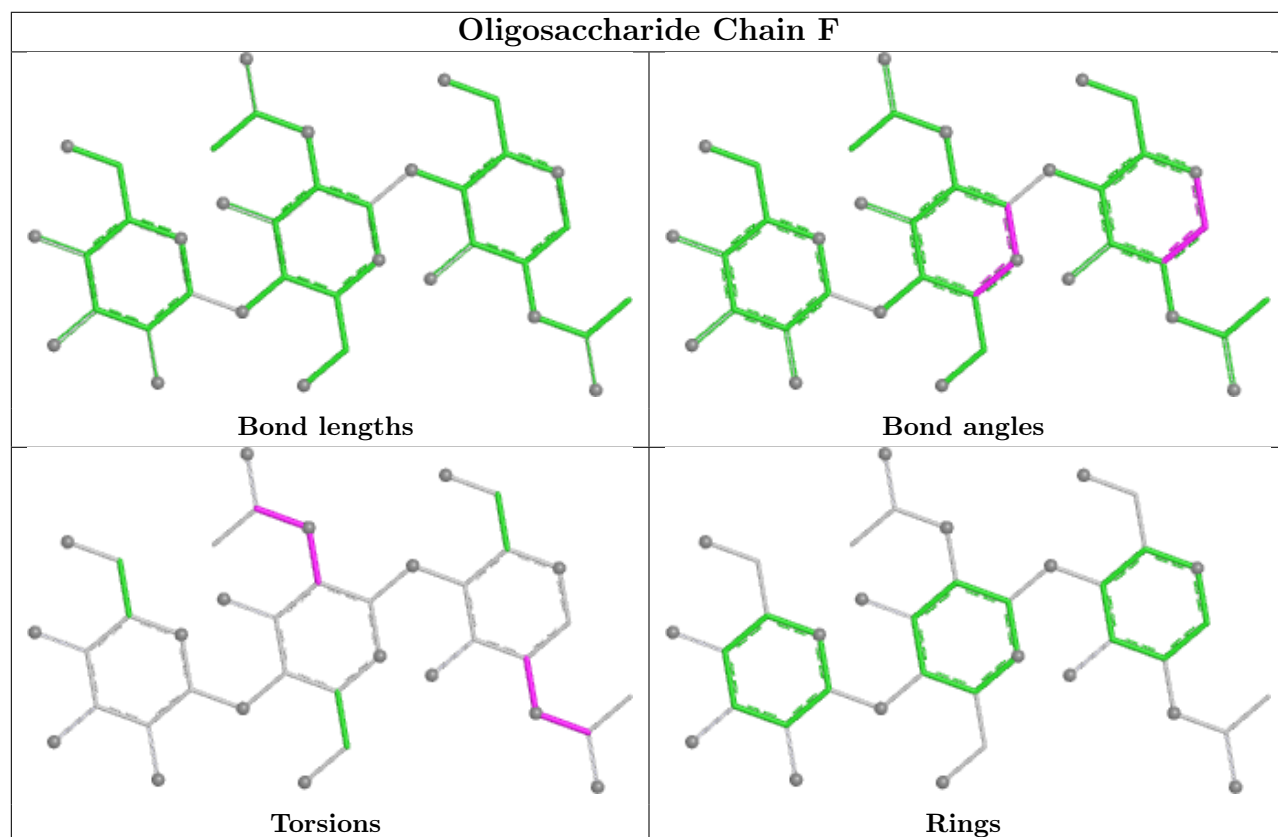
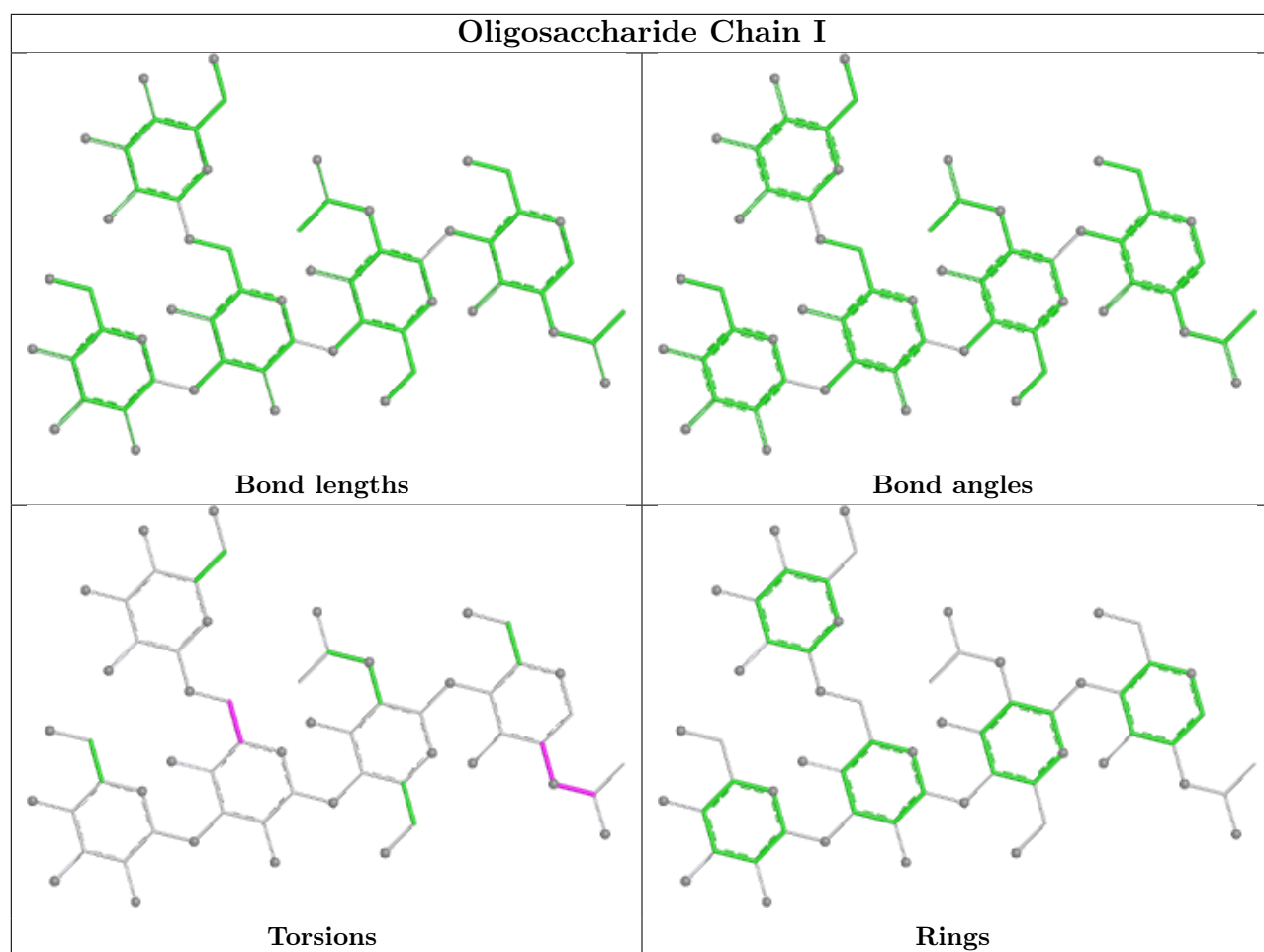
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

