Full wwPDB EM Validation Report

Mar 20, 2026 – 06:31 AM UTC

PDB ID	:	9ATZ / pdb_00009atz
EMDB ID	:	EMD-43838
Title	:	HIV 16055.v8.3 SOSIP Env in Complex with V2 Epitope and Anti-Immune Complex pAbs from Rabbit 2464
Authors	:	Brown, S.; Antansijevic, A.; Ward, A.B.
Deposited on	:	2024-02-27
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

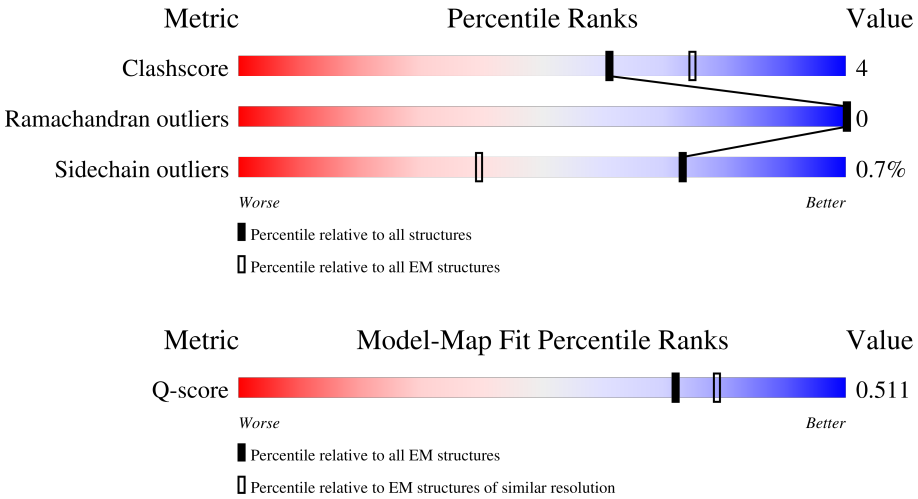
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	108	100%
1	F	108	100%
1	N	108	99%
2	B	112	100%

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Mol	Chain	Length	Quality of chain
2	G	112	100%
2	K	112	100%
3	C	125	100%
3	H	125	100%
3	L	125	100%
4	D	514	75% 9% 16%
4	I	514	78% 6% 16%
4	M	514	77% 7% 16%
5	E	111	100%
5	J	111	100%
5	R	111	100%
6	O	155	14% 65% 17% 18%
6	P	155	12% 71% 12% 17%
6	Q	155	15% 70% 12% 17%
7	S	2	50% 100%
7	T	2	50% 50% 50%
7	U	2	100%
7	W	2	50% 100%
7	X	2	50% 50% 50%
7	Y	2	50% 50%
7	Z	2	100%
7	b	2	50% 100%
7	c	2	50% 50% 50%
7	d	2	50% 50%
7	f	2	50% 50% 50%

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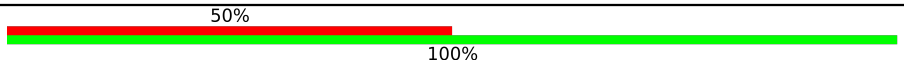
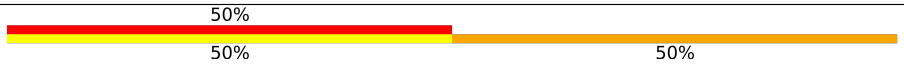
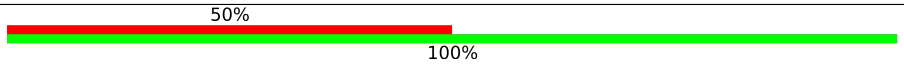
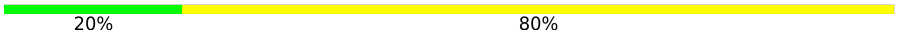
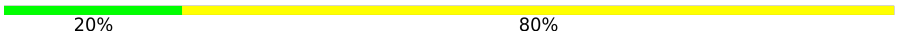
Mol	Chain	Length	Quality of chain
7	g	2	
7	h	2	
7	i	2	
8	V	5	
8	a	5	
8	e	5	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 21190 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 Rabbit V2 Polyclonal Antibody - Predicted Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	108	Total 539	C 323	N 108	O 108	0	0
1	F	108	Total 539	C 323	N 108	O 108	0	0
1	N	108	Total 539	C 323	N 108	O 108	0	0

- Molecule 2 is a protein called Rabbit Anti-Immune Complex Antibody - Predicted Light Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	112	Total 558	C 334	N 112	O 112	0	0
2	G	112	Total 558	C 334	N 112	O 112	0	0
2	K	112	Total 558	C 334	N 112	O 112	0	0

- Molecule 3 is a protein called Rabbit V2 Polyclonal Antibody - Predicted Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	125	Total 622	C 372	N 125	O 125	0	0
3	H	125	Total 622	C 372	N 125	O 125	0	0
3	L	125	Total 622	C 372	N 125	O 125	0	0

- Molecule 4 is a protein called Surface protein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	431	Total 3443	C 2175	N 606	O 635	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	431	Total	C	N	O	S	0	0
			3443	2175	606	635	27		
4	M	431	Total	C	N	O	S	0	0
			3443	2175	606	635	27		

