



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:54 AM UTC

PDB ID : 9E8C / pdb_00009e8c
EMDB ID : EMD-47716
Title : Integrin α IIb β 3 dimer conformation from human platelet membrane crude preparation
Authors : Han, X.; Nieman, M.T.
Deposited on : 2024-11-05
Resolution : 3.00 Å(reported)

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

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<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

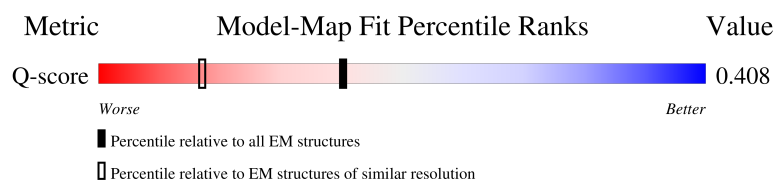
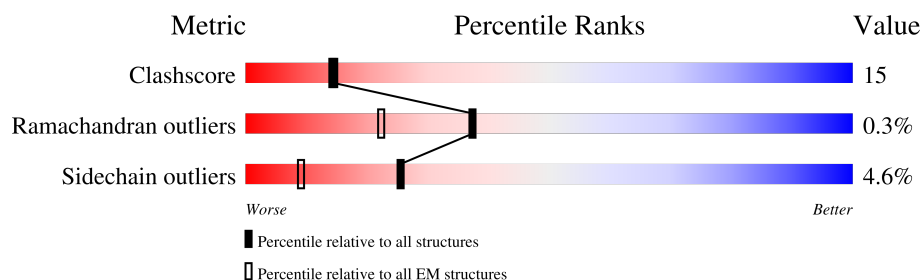
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

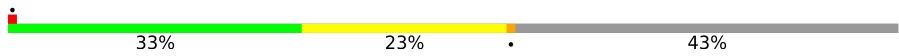
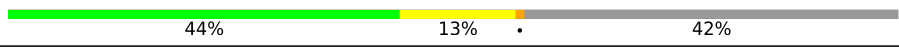
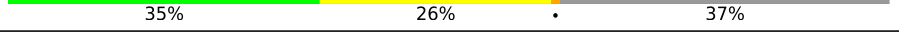
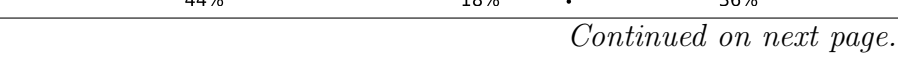
The reported resolution of this entry is 3.00 Å.

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	14081 (2.50 - 3.50)

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	1039	
1	C	1039	
2	B	788	
2	D	788	

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Mol	Chain	Length	Quality of chain
3	E	3	 100%
3	K	3	 67% 33%
4	G	2	 50% 50%
4	M	2	 50% 50%
5	H	3	 33% 67%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17076 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.

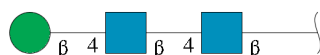
- Molecule 1 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	595	Total	C	N	O	S	0	0
			4525	2866	785	859	15		
1	C	602	Total	C	N	O	S	0	0
			4599	2908	803	872	16		

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	493	Total	C	N	O	S	0	0
			3762	2333	637	752	40		
2	D	506	Total	C	N	O	S	0	0
			3891	2407	668	776	40		

- 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.



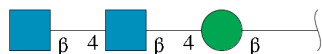
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		

- 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
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose.



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	4	Total	Ca	0
			4	4	
6	B	2	Total	Ca	0
			2	2	
6	C	4	Total	Ca	0
			4	4	
6	D	2	Total	Ca	0
			2	2	

- 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	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	

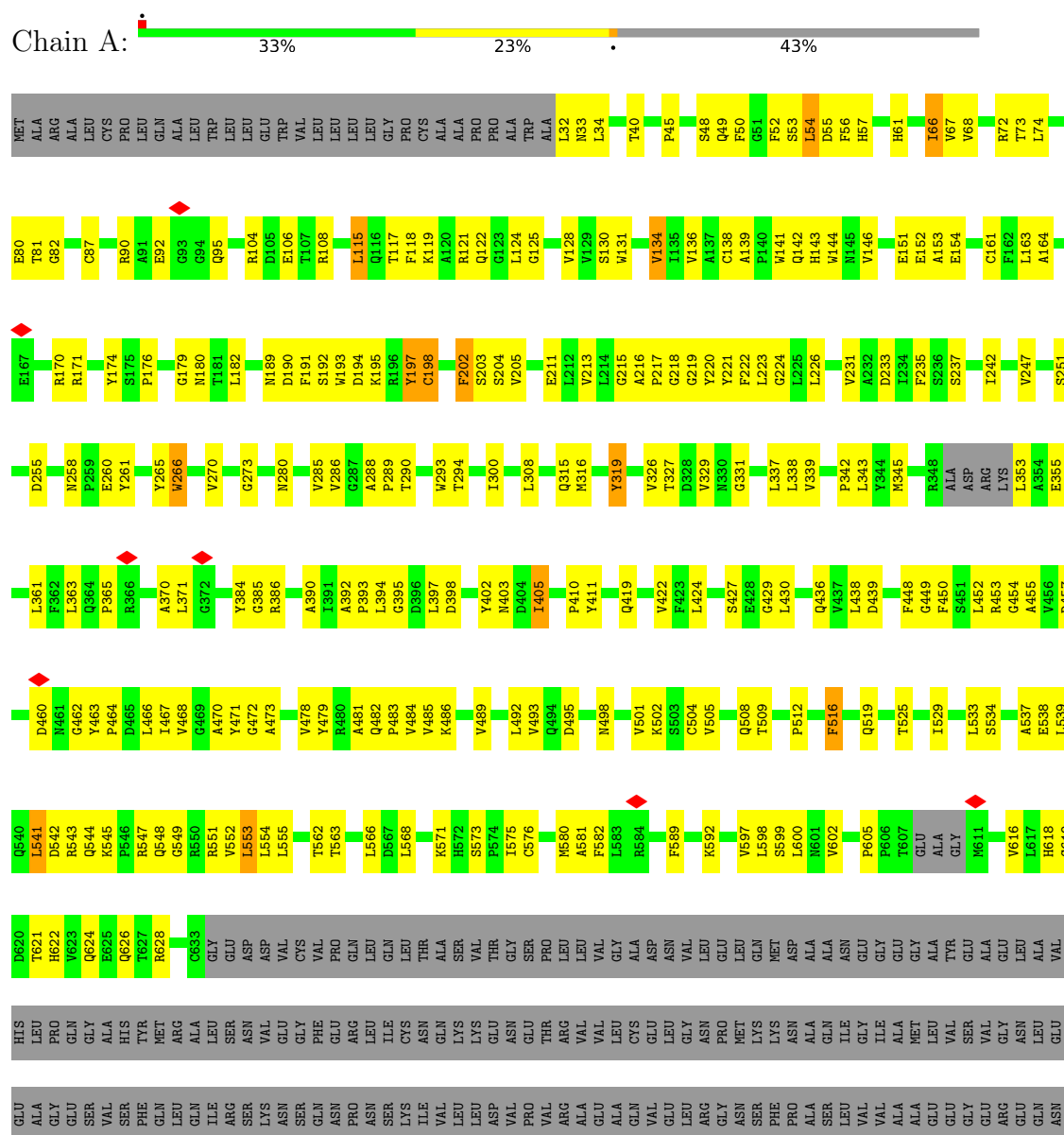
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	
8	D	1	Total	Mg	0
			1	1	