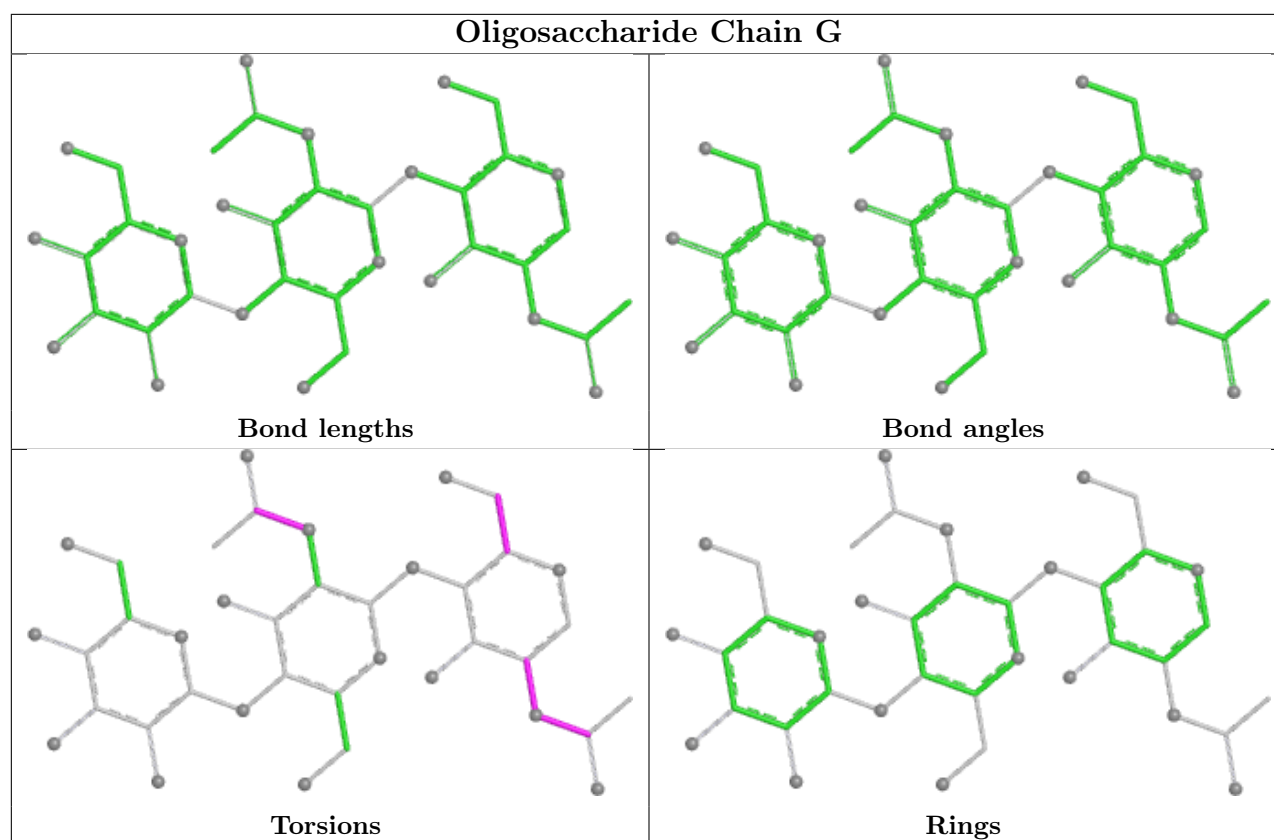












5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 20 are monoatomic - leaving 6 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	A2G	B	4705	2	14,14,15	0.41	0	17,19,21	0.58	0
8	NAG	B	4701	2	14,14,15	0.41	0	17,19,21	0.96	1 (5%)
9	A2G	B	4704	2	14,14,15	0.43	0	17,19,21	0.89	1 (5%)
9	A2G	B	4703	-	14,14,15	0.41	0	17,19,21	2.53	3 (17%)
9	A2G	B	4706	2	14,14,15	0.45	0	17,19,21	0.90	1 (5%)
8	NAG	B	4702	2	14,14,15	0.54	0	17,19,21	1.36	3 (17%)

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	A2G	B	4705	2	-	1/6/23/26	0/1/1/1
8	NAG	B	4701	2	-	0/6/23/26	0/1/1/1
9	A2G	B	4704	2	-	2/6/23/26	0/1/1/1
9	A2G	B	4703	-	-	0/6/23/26	0/1/1/1
9	A2G	B	4706	2	-	2/6/23/26	0/1/1/1
8	NAG	B	4702	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	4703	A2G	O5-C1-C2	9.28	125.65	111.29
8	B	4702	NAG	C4-C3-C2	-3.63	105.70	111.02
9	B	4704	A2G	O5-C1-C2	-3.44	105.97	111.29
9	B	4703	A2G	C1-C2-N2	3.42	115.82	110.43
8	B	4702	NAG	O5-C5-C6	3.21	113.91	107.66
9	B	4706	A2G	O5-C1-C2	-3.05	106.57	111.29
9	B	4703	A2G	C1-O5-C5	3.03	116.25	112.19
8	B	4701	NAG	C1-O5-C5	2.76	115.89	112.19
8	B	4702	NAG	C1-O5-C5	-2.12	109.35	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	4704	A2G	C8-C7-N2-C2
9	B	4705	A2G	O5-C5-C6-O6
9	B	4704	A2G	O7-C7-N2-C2
9	B	4706	A2G	C1-C2-N2-C7
9	B	4706	A2G	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	4703	A2G	6	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.

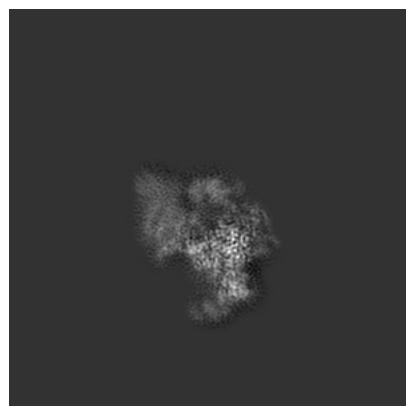
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36699. These allow visual inspection of the internal detail of the map and identification of artifacts.

