wwPDB EM Validation Summary Report

Nov 10, 2024 – 11:03 PM EST

PDB ID	:	8T5C
EMDB ID	:	EMD-41048
Title	:	Lassa GPC Trimer in complex with Fab 8.11G and nanobody D5
Authors	:	Gorman, J.; Kwong, P.D.
Deposited on	:	2023-06-13
Resolution	:	4.70 Å(reported)
Based on initial model	:	5VK2

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:

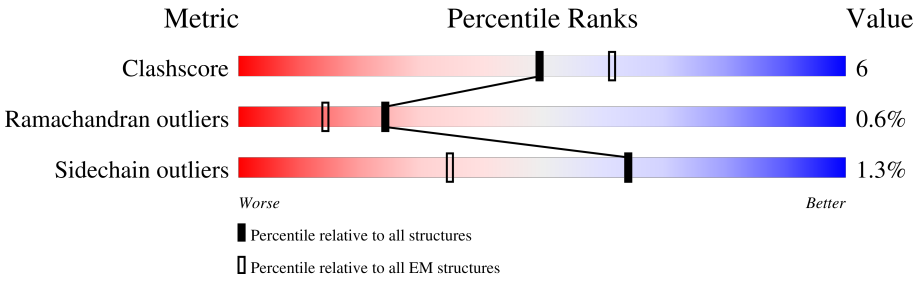
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.70 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	202	77% 20%
1	B	202	89% 10%
1	C	202	90% 10%
2	a	194	80% 18%
2	b	194	79% 18%
2	c	194	80% 18%
3	D	120	87% 8%
4	E	120	88% 10%

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Mol	Chain	Length	Quality of chain
4	H	120	88% 11%
5	I	109	90% 9%
5	L	109	76% 24%
6	F	8	12% 62% 25%
7	G	3	100%
7	Q	3	100%
7	U	3	67% 33%
7	X	3	100%
8	J	2	100%
8	K	2	50% 50%
8	V	2	100%
9	M	6	50% 50%
9	R	6	50% 50%
9	W	6	100%
10	N	5	40% 60%
10	S	5	20% 60% 20%
11	O	5	60% 40%
12	P	3	67% 33%
13	T	6	17% 83%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 14189 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 Glycoprotein G1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	202	Total	C	N	O	S	0	0
			1581	992	269	304	16		
1	A	198	Total	C	N	O	S	0	0
			1548	971	262	299	16		
1	C	202	Total	C	N	O	S	0	0
			1599	1001	278	304	16		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206A	GLY	ARG	conflict	UNP P08669
B	207	CYS	-	insertion	UNP P08669
B	258	ARG	-	expression tag	UNP P08669
B	259	ARG	-	expression tag	UNP P08669
A	206A	GLY	ARG	conflict	UNP P08669
A	207	CYS	-	insertion	UNP P08669
A	258	ARG	-	expression tag	UNP P08669
A	259	ARG	-	expression tag	UNP P08669
C	206A	GLY	ARG	conflict	UNP P08669
C	207	CYS	-	insertion	UNP P08669
C	258	ARG	-	expression tag	UNP P08669
C	259	ARG	-	expression tag	UNP P08669

- Molecule 2 is a protein called Glycoprotein G2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	159	Total	C	N	O	S	0	0
			1282	806	217	245	14		
2	a	159	Total	C	N	O	S	0	0
			1282	806	217	245	14		
2	c	159	Total	C	N	O	S	0	0
			1282	806	217	245	14		

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	326	CYS	LEU	conflict	UNP P08669
b	329	PRO	GLU	conflict	UNP P08669
b	419	GLY	-	expression tag	UNP P08669
b	420	GLY	-	expression tag	UNP P08669
b	421	GLY	-	expression tag	UNP P08669
b	422	TYR	-	expression tag	UNP P08669
b	423	ILE	-	expression tag	UNP P08669
b	424	PRO	-	expression tag	UNP P08669
b	425	GLU	-	expression tag	UNP P08669
b	426	ALA	-	expression tag	UNP P08669
b	427	PRO	-	expression tag	UNP P08669
b	428	ARG	-	expression tag	UNP P08669
b	429	ASP	-	expression tag	UNP P08669
b	430	GLY	-	expression tag	UNP P08669
b	431	GLN	-	expression tag	UNP P08669
b	432	ALA	-	expression tag	UNP P08669
b	433	TYR	-	expression tag	UNP P08669
b	434	VAL	-	expression tag	UNP P08669
b	435	ARG	-	expression tag	UNP P08669
b	436	LYS	-	expression tag	UNP P08669
b	437	ASP	-	expression tag	UNP P08669
b	438	GLY	-	expression tag	UNP P08669
b	439	GLU	-	expression tag	UNP P08669
b	440	TRP	-	expression tag	UNP P08669
b	441	VAL	-	expression tag	UNP P08669
b	442	LEU	-	expression tag	UNP P08669
b	443	LEU	-	expression tag	UNP P08669
b	444	SER	-	expression tag	UNP P08669
b	445	THR	-	expression tag	UNP P08669
b	446	PHE	-	expression tag	UNP P08669
b	447	LEU	-	expression tag	UNP P08669
b	448	GLY	-	expression tag	UNP P08669
b	449	GLY	-	expression tag	UNP P08669
b	450	LEU	-	expression tag	UNP P08669
b	451	VAL	-	expression tag	UNP P08669
b	452	PRO	-	expression tag	UNP P08669
b	453	ARG	-	expression tag	UNP P08669
a	326	CYS	LEU	conflict	UNP P08669
a	329	PRO	GLU	conflict	UNP P08669
a	419	GLY	-	expression tag	UNP P08669
a	420	GLY	-	expression tag	UNP P08669
a	421	GLY	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
a	422	TYR	-	expression tag	UNP P08669
a	423	ILE	-	expression tag	UNP P08669
a	424	PRO	-	expression tag	UNP P08669
a	425	GLU	-	expression tag	UNP P08669
a	426	ALA	-	expression tag	UNP P08669
a	427	PRO	-	expression tag	UNP P08669
a	428	ARG	-	expression tag	UNP P08669
a	429	ASP	-	expression tag	UNP P08669
a	430	GLY	-	expression tag	UNP P08669
a	431	GLN	-	expression tag	UNP P08669
a	432	ALA	-	expression tag	UNP P08669
a	433	TYR	-	expression tag	UNP P08669
a	434	VAL	-	expression tag	UNP P08669
a	435	ARG	-	expression tag	UNP P08669
a	436	LYS	-	expression tag	UNP P08669
a	437	ASP	-	expression tag	UNP P08669
a	438	GLY	-	expression tag	UNP P08669
a	439	GLU	-	expression tag	UNP P08669
a	440	TRP	-	expression tag	UNP P08669
a	441	VAL	-	expression tag	UNP P08669
a	442	LEU	-	expression tag	UNP P08669
a	443	LEU	-	expression tag	UNP P08669
a	444	SER	-	expression tag	UNP P08669
a	445	THR	-	expression tag	UNP P08669
a	446	PHE	-	expression tag	UNP P08669
a	447	LEU	-	expression tag	UNP P08669
a	448	GLY	-	expression tag	UNP P08669
a	449	GLY	-	expression tag	UNP P08669
a	450	LEU	-	expression tag	UNP P08669
a	451	VAL	-	expression tag	UNP P08669
a	452	PRO	-	expression tag	UNP P08669
a	453	ARG	-	expression tag	UNP P08669
c	326	CYS	LEU	conflict	UNP P08669
c	329	PRO	GLU	conflict	UNP P08669
c	419	GLY	-	expression tag	UNP P08669
c	420	GLY	-	expression tag	UNP P08669
c	421	GLY	-	expression tag	UNP P08669
c	422	TYR	-	expression tag	UNP P08669
c	423	ILE	-	expression tag	UNP P08669
c	424	PRO	-	expression tag	UNP P08669
c	425	GLU	-	expression tag	UNP P08669
c	426	ALA	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	427	PRO	-	expression tag	UNP P08669
c	428	ARG	-	expression tag	UNP P08669
c	429	ASP	-	expression tag	UNP P08669
c	430	GLY	-	expression tag	UNP P08669
c	431	GLN	-	expression tag	UNP P08669
c	432	ALA	-	expression tag	UNP P08669
c	433	TYR	-	expression tag	UNP P08669
c	434	VAL	-	expression tag	UNP P08669
c	435	ARG	-	expression tag	UNP P08669
c	436	LYS	-	expression tag	UNP P08669
c	437	ASP	-	expression tag	UNP P08669
c	438	GLY	-	expression tag	UNP P08669
c	439	GLU	-	expression tag	UNP P08669
c	440	TRP	-	expression tag	UNP P08669
c	441	VAL	-	expression tag	UNP P08669
c	442	LEU	-	expression tag	UNP P08669
c	443	LEU	-	expression tag	UNP P08669
c	444	SER	-	expression tag	UNP P08669
c	445	THR	-	expression tag	UNP P08669
c	446	PHE	-	expression tag	UNP P08669
c	447	LEU	-	expression tag	UNP P08669
c	448	GLY	-	expression tag	UNP P08669
c	449	GLY	-	expression tag	UNP P08669
c	450	LEU	-	expression tag	UNP P08669
c	451	VAL	-	expression tag	UNP P08669
c	452	PRO	-	expression tag	UNP P08669
c	453	ARG	-	expression tag	UNP P08669

- Molecule 3 is a protein called D5 nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	116	Total	C	N	O	S	0	0
			906	557	165	180	4		

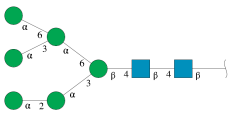
- Molecule 4 is a protein called 8.11G Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	119	Total	C	N	O	S	0	0
			928	593	148	185	2		
4	E	119	Total	C	N	O	S	0	0
			928	593	148	185	2		

- Molecule 5 is a protein called 8.11G Light Chain.

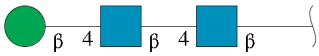
Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	109	Total	C	N	O	S	0	0
			851	532	153	163	3		
5	I	109	Total	C	N	O	S	0	0
			851	532	153	163	3		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	F	8	Total	C	N	O	0	0
			94	52	2	40		

- 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.

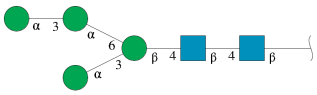


Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	3	Total	C	N	O	0	0
			39	22	2	15		
7	Q	3	Total	C	N	O	0	0
			39	22	2	15		
7	U	3	Total	C	N	O	0	0
			39	22	2	15		
7	X	3	Total	C	N	O	0	0
			39	22	2	15		

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

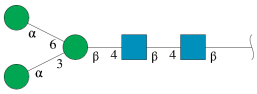
Mol	Chain	Residues	Atoms	AltConf	Trace
8	J	2	Total C N O 25 14 1 10	0	0
8	K	2	Total C N O 25 14 1 10	0	0
8	V	2	Total C N O 25 14 1 10	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



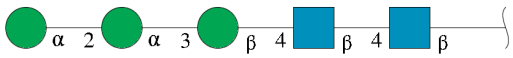
Mol	Chain	Residues	Atoms	AltConf	Trace
9	M	6	Total C N O 72 40 2 30	0	0
9	R	6	Total C N O 72 40 2 30	0	0
9	W	6	Total C N O 72 40 2 30	0	0

- Molecule 10 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.



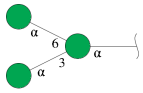
Mol	Chain	Residues	Atoms	AltConf	Trace
10	N	5	Total C N O 61 34 2 25	0	0
10	S	5	Total C N O 61 34 2 25	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



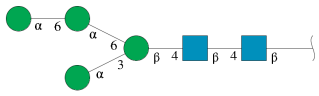
Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose.



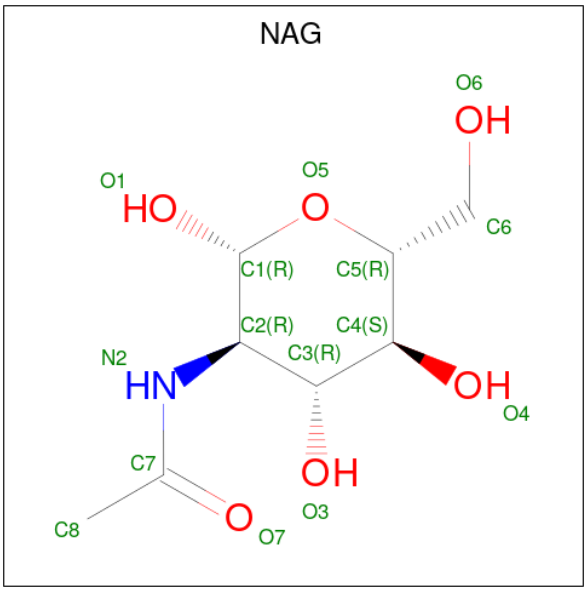
Mol	Chain	Residues	Atoms			AltConf	Trace
12	P	3	Total	C	O	0	0
			33	18	15		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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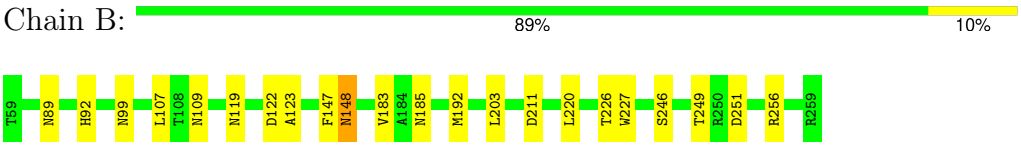
Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	N	O	0
			14	8	1	5	
14	C	1	Total	C	N	O	0
			14	8	1	5	
14	C	1	Total	C	N	O	0
			14	8	1	5	
14	C	1	Total	C	N	O	0
			14	8	1	5	
14	C	1	Total	C	N	O	0
			14	8	1	5	
14	c	1	Total	C	N	O	0
			14	8	1	5	
14	c	1	Total	C	N	O	0
			14	8	1	5	
14	L	1	Total	C	N	O	0
			14	8	1	5	
14	I	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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.

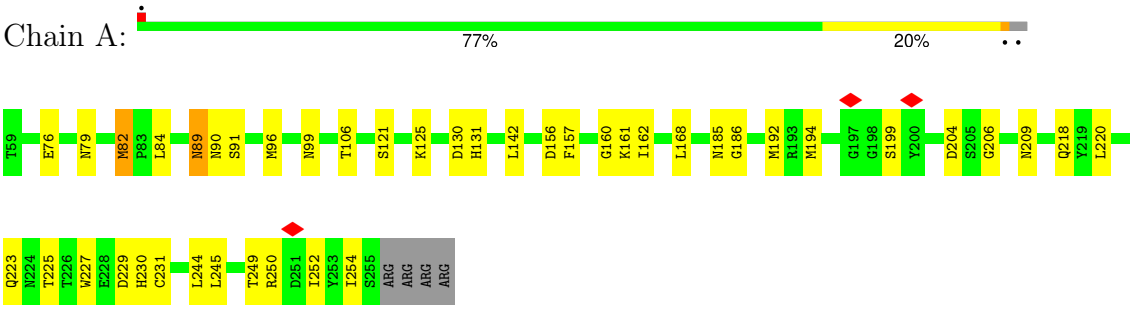
• Molecule 1: Glycoprotein G1

Chain B:



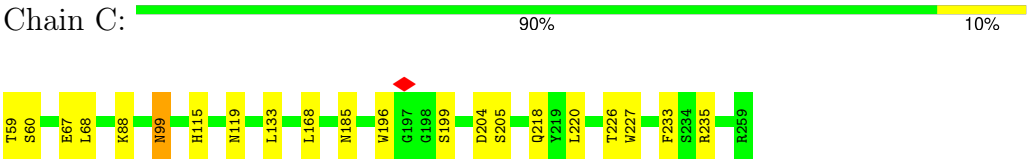
• Molecule 1: Glycoprotein G1

Chain A:



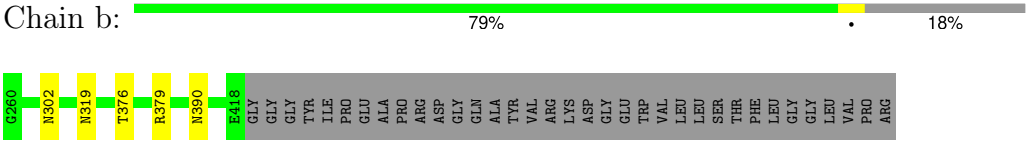
• Molecule 1: Glycoprotein G1

Chain C:



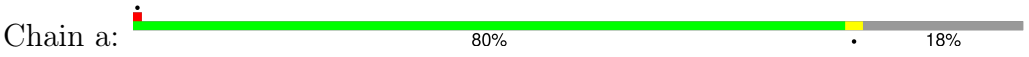
• Molecule 2: Glycoprotein G2

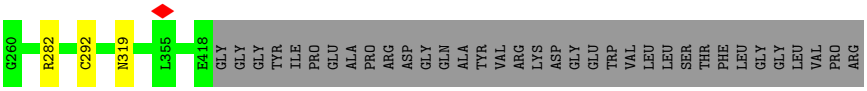
Chain b:



• Molecule 2: Glycoprotein G2

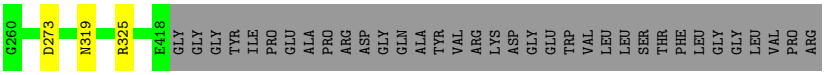
Chain a:





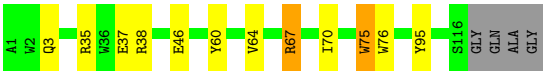
• Molecule 2: Glycoprotein G2

Chain c:



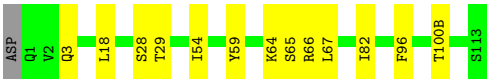
• Molecule 3: D5 nanobody

Chain D:



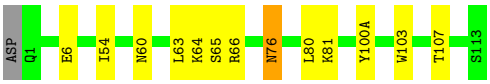
• Molecule 4: 8.11G Heavy Chain

Chain H:



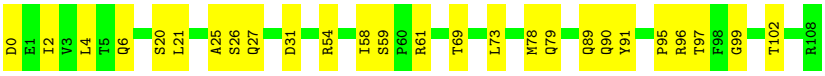
• Molecule 4: 8.11G Heavy Chain

Chain E:



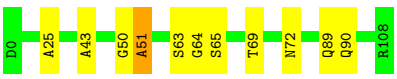
• Molecule 5: 8.11G Light Chain

Chain L:



• Molecule 5: 8.11G Light Chain

Chain I:



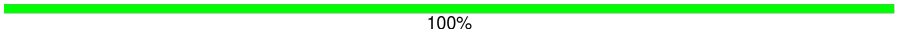
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1

-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain F:

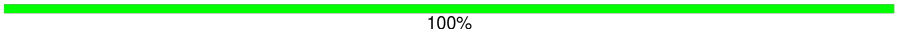
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain Q:

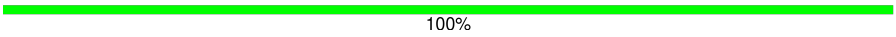


• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain U:

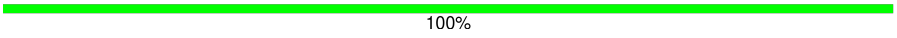
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain X:



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

Chain J:



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

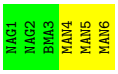
Chain K:

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

Chain V:

• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

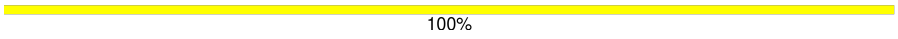


• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

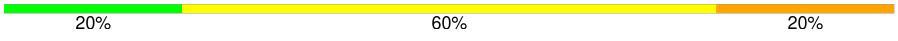


• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• Molecule 10: 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 S:

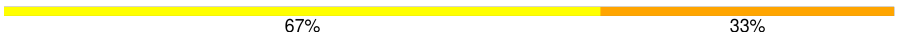


• Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

• Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose

Chain P:



• Molecule 13: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109878	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 ($e^-/Å^2$)	51.15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.547	Depositor
Minimum map value	-1.400	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	322.8, 322.8, 322.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	A	0.25	0/1583	0.53	0/2147
1	B	0.24	0/1617	0.49	0/2193
1	C	0.25	0/1635	0.52	0/2214
2	a	0.24	0/1309	0.52	1/1768 (0.1%)
2	b	0.28	0/1309	0.51	0/1768
2	c	0.25	0/1309	0.47	0/1768
3	D	0.24	0/925	0.56	0/1249
4	E	0.27	0/953	0.51	0/1301
4	H	0.25	0/953	0.49	0/1301
5	I	0.26	0/870	0.55	0/1176
5	L	0.27	0/870	0.56	0/1176
All	All	0.25	0/13333	0.52	1/18061 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	292	CYS	CA-CB-SG	8.68	129.62	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	379	ARG	Sidechain

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	1548	0	1463	28	0
1	B	1581	0	1489	12	0
1	C	1599	0	1522	14	0
2	a	1282	0	1229	0	0
2	b	1282	0	1229	0	0
2	c	1282	0	1229	0	0
3	D	906	0	868	9	0
4	E	928	0	890	10	0
4	H	928	0	890	8	0
5	I	851	0	831	6	0
5	L	851	0	831	15	0
6	F	94	0	79	4	0
7	G	39	0	34	0	0
7	Q	39	0	34	0	0
7	U	39	0	34	1	0
7	X	39	0	34	0	0
8	J	25	0	22	0	0
8	K	25	0	22	0	0
8	V	25	0	22	0	0
9	M	72	0	61	0	0
9	R	72	0	61	0	0
9	W	72	0	61	2	0
10	N	61	0	52	0	0
10	S	61	0	52	1	0
11	O	61	0	52	0	0
12	P	33	0	28	1	0
13	T	72	0	61	0	0
14	A	70	0	65	6	0
14	B	70	0	65	1	0
14	C	70	0	65	2	0
14	I	14	0	13	0	0
14	L	14	0	13	1	0
14	a	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	28	0	26	0	0
14	c	28	0	26	0	0
All	All	14189	0	13479	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 101 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:A:229:ASP:OD2	5:L:61:ARG:NH2	2.13	0.82
5:I:25:ALA:O	5:I:69:THR:OG1	2.04	0.75
5:L:89:GLN:NE2	5:L:90:GLN:O	2.23	0.72
1:C:99:ASN:OD1	14:C:301:NAG:N2	2.25	0.70
1:A:245:LEU:O	1:A:249:THR:OG1	2.08	0.69

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	196/202 (97%)	166 (85%)	29 (15%)	1 (0%)	25 64
1	B	200/202 (99%)	164 (82%)	35 (18%)	1 (0%)	25 64
1	C	200/202 (99%)	160 (80%)	40 (20%)	0	100 100
2	a	157/194 (81%)	140 (89%)	17 (11%)	0	100 100
2	b	157/194 (81%)	130 (83%)	26 (17%)	1 (1%)	22 60
2	c	157/194 (81%)	146 (93%)	9 (6%)	2 (1%)	10 42
3	D	114/120 (95%)	104 (91%)	9 (8%)	1 (1%)	14 51
4	E	117/120 (98%)	97 (83%)	20 (17%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	H	117/120 (98%)	107 (92%)	10 (8%)	0	100 100
5	I	107/109 (98%)	92 (86%)	14 (13%)	1 (1%)	14 51
5	L	107/109 (98%)	94 (88%)	11 (10%)	2 (2%)	6 32
All	All	1629/1766 (92%)	1400 (86%)	220 (14%)	9 (1%)	24 60

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	256	ARG
2	b	376	THR
1	A	227	TRP
2	c	325	ARG
5	L	58	ILE

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	173/178 (97%)	168 (97%)	5 (3%)	37 58
1	B	175/178 (98%)	171 (98%)	4 (2%)	45 65
1	C	178/178 (100%)	176 (99%)	2 (1%)	70 80
2	a	142/168 (84%)	140 (99%)	2 (1%)	62 76
2	b	142/168 (84%)	139 (98%)	3 (2%)	48 67
2	c	142/168 (84%)	141 (99%)	1 (1%)	81 87
3	D	100/101 (99%)	99 (99%)	1 (1%)	73 82
4	E	104/105 (99%)	103 (99%)	1 (1%)	73 82
4	H	104/105 (99%)	104 (100%)	0	100 100
5	I	92/92 (100%)	92 (100%)	0	100 100
5	L	92/92 (100%)	92 (100%)	0	100 100
All	All	1444/1533 (94%)	1425 (99%)	19 (1%)	64 77

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	99	ASN
3	D	67	ARG
4	E	76	ASN
2	c	319	ASN
1	A	89	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
2	c	305	HIS

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

68 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	$\#\|Z\| > 2$
6	NAG	F	1	6,1	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	F	2	6	14,14,15	0.20	0	17,19,21	0.51	0
6	BMA	F	3	6	11,11,12	0.56	0	15,15,17	0.98	0
6	MAN	F	4	6	11,11,12	0.56	0	15,15,17	0.93	1 (6%)
6	MAN	F	5	6	11,11,12	0.59	0	15,15,17	1.09	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	F	6	6	11,11,12	0.64	0	15,15,17	1.07	0
6	MAN	F	7	6	11,11,12	0.71	0	15,15,17	0.92	2 (13%)
6	MAN	F	8	6	11,11,12	0.67	0	15,15,17	0.87	1 (6%)
7	NAG	G	1	1,7	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	G	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	BMA	G	3	7	11,11,12	0.54	0	15,15,17	0.70	0
8	NAG	J	1	8	14,14,15	0.20	0	17,19,21	0.43	0
8	BMA	J	2	8	11,11,12	0.54	0	15,15,17	0.69	0
8	NAG	K	1	8	14,14,15	0.23	0	17,19,21	0.54	0
8	BMA	K	2	8	11,11,12	0.80	1 (9%)	15,15,17	0.76	0
9	NAG	M	1	2,9	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	M	2	9	14,14,15	0.19	0	17,19,21	0.42	0
9	BMA	M	3	9	11,11,12	0.57	0	15,15,17	0.85	0
9	MAN	M	4	9	11,11,12	0.71	0	15,15,17	1.11	1 (6%)
9	MAN	M	5	9	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
9	MAN	M	6	9	11,11,12	0.77	1 (9%)	15,15,17	1.04	2 (13%)
10	NAG	N	1	2,10	14,14,15	0.20	0	17,19,21	0.44	0
10	NAG	N	2	10	14,14,15	0.24	0	17,19,21	0.64	0
10	BMA	N	3	10	11,11,12	0.92	0	15,15,17	1.05	1 (6%)
10	MAN	N	4	10	11,11,12	0.61	0	15,15,17	1.04	2 (13%)
10	MAN	N	5	10	11,11,12	0.71	0	15,15,17	0.90	1 (6%)
11	NAG	O	1	11,1	14,14,15	0.31	0	17,19,21	0.42	0
11	NAG	O	2	11	14,14,15	0.18	0	17,19,21	0.41	0
11	BMA	O	3	11	11,11,12	0.52	0	15,15,17	0.77	0
11	MAN	O	4	11	11,11,12	1.18	1 (9%)	15,15,17	1.08	2 (13%)
11	MAN	O	5	11	11,11,12	0.75	1 (9%)	15,15,17	0.85	1 (6%)
12	MAN	P	1	12	11,11,12	0.68	0	15,15,17	0.99	1 (6%)
12	MAN	P	2	12	11,11,12	0.85	1 (9%)	15,15,17	0.83	1 (6%)
12	MAN	P	3	12	11,11,12	0.61	0	15,15,17	0.91	2 (13%)
7	NAG	Q	1	1,7	14,14,15	0.28	0	17,19,21	0.47	0
7	NAG	Q	2	7	14,14,15	0.23	0	17,19,21	0.41	0
7	BMA	Q	3	7	11,11,12	0.54	0	15,15,17	0.73	0
9	NAG	R	1	2,9	14,14,15	0.19	0	17,19,21	0.50	0
9	NAG	R	2	9	14,14,15	0.18	0	17,19,21	0.44	0
9	BMA	R	3	9	11,11,12	0.58	0	15,15,17	0.85	0
9	MAN	R	4	9	11,11,12	0.71	0	15,15,17	1.11	1 (6%)
9	MAN	R	5	9	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
9	MAN	R	6	9	11,11,12	0.77	1 (9%)	15,15,17	1.05	2 (13%)
10	NAG	S	1	2,10	14,14,15	0.23	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	S	2	10	14,14,15	0.18	0	17,19,21	0.45	0
10	BMA	S	3	10	11,11,12	0.67	0	15,15,17	0.98	1 (6%)
10	MAN	S	4	10	11,11,12	0.64	0	15,15,17	0.99	2 (13%)
10	MAN	S	5	10	11,11,12	0.66	0	15,15,17	0.94	2 (13%)
13	NAG	T	1	1,13	14,14,15	0.57	1 (7%)	17,19,21	0.63	0
13	NAG	T	2	13	14,14,15	0.40	0	17,19,21	0.79	1 (5%)
13	BMA	T	3	13	11,11,12	0.71	0	15,15,17	0.88	0
13	MAN	T	4	13	11,11,12	1.02	1 (9%)	15,15,17	1.57	1 (6%)
13	MAN	T	5	13	11,11,12	0.65	0	15,15,17	0.94	2 (13%)
13	MAN	T	6	13	11,11,12	0.78	0	15,15,17	1.05	2 (13%)
7	NAG	U	1	1,7	14,14,15	0.39	0	17,19,21	0.47	0
7	NAG	U	2	7	14,14,15	0.22	0	17,19,21	0.44	0
7	BMA	U	3	7	11,11,12	0.55	0	15,15,17	0.70	0
8	NAG	V	1	8	14,14,15	0.26	0	17,19,21	0.66	0
8	BMA	V	2	8	11,11,12	0.61	0	15,15,17	0.70	0
9	NAG	W	1	2,9	14,14,15	0.21	0	17,19,21	0.38	0
9	NAG	W	2	9	14,14,15	0.23	0	17,19,21	0.45	0
9	BMA	W	3	9	11,11,12	0.75	0	15,15,17	0.84	1 (6%)
9	MAN	W	4	9	11,11,12	0.71	0	15,15,17	1.11	1 (6%)
9	MAN	W	5	9	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
9	MAN	W	6	9	11,11,12	0.59	0	15,15,17	0.95	2 (13%)
7	NAG	X	1	2,7	14,14,15	0.28	0	17,19,21	0.45	0
7	NAG	X	2	7	14,14,15	0.26	0	17,19,21	0.45	0
7	BMA	X	3	7	11,11,12	0.57	0	15,15,17	0.63	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
6	NAG	F	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	0/2/19/22	0/1/1/1
6	MAN	F	5	6	-	2/2/19/22	0/1/1/1
6	MAN	F	6	6	-	2/2/19/22	0/1/1/1
6	MAN	F	7	6	-	0/2/19/22	0/1/1/1
6	MAN	F	8	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	1/6/23/26	0/1/1/1
7	BMA	G	3	7	-	1/2/19/22	0/1/1/1
8	NAG	J	1	8	-	4/6/23/26	0/1/1/1
8	BMA	J	2	8	-	0/2/19/22	0/1/1/1
8	NAG	K	1	8	-	2/6/23/26	0/1/1/1
8	BMA	K	2	8	-	0/2/19/22	0/1/1/1
9	NAG	M	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	BMA	M	3	9	-	2/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	0/2/19/22	0/1/1/1
9	MAN	M	6	9	-	1/2/19/22	1/1/1/1
10	NAG	N	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	N	2	10	-	2/6/23/26	0/1/1/1
10	BMA	N	3	10	-	2/2/19/22	0/1/1/1
10	MAN	N	4	10	-	0/2/19/22	0/1/1/1
10	MAN	N	5	10	-	0/2/19/22	0/1/1/1
11	NAG	O	1	11,1	-	1/6/23/26	0/1/1/1
11	NAG	O	2	11	-	1/6/23/26	0/1/1/1
11	BMA	O	3	11	-	2/2/19/22	0/1/1/1
11	MAN	O	4	11	-	2/2/19/22	0/1/1/1
11	MAN	O	5	11	-	2/2/19/22	0/1/1/1
12	MAN	P	1	12	-	2/2/19/22	0/1/1/1
12	MAN	P	2	12	-	0/2/19/22	0/1/1/1
12	MAN	P	3	12	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	1/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	1/2/19/22	0/1/1/1
9	NAG	R	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	0/6/23/26	0/1/1/1
9	BMA	R	3	9	-	2/2/19/22	0/1/1/1
9	MAN	R	4	9	-	0/2/19/22	0/1/1/1
9	MAN	R	5	9	-	0/2/19/22	0/1/1/1
9	MAN	R	6	9	-	1/2/19/22	1/1/1/1
10	NAG	S	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
10	BMA	S	3	10	-	2/2/19/22	0/1/1/1
10	MAN	S	4	10	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	S	5	10	-	0/2/19/22	0/1/1/1
13	NAG	T	1	1,13	-	2/6/23/26	0/1/1/1
13	NAG	T	2	13	-	2/6/23/26	0/1/1/1
13	BMA	T	3	13	-	2/2/19/22	0/1/1/1
13	MAN	T	4	13	-	2/2/19/22	0/1/1/1
13	MAN	T	5	13	-	0/2/19/22	0/1/1/1
13	MAN	T	6	13	-	0/2/19/22	1/1/1/1
7	NAG	U	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	1/6/23/26	0/1/1/1
7	BMA	U	3	7	-	1/2/19/22	0/1/1/1
8	NAG	V	1	8	-	2/6/23/26	0/1/1/1
8	BMA	V	2	8	-	0/2/19/22	0/1/1/1
9	NAG	W	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	W	2	9	-	1/6/23/26	0/1/1/1
9	BMA	W	3	9	-	2/2/19/22	0/1/1/1
9	MAN	W	4	9	-	0/2/19/22	0/1/1/1
9	MAN	W	5	9	-	0/2/19/22	0/1/1/1
9	MAN	W	6	9	-	1/2/19/22	0/1/1/1
7	NAG	X	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	2/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	4	MAN	C2-C3	2.93	1.57	1.52
8	K	2	BMA	C1-C2	2.34	1.57	1.52
12	P	2	MAN	O5-C1	-2.11	1.40	1.43
9	R	6	MAN	C1-C2	2.04	1.57	1.52
11	O	5	MAN	O5-C1	-2.02	1.40	1.43

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	4	MAN	C1-O5-C5	5.15	119.09	112.19
6	F	5	MAN	C1-O5-C5	3.09	116.33	112.19
13	T	6	MAN	C1-O5-C5	3.07	116.30	112.19
9	R	6	MAN	C1-O5-C5	3.03	116.25	112.19
9	M	6	MAN	C1-O5-C5	2.92	116.09	112.19