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: Integrin alpha-IIb



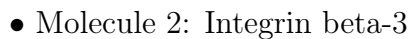
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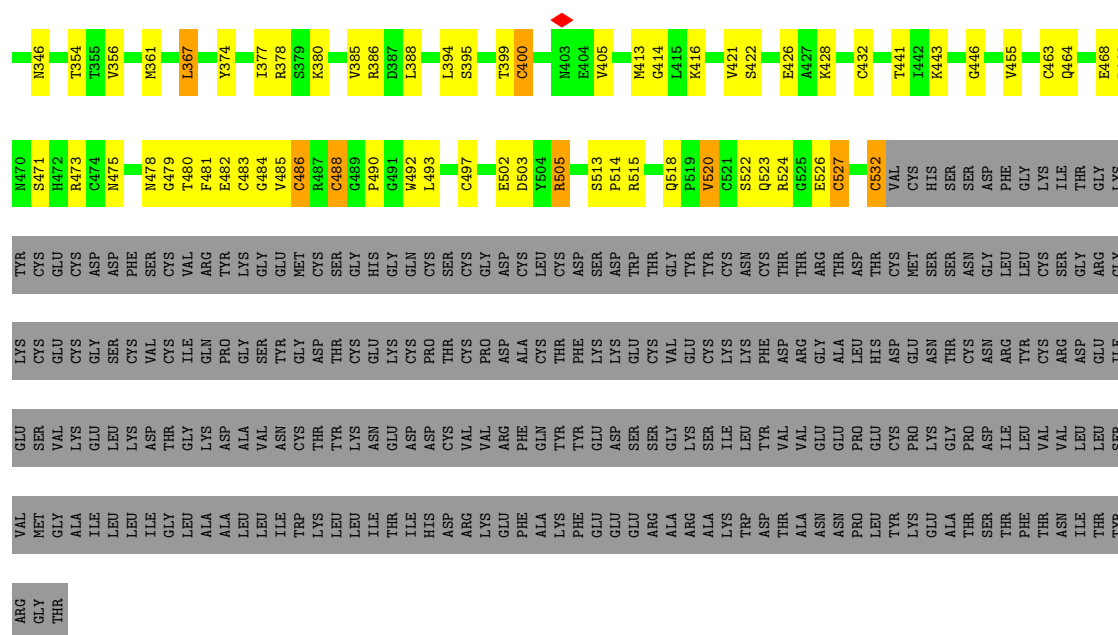
- Molecule 1: Integrin alpha-IIb



ARG	LEU	PRO	ILE	PHE	LYS	MET	L583	L491	T290	L124	MET
ARG	PRO	VAL	LEU	ALA	ASN	ASP	L584	L492	ALA	ALA	ARG
ARG	TYR	LEU	ASP	PRO	ALA	ALA	D585	L493	ALA	ARG	ALA
PRO	ALA	VAL	ILE	SER	GLN	ASN	E586	Q494	ALA	C138	LEU
LEU	PRO	CYS	PRO	VAL	GLY	GLY	F589	L497	T300	W144	CYS
GLU	PRO	ASP	GLN	VAL	ILE	GLY	F590	M498	L301	W147	PRO
GLU	LEU	SER	GLY	ALA	ALA	GLU	D591	P499	L302	L147	LEU
ASP	SER	ALA	GLY	ALA	MET	GLY	A500	S303	GLN	E154	GLN
GLU	ASP	LEU	LEU	GLU	LEU	ALA	S594	V501	Y304	E154	ALA
GLU	GLU	CYS	GLN	GLY	VAL	TYR	E594	V501	Y305	E154	LEU
ARG	ARG	THR	CYS	GLY	SER	GLY	L598	C504	Q306	C161	TRP
GLY	GLY	VAL	PHE	GLU	VAL	ALA	S599	V505	R307	C161	LEU
GLU	GLU	VAL	GLU	ARG	VAL	GLU	L600	L506	Y319	T185	LEU
ALA	ALA	GLN	GLN	GLU	ASN	LEU	N601	P507	Y319	Y186	GLU
GLN	CYS	PRO	PRO	GLN	LEU	ALA	N601	P507	Y319	Y186	TRP
CYS	PRO	ASP	PRO	ASN	GLU	VAL	P605	Q508	D328	M189	VAL
VAL	VAL	LEU	VAL	SER	GLU	HIS	P606	S514	V329	D190	LEU
TRP	TRP	GLN	ASN	LEU	ALA	LEU	T607	C515	N330	F191	LEU
GLN	THR	GLN	PRO	ASP	GLY	PRO	E608	C515	N330	F191	LEU
LEU	LEU	MET	LEU	SER	GLU	GLY	E608	M520	A354	W193	LEU
LEU	LEU	ALA	LYS	TRP	SER	GLN	E608	M520	A354	W193	GLY
ARG	ARG	ARG	VAL	GLY	VAL	ALA	M611	N528	L361	Y197	PRO
ALA	ALA	GLY	ASP	PRO	SER	HIS	M611	N528	L361	Y197	CYS
LEU	LEU	GLN	TRP	LYS	PHE	TYR	L617	1529	F362	G201	ALA
GLU	GLU	GLN	GLY	VAL	LEU	MET	R628	S534	L371	T207	PRO
GLU	GLU	ALA	GLU	GLU	LEU	ARG	R628	L535	L376	T207	PRO
ARG	ARG	MET	PRO	HIS	GLN	ALA	C633	L535	ALA	A216	ALA
ALA	ALA	ILE	ILE	THR	ILE	LEU	C633	E538	L383	A216	TRP
TRP	TRP	THR	PRO	TYR	ARG	SER	GLY	L539	L383	P217	ALA
PRO	PRO	VAL	SER	GLU	SER	ASN	GLU	Q540	L383	P217	ALA
PRO	ILE	VAL	PRO	LEU	SER	ASN	ASP	L541	A392	G218	ALA
TRP	TRP	ALA	SER	HIS	ASN	GLY	VAL	ASP	A392	G218	ALA
VAL	VAL	PHE	PRO	ASN	SER	GLY	VAL	L223	L394	F222	ALA
LEU	LEU	LEU	ILE	ASN	SER	PHE	CYS	K545	L394	F222	N33
LEU	LEU	LEU	ILE	GLY	GLN	GLU	VAL	P946	L394	G224	T40
VAL	VAL	THR	HIS	GLY	ASN	GLU	VAL	R946	N403	G224	T40
GLY	GLY	PRO	PRO	PRO	ASN	ARG	GLN	R547	N403	Q228	L54
GLY	VAL	GLY	ALA	GLY	ASN	ARG	GLN	Q548	D404	Q228	L54
VAL	VAL	THR	HIS	THR	ASN	ILE	LEU	G549	L408	D233	D55
LEU	LEU	LEU	HIS	VAL	SER	ILE	GLN	R550	A408	D233	D55
GLY	GLY	TYR	LYS	ASN	LYS	CYS	LEU	R551	A408	D233	D55
GLY	GLY	GLN	LYS	ASN	ILE	ASN	THR	S551	G425	S249	S60
LEU	LEU	ARG	ASP	LEU	VAL	ASN	THR	V552	G425	S249	S60
LEU	LEU	PRO	ARG	LEU	LEU	ASN	THR	L553	L430	Q250	R72
LEU	LEU	PRO	ARG	HIS	LYS	VAL	THR	L554	L430	S251	R72
THR	THR	GLN	ILE	HIS	VAL	ASN	THR	L555	L452	N258	G82
ILE	PHE	PHE	PHE	HIS	VAL	THR	GLY	Q558	L452	N258	G82
VAL	VAL	VAL	VAL	ILE	PRO	ASN	SER	Q559	R453	P259	E92
VAL	VAL	VAL	GLY	VAL	PRO	GLY	THR	A560	D457	E260	E92
LEU	LEU	GLN	GLY	GLU	ARG	VAL	LEU	L566	L458	E260	E92
ALA	ALA	SER	PRO	GLY	VAL	VAL	VAL	D460	D459	E261	Q95
MET	MET	GLY	GLY	ALA	ALA	LEU	GLY	N461	L461	E261	Q95
TRP	TRP	HIS	GLN	SER	GLN	CYS	ALA	D567	G462	E262	Q95
ALA	ALA	VAL	VAL	GLN	VAL	GLY	ASP	H572	V266	D263	R104
LYS	LYS	PRO	GLU	VAL	GLY	ASN	ASP	H572	L466	D263	R104
THR	THR	PRO	GLU	GLY	LEU	ASN	ASN	H572	L466	V272	N109
PHE	PHE	SER	SER	GLY	LEU	GLY	VAL	1575	L466	L279	T114
GLY	GLY	ASN	ARG	ASP	VAL	ASN	VAL	C576	V478	L279	L115
VAL	VAL	VAL	GLY	LEU	ARG	PRO	LEU	H577	V478	E284	Q116
PHE	PHE	VAL	LEU	LEU	GLY	PRO	GLU	H577	V478	E284	T117
PHE	PHE	SER	GLN	THR	ASN	MET	LEU	H577	V485	E285	F118
LYS	LYS	SER	ASN	VAL	ASN	LYS	LEU	H577	V485	E285	F118