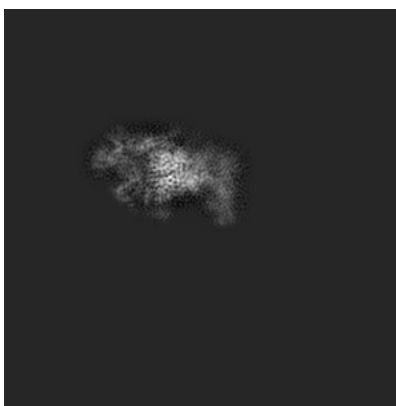
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

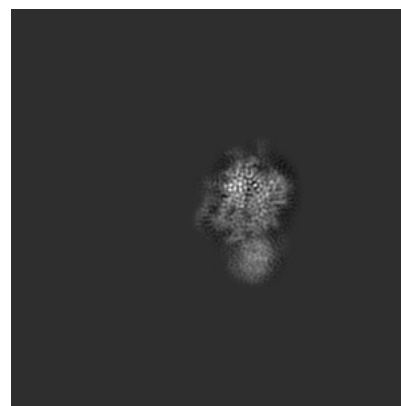
6.1.1 Primary map



X

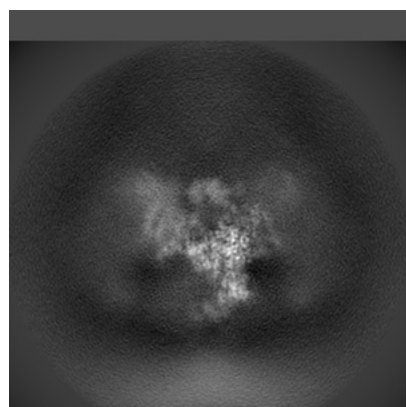


Y

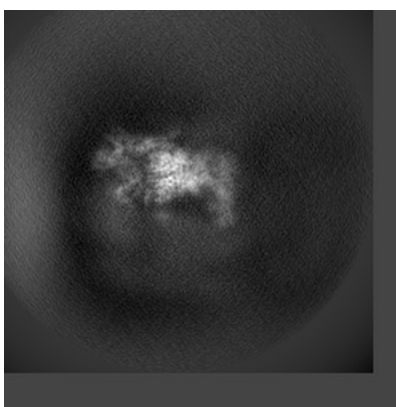


Z

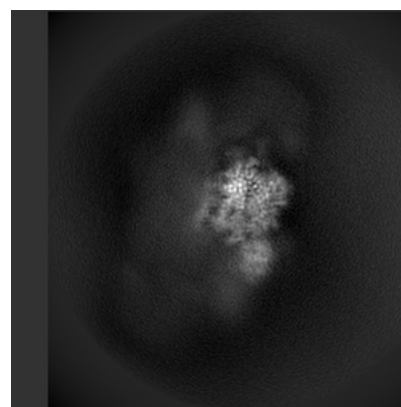
6.1.2 Raw map



X



Y

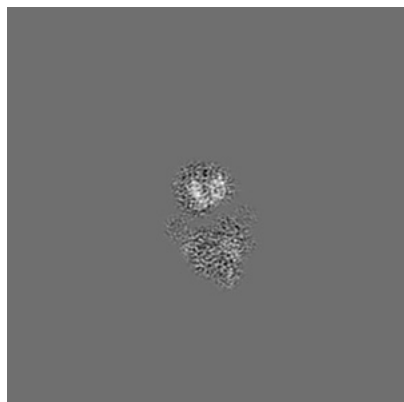


Z

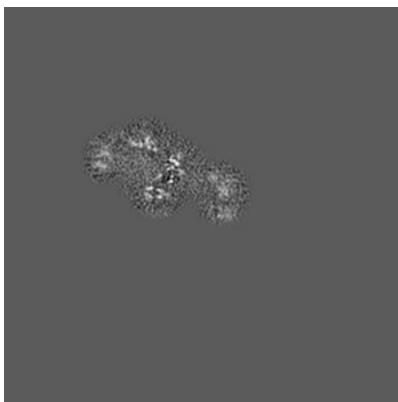
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

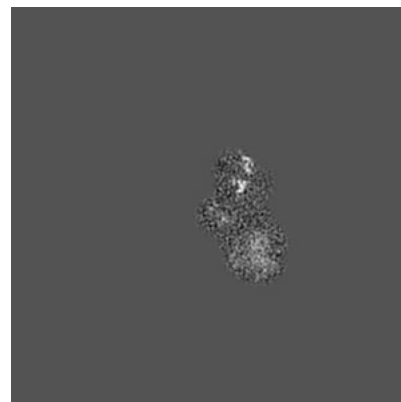
6.2.1 Primary map



X Index: 130

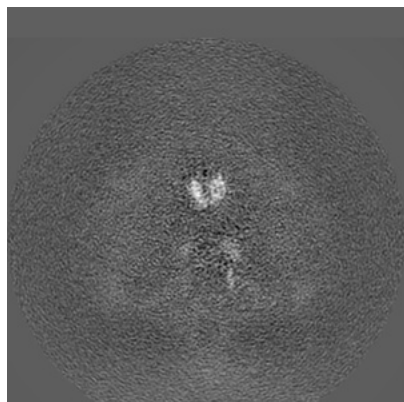


Y Index: 130

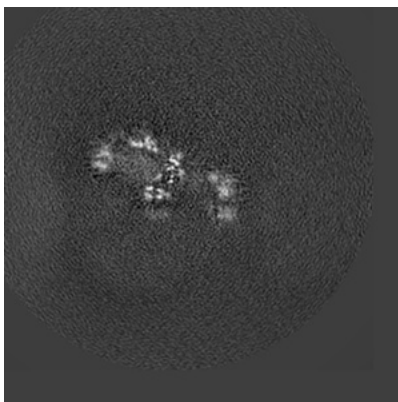


Z Index: 130

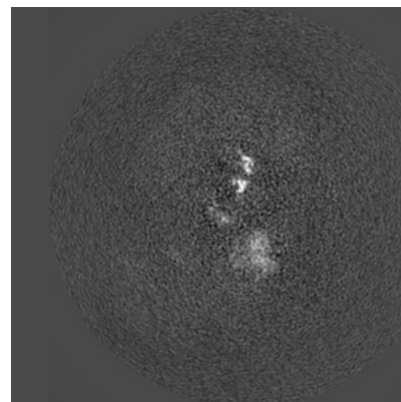
6.2.2 Raw map



X Index: 130



Y Index: 130

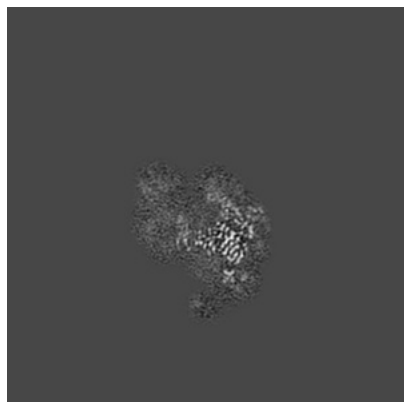


Z Index: 130

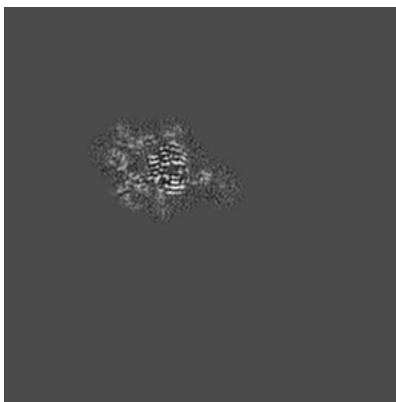
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