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	W	1	NAG	O5-C5-C6-O6
9	R	1	NAG	C4-C5-C6-O6
9	W	3	BMA	C4-C5-C6-O6
9	R	1	NAG	O5-C5-C6-O6
9	R	3	BMA	C4-C5-C6-O6

All (3) ring outliers are listed below:

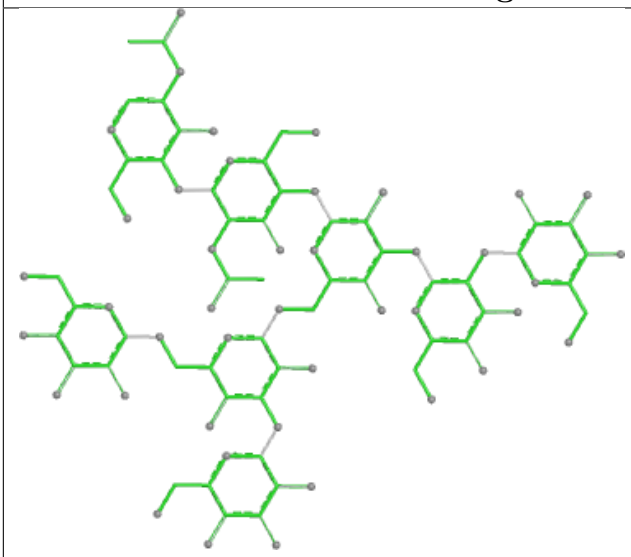
Mol	Chain	Res	Type	Atoms
13	T	6	MAN	C1-C2-C3-C4-C5-O5
9	M	6	MAN	C1-C2-C3-C4-C5-O5
9	R	6	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 9 short contacts:

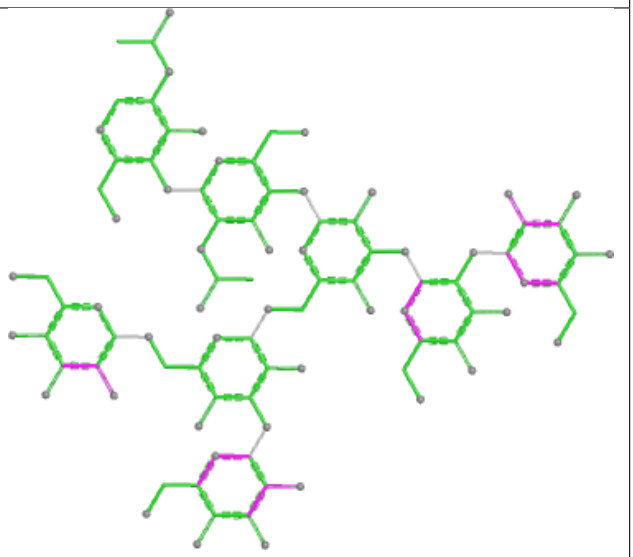
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	S	2	NAG	1	0
6	F	7	MAN	1	0
6	F	2	NAG	1	0
6	F	6	MAN	1	0
7	U	1	NAG	1	0
10	S	3	BMA	1	0
9	W	2	NAG	1	0
6	F	1	NAG	1	0
12	P	2	MAN	1	0
6	F	5	MAN	2	0
9	W	1	NAG	1	0