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	MET	-	initiating methionine	UNP A1EAI1
D	-3	ASP	-	expression tag	UNP A1EAI1
D	-2	ALA	-	expression tag	UNP A1EAI1
D	-1	MET	-	expression tag	UNP A1EAI1
D	0	LYS	-	expression tag	UNP A1EAI1
D	1	ARG	-	expression tag	UNP A1EAI1
D	2	GLY	-	expression tag	UNP A1EAI1
D	3	LEU	-	expression tag	UNP A1EAI1
D	4	CYS	-	expression tag	UNP A1EAI1
D	5	CYS	-	expression tag	UNP A1EAI1
D	6	VAL	-	expression tag	UNP A1EAI1
D	7	LEU	-	expression tag	UNP A1EAI1
D	8	LEU	-	expression tag	UNP A1EAI1
D	9	LEU	-	expression tag	UNP A1EAI1
D	10	CYS	-	expression tag	UNP A1EAI1
D	11	GLY	-	expression tag	UNP A1EAI1
D	12	ALA	-	expression tag	UNP A1EAI1
D	13	VAL	-	expression tag	UNP A1EAI1
D	14	PHE	-	expression tag	UNP A1EAI1
D	15	VAL	-	expression tag	UNP A1EAI1
D	16	SER	-	expression tag	UNP A1EAI1
D	17	PRO	-	expression tag	UNP A1EAI1
D	18	SER	-	expression tag	UNP A1EAI1
D	19	GLN	-	expression tag	UNP A1EAI1
D	20	GLU	-	expression tag	UNP A1EAI1
D	21	ILE	-	expression tag	UNP A1EAI1
D	22	HIS	-	expression tag	UNP A1EAI1
D	23	ALA	-	expression tag	UNP A1EAI1
D	24	ARG	-	expression tag	UNP A1EAI1
D	25	PHE	-	expression tag	UNP A1EAI1
D	26	ARG	-	expression tag	UNP A1EAI1
D	27	ARG	-	expression tag	UNP A1EAI1
D	28	GLY	-	expression tag	UNP A1EAI1
D	29	ALA	-	expression tag	UNP A1EAI1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	30	ARG	-	expression tag	UNP A1EAI1
D	47	ASP	GLU	conflict	UNP A1EAI1
D	49	GLU	LYS	conflict	UNP A1EAI1
D	65	LYS	VAL	conflict	UNP A1EAI1
D	66	ARG	HIS	conflict	UNP A1EAI1
D	73	CYS	ALA	conflict	UNP A1EAI1
D	165	LEU	ILE	conflict	UNP A1EAI1
D	304	VAL	ARG	conflict	UNP A1EAI1
D	314	TRP	THR	conflict	UNP A1EAI1
D	317	TYR	ALA	conflict	UNP A1EAI1
D	360	GLN	SER	conflict	UNP A1EAI1
D	426	ARG	GLU	conflict	UNP A1EAI1
D	429	GLN	ARG	conflict	UNP A1EAI1
D	497	ARG	ALA	conflict	UNP A1EAI1
D	498	CYS	ALA	conflict	UNP A1EAI1
D	506	ARG	GLU	conflict	UNP A1EAI1
D	507	ARG	LYS	conflict	UNP A1EAI1
I	-4	MET	-	initiating methionine	UNP A1EAI1
I	-3	ASP	-	expression tag	UNP A1EAI1
I	-2	ALA	-	expression tag	UNP A1EAI1
I	-1	MET	-	expression tag	UNP A1EAI1
I	0	LYS	-	expression tag	UNP A1EAI1
I	1	ARG	-	expression tag	UNP A1EAI1
I	2	GLY	-	expression tag	UNP A1EAI1
I	3	LEU	-	expression tag	UNP A1EAI1
I	4	CYS	-	expression tag	UNP A1EAI1
I	5	CYS	-	expression tag	UNP A1EAI1
I	6	VAL	-	expression tag	UNP A1EAI1
I	7	LEU	-	expression tag	UNP A1EAI1
I	8	LEU	-	expression tag	UNP A1EAI1
I	9	LEU	-	expression tag	UNP A1EAI1
I	10	CYS	-	expression tag	UNP A1EAI1
I	11	GLY	-	expression tag	UNP A1EAI1
I	12	ALA	-	expression tag	UNP A1EAI1
I	13	VAL	-	expression tag	UNP A1EAI1
I	14	PHE	-	expression tag	UNP A1EAI1
I	15	VAL	-	expression tag	UNP A1EAI1
I	16	SER	-	expression tag	UNP A1EAI1
I	17	PRO	-	expression tag	UNP A1EAI1
I	18	SER	-	expression tag	UNP A1EAI1
I	19	GLN	-	expression tag	UNP A1EAI1
I	20	GLU	-	expression tag	UNP A1EAI1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	21	ILE	-	expression tag	UNP A1EAI1
I	22	HIS	-	expression tag	UNP A1EAI1
I	23	ALA	-	expression tag	UNP A1EAI1
I	24	ARG	-	expression tag	UNP A1EAI1
I	25	PHE	-	expression tag	UNP A1EAI1
I	26	ARG	-	expression tag	UNP A1EAI1
I	27	ARG	-	expression tag	UNP A1EAI1
I	28	GLY	-	expression tag	UNP A1EAI1
I	29	ALA	-	expression tag	UNP A1EAI1
I	30	ARG	-	expression tag	UNP A1EAI1
I	47	ASP	GLU	conflict	UNP A1EAI1
I	49	GLU	LYS	conflict	UNP A1EAI1
I	65	LYS	VAL	conflict	UNP A1EAI1
I	66	ARG	HIS	conflict	UNP A1EAI1
I	73	CYS	ALA	conflict	UNP A1EAI1
I	165	LEU	ILE	conflict	UNP A1EAI1
I	304	VAL	ARG	conflict	UNP A1EAI1
I	314	TRP	THR	conflict	UNP A1EAI1
I	317	TYR	ALA	conflict	UNP A1EAI1
I	360	GLN	SER	conflict	UNP A1EAI1
I	426	ARG	GLU	conflict	UNP A1EAI1
I	429	GLN	ARG	conflict	UNP A1EAI1
I	497	ARG	ALA	conflict	UNP A1EAI1
I	498	CYS	ALA	conflict	UNP A1EAI1
I	506	ARG	GLU	conflict	UNP A1EAI1
I	507	ARG	LYS	conflict	UNP A1EAI1
M	-4	MET	-	initiating methionine	UNP A1EAI1
M	-3	ASP	-	expression tag	UNP A1EAI1
M	-2	ALA	-	expression tag	UNP A1EAI1
M	-1	MET	-	expression tag	UNP A1EAI1
M	0	LYS	-	expression tag	UNP A1EAI1
M	1	ARG	-	expression tag	UNP A1EAI1
M	2	GLY	-	expression tag	UNP A1EAI1
M	3	LEU	-	expression tag	UNP A1EAI1
M	4	CYS	-	expression tag	UNP A1EAI1
M	5	CYS	-	expression tag	UNP A1EAI1
M	6	VAL	-	expression tag	UNP A1EAI1
M	7	LEU	-	expression tag	UNP A1EAI1
M	8	LEU	-	expression tag	UNP A1EAI1
M	9	LEU	-	expression tag	UNP A1EAI1
M	10	CYS	-	expression tag	UNP A1EAI1
M	11	GLY	-	expression tag	UNP A1EAI1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	12	ALA	-	expression tag	UNP A1EAI1
M	13	VAL	-	expression tag	UNP A1EAI1
M	14	PHE	-	expression tag	UNP A1EAI1
M	15	VAL	-	expression tag	UNP A1EAI1
M	16	SER	-	expression tag	UNP A1EAI1
M	17	PRO	-	expression tag	UNP A1EAI1
M	18	SER	-	expression tag	UNP A1EAI1
M	19	GLN	-	expression tag	UNP A1EAI1
M	20	GLU	-	expression tag	UNP A1EAI1
M	21	ILE	-	expression tag	UNP A1EAI1
M	22	HIS	-	expression tag	UNP A1EAI1
M	23	ALA	-	expression tag	UNP A1EAI1
M	24	ARG	-	expression tag	UNP A1EAI1
M	25	PHE	-	expression tag	UNP A1EAI1
M	26	ARG	-	expression tag	UNP A1EAI1
M	27	ARG	-	expression tag	UNP A1EAI1
M	28	GLY	-	expression tag	UNP A1EAI1
M	29	ALA	-	expression tag	UNP A1EAI1
M	30	ARG	-	expression tag	UNP A1EAI1
M	47	ASP	GLU	conflict	UNP A1EAI1
M	49	GLU	LYS	conflict	UNP A1EAI1
M	65	LYS	VAL	conflict	UNP A1EAI1
M	66	ARG	HIS	conflict	UNP A1EAI1
M	73	CYS	ALA	conflict	UNP A1EAI1
M	165	LEU	ILE	conflict	UNP A1EAI1
M	304	VAL	ARG	conflict	UNP A1EAI1
M	314	TRP	THR	conflict	UNP A1EAI1
M	317	TYR	ALA	conflict	UNP A1EAI1
M	360	GLN	SER	conflict	UNP A1EAI1
M	426	ARG	GLU	conflict	UNP A1EAI1
M	429	GLN	ARG	conflict	UNP A1EAI1
M	497	ARG	ALA	conflict	UNP A1EAI1
M	498	CYS	ALA	conflict	UNP A1EAI1
M	506	ARG	GLU	conflict	UNP A1EAI1
M	507	ARG	LYS	conflict	UNP A1EAI1