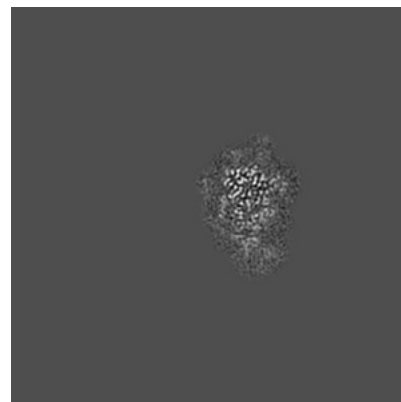
6.3.1 Primary map



X Index: 149

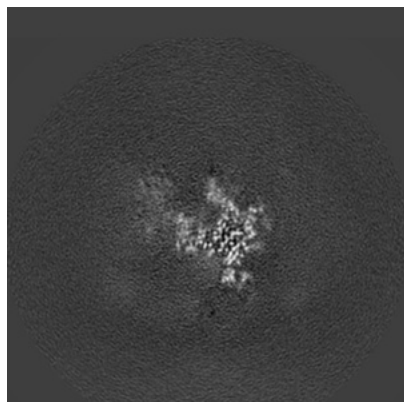


Y Index: 145

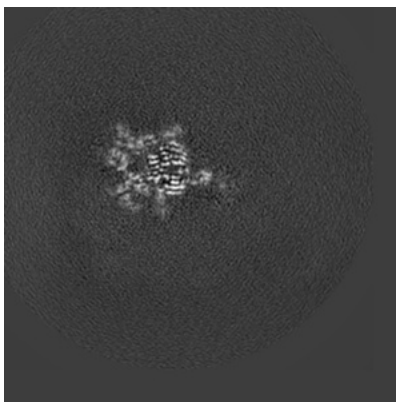


Z Index: 106

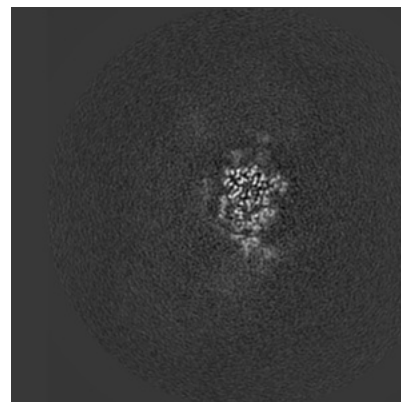
6.3.2 Raw map



X Index: 148



Y Index: 145

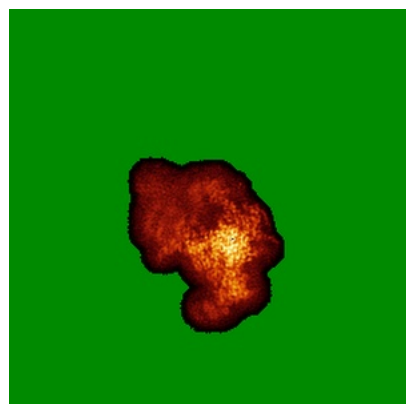


Z Index: 106

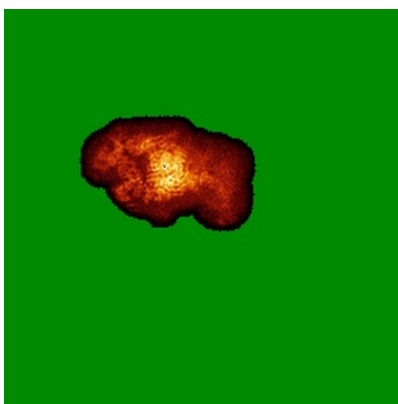
The images above show the largest variance slices of the map in three orthogonal directions.

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

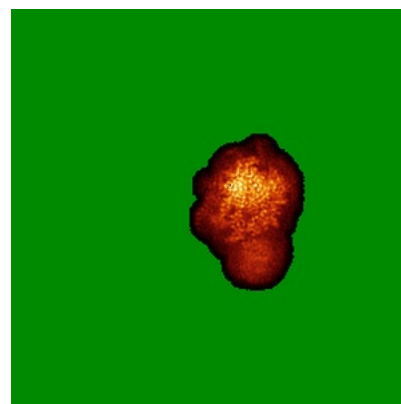
6.4.1 Primary map



X

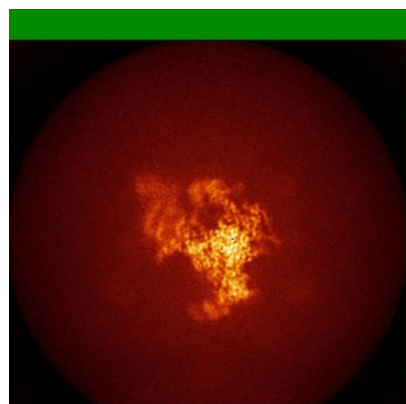


Y

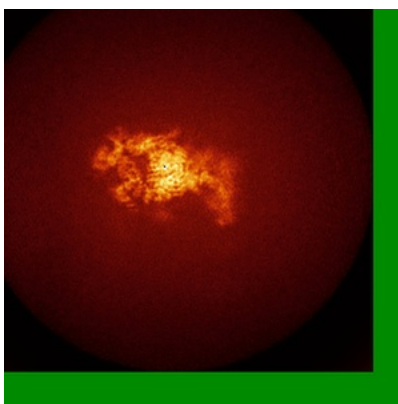


Z

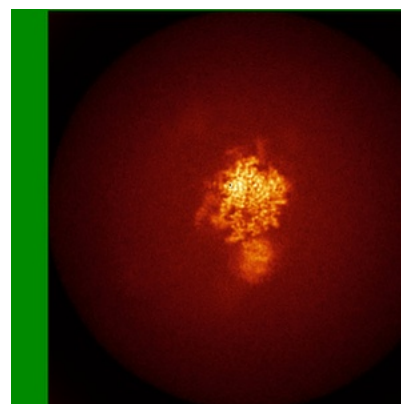
6.4.2 Raw map



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.

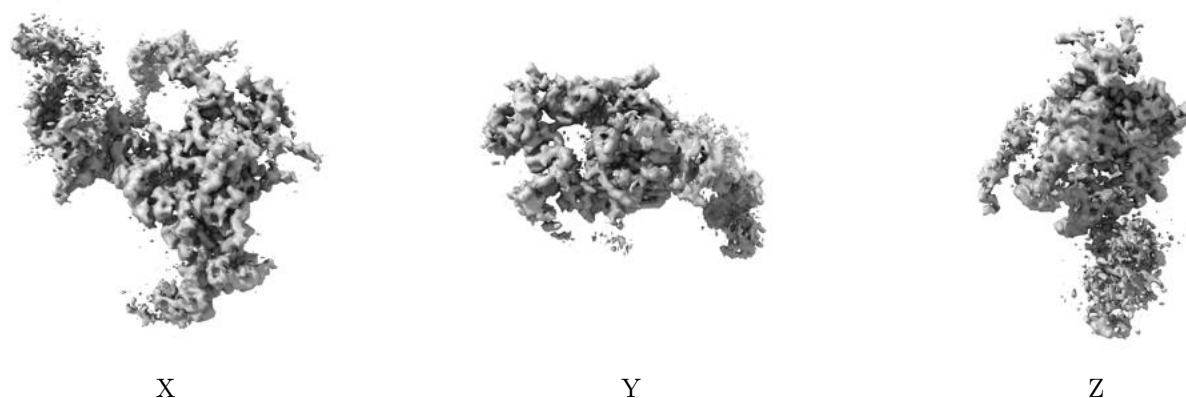
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0271. 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.