- Molecule 2: Integrin beta-3





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

Chain E: 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 K: 67%



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

Chain G: 50%



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

Chain M: 50%



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

Chain H:  33% 67%

 MAG1
MAG2
MAG3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	274866	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 ($e^-/\text{\AA}^2$)	36.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.800	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: MG, NAG, BMA, CA

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	0/4637	0.39	0/6321
1	C	0.21	0/4713	0.36	0/6420
2	B	0.21	0/3825	0.41	1/5180 (0.0%)
2	D	0.25	0/3962	0.44	0/5369
All	All	0.22	0/17137	0.40	1/23290 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	512	CYS	N-CA-C	-5.35	105.85	112.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	515	ARG	Sidechain
2	D	473	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	4525	0	4367	174	0
1	C	4599	0	4462	96	0
2	B	3762	0	3611	163	0
2	D	3891	0	3768	103	0
3	E	39	0	34	0	0
3	K	39	0	34	1	0
4	G	28	0	25	1	0
4	M	28	0	25	1	0
5	H	39	0	34	1	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
7	A	42	0	39	2	0
7	B	14	0	13	1	0
7	C	42	0	39	0	0
7	D	14	0	13	1	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
All	All	17076	0	16464	514	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 15.

The worst 5 of 514 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:D:469:PRO:HA	2:D:480:THR:HA	1.42	1.02
2:B:522:SER:HB3	2:B:527:CYS:HA	1.57	0.85
1:A:220:TYR:CE1	1:A:255:ASP:HB2	2.17	0.78
2:D:167:GLN:HG3	2:D:367:LEU:HD11	1.65	0.78
1:A:73:THR:HG22	1:A:74:LEU:N	1.97	0.78

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	A	589/1039 (57%)	549 (93%)	39 (7%)	1 (0%)	43	76
1	C	600/1039 (58%)	569 (95%)	30 (5%)	1 (0%)	43	76
2	B	477/788 (60%)	430 (90%)	44 (9%)	3 (1%)	21	56
2	D	504/788 (64%)	459 (91%)	43 (8%)	2 (0%)	30	65
All	All	2170/3654 (59%)	2007 (92%)	156 (7%)	7 (0%)	37	70

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	63	ARG
2	D	484	GLY
2	D	520	VAL
1	A	154	GLU
1	C	154	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	482/864 (56%)	456 (95%)	26 (5%)	20	53
1	C	491/864 (57%)	468 (95%)	23 (5%)	23	58
2	B	431/690 (62%)	412 (96%)	19 (4%)	25	60
2	D	448/690 (65%)	431 (96%)	17 (4%)	29	63
All	All	1852/3108 (60%)	1767 (95%)	85 (5%)	25	58

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	508	GLN
2	D	133	VAL
1	C	547	ARG
1	C	591	ASP
2	D	213	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	527	HIS
2	D	368	GLN
2	D	236	GLN
2	D	402	ASN
2	B	108	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	E	1	2,3	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.39	0
3	BMA	E	3	3	11,11,12	0.61	0	15,15,17	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	1	4	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.45	0
5	BMA	H	1	5	11,11,12	0.61	0	15,15,17	0.72	0
5	NAG	H	2	5	14,14,15	0.32	0	17,19,21	0.73	1 (5%)
5	NAG	H	3	5	14,14,15	0.76	1 (7%)	17,19,21	0.39	0
3	NAG	K	1	2,3	14,14,15	0.28	0	17,19,21	0.44	0
3	NAG	K	2	3	14,14,15	0.24	0	17,19,21	0.41	0
3	BMA	K	3	3	11,11,12	0.58	0	15,15,17	0.69	0
4	NAG	M	1	4	14,14,15	0.23	0	17,19,21	0.56	0
4	NAG	M	2	4	14,14,15	0.21	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	BMA	H	1	5	-	1/2/19/22	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	NAG	H	3	5	-	1/6/23/26	0/1/1/1
3	NAG	K	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
4	NAG	M	1	4	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	NAG	O5-C1	2.19	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	NAG	O4-C4-C3	2.32	115.84	110.38

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

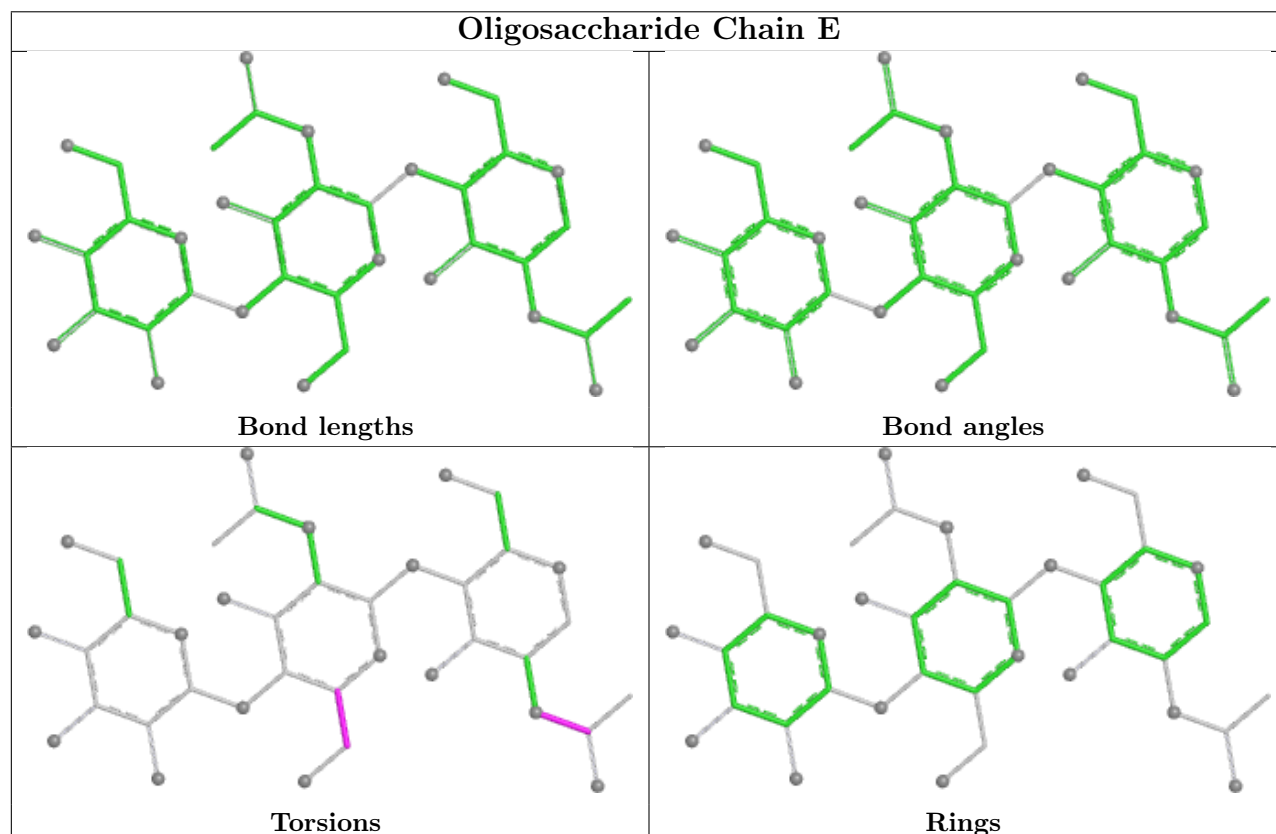
Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2