- Molecule 5 is a protein called Rabbit Anti-Immune Complex Antibody - Predicted Heavy Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	111	Total	C	N	O	0	0
			555	333	111	111		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	111	Total	C	N	O	0	0
			555	333	111	111		
5	R	111	Total	C	N	O	0	0
			555	333	111	111		

- Molecule 6 is a protein called Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	127	Total	C	N	O	S	0	0
			1014	637	179	192	6		
6	P	128	Total	C	N	O	S	0	0
			1023	642	181	194	6		
6	Q	128	Total	C	N	O	S	0	0
			1021	642	180	193	6		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	507	ARG	LYS	conflict	UNP A0A0B5KUY7
O	516	SER	ILE	conflict	UNP A0A0B5KUY7
O	556	PRO	ILE	conflict	UNP A0A0B5KUY7
O	558	CYS	ALA	conflict	UNP A0A0B5KUY7
O	565	ASP	LEU	conflict	UNP A0A0B5KUY7
O	566	GLY	THR	conflict	UNP A0A0B5KUY7
O	567	HIS	VAL	conflict	UNP A0A0B5KUY7
O	582	HIS	ARG	conflict	UNP A0A0B5KUY7
O	602	CYS	THR	conflict	UNP A0A0B5KUY7
P	507	ARG	LYS	conflict	UNP A0A0B5KUY7
P	516	SER	ILE	conflict	UNP A0A0B5KUY7
P	556	PRO	ILE	conflict	UNP A0A0B5KUY7
P	558	CYS	ALA	conflict	UNP A0A0B5KUY7
P	565	ASP	LEU	conflict	UNP A0A0B5KUY7
P	566	GLY	THR	conflict	UNP A0A0B5KUY7
P	567	HIS	VAL	conflict	UNP A0A0B5KUY7
P	582	HIS	ARG	conflict	UNP A0A0B5KUY7
P	602	CYS	THR	conflict	UNP A0A0B5KUY7
Q	507	ARG	LYS	conflict	UNP A0A0B5KUY7
Q	516	SER	ILE	conflict	UNP A0A0B5KUY7
Q	556	PRO	ILE	conflict	UNP A0A0B5KUY7
Q	558	CYS	ALA	conflict	UNP A0A0B5KUY7
Q	565	ASP	LEU	conflict	UNP A0A0B5KUY7
Q	566	GLY	THR	conflict	UNP A0A0B5KUY7