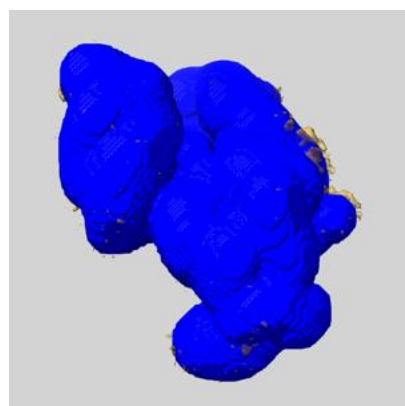
6.6 Mask visualisation [i](#)

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

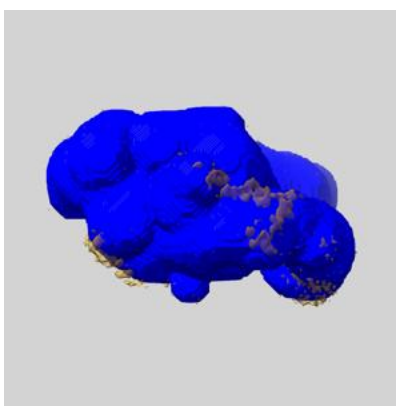
A mask typically either:

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

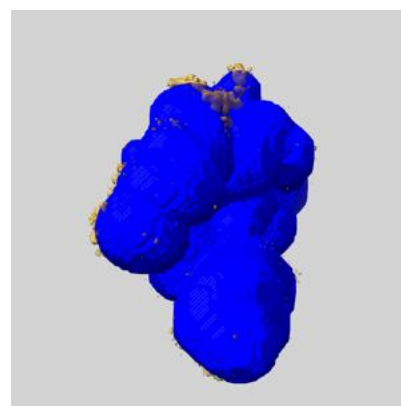
6.6.1 emd_36699_msk_1.map [i](#)