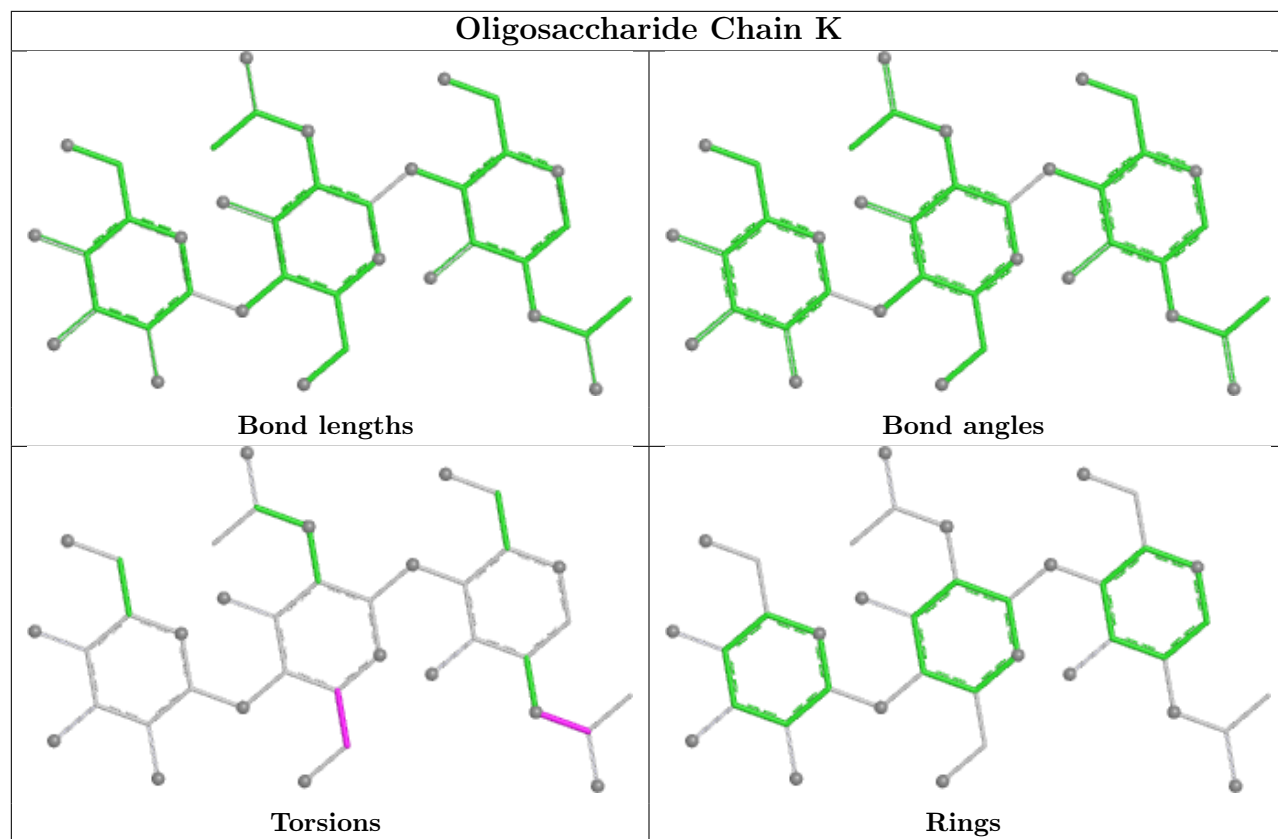
There are no ring outliers.

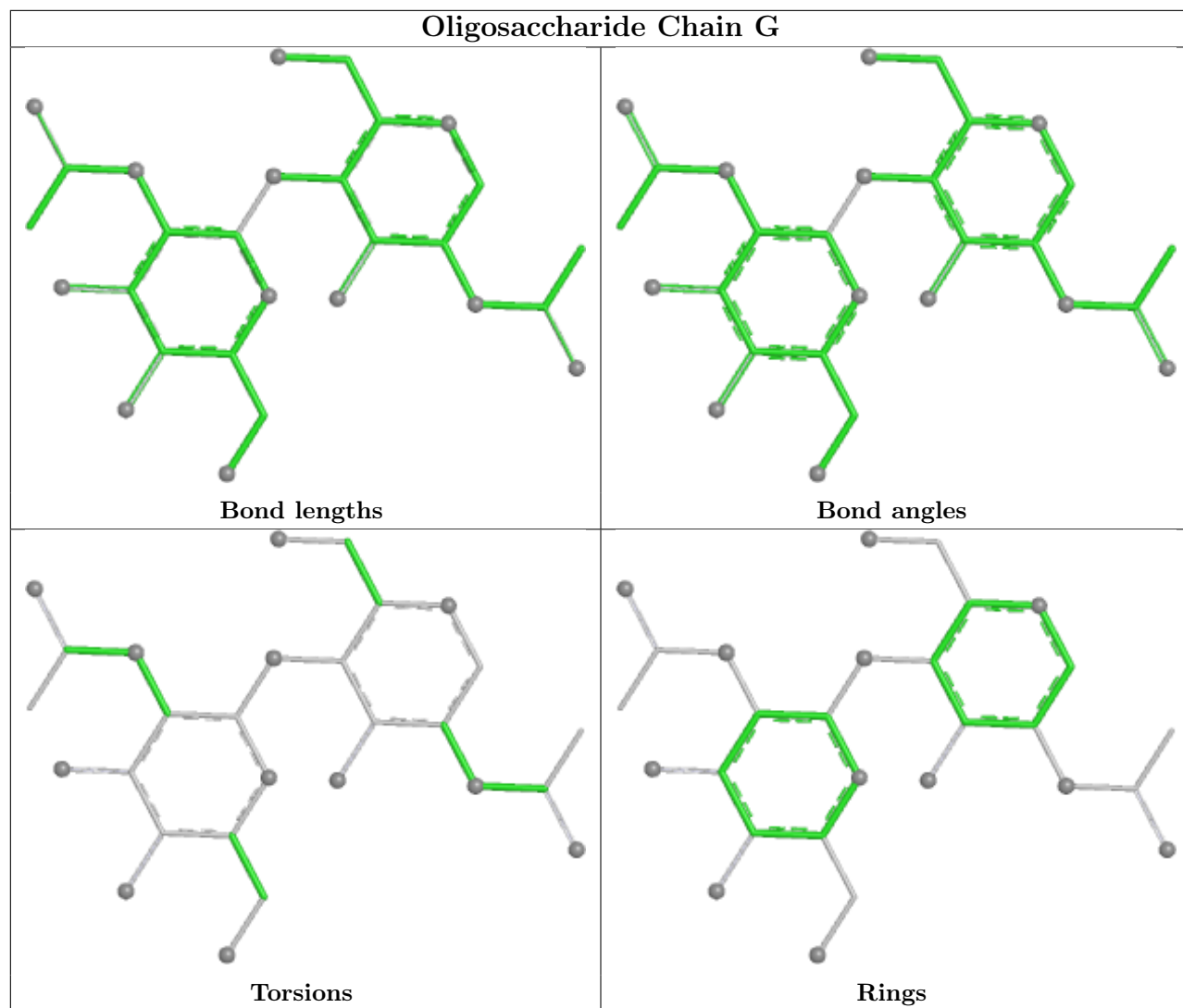
5 monomers are involved in 4 short contacts:

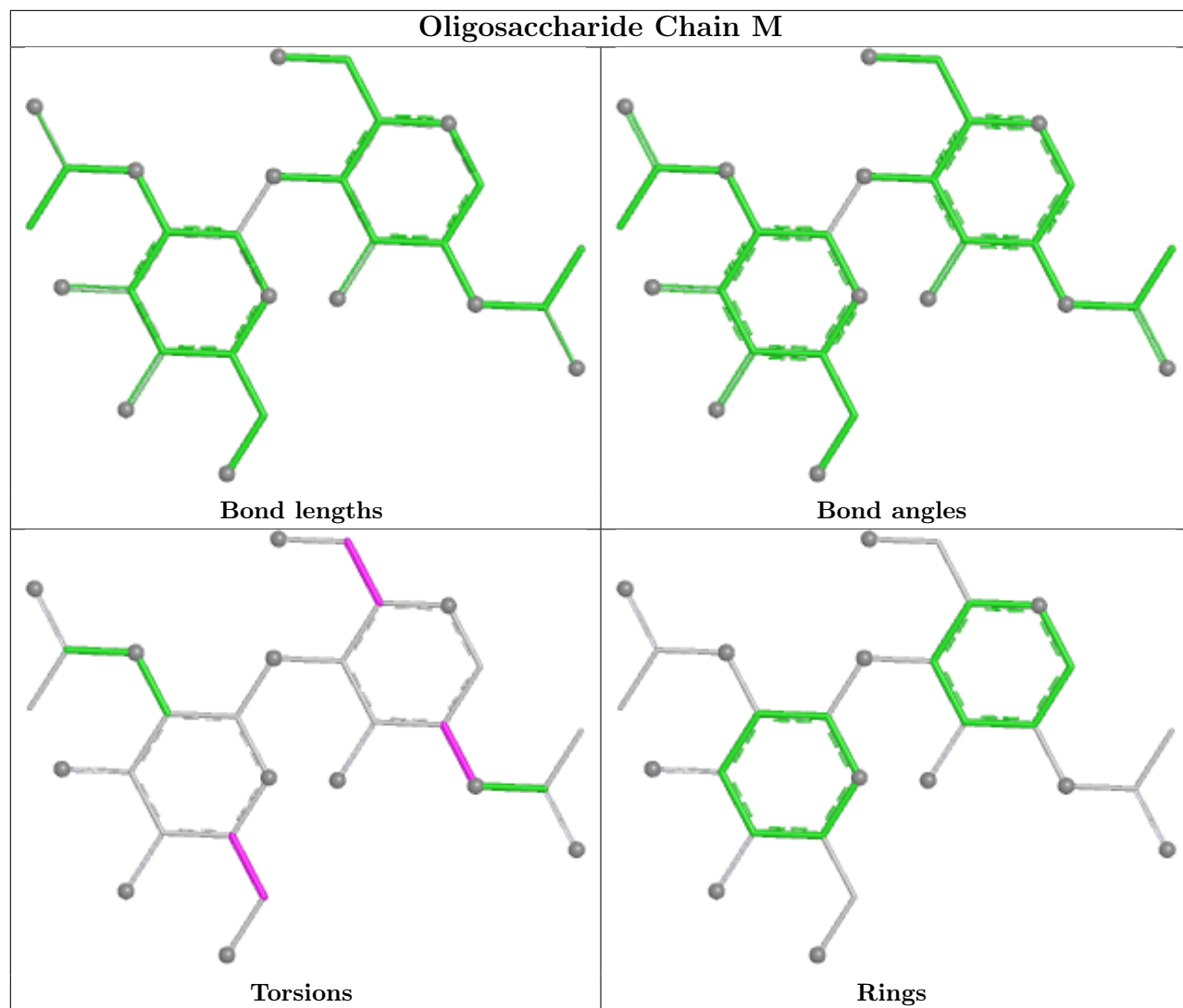
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	3	NAG	1	0
4	G	1	NAG	1	0
4	M	2	NAG	1	0
5	H	2	NAG	1	0
3	K	1	NAG	1	0

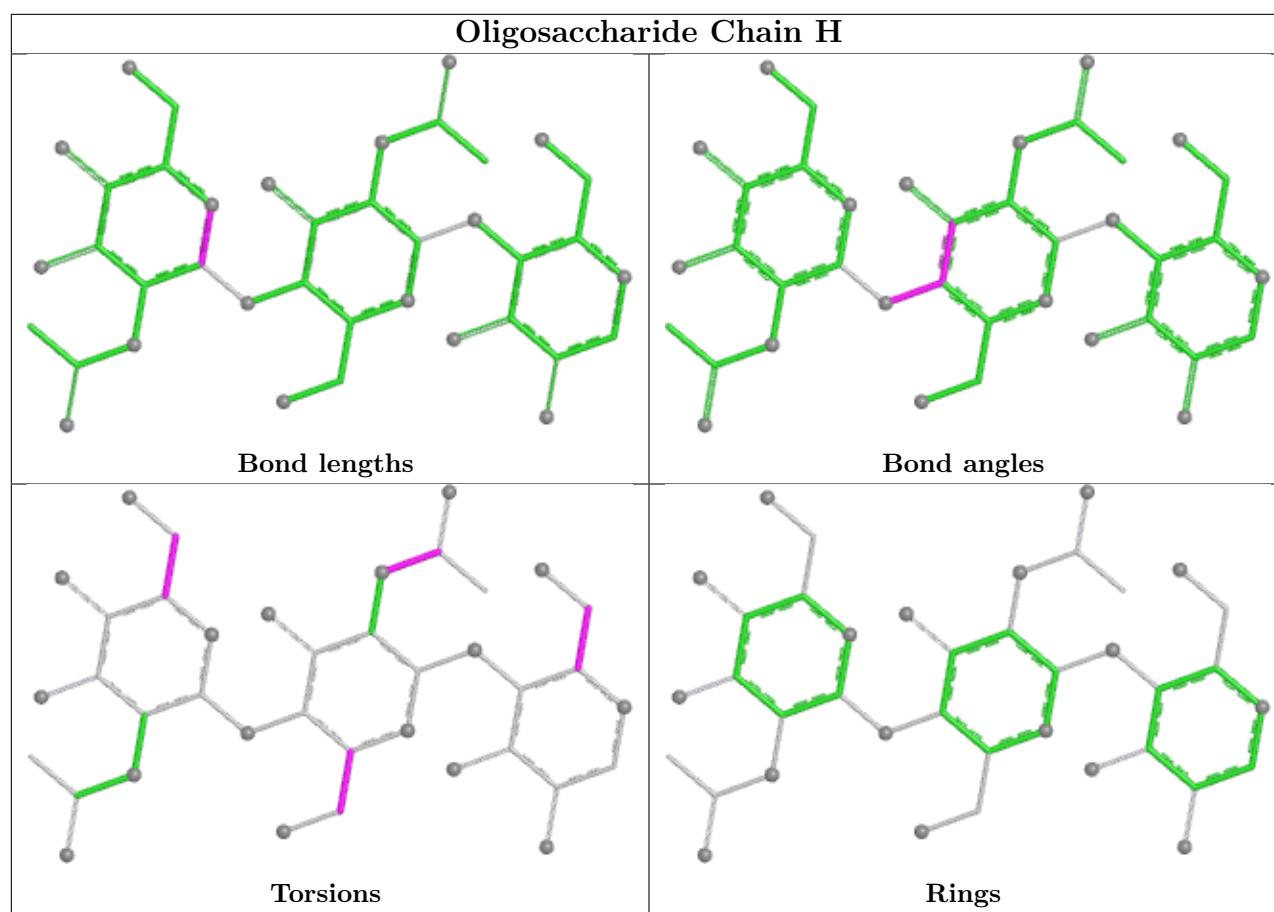
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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	$\# Z > 2$
7	NAG	A	1107	-	14,14,15	0.18	0	17,19,21	0.46	0
7	NAG	A	1106	-	14,14,15	0.20	0	17,19,21	0.42	0
7	NAG	A	1105	1	14,14,15	0.84	1 (7%)	17,19,21	0.97	1 (5%)
7	NAG	D	804	-	14,14,15	0.36	0	17,19,21	0.78	1 (5%)
7	NAG	C	1105	1	14,14,15	0.24	0	17,19,21	0.48	0
7	NAG	C	1107	-	14,14,15	0.20	0	17,19,21	0.44	0
7	NAG	B	804	-	14,14,15	0.22	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	1106	-	14,14,15	0.57	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1107	-	-	0/6/23/26	0/1/1/1
7	NAG	A	1106	-	-	0/6/23/26	0/1/1/1
7	NAG	A	1105	1	-	2/6/23/26	0/1/1/1
7	NAG	D	804	-	-	2/6/23/26	0/1/1/1
7	NAG	C	1105	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1107	-	-	2/6/23/26	0/1/1/1
7	NAG	B	804	-	-	2/6/23/26	0/1/1/1
7	NAG	C	1106	-	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1105	NAG	O5-C1	2.58	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1105	NAG	C1-O5-C5	3.71	117.16	112.19
7	D	804	NAG	C1-O5-C5	2.50	115.54	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	804	NAG	O5-C5-C6-O6
7	C	1107	NAG	O5-C5-C6-O6
7	C	1107	NAG	C4-C5-C6-O6
7	B	804	NAG	C4-C5-C6-O6
7	C	1105	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1106	NAG	1	0
7	A	1105	NAG	1	0
7	D	804	NAG	1	0
7	B	804	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

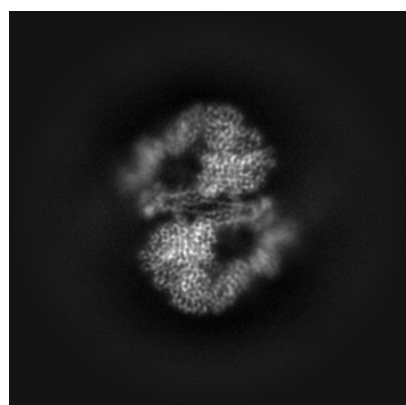
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47716. These allow visual inspection of the internal detail of the map and identification of artifacts.