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

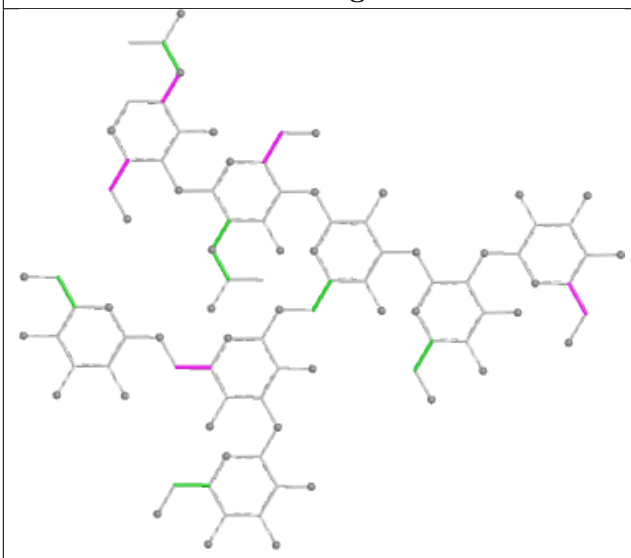
Oligosaccharide Chain F



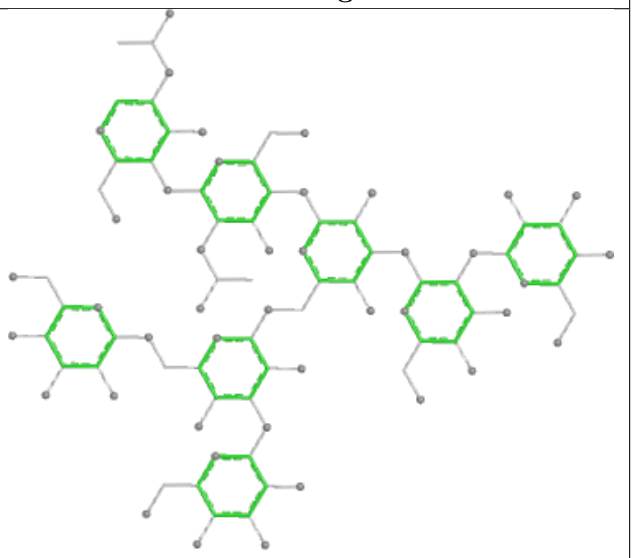
Bond lengths



Bond angles

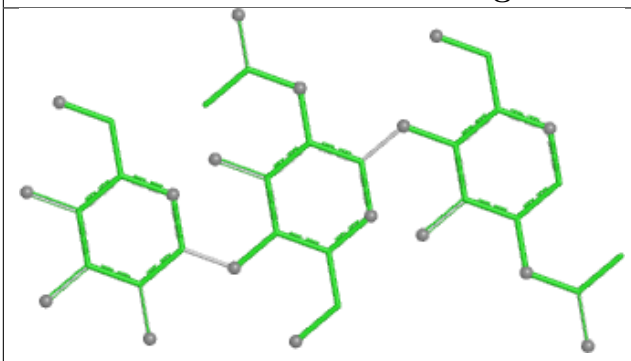


Torsions

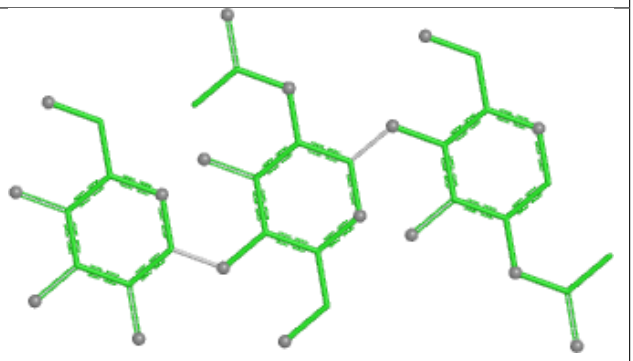


Rings

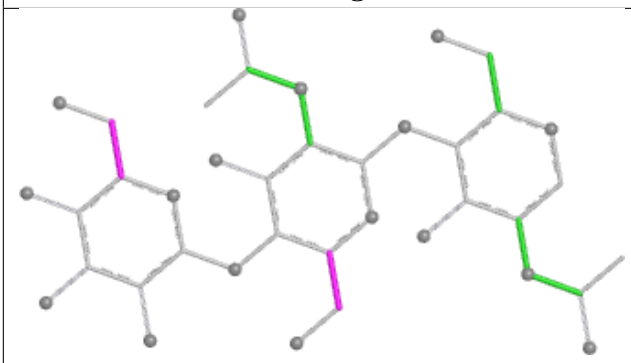
Oligosaccharide Chain G



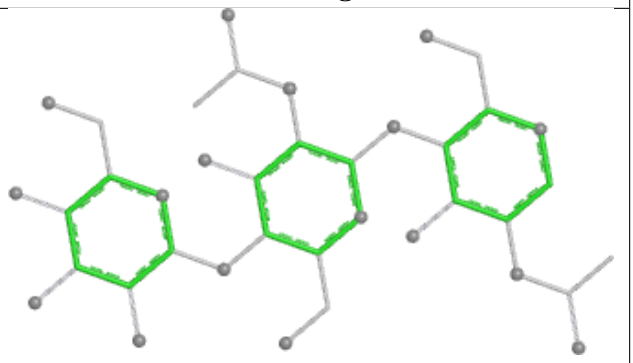
Bond lengths



Bond angles

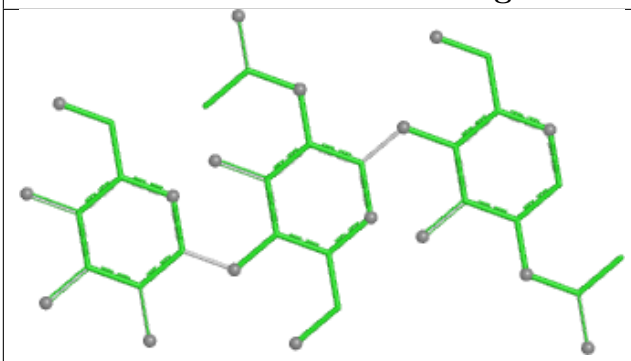


Torsions

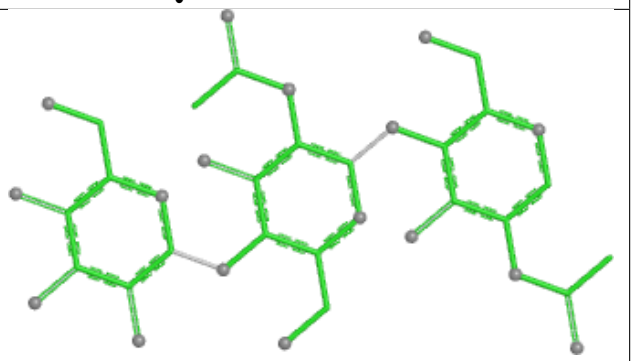


Rings

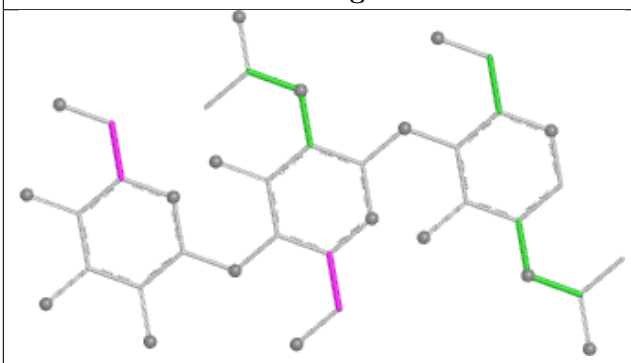
Oligosaccharide Chain Q



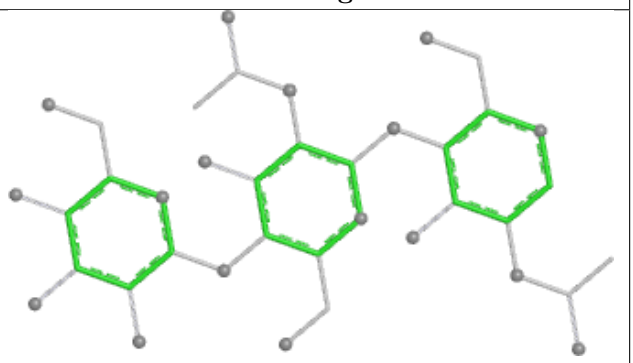
Bond lengths



Bond angles

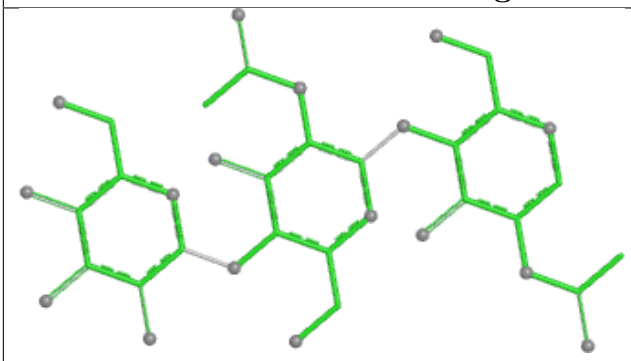


Torsions

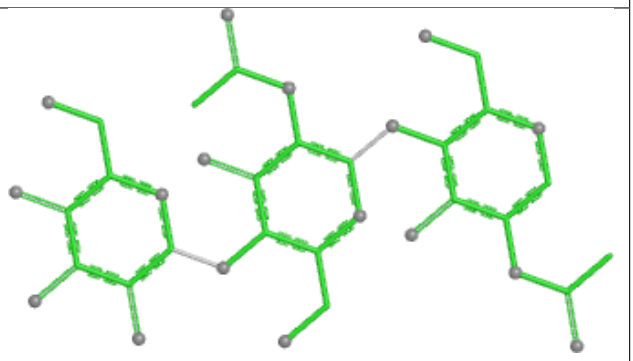


Rings

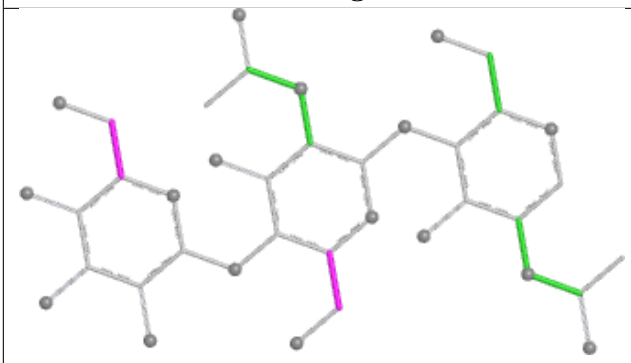
Oligosaccharide Chain U



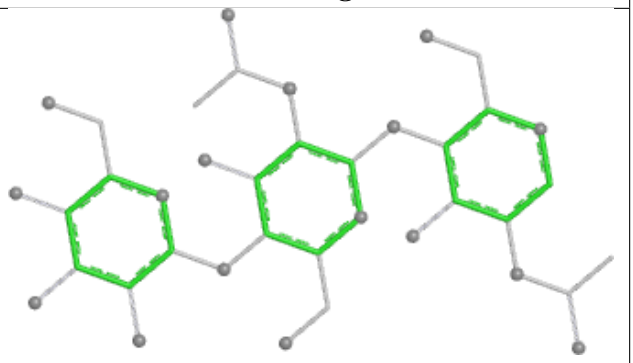
Bond lengths



Bond angles

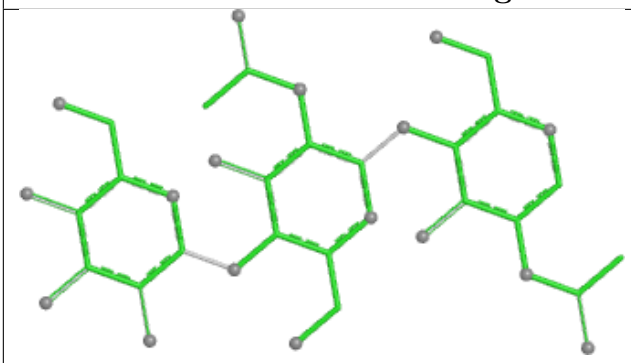


Torsions

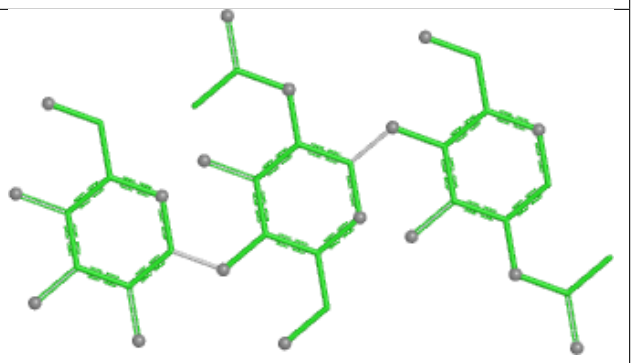


Rings

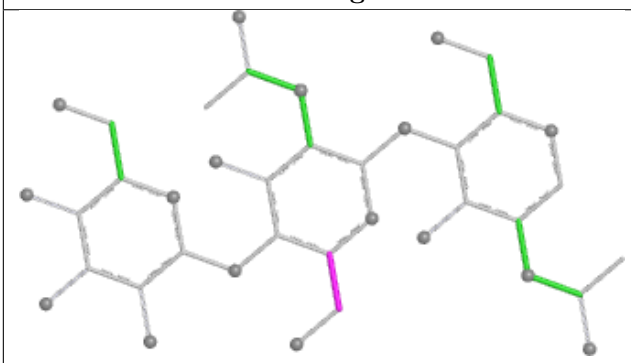
Oligosaccharide Chain X



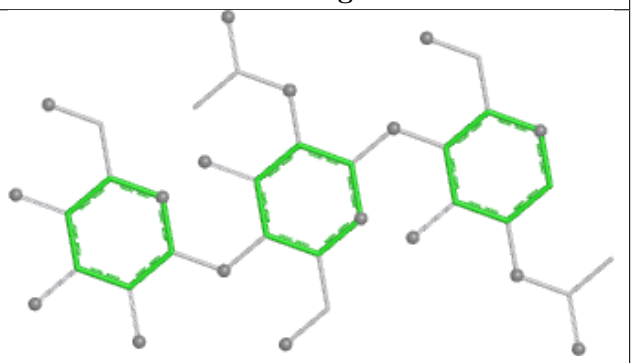
Bond lengths



Bond angles

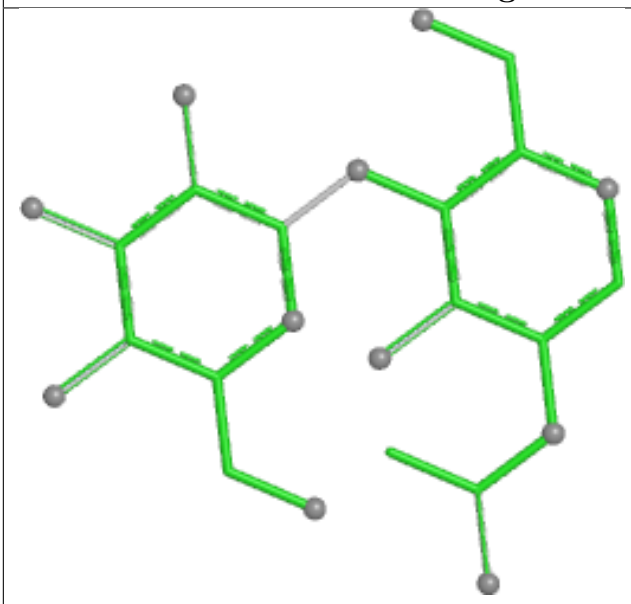


Torsions

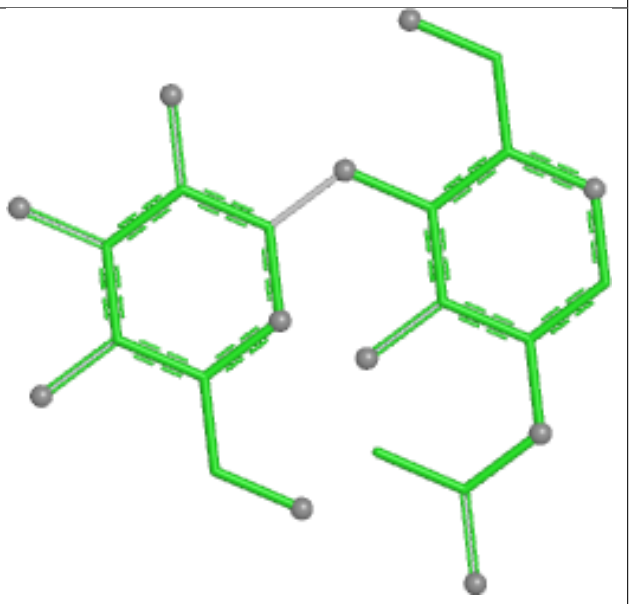


Rings

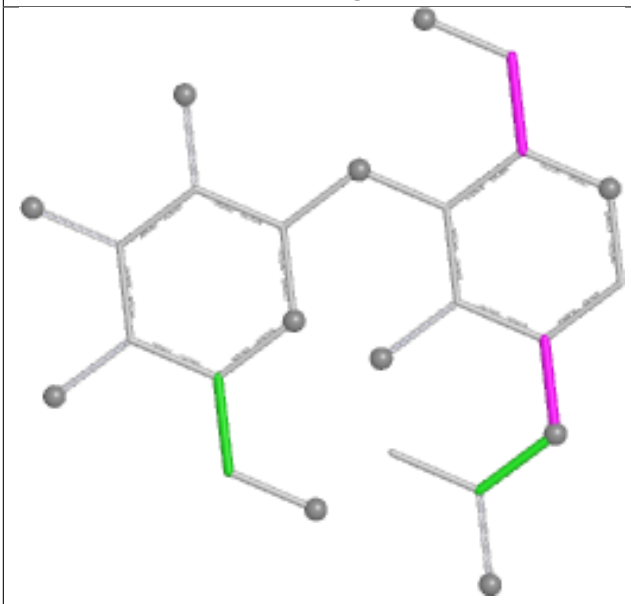
Oligosaccharide Chain J



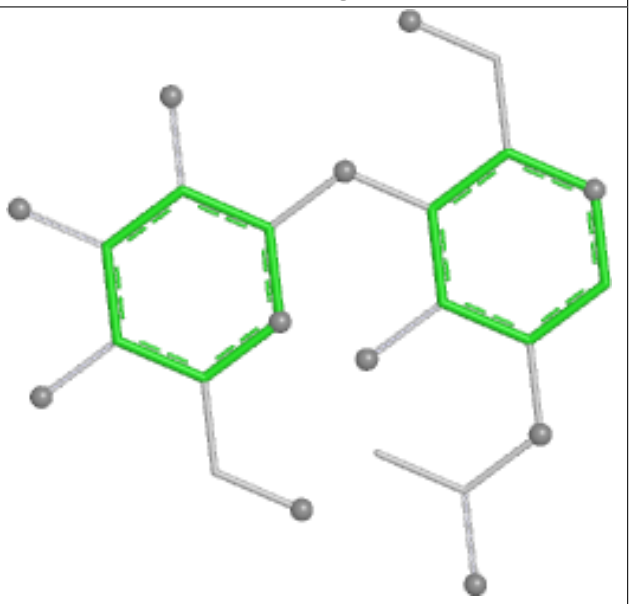
Bond lengths



Bond angles

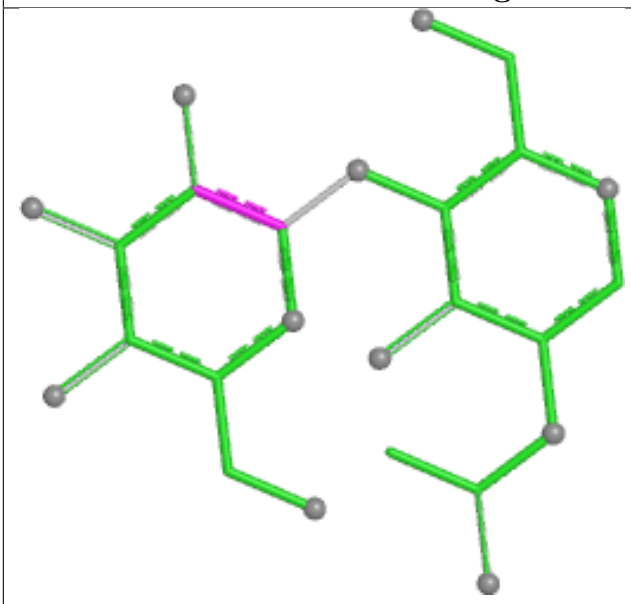


Torsions

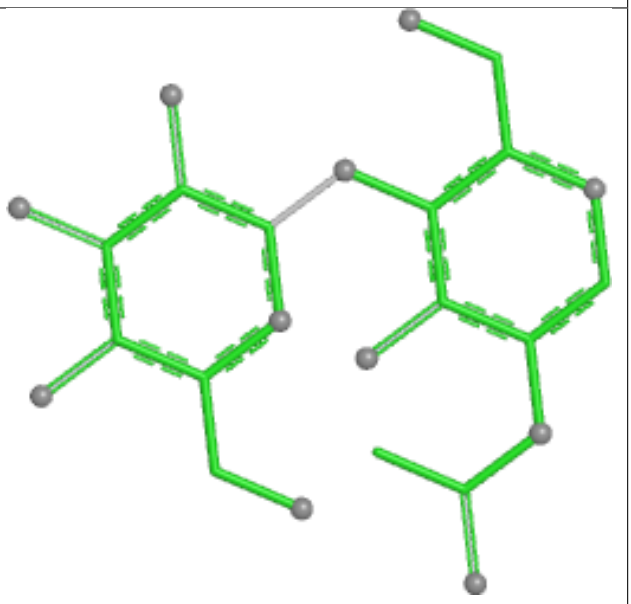


Rings

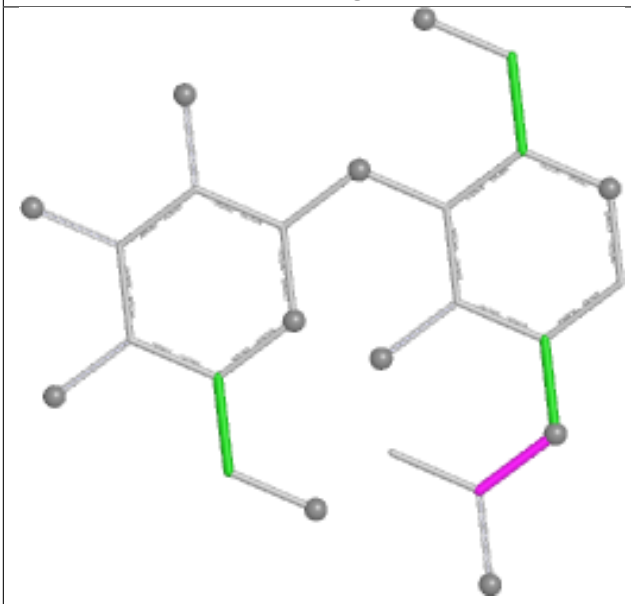
Oligosaccharide Chain K



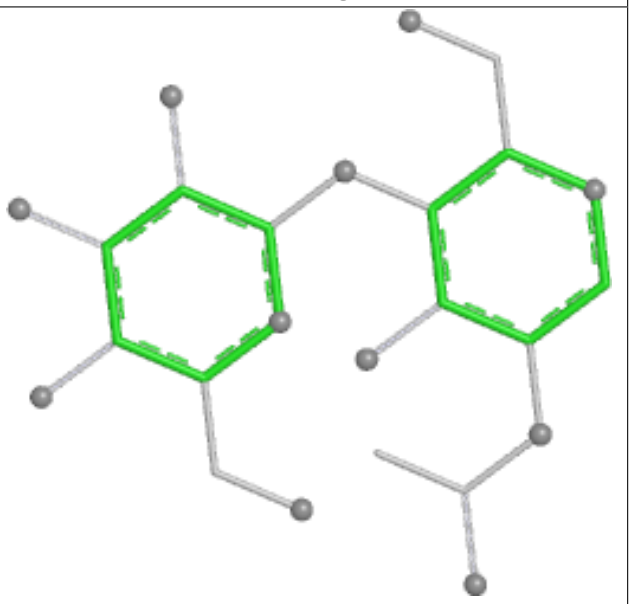
Bond lengths



Bond angles

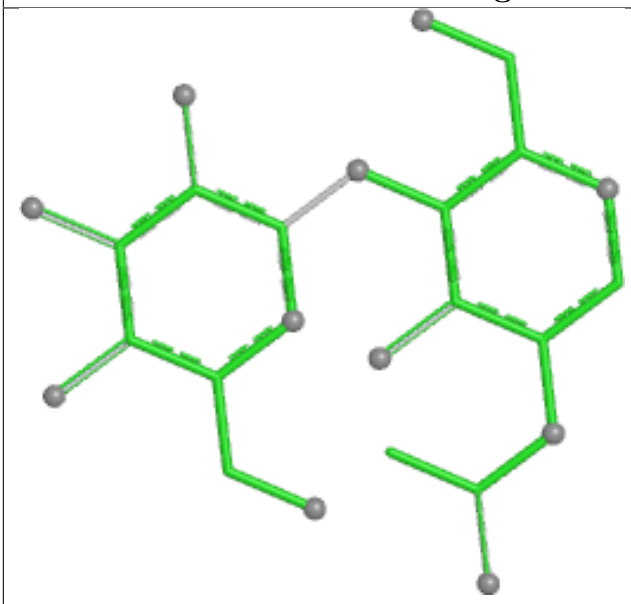


Torsions

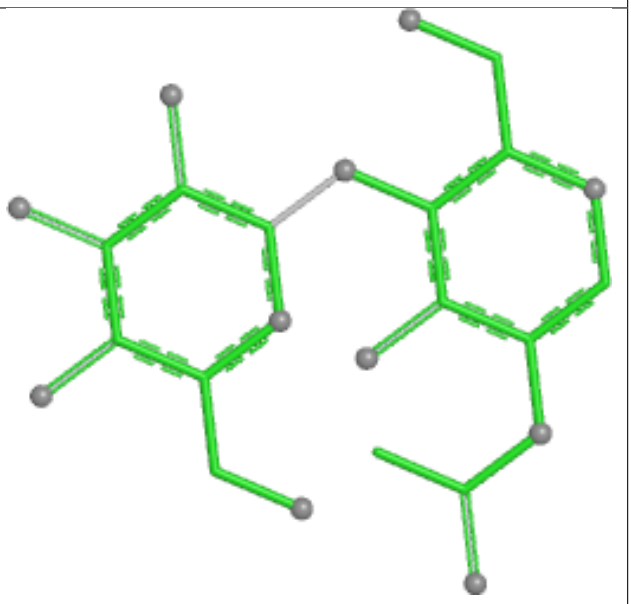


Rings

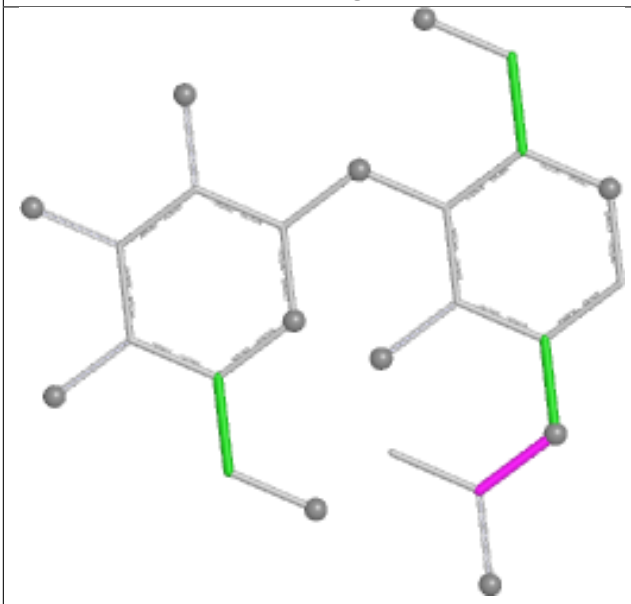
Oligosaccharide Chain V



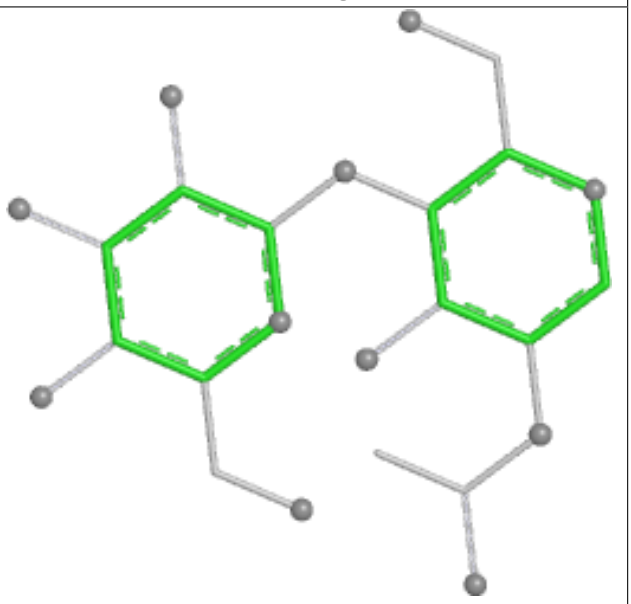
Bond lengths



Bond angles

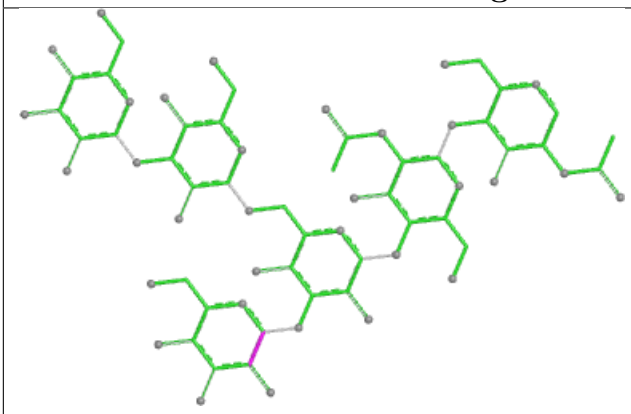


Torsions

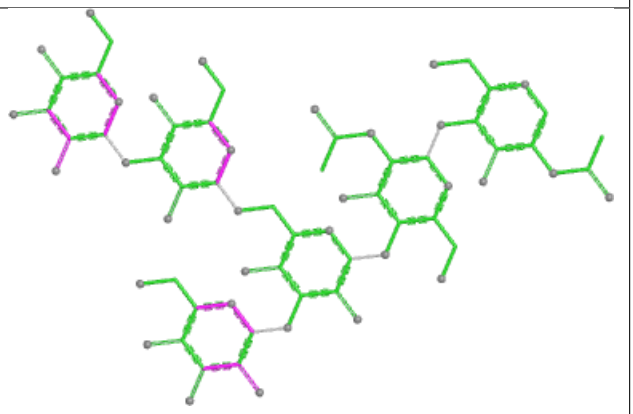


Rings

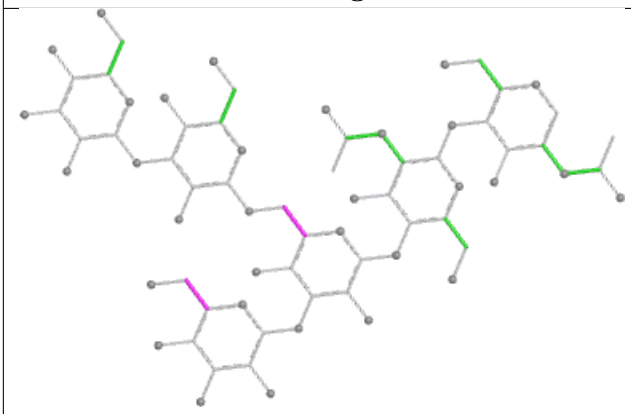
Oligosaccharide Chain M



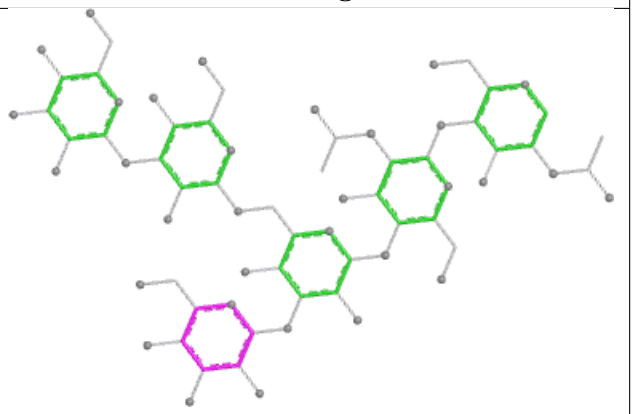
Bond lengths



Bond angles

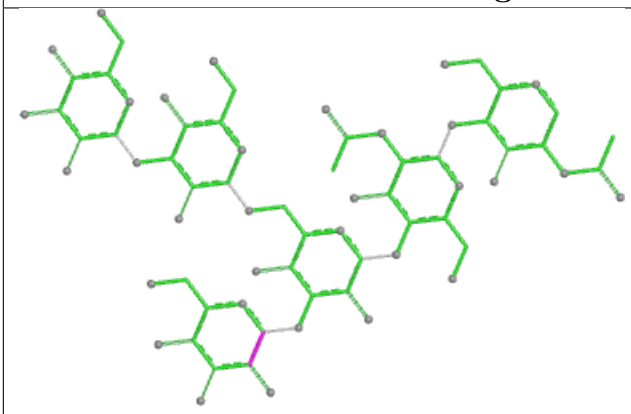


Torsions

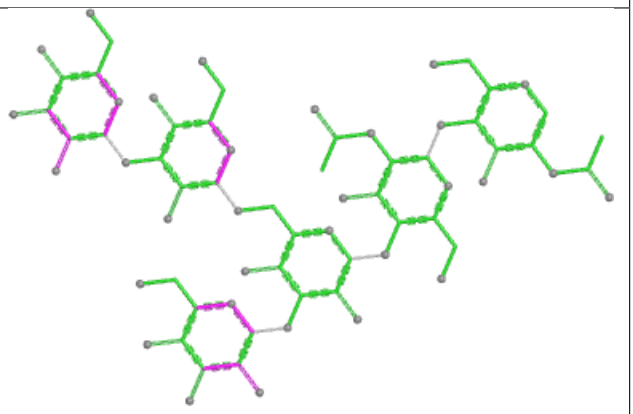


Rings

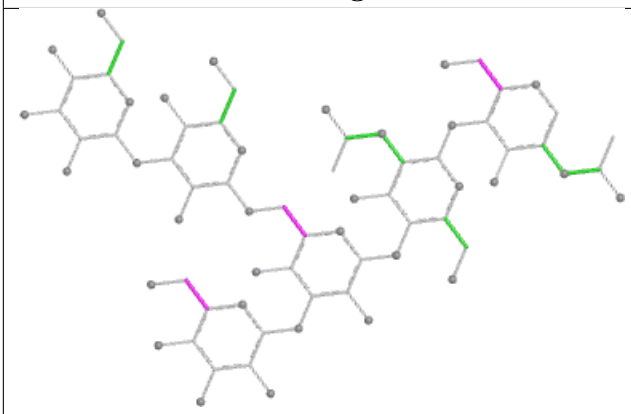