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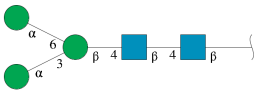
Chain	Residue	Modelled	Actual	Comment	Reference
Q	567	HIS	VAL	conflict	UNP A0A0B5KUY7
Q	582	HIS	ARG	conflict	UNP A0A0B5KUY7
Q	602	CYS	THR	conflict	UNP A0A0B5KUY7

- Molecule 7 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
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	f	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	h	2	Total	C	N	O	0	0
			28	16	2	10		
7	i	2	Total	C	N	O	0	0
			28	16	2	10		

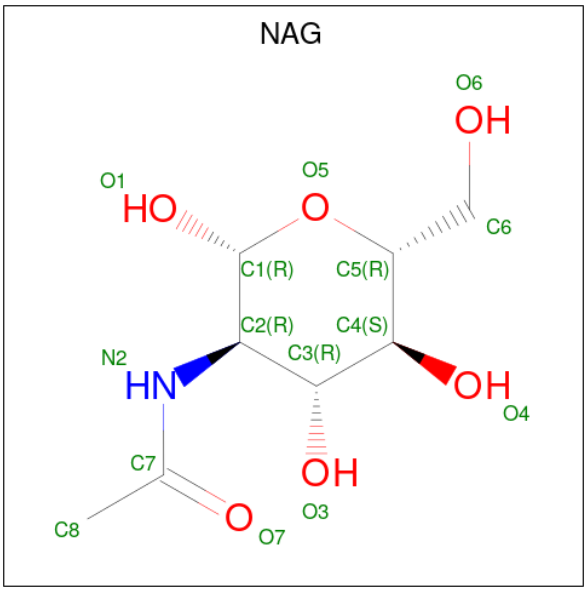
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(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
8	V	5	Total	C	N	O	0	0
			61	34	2	25		
8	a	5	Total	C	N	O	0	0
			61	34	2	25		
8	e	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	N	O	0
			14	8	1	5	
9	D	1	Total	C	N	O	0
			14	8	1	5	
9	D	1	Total	C	N	O	0
			14	8	1	5	
9	D	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	

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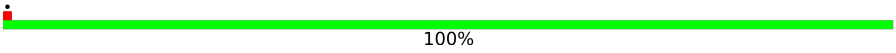
Mol	Chain	Residues	Atoms				AltConf
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	

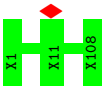
3 Residue-property plots (i)

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: Rabbit V2 Polyclonal Antibody - Predicted Light Chain

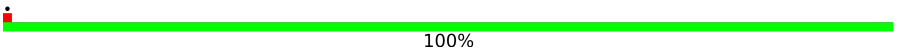
Chain A:

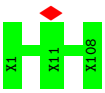




• Molecule 1: Rabbit V2 Polyclonal Antibody - Predicted Light Chain

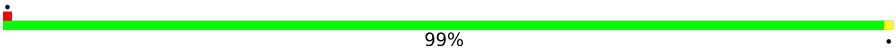
Chain F:

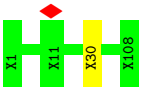




• Molecule 1: Rabbit V2 Polyclonal Antibody - Predicted Light Chain

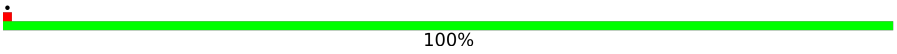
Chain N:

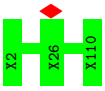




• Molecule 2: Rabbit Anti-Immune Complex Antibody - Predicted Light Chain

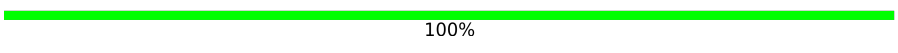
Chain B:





• Molecule 2: Rabbit Anti-Immune Complex Antibody - Predicted Light Chain

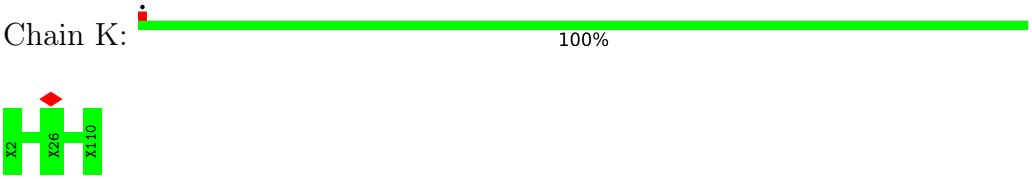
Chain G:



There are no outlier residues recorded for this chain.

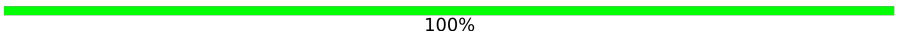
• Molecule 2: Rabbit Anti-Immune Complex Antibody - Predicted Light Chain

Chain K:



• Molecule 3: Rabbit V2 Polyclonal Antibody - Predicted Heavy Chain

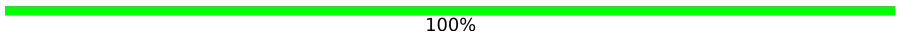
Chain C:



There are no outlier residues recorded for this chain.