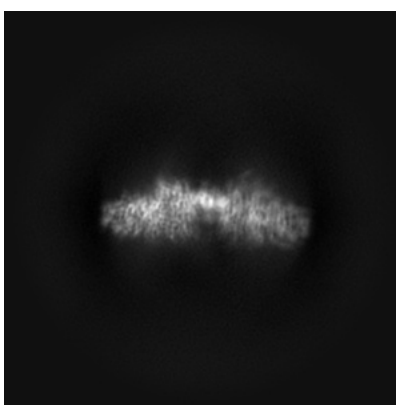
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

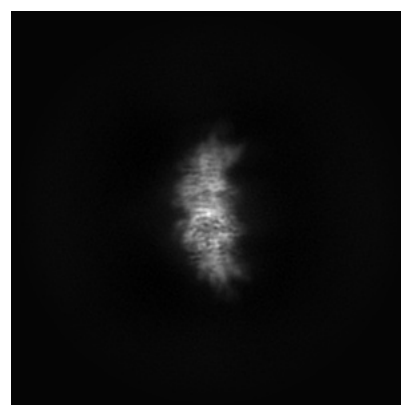
6.1.1 Primary map



X



Y

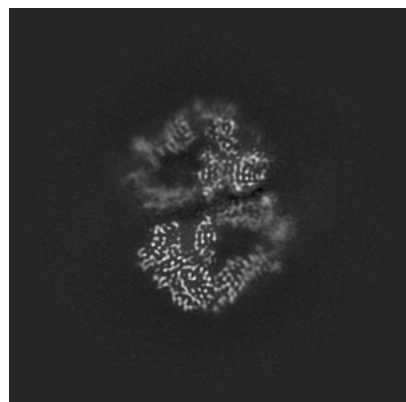


Z

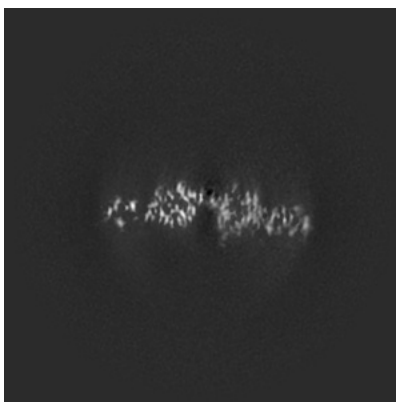
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

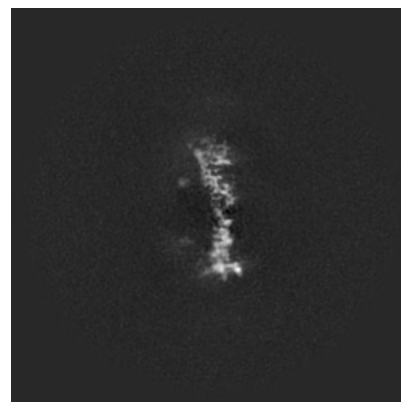
6.2.1 Primary map



X Index: 150



Y Index: 150

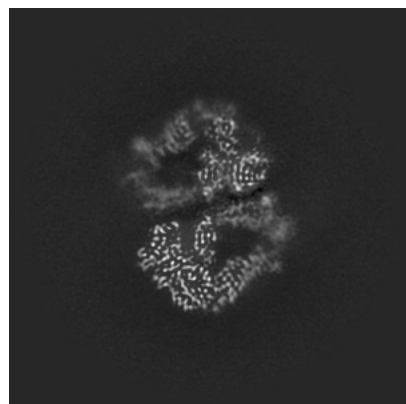


Z Index: 150

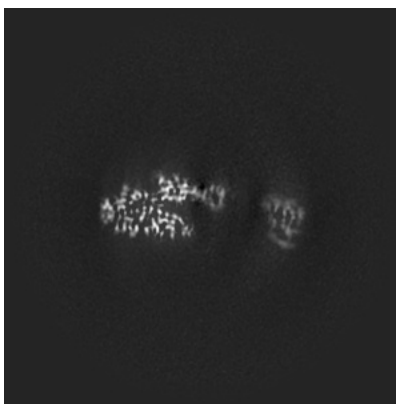
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

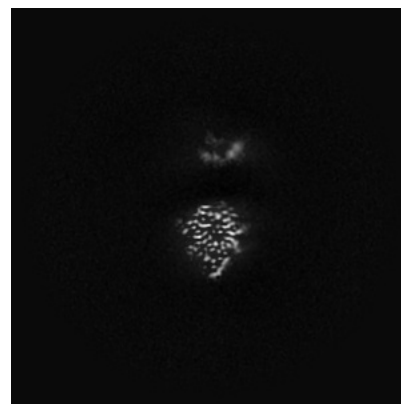
6.3.1 Primary map



X Index: 150



Y Index: 132

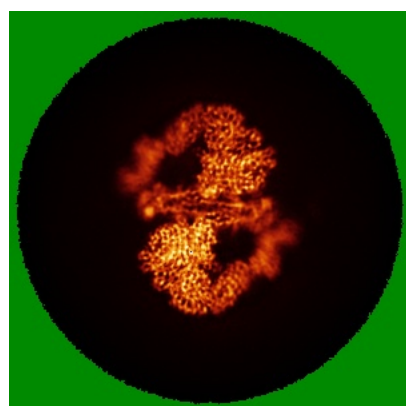


Z Index: 118

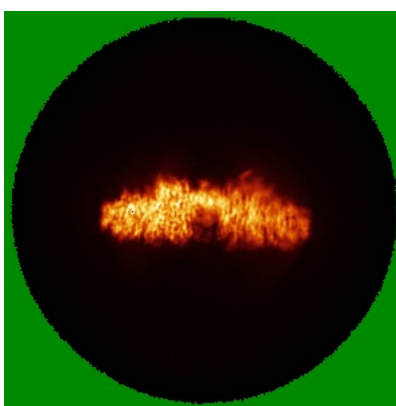
The images above show the largest variance slices of the map in three orthogonal directions.