X



Y

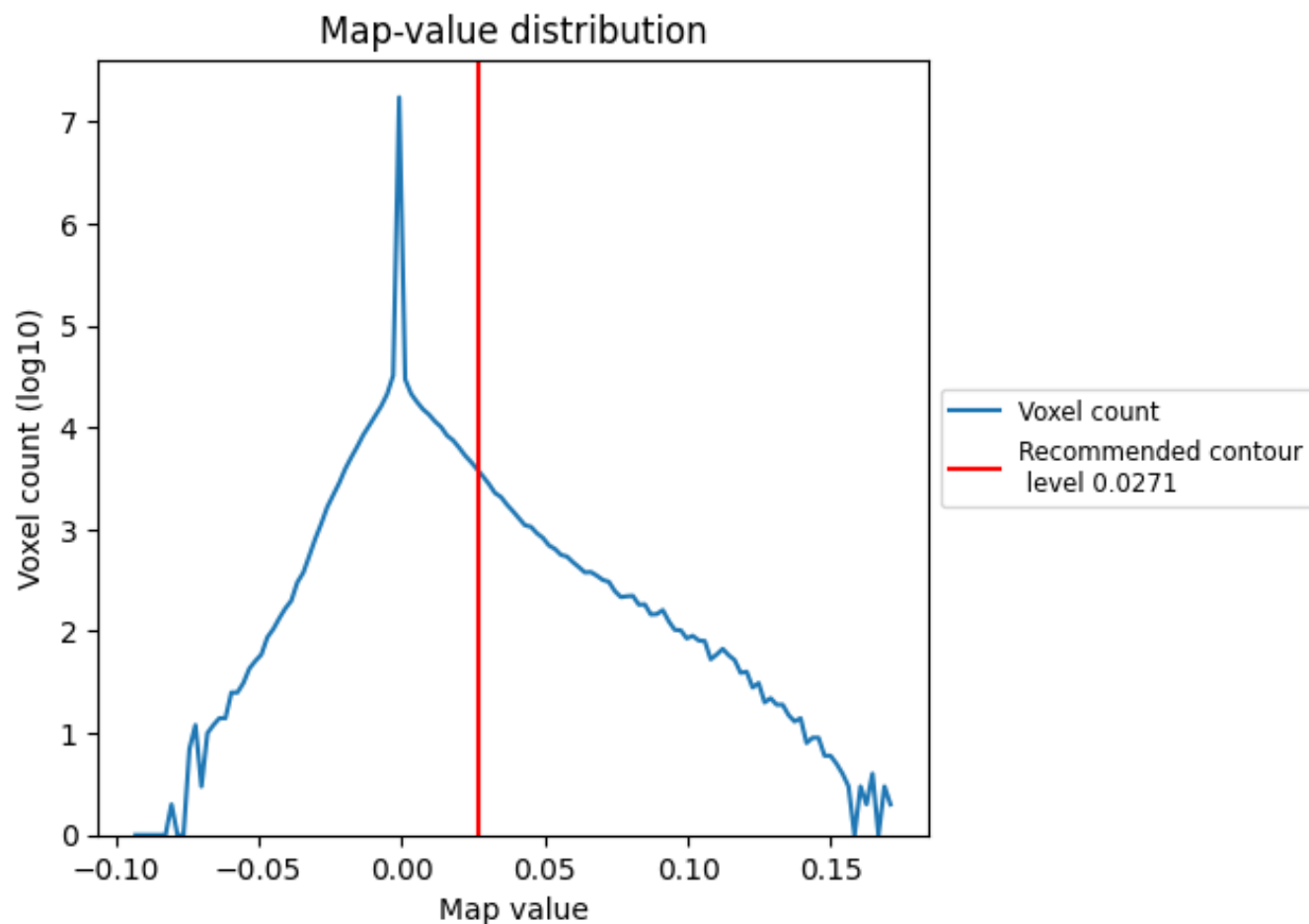


Z

7 Map analysis [i](#)

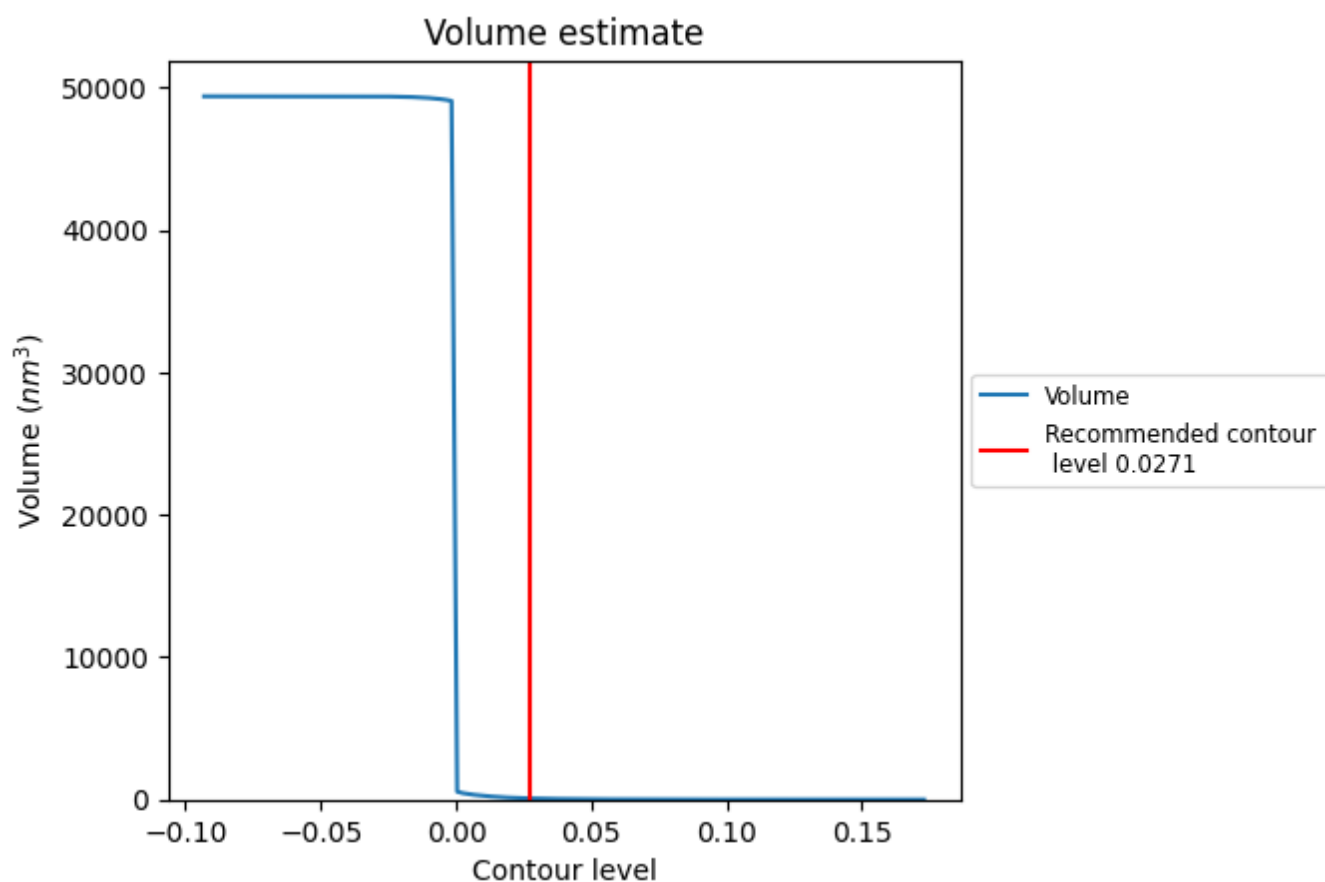
This section contains the results of statistical analysis of the map.

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.

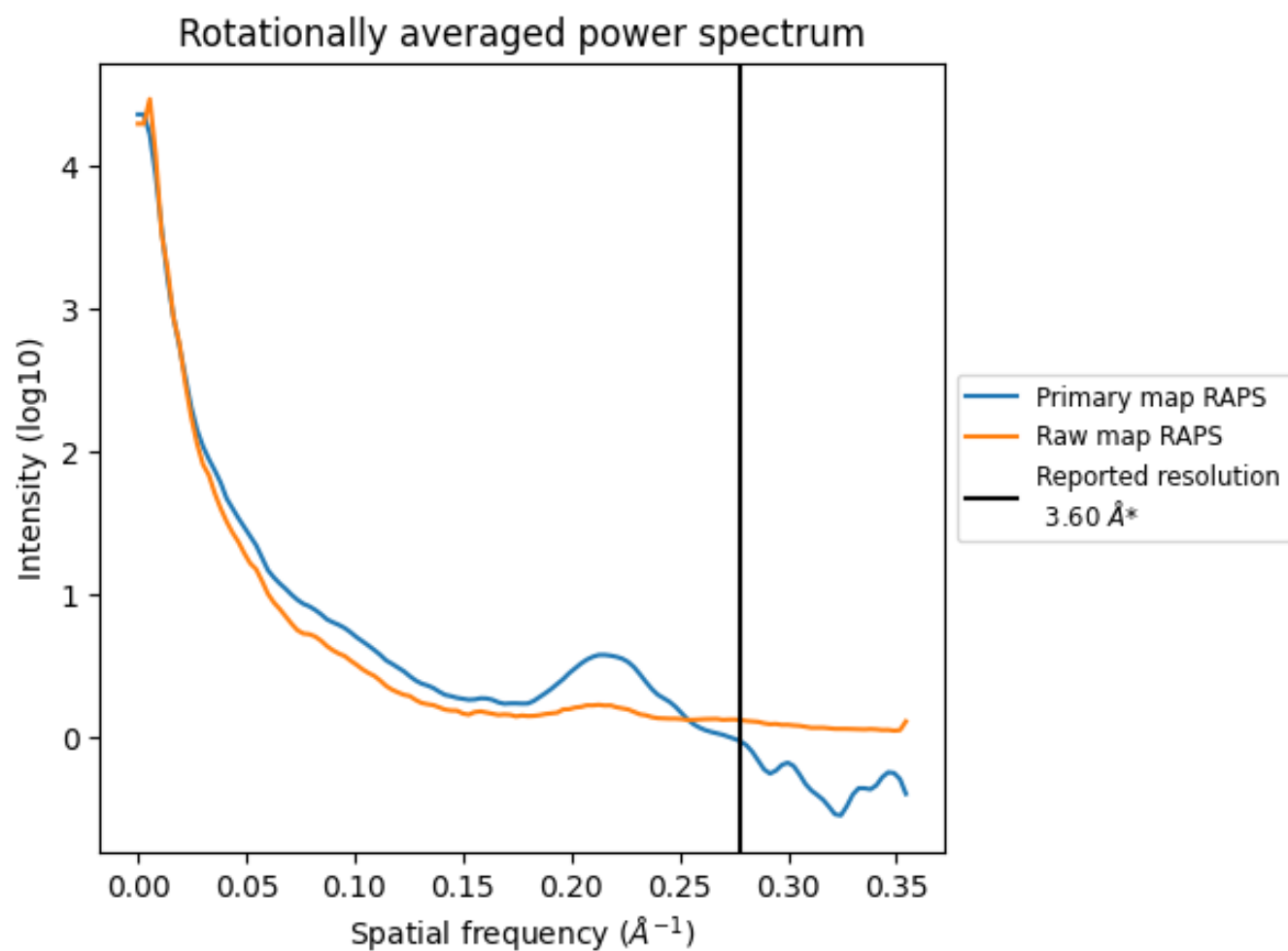
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm³; this corresponds to an approximate mass of 74 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 ⓘ