• Molecule 3: Rabbit V2 Polyclonal Antibody - Predicted Heavy Chain

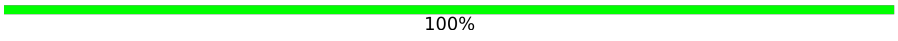
Chain H:



There are no outlier residues recorded for this chain.

• Molecule 3: Rabbit V2 Polyclonal Antibody - Predicted Heavy Chain

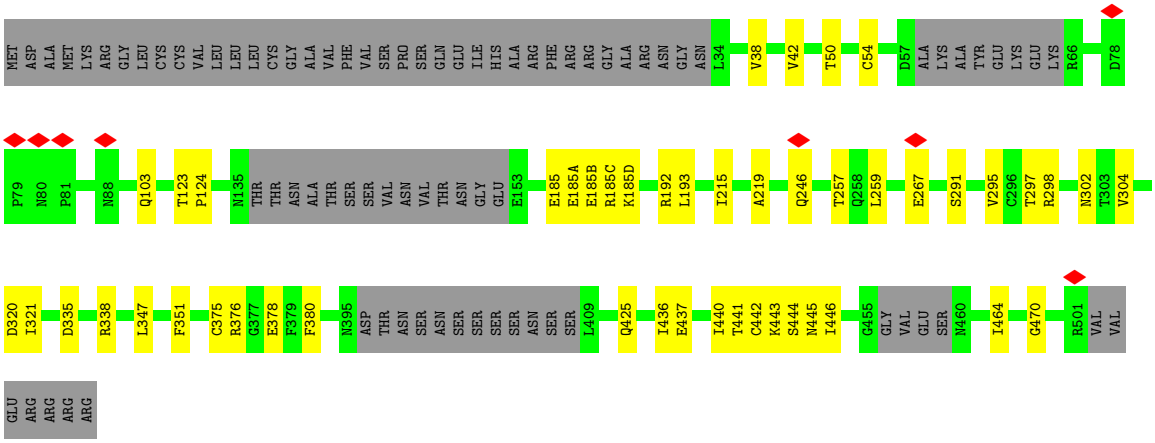
Chain L:



There are no outlier residues recorded for this chain.

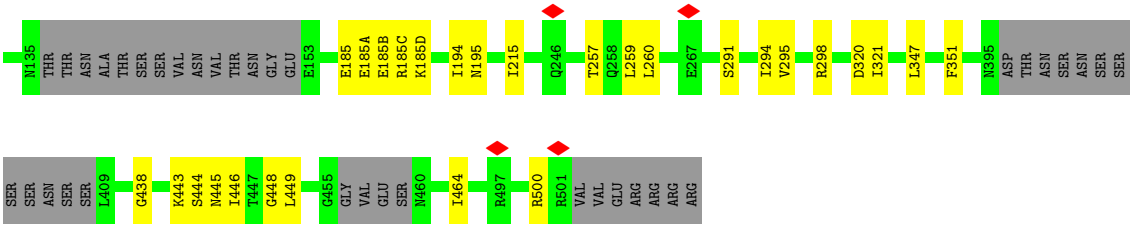
• Molecule 4: Surface protein gp120

Chain D:

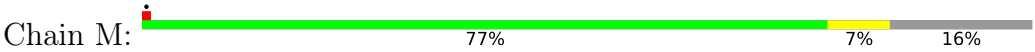


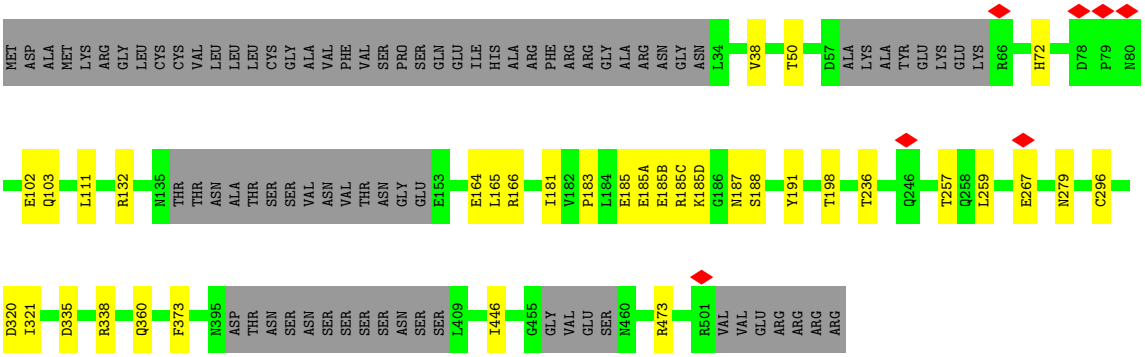
• Molecule 4: Surface protein gp120

Chain I:



• Molecule 4: Surface protein gp120





• Molecule 5: Rabbit Anti-Immune Complex Antibody - Predicted Heavy Chain

There are no outlier residues recorded for this chain.

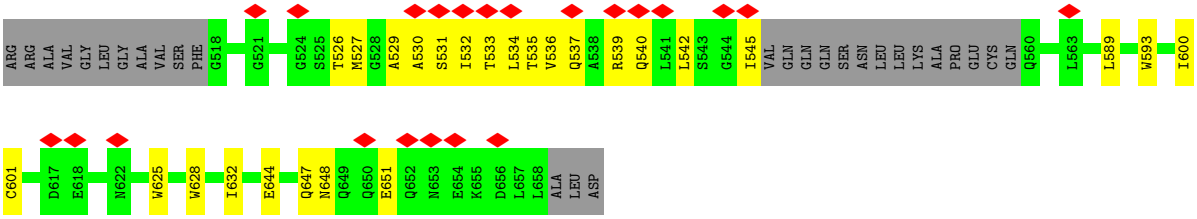
• Molecule 5: Rabbit Anti-Immune Complex Antibody - Predicted Heavy Chain

There are no outlier residues recorded for this chain.