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

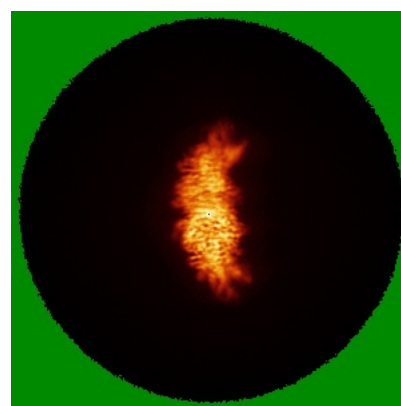
6.4.1 Primary map



X



Y



Z

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

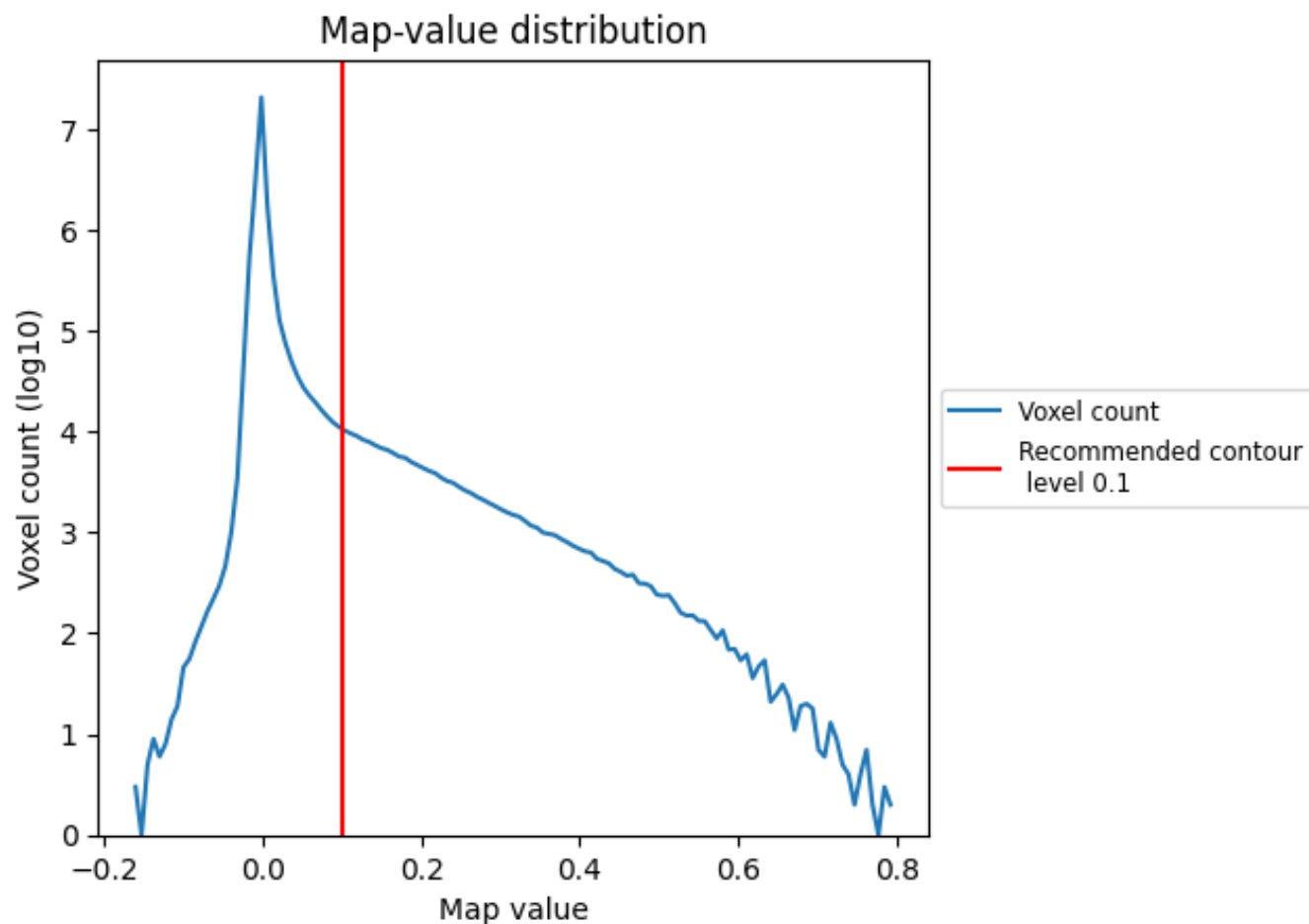
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

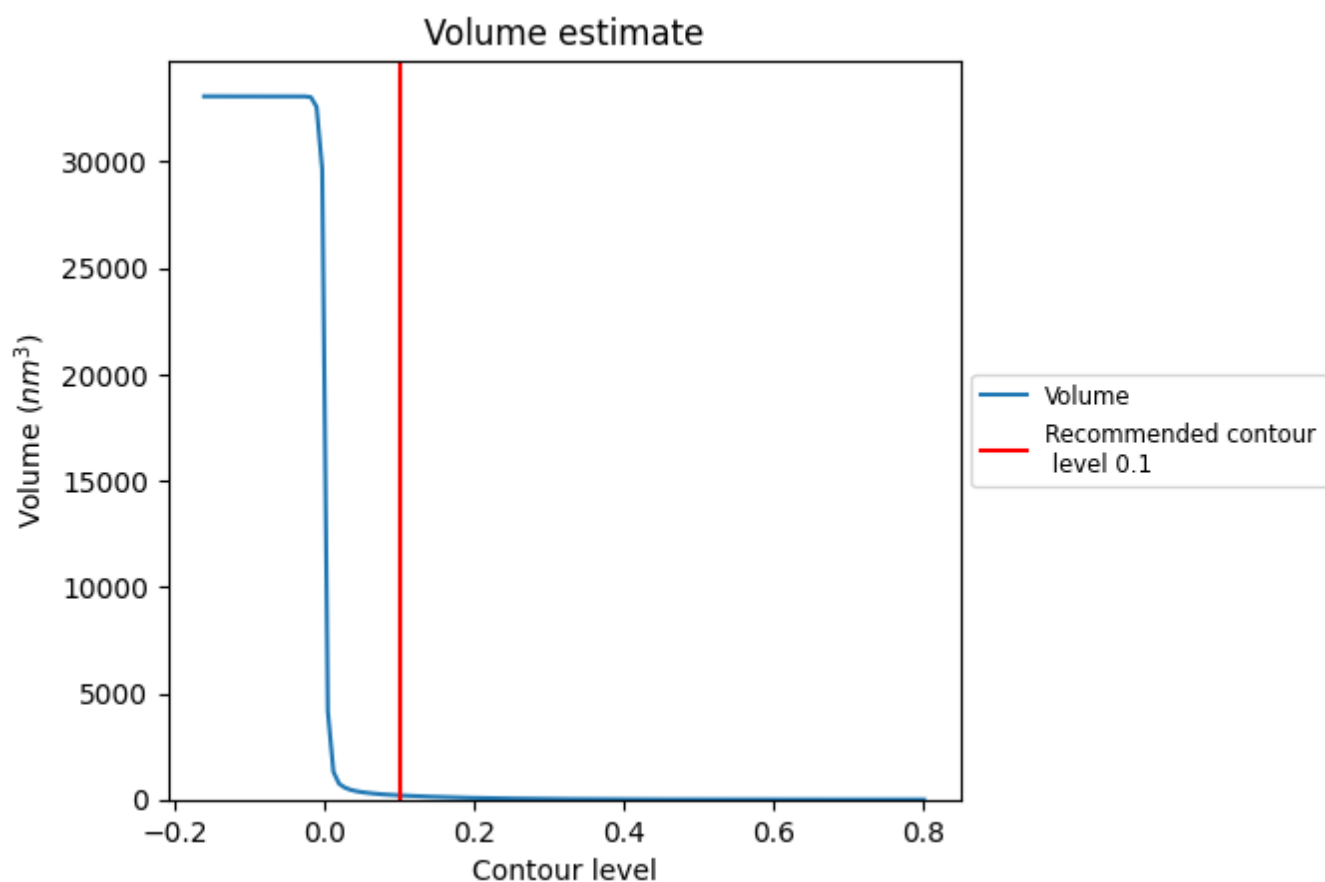
This section contains the results of statistical analysis of the map.

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.

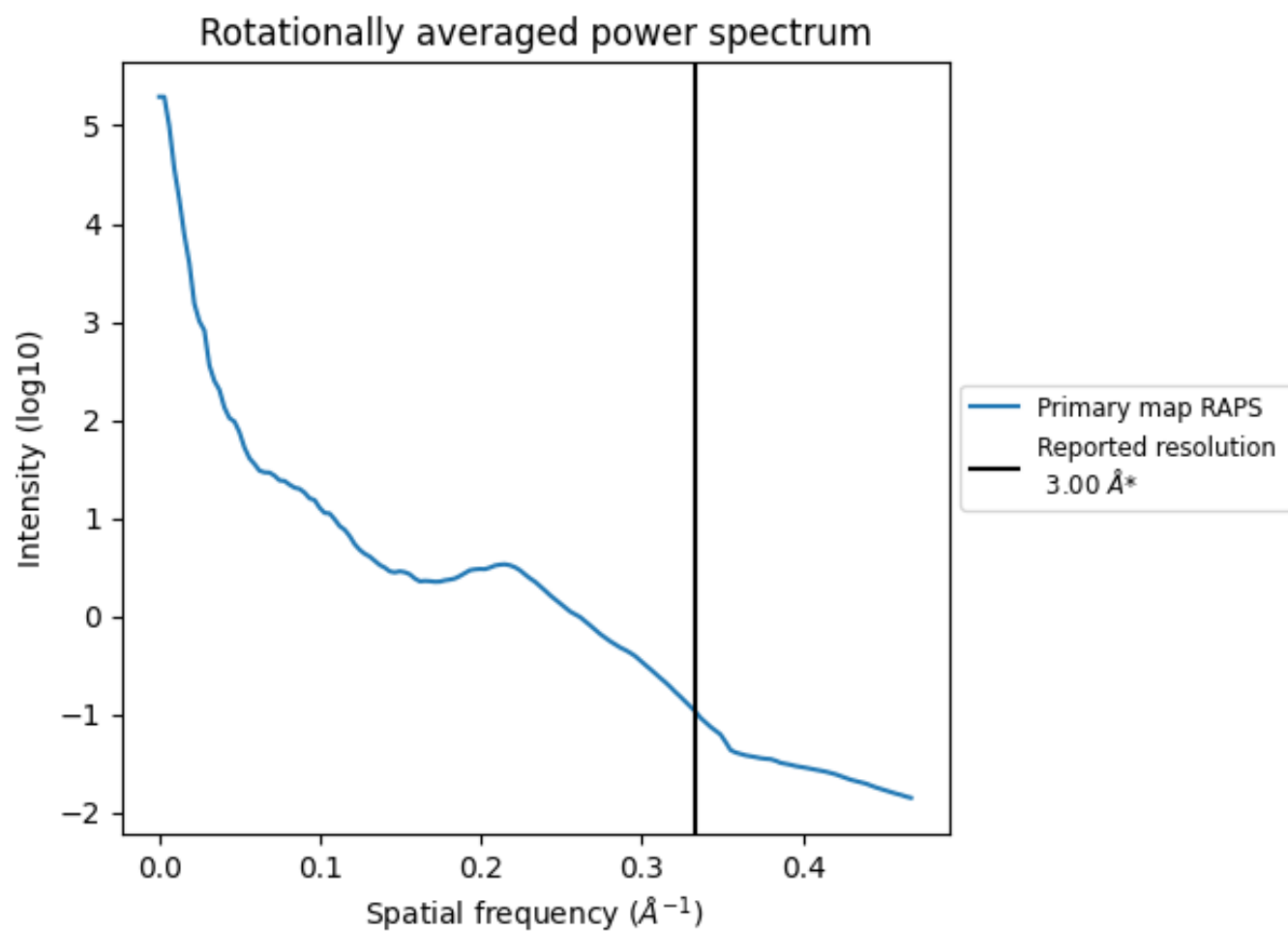
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm^3 ; this corresponds to an approximate mass of 178 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 0.333 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

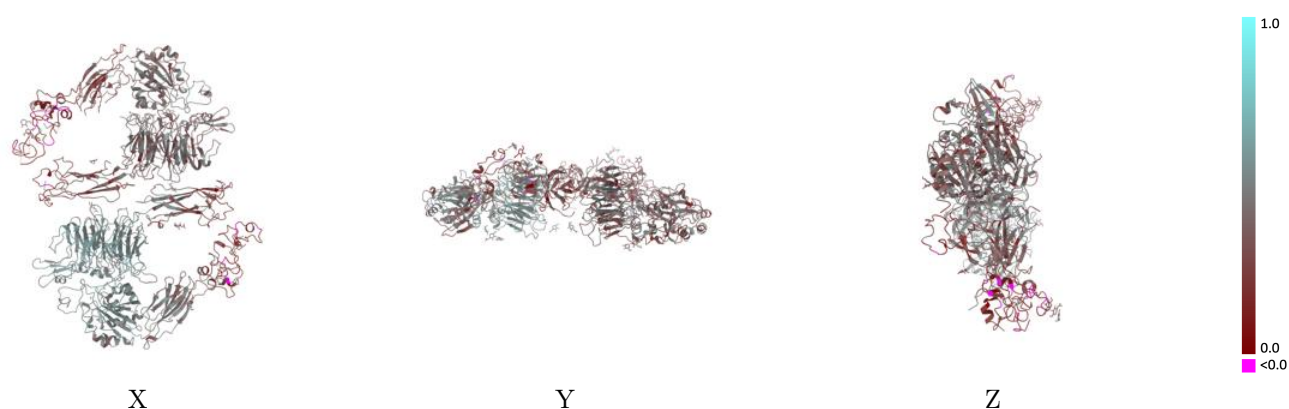
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47716 and PDB model 9E8C. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

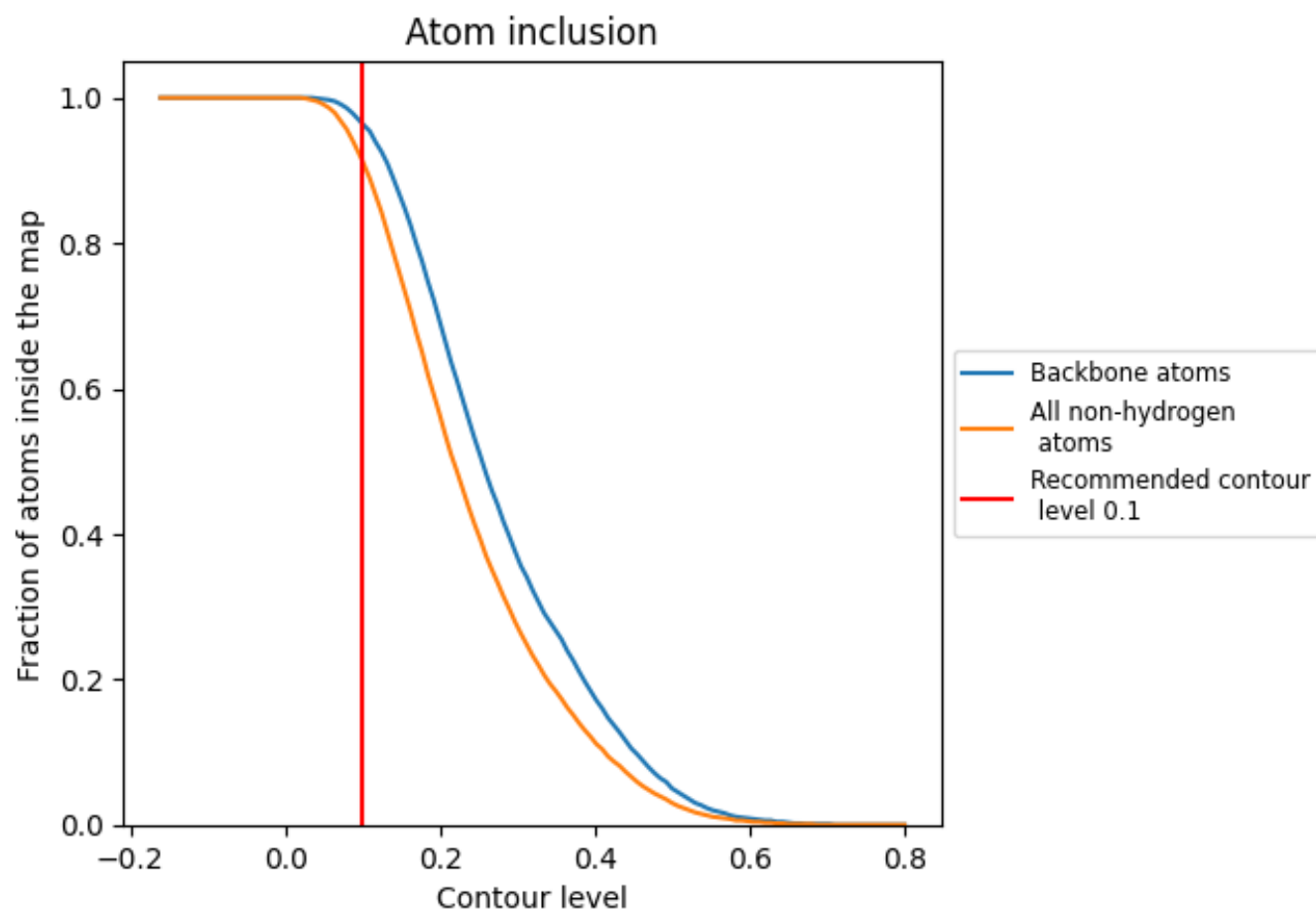


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.





















9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.4080
A	 0.8990	 0.3840
B	 0.8320	 0.3200
C	 0.9640	 0.4870
D	 0.9460	 0.4320
E	 0.8460	 0.3540
G	 0.9290	 0.2940
H	 0.9740	 0.3550
K	 0.9230	 0.4620
M	 0.8930	 0.2320