Oligosaccharide Chain R



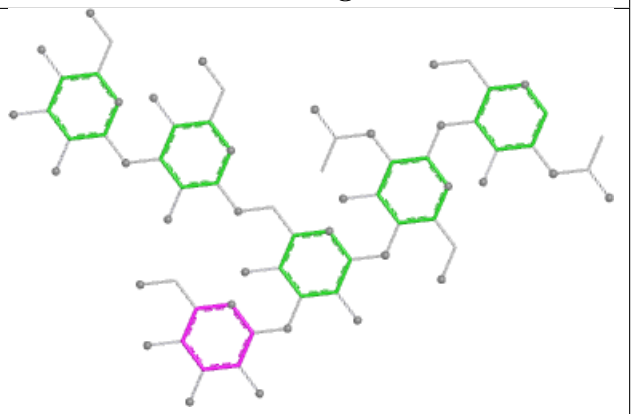
Bond lengths



Bond angles

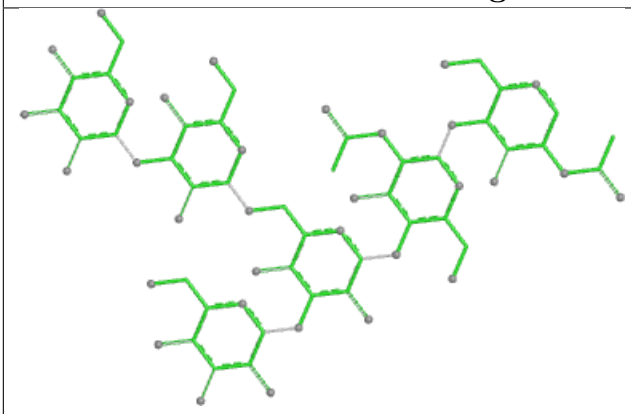


Torsions

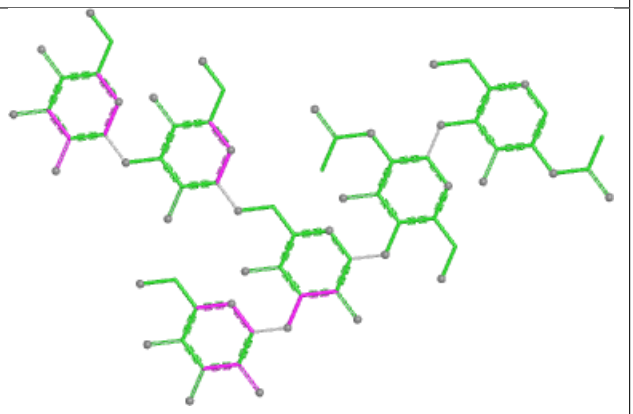


Rings

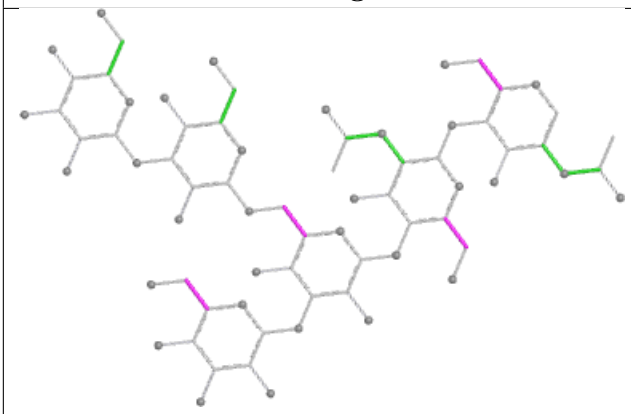
Oligosaccharide Chain W



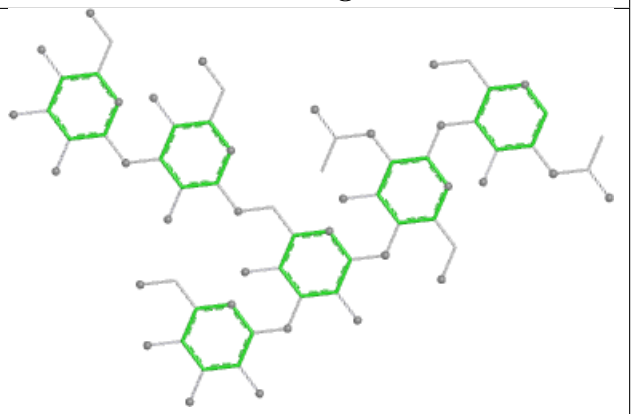
Bond lengths



Bond angles

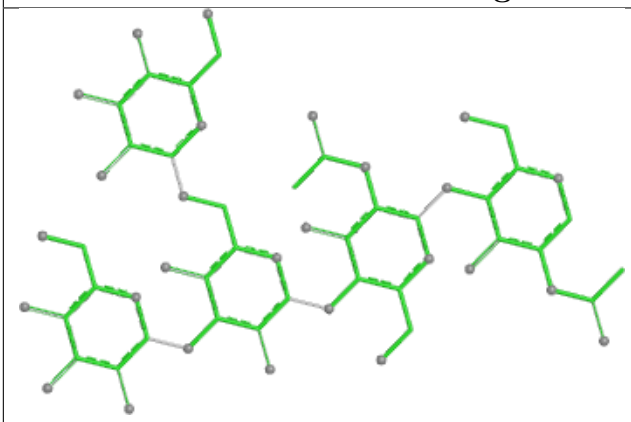


Torsions

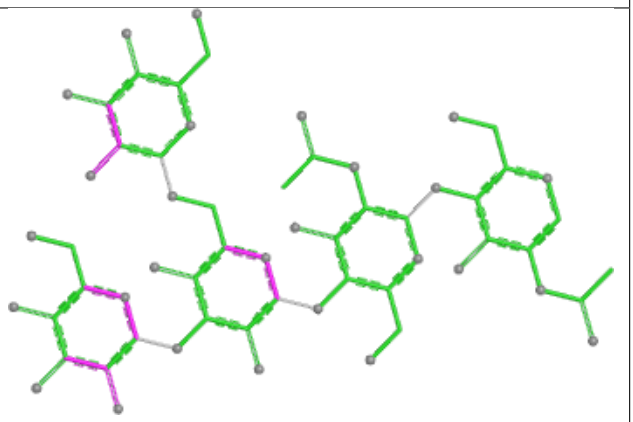


Rings

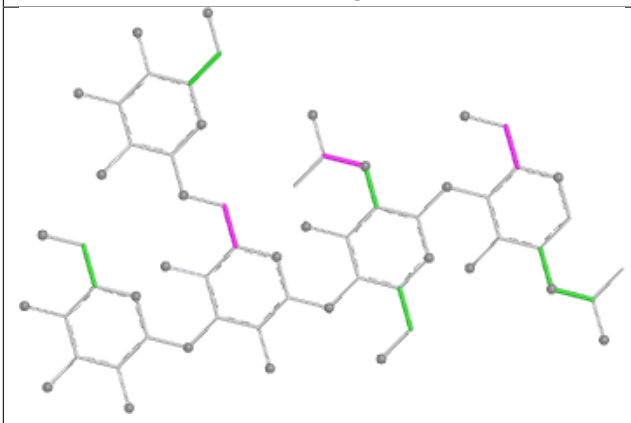
Oligosaccharide Chain N



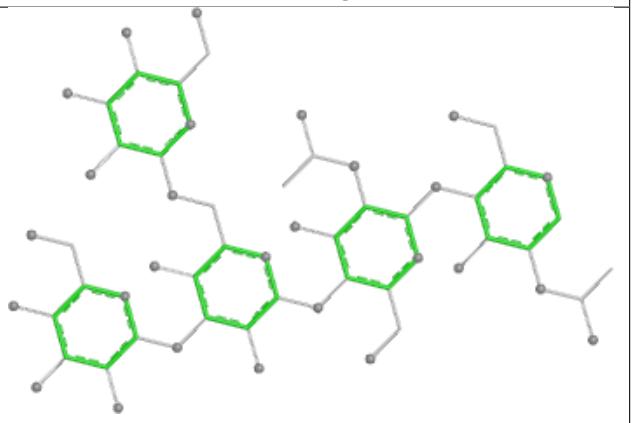
Bond lengths



Bond angles

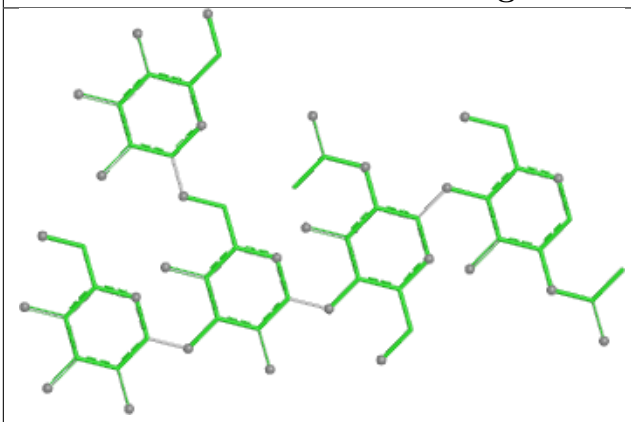


Torsions

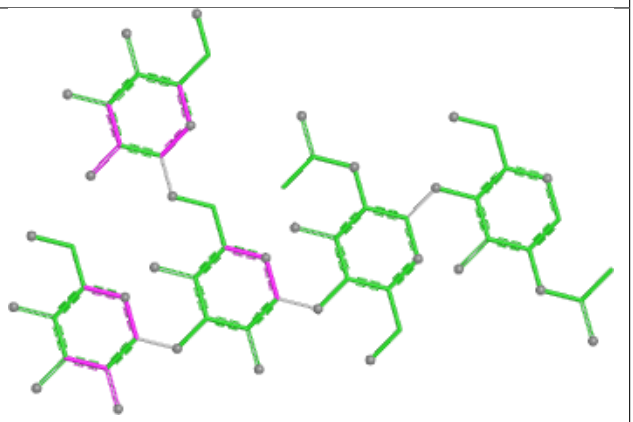


Rings

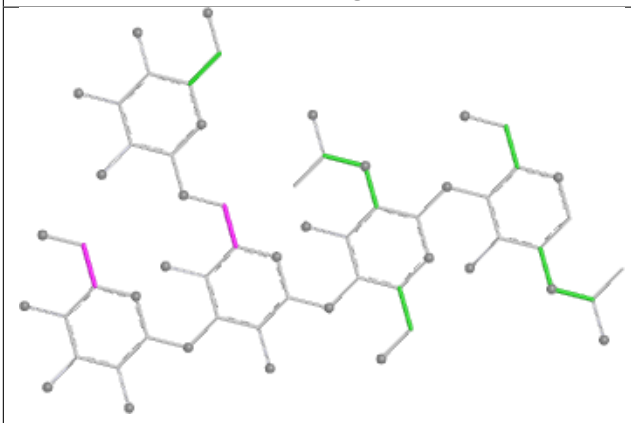
Oligosaccharide Chain S



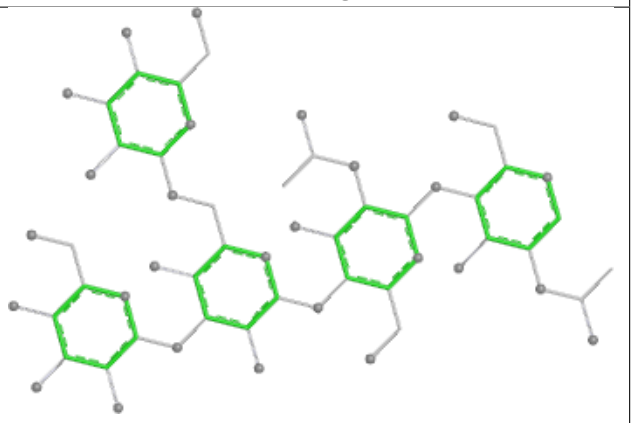
Bond lengths



Bond angles

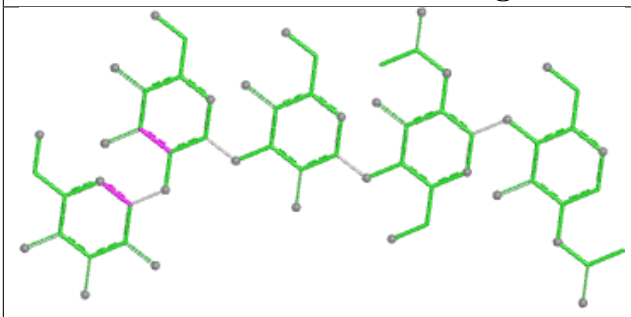


Torsions

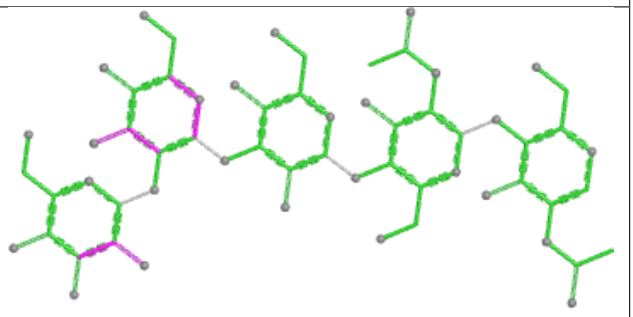


Rings

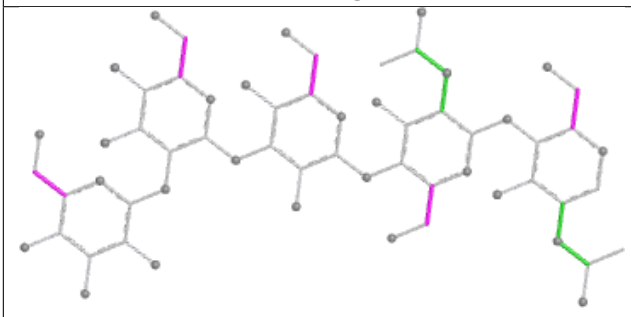
Oligosaccharide Chain O



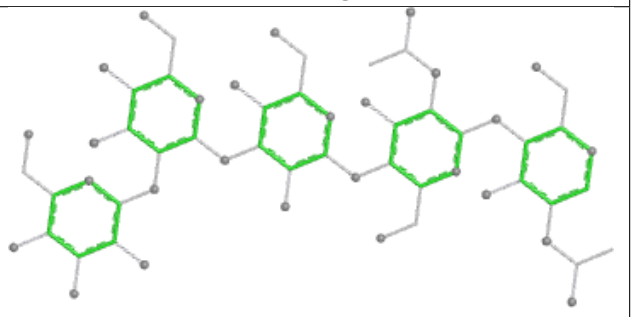
Bond lengths



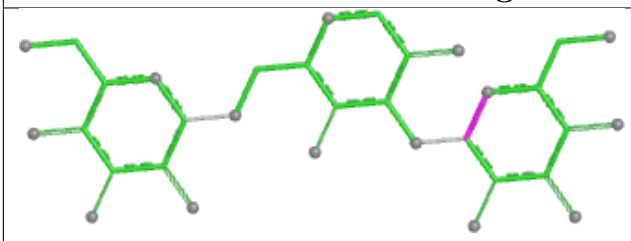
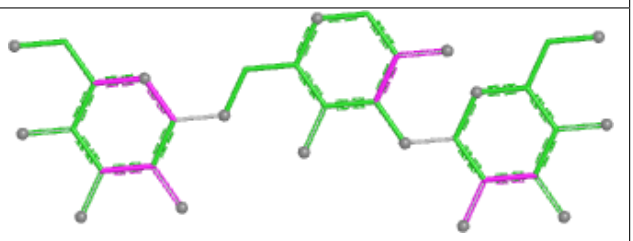
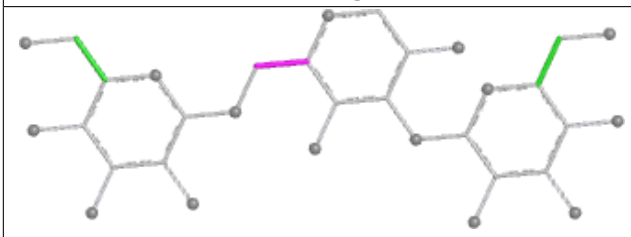
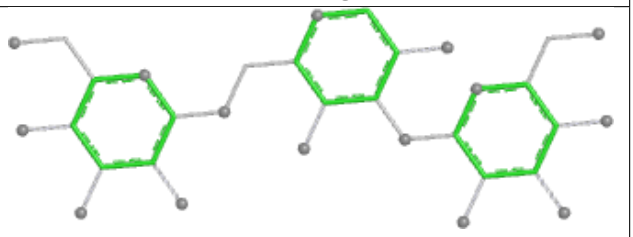
Bond angles



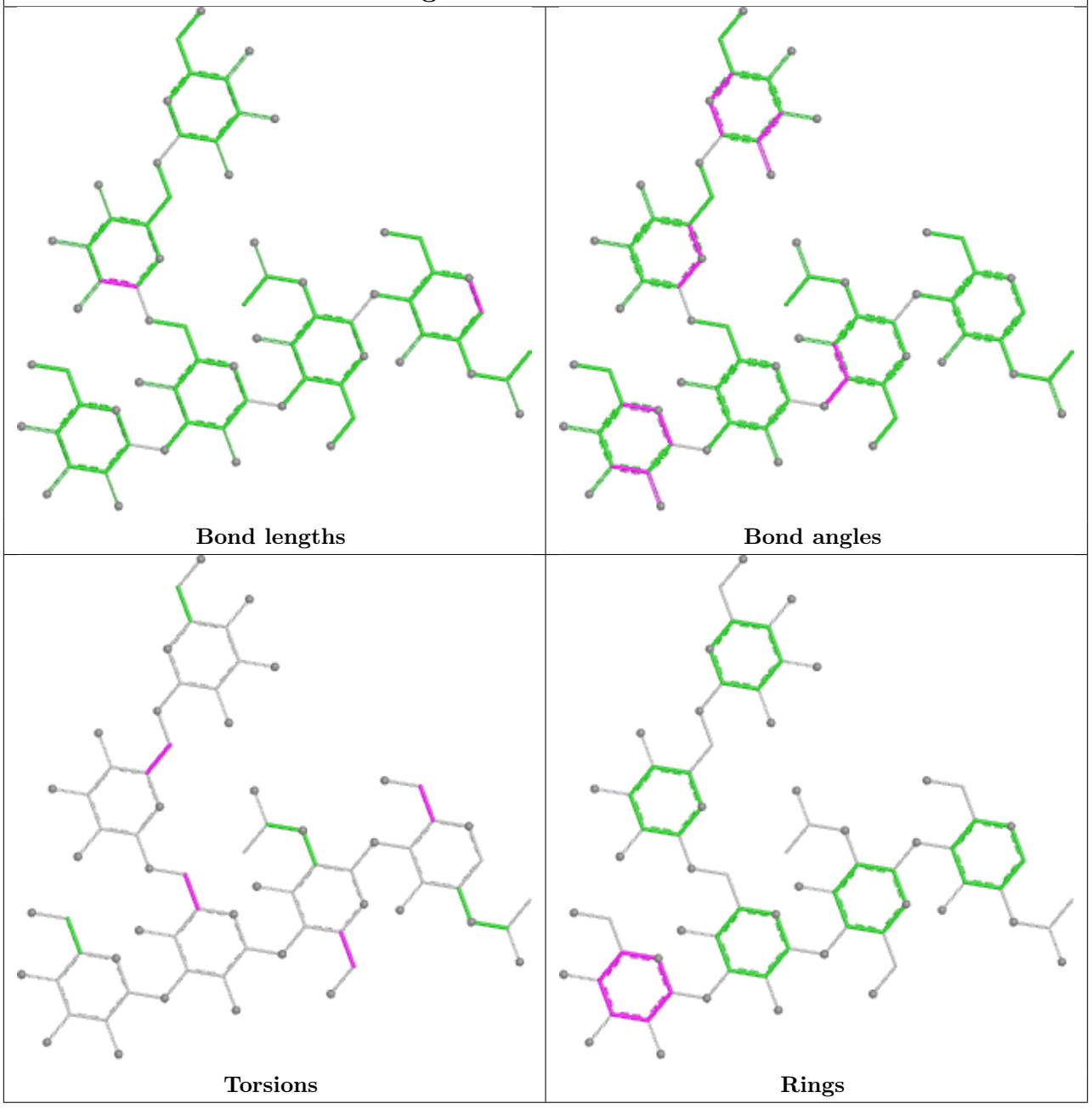
Torsions



Rings

Oligosaccharide Chain P	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain T



5.6 Ligand geometry (i)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	NAG	B	304	1	14,14,15	0.25	0	17,19,21	0.67	0
14	NAG	C	302	1	14,14,15	0.25	0	17,19,21	0.43	0
14	NAG	a	501	2	14,14,15	0.23	0	17,19,21	0.46	0
14	NAG	A	303	1	14,14,15	0.44	0	17,19,21	0.54	0
14	NAG	B	303	1	14,14,15	0.44	0	17,19,21	0.74	0
14	NAG	A	304	1	14,14,15	0.40	0	17,19,21	0.84	1 (5%)
14	NAG	A	305	1	14,14,15	0.24	0	17,19,21	0.46	0
14	NAG	L	201	5	14,14,15	0.23	0	17,19,21	0.42	0
14	NAG	C	304	1	14,14,15	0.23	0	17,19,21	0.47	0
14	NAG	c	502	2	14,14,15	0.22	0	17,19,21	0.44	0
14	NAG	c	501	2	14,14,15	0.29	0	17,19,21	0.41	0
14	NAG	b	502	2	14,14,15	0.24	0	17,19,21	0.44	0
14	NAG	B	305	1	14,14,15	0.39	0	17,19,21	0.79	1 (5%)
14	NAG	C	301	1	14,14,15	0.46	0	17,19,21	0.51	0
14	NAG	b	501	2	14,14,15	0.25	0	17,19,21	0.43	0
14	NAG	B	302	1	14,14,15	0.26	0	17,19,21	0.46	0
14	NAG	B	301	1	14,14,15	0.32	0	17,19,21	0.45	0