• Molecule 5: Rabbit Anti-Immune Complex Antibody - Predicted Heavy Chain

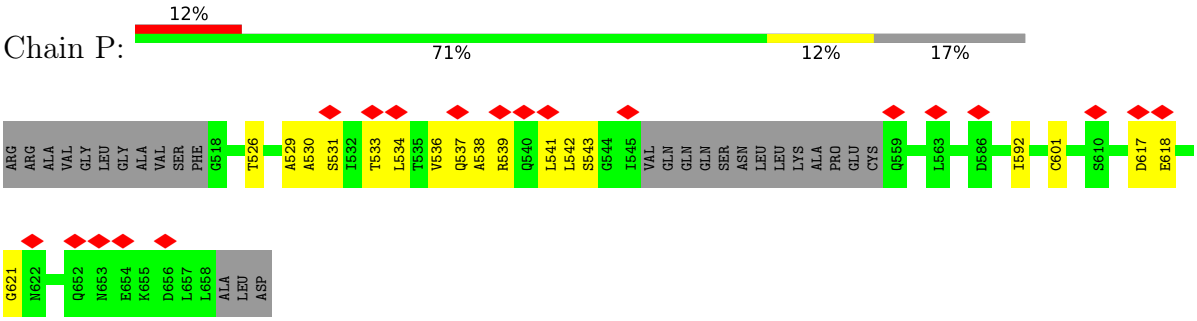
There are no outlier residues recorded for this chain.

• Molecule 6: Transmembrane protein gp41



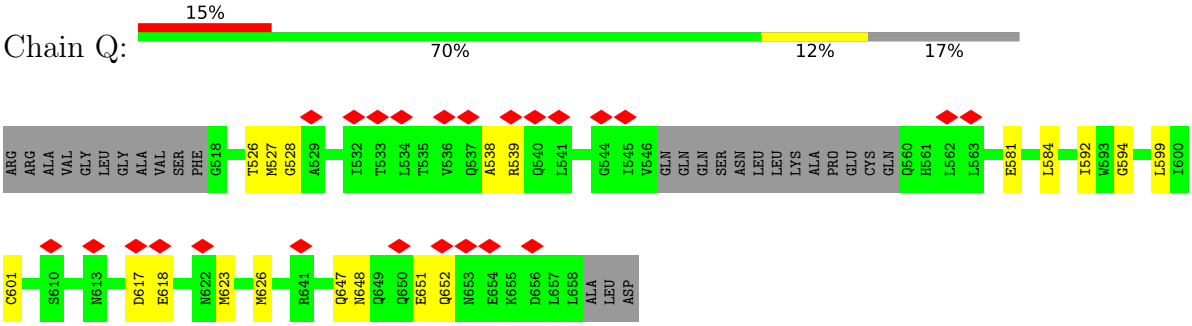
• Molecule 6: Transmembrane protein gp41

Chain P:



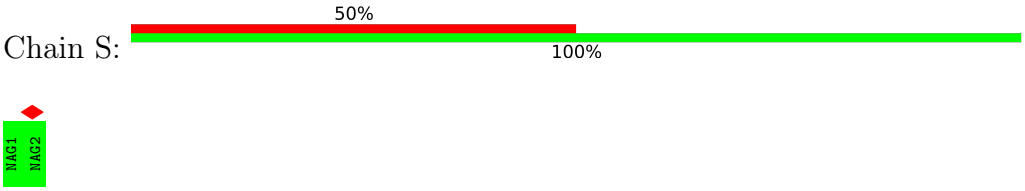
• Molecule 6: Transmembrane protein gp41

Chain Q:



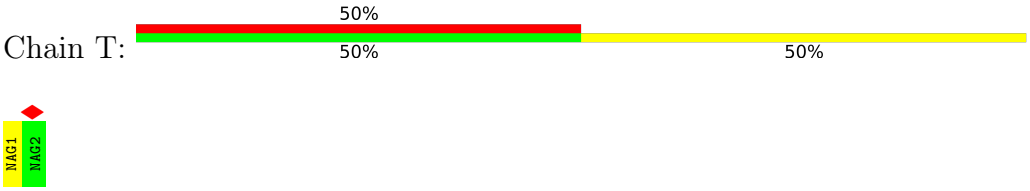
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



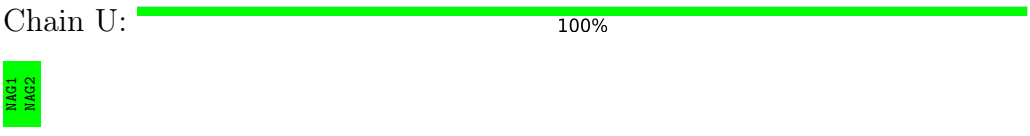
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



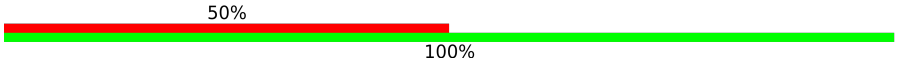
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



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

Chain W:



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

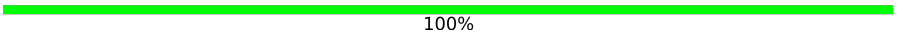
Chain X:

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

Chain Y:

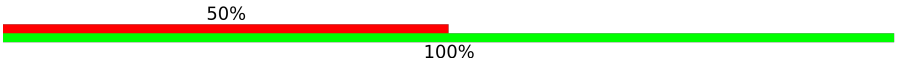
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain b:



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

Chain c:

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

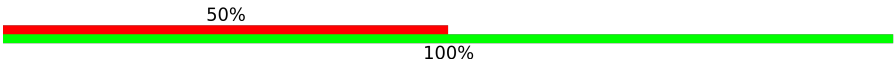
Chain d:

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

Chain f:

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

Chain g:

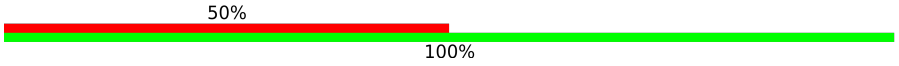


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

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

Chain i:



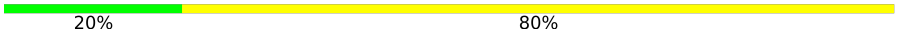
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

• Molecule 8: 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-glucopyra

nose

Chain a:



• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23375	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	376.19998, 376.19998, 376.19998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA

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	$\#\|Z\| > 5$
4	D	0.29	0/3516	0.47	0/4773
4	I	0.26	0/3516	0.44	0/4773
4	M	0.34	0/3516	0.50	0/4773
6	O	0.47	0/1035	0.68	0/1402
6	P	0.31	0/1044	0.52	0/1414
6	Q	0.26	0/1042	0.44	0/1412
All	All	0.31	0/13669	0.49	0/18547

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	539	0	123	0	0
1	F	539	0	123	0	0
1	N	539	0	123	1	0
2	B	558	0	125	0	0
2	G	558	0	127	0	0
2	K	558	0	123	0	0
3	C	622	0	135	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	622	0	134	0	0
3	L	622	0	134	0	0
4	D	3443	0	3398	35	0
4	I	3443	0	3398	18	0
4	M	3443	0	3402	33	0
5	E	555	0	128	0	0
5	J	555	0	128	0	0
5	R	555	0	127	0	0
6	O	1014	0	978	50	0
6	P	1023	0	986	14	0
6	Q	1021	0	986	31	0
7	S	28	0	25	0	0
7	T	28	0	25	1	0
7	U	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	1	0
7	Y	28	0	25	0	0
7	Z	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	1	0
7	d	28	0	25	0	0
7	f	28	0	25	0	0
7	g	28	0	25	0	0
7	h	28	0	25	2	0
7	i	28	0	25	0	0
8	V	61	0	52	0	0
8	a	61	0	52	2	0
8	e	61	0	52	0	0
9	D	126	0	117	2	0
9	I	140	0	130	3	0
9	M	140	0	130	8	0
All	All	21190	0	15561	161	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 4.