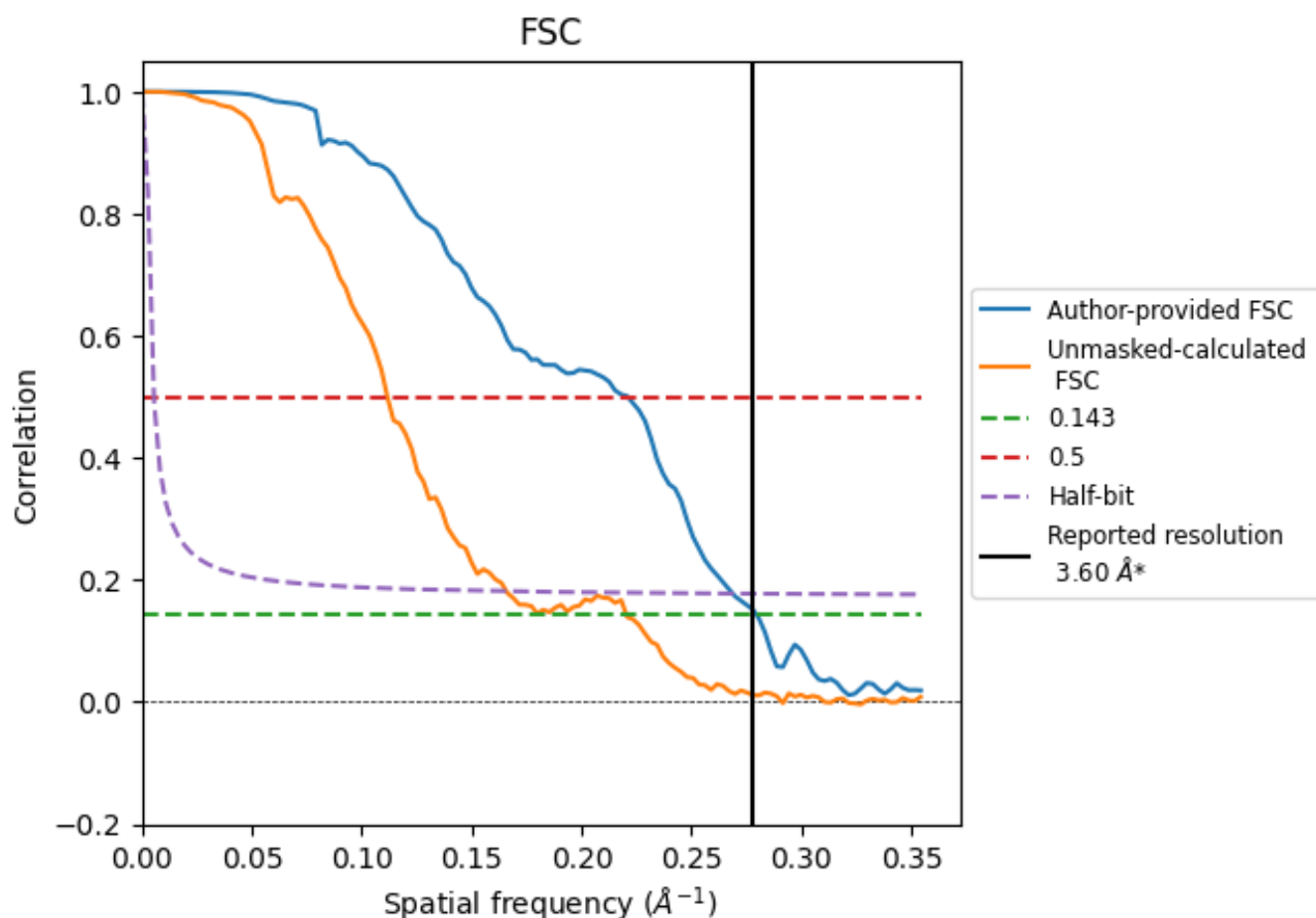


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

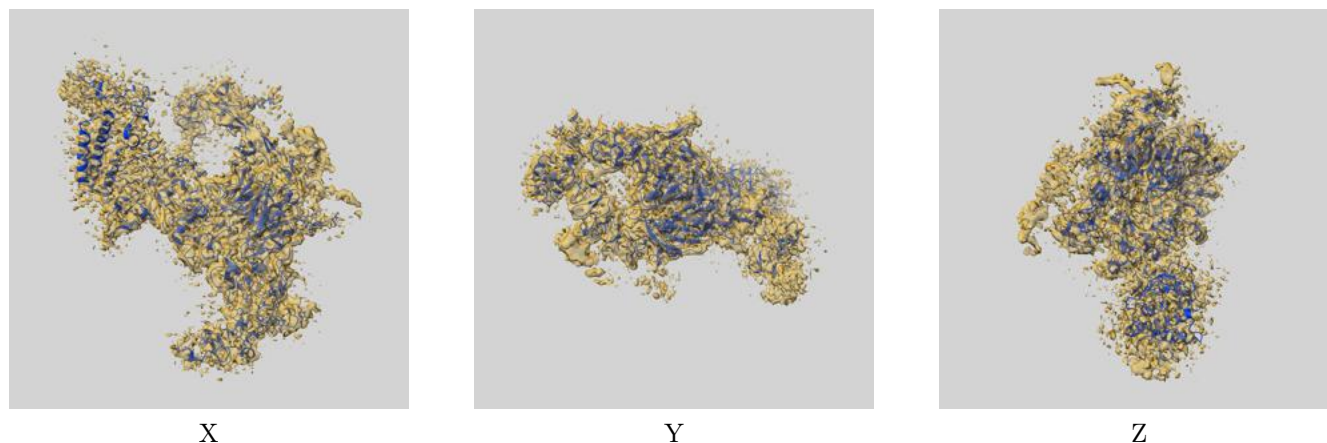
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.52	3.72
Unmasked-calculated*	4.54	8.96	6.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.54 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