14	NAG	a	502	2	14,14,15	0.28	0	17,19,21	0.41	0
14	NAG	C	305	1	14,14,15	0.22	0	17,19,21	0.50	0
14	NAG	A	302	1	14,14,15	0.30	0	17,19,21	0.48	0
14	NAG	C	303	1	14,14,15	0.33	0	17,19,21	0.66	0
14	NAG	I	201	5	14,14,15	0.23	0	17,19,21	0.40	0
14	NAG	A	301	1	14,14,15	0.32	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
14	NAG	B	304	1	-	3/6/23/26	0/1/1/1
14	NAG	C	302	1	-	0/6/23/26	0/1/1/1
14	NAG	a	501	2	-	2/6/23/26	0/1/1/1
14	NAG	A	303	1	-	4/6/23/26	0/1/1/1
14	NAG	B	303	1	-	2/6/23/26	0/1/1/1
14	NAG	A	304	1	-	4/6/23/26	0/1/1/1
14	NAG	A	305	1	-	4/6/23/26	0/1/1/1
14	NAG	L	201	5	-	2/6/23/26	0/1/1/1
14	NAG	C	304	1	-	4/6/23/26	0/1/1/1
14	NAG	c	502	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	c	501	2	-	4/6/23/26	0/1/1/1
14	NAG	b	502	2	-	0/6/23/26	0/1/1/1
14	NAG	B	305	1	-	4/6/23/26	0/1/1/1
14	NAG	C	301	1	-	1/6/23/26	0/1/1/1
14	NAG	b	501	2	-	4/6/23/26	0/1/1/1
14	NAG	B	302	1	-	0/6/23/26	0/1/1/1
14	NAG	B	301	1	-	2/6/23/26	0/1/1/1
14	NAG	a	502	2	-	2/6/23/26	0/1/1/1
14	NAG	C	305	1	-	2/6/23/26	0/1/1/1
14	NAG	A	302	1	-	0/6/23/26	0/1/1/1
14	NAG	C	303	1	-	4/6/23/26	0/1/1/1
14	NAG	I	201	5	-	0/6/23/26	0/1/1/1
14	NAG	A	301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	304	NAG	C2-N2-C7	2.54	126.31	122.90
14	B	305	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	305	NAG	C1-C2-N2-C7
14	A	305	NAG	C4-C5-C6-O6
14	B	301	NAG	C4-C5-C6-O6
14	B	301	NAG	O5-C5-C6-O6
14	A	305	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	303	NAG	3	0
14	B	303	NAG	1	0
14	A	304	NAG	3	0
14	L	201	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	301	NAG	1	0
14	C	305	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.

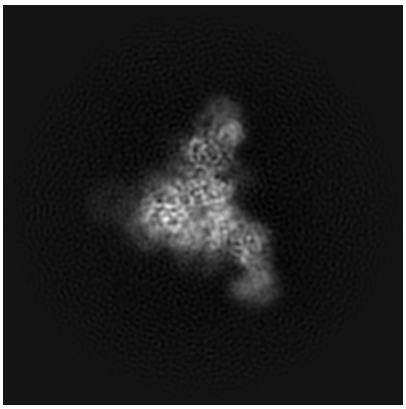
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41048. These allow visual inspection of the internal detail of the map and identification of artifacts.

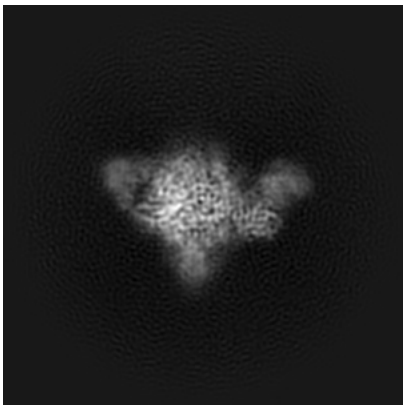
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

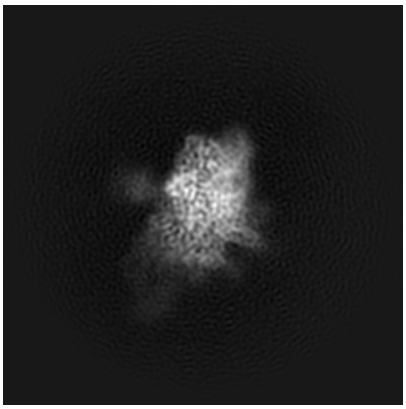
6.1.1 Primary map



X

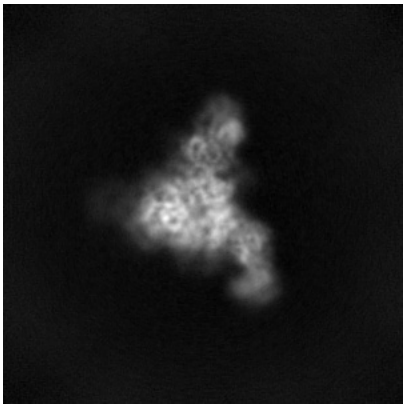


Y

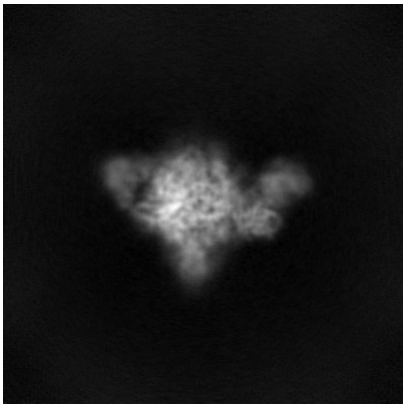


Z

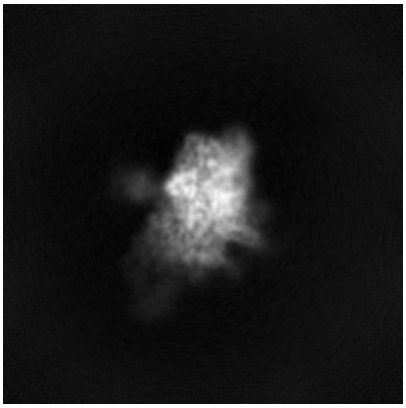
6.1.2 Raw map



X



Y

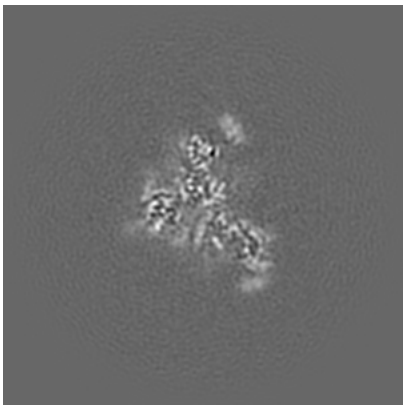


Z

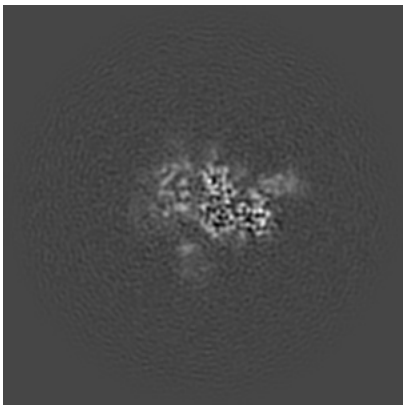
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