All (161) 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)
4:D:376:ARG:HG3	4:D:440:ILE:HG23	1.51	0.89
6:P:531:SER:HA	6:P:534:LEU:HG	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:259:LEU:HD13	4:M:446:ILE:HD13	1.62	0.80
4:M:38:VAL:HB	6:P:601:CYS:SG	2.23	0.79
4:D:259:LEU:HD13	4:D:446:ILE:HD13	1.65	0.79
4:D:378:GLU:HG3	4:D:440:ILE:HD12	1.63	0.79
4:I:38:VAL:HB	6:Q:601:CYS:SG	2.22	0.78
4:M:296:CYS:SG	4:M:373:PHE:CZ	2.76	0.76
4:D:38:VAL:HB	6:O:601:CYS:SG	2.27	0.75
4:D:378:GLU:HG2	4:D:440:ILE:CD1	2.17	0.74
6:O:536:VAL:CG2	6:Q:648:ASN:ND2	2.52	0.72
6:O:545:ILE:HG12	6:Q:584:LEU:HB2	1.71	0.72
4:D:378:GLU:CG	4:D:440:ILE:HD12	2.19	0.71
6:O:527:MET:HE3	6:O:625:TRP:CZ3	2.26	0.70
4:M:335:ASP:OD1	4:M:338:ARG:NH2	2.25	0.70
6:O:628:TRP:CZ2	6:O:632:ILE:HD13	2.27	0.69
6:O:536:VAL:HG22	6:Q:648:ASN:ND2	2.08	0.68
6:O:530:ALA:O	6:O:534:LEU:HG	1.93	0.68
6:Q:526:THR:HG22	6:Q:527:MET:N	2.08	0.68
4:D:378:GLU:CG	4:D:440:ILE:CD1	2.72	0.68
6:O:535:THR:O	6:O:539:ARG:HG2	1.94	0.67
6:O:545:ILE:HG12	6:Q:584:LEU:CB	2.26	0.66
6:O:534:LEU:HA	6:O:537:GLN:HB2	1.78	0.66
4:I:298:ARG:NH2	4:I:438:GLY:O	2.29	0.65
4:M:185(B):GLU:O	4:M:185(C):ARG:HG3	1.97	0.65
4:I:500:ARG:NH1	6:Q:647:GLN:OE1	2.30	0.65
4:D:378:GLU:HG2	4:D:440:ILE:HD13	1.77	0.64
4:D:376:ARG:CG	4:D:440:ILE:HG23	2.26	0.64
4:D:436:ILE:HB	4:D:440:ILE:HD11	1.82	0.62
6:O:530:ALA:O	6:O:534:LEU:N	2.24	0.61
4:D:42:VAL:HA	6:O:534:LEU:HD22	1.83	0.61
4:M:198:THR:HA	9:M:606:NAG:H82	1.83	0.60
6:P:530:ALA:O	6:P:534:LEU:N	2.34	0.60
6:O:527:MET:HE3	6:O:625:TRP:CE3	2.36	0.60
4:D:298:ARG:HH21	4:D:440:ILE:CD1	2.14	0.60
4:I:295:VAL:HG22	4:I:443:LYS:HG2	1.84	0.59
6:O:531:SER:O	6:O:535:THR:HG23	2.02	0.59
6:P:531:SER:HA	6:P:534:LEU:CG	2.31	0.58
4:M:279:ASN:HA	9:M:604:NAG:H83	1.86	0.58
4:D:123:THR:O	4:M:166:ARG:HD2	2.03	0.58
6:O:593:TRP:HE1	6:O:644:GLU:HG3	1.69	0.58
4:D:375:CYS:HB3	4:D:380:PHE:CE1	2.39	0.57
6:O:527:MET:HE1	6:O:628:TRP:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:259:LEU:HD13	4:I:446:ILE:HD13	1.87	0.56
6:O:527:MET:HA	6:O:625:TRP:CD1	2.40	0.56
4:D:124:PRO:HA	4:M:166:ARG:CZ	2.36	0.56
6:O:600:ILE:HD11	6:Q:651:GLU:C	2.30	0.55
6:O:534:LEU:HD12	6:O:535:THR:N	2.22	0.55
6:P:541:LEU:HG	6:P:543:SER:HB3	1.88	0.55
4:M:181:ILE:CG2	4:M:191:TYR:HB3	2.37	0.55
6:Q:526:THR:HG22	6:Q:527:MET:H	1.72	0.54
6:O:539:ARG:HH11	6:Q:592:ILE:HG23	1.72	0.54
4:M:185(B):GLU:C	4:M:185(C):ARG:HG3	2.33	0.54
6:O:536:VAL:HG23	6:Q:648:ASN:ND2	2.22	0.54
6:O:536:VAL:HG23	6:Q:648:ASN:HD21	1.73	0.54
7:T:1:NAG:O7	7:T:1:NAG:O3	2.26	0.54
6:O:542:LEU:HD22	6:Q:592:ILE:HD13	1.89	0.53
6:P:526:THR:O	6:P:529:ALA:N	2.42	0.53
6:P:526:THR:HG23	6:P:621:GLY:O	2.07	0.53
4:I:260:LEU:HD12	4:I:448:GLY:HA3	1.91	0.52
4:D:444:SER:HA	9:D:609:NAG:H81	1.90	0.52
6:O:539:ARG:HG3	6:Q:648:ASN:HB2	1.91	0.52
9:M:610:NAG:C1	9:M:610:NAG:O7	2.58	0.52
6:O:545:ILE:HD11	6:Q:581:GLU:HA	1.91	0.52
6:P:534:LEU:O	6:P:538:ALA:HB2	2.10	0.52
4:M:185(C):ARG:HH22	9:M:601:NAG:H82	1.75	0.51
6:O:527:MET:CE	6:O:628:TRP:CD1	2.93	0.50
6:O:536:VAL:HA	6:O:539:ARG:HB2	1.92	0.50
6:O:600:ILE:HD11	6:Q:651:GLU:O	2.12	0.50
6:O:628:TRP:CH2	6:O:632:ILE:HG21	2.46	0.50
4:D:376:ARG:HG2	4:D:442:CYS:SG	2.51	0.50
6:O:530:ALA:HA	6:O:533:THR:OG1	2.10	0.50
6:Q:526:THR:CG2	6:Q:527:MET:N	2.73	0.50
4:M:181:ILE:HG22	4:M:191:TYR:HB3	1.93	0.50
6:O:530:ALA:O	6:O:534:LEU:CG	2.58	0.49
4:D:295:VAL:HG13	4:D:443:LYS:HG2	1.92	0.49
4:I:320:ASP:OD1	4:I:321:ILE:N	2.45	0.49
4:D:297:THR:HB	4:D:441:THR:HG23	1.95	0.49
4:I:448:GLY:C	4:I:449:LEU:HD12	2.37	0.49
4:M:185(B):GLU:O	4:M:185(C):ARG:CG	2.60	0.49
4:D:335:ASP:OD1	4:D:338:ARG:NH2	2.43	0.49
4:M:132:ARG:HB3	4:M:188:SER:HB3	1.93	0.49
6:Q:526:THR:HG22	6:Q:528:GLY:H	1.78	0.49
4:I:194:ILE:HG12	4:I:195:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:183:PRO:HA	4:M:191:TYR:CD2	2.48	0.48
4:D:320:ASP:OD1	4:D:321:ILE:N	2.45	0.48
9:I:610:NAG:C1	9:I:610:NAG:O7	2.62	0.48
4:D:192:ARG:NH1	4:D:193:LEU:O	2.47	0.48
4:D:425:GLN:NE2	4:D:470:GLY:O	2.44	0.48
4:I:295:VAL:HG13	4:I:443:LYS:HG2	1.95	0.48
6:O:533:THR:O	6:O:537:GLN:N	2.28	0.47
6:O:532:ILE:HG23	6:Q:652:GLN:HE22	1.79	0.47
4:I:294:ILE:HG22	4:I:444:SER:O	2.15	0.47
4:M:320:ASP:OD1	4:M:321:ILE:N	2.46	0.47
6:O:531:SER:HA	6:O:534:LEU:HD21	1.96	0.47
6:P:539:ARG:O	6:P:542:LEU:HG	2.15	0.47
4:D:291:SER:HB2