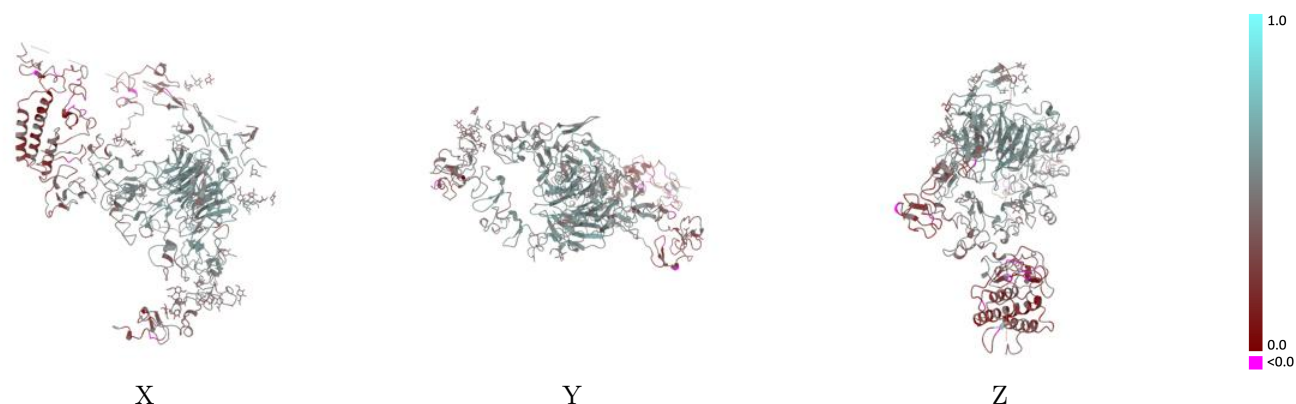
This section contains information regarding the fit between EMDB map EMD-36699 and PDB model 8JXF. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



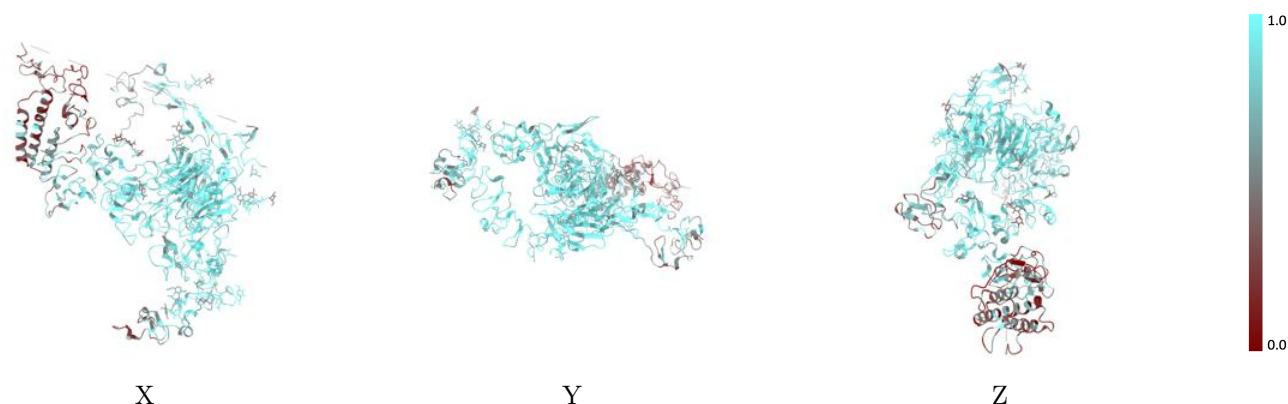
The images above show the 3D surface view of the map at the recommended contour level 0.0271 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



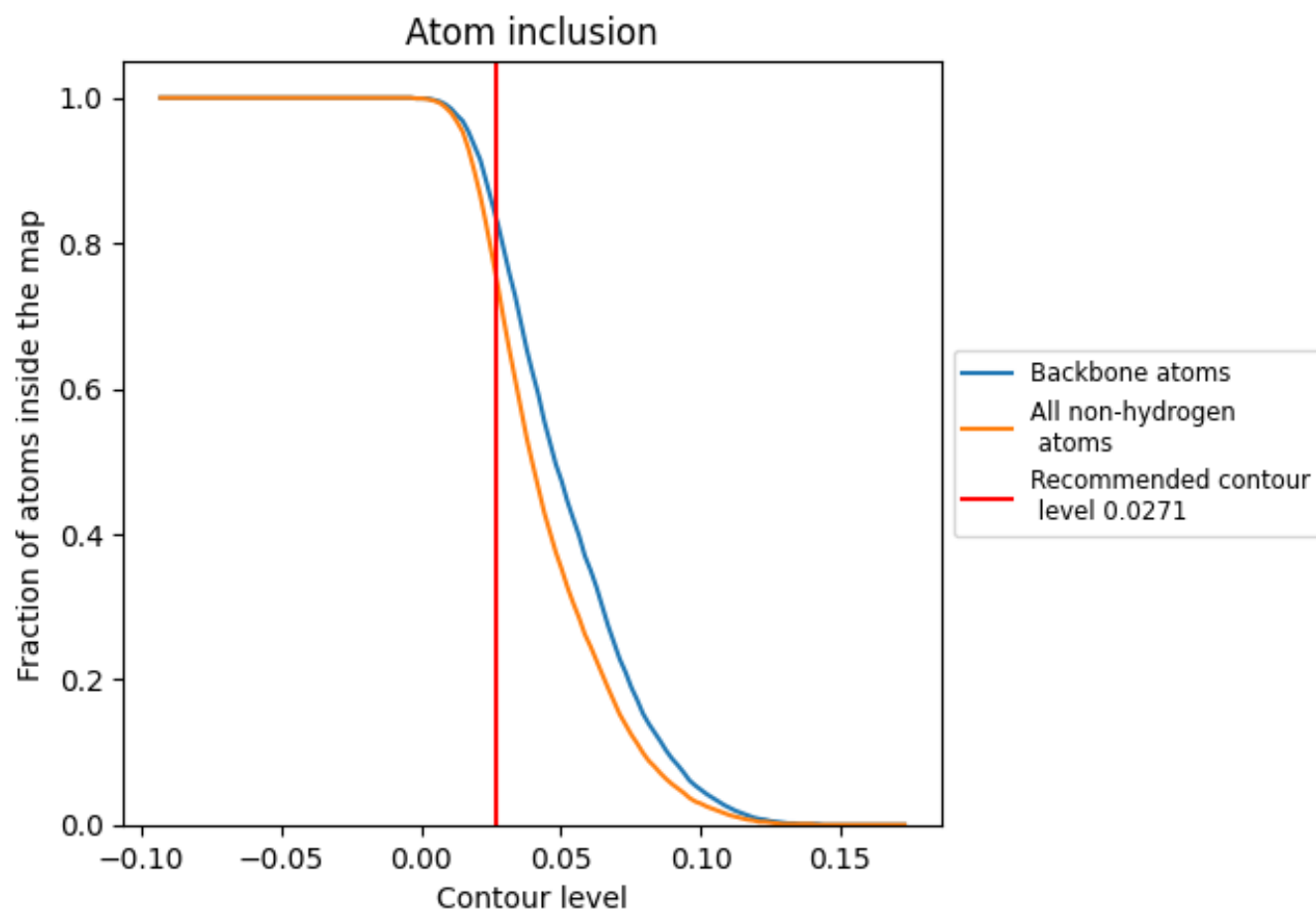
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0271).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 75% 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 (0.0271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4440
A	0.6410	0.3410
B	0.7770	0.4570
C	0.4080	0.2680
D	0.6920	0.4270
E	0.7870	0.4840
F	0.4620	0.3860
G	0.5380	0.4950
H	0.7050	0.3520
I	0.7380	0.4130
O	1.0000	0.6020

1.0

0.0

<0.0