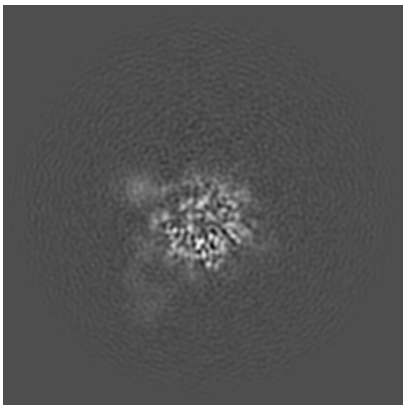
6.2.1 Primary map



X Index: 150

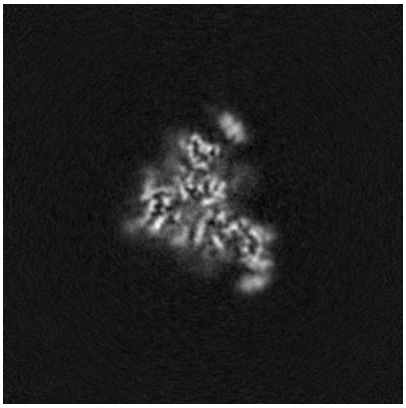


Y Index: 150

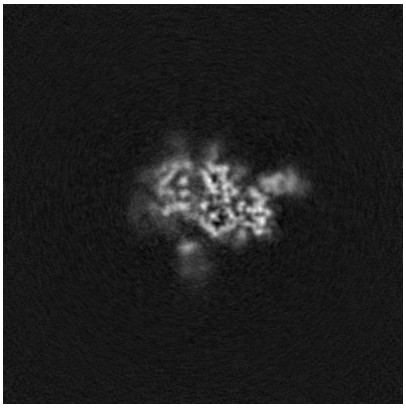


Z Index: 150

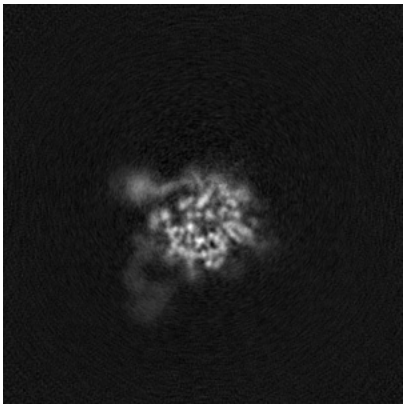
6.2.2 Raw map



X Index: 150



Y Index: 150

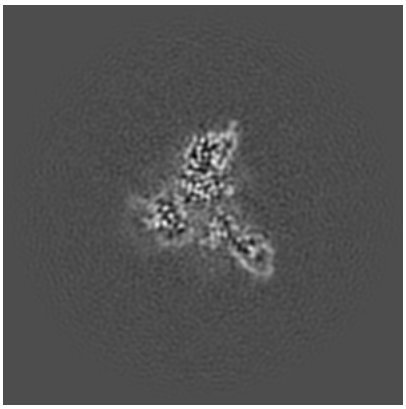


Z Index: 150

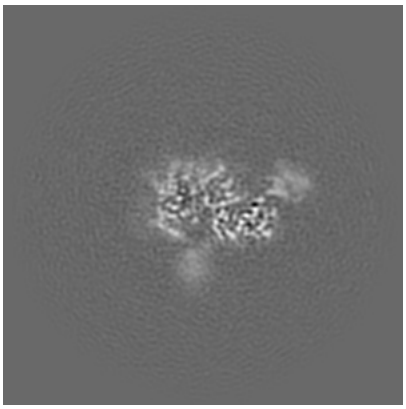
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

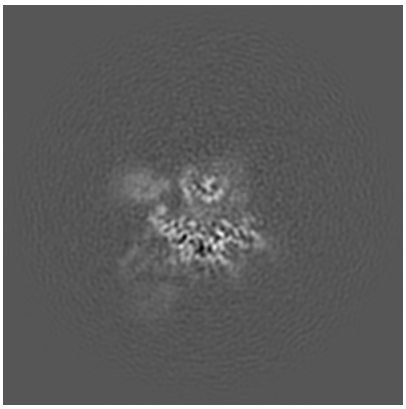
6.3.1 Primary map



X Index: 142

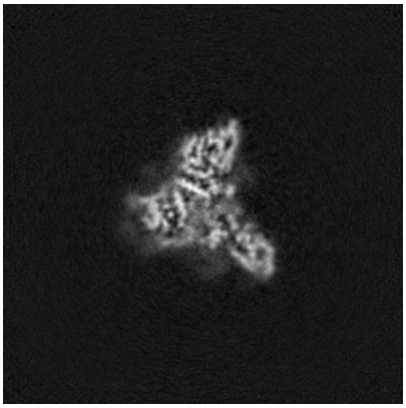


Y Index: 157

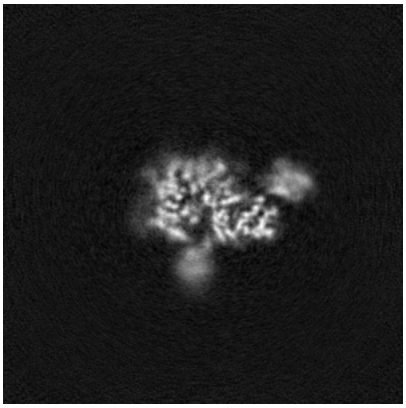


Z Index: 143

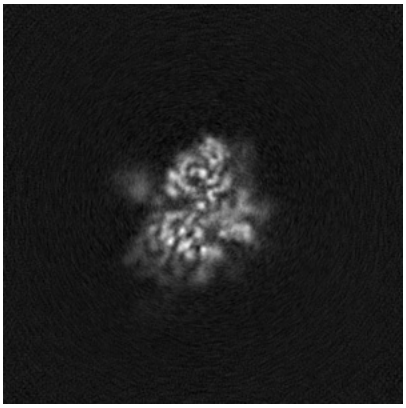
6.3.2 Raw map



X Index: 141



Y Index: 158

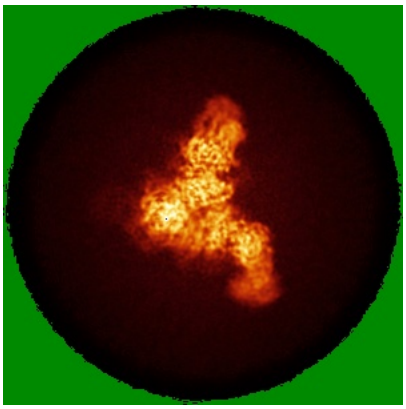


Z Index: 132

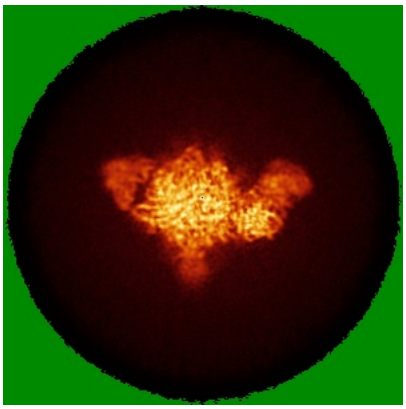
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

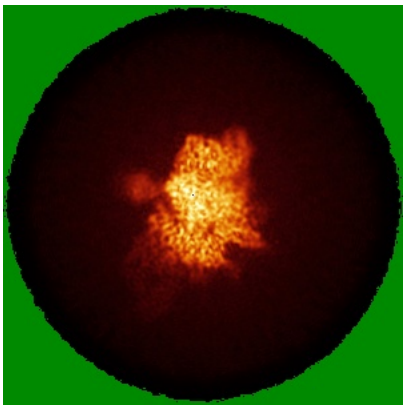
6.4.1 Primary map



X

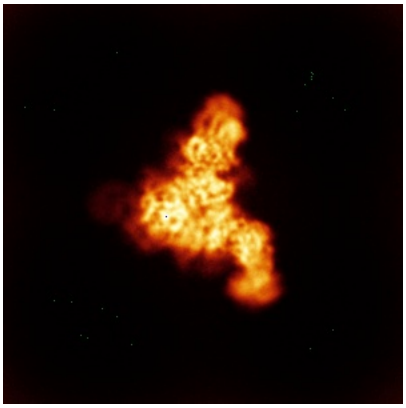


Y

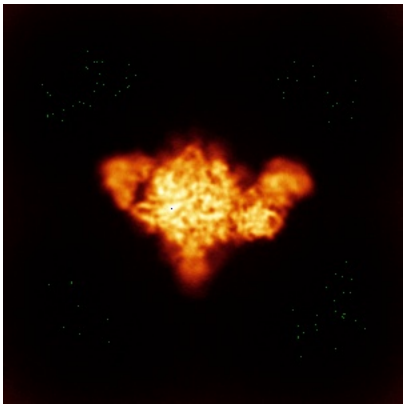


Z

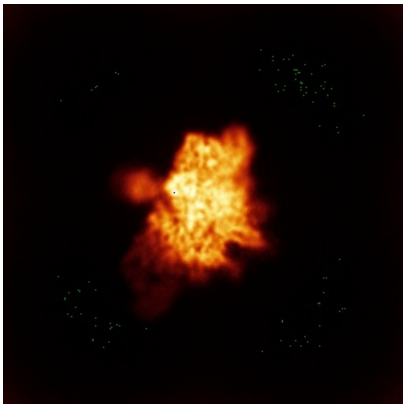
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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

X Y Z

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.

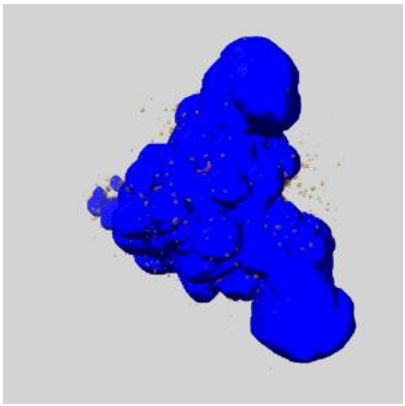
6.6 Mask visualisation (i)

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

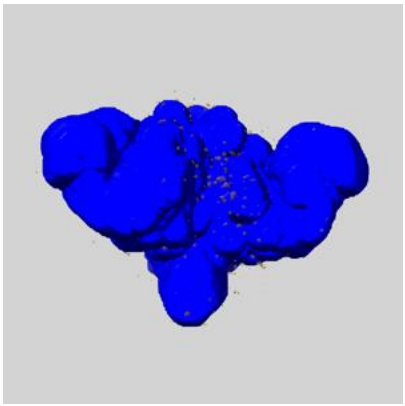
A mask typically either:

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

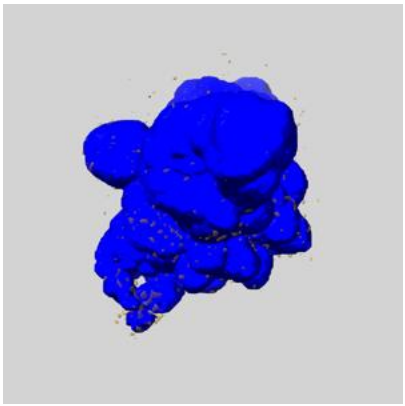
6.6.1 emd_41048_msk_1.map (i)



X



Y

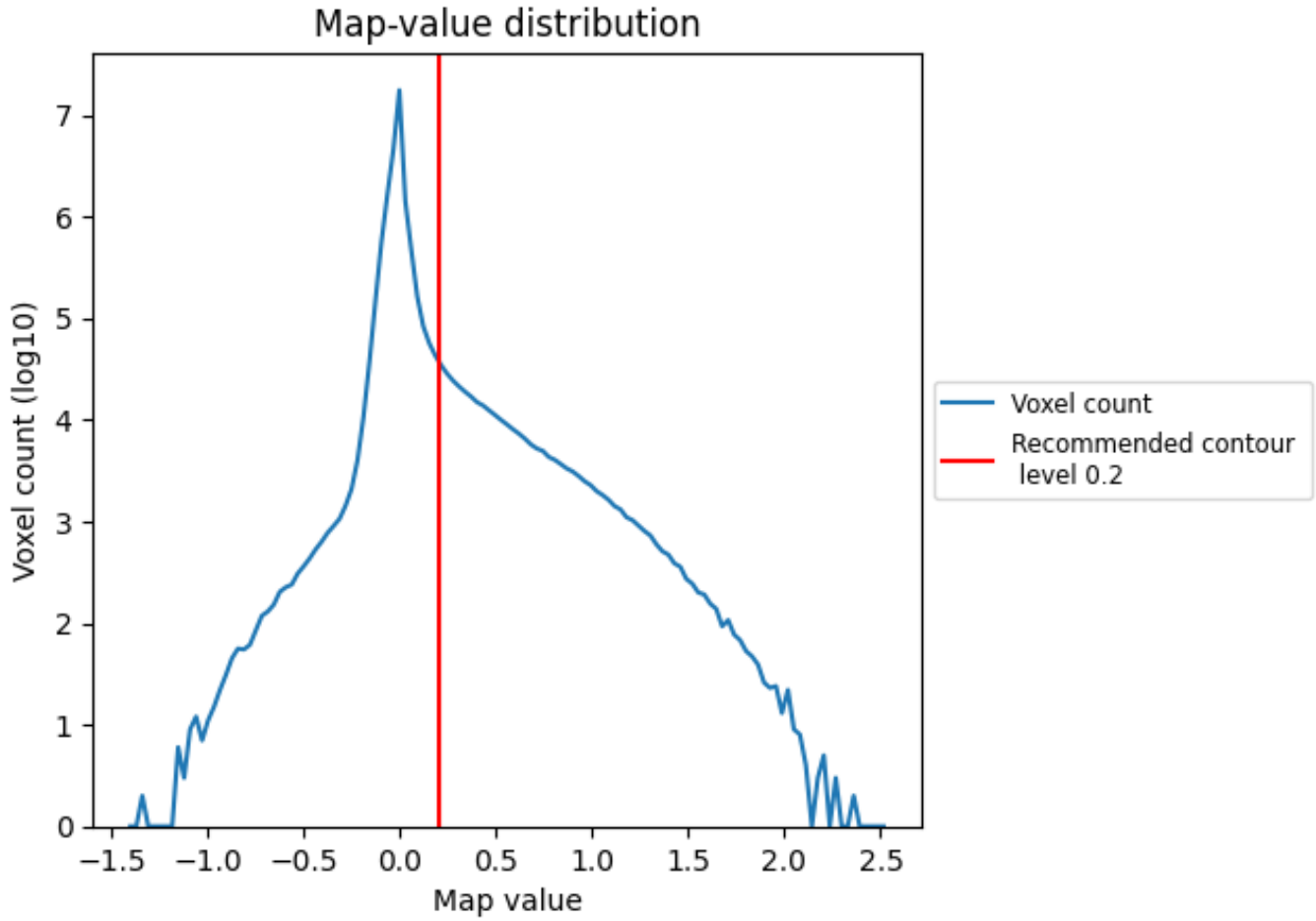


Z

7 Map analysis

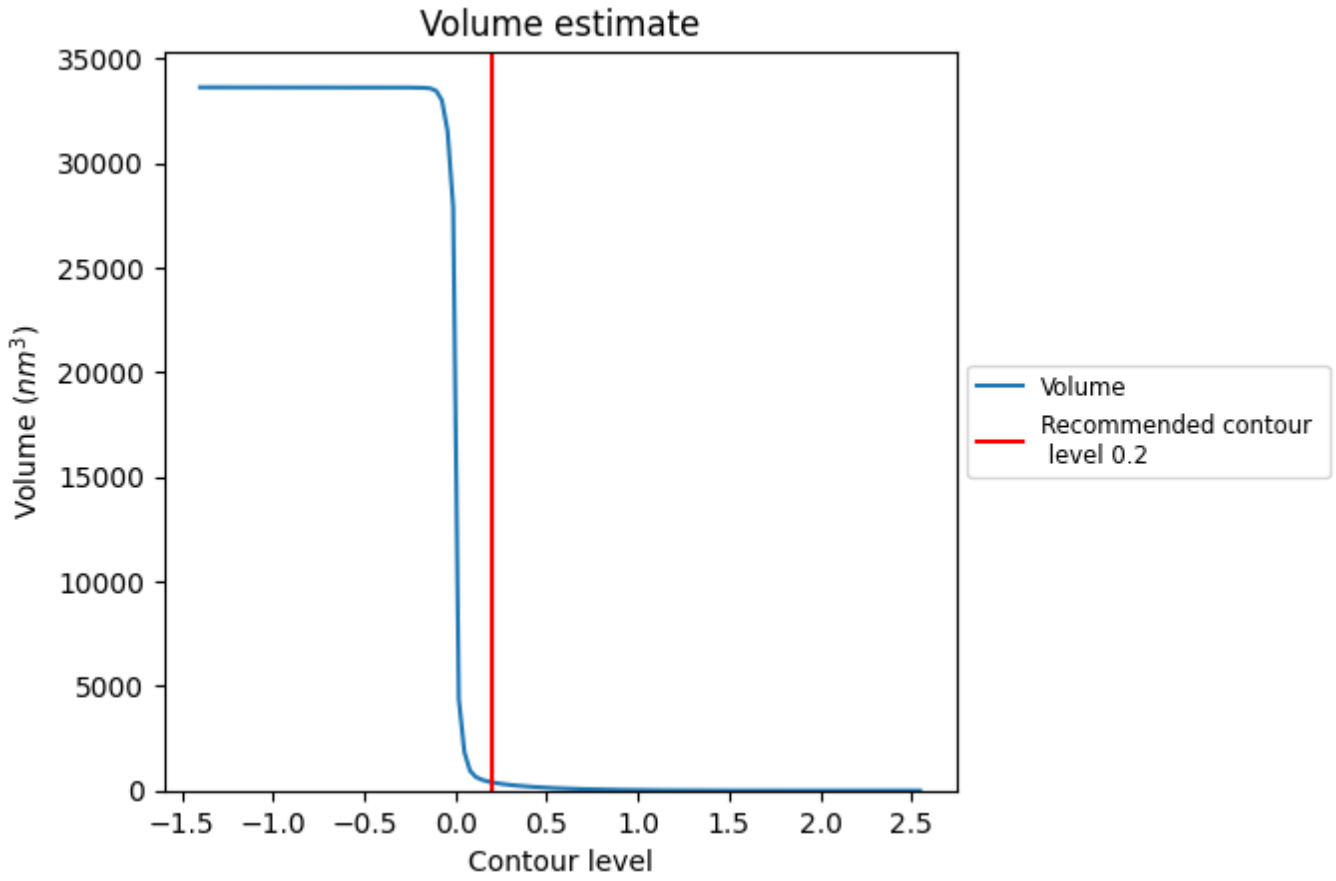
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

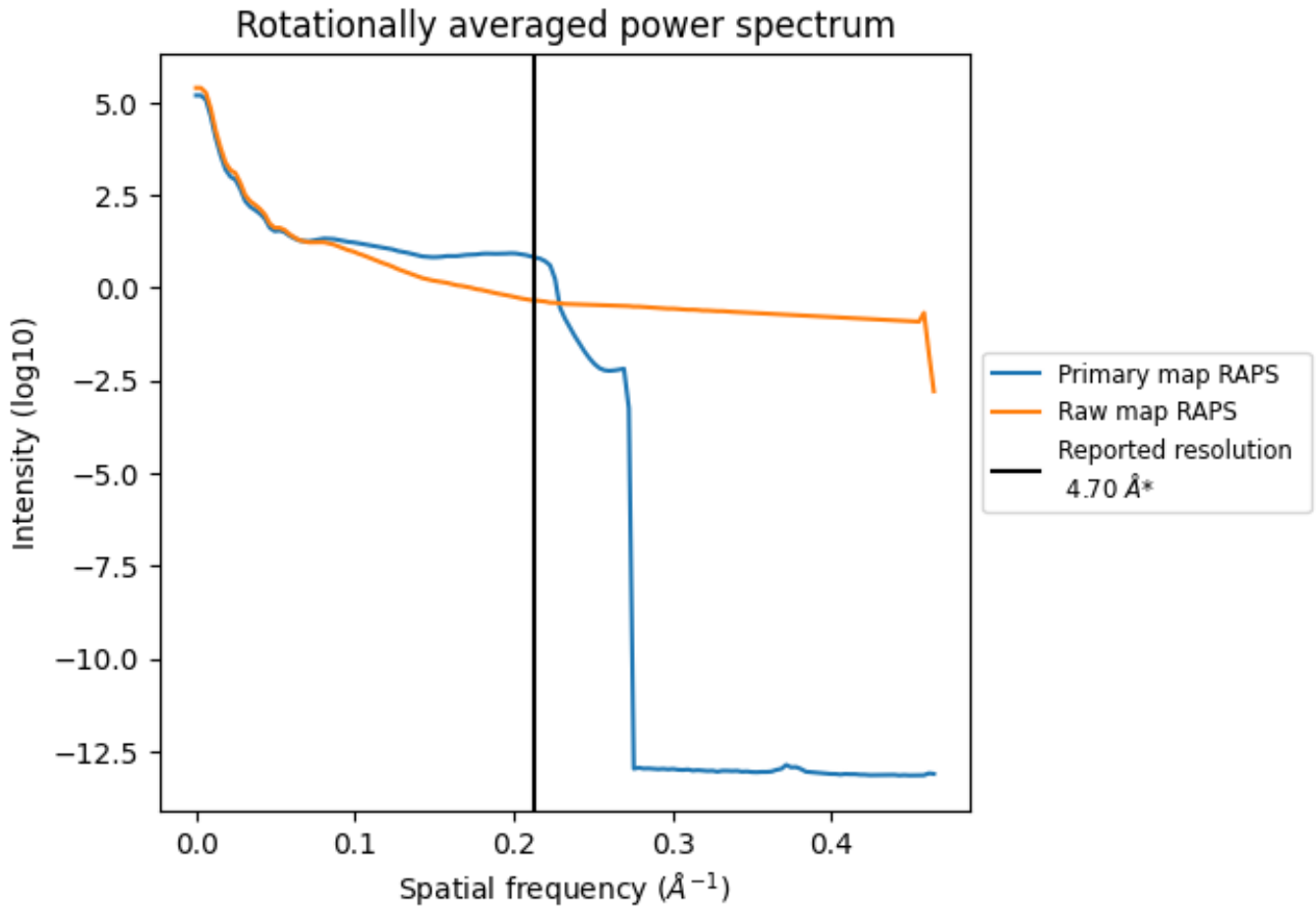
7.2 Volume estimate (i)



The volume at the recommended contour level is 396 nm^3; this corresponds to an approximate mass of 357 kDa.

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

7.3 Rotationally averaged power spectrum (i)

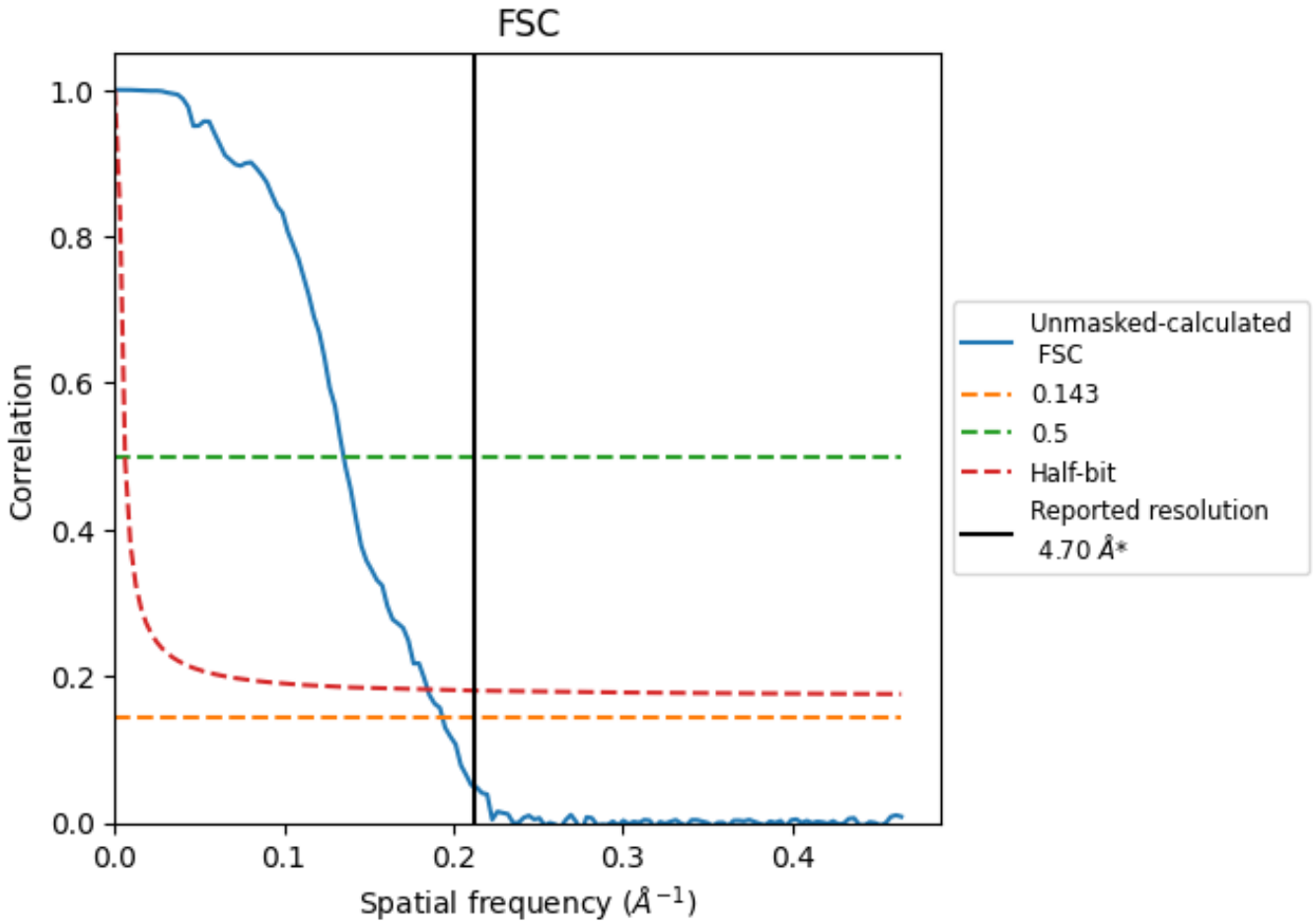


*Reported resolution corresponds to spatial frequency of 0.213 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8.2 Resolution estimates (i)

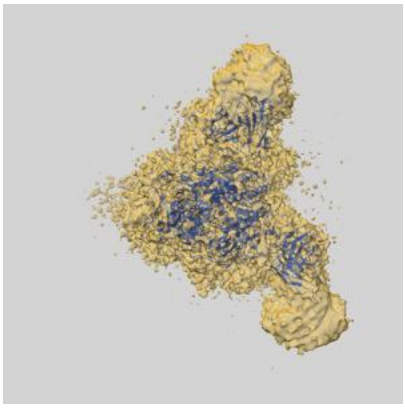
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.17	7.40	5.41

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

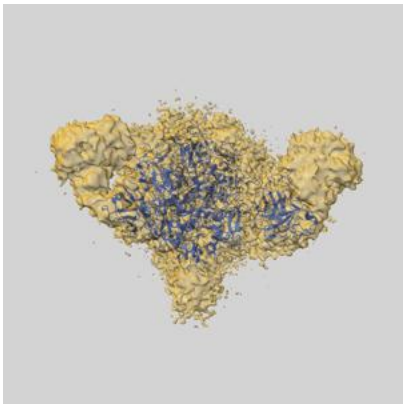
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41048 and PDB model 8T5C. Per-residue inclusion information can be found in section 3 on page 13.

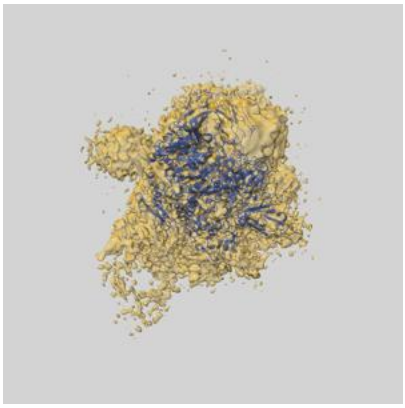
9.1 Map-model overlay



X



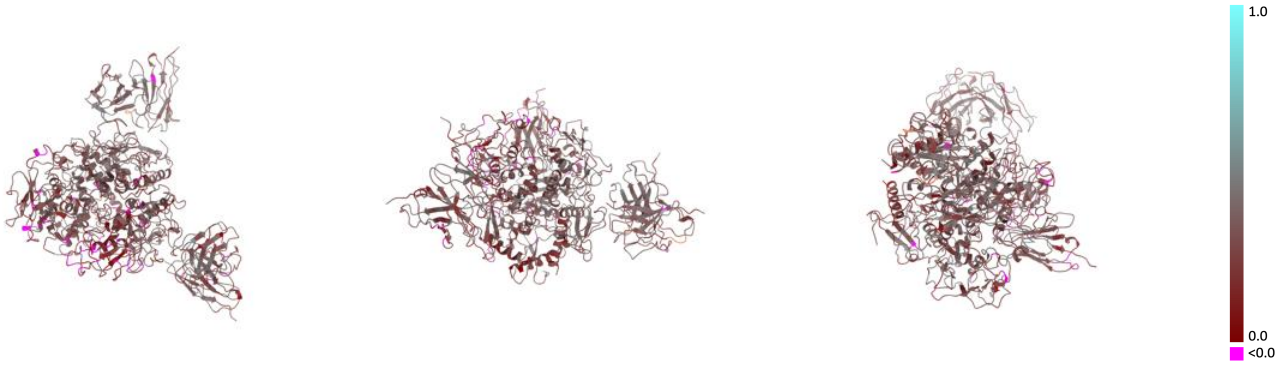
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

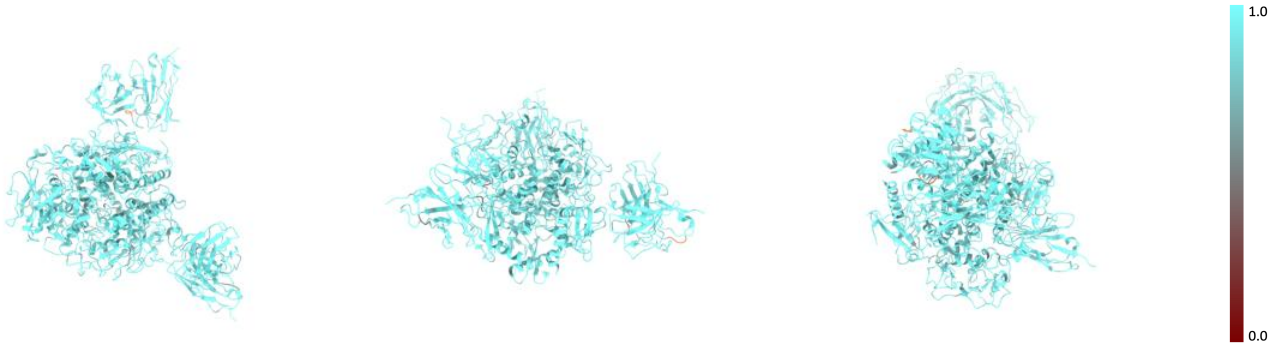
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

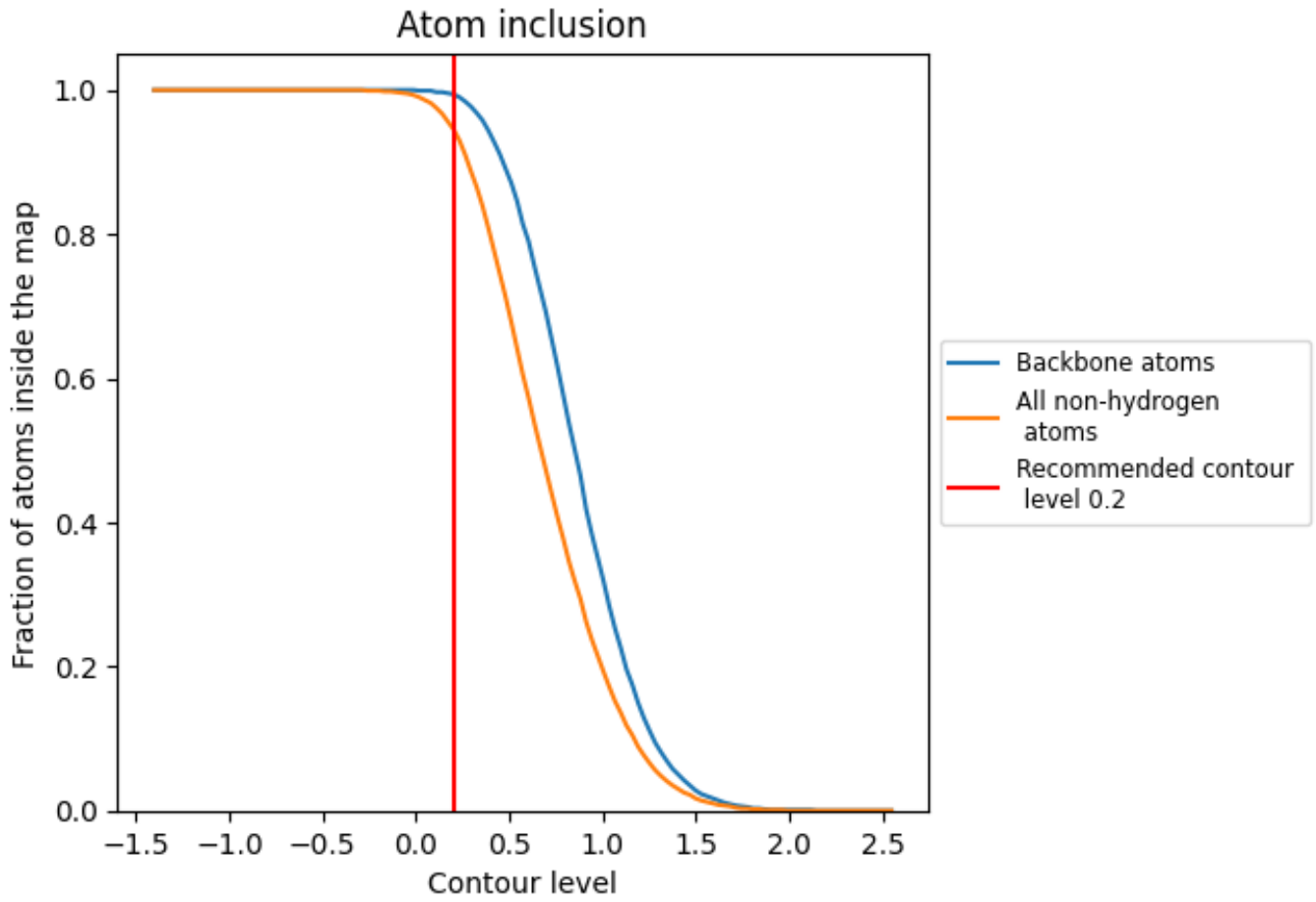
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.3010
A	0.9300	0.2020
B	0.9520	0.3260
C	0.9450	0.3010
D	0.9360	0.2940
E	0.9460	0.3350
F	0.9790	0.3920
G	1.0000	0.3760
H	0.9520	0.2930
I	0.9540	0.3590
J	0.9600	0.2730
K	0.8400	0.1490
L	0.9500	0.3360
M	0.9580	0.3650
N	0.9670	0.3780
O	0.9510	0.3660
P	0.7880	0.2550
Q	0.9490	0.2370
R	0.9860	0.3820
S	0.9340	0.3380
T	0.9860	0.3600
U	0.9230	0.1790
V	1.0000	0.2330
W	0.9580	0.3670
X	0.9740	0.3300
a	0.9400	0.2950
b	0.9570	0.3330
c	0.9490	0.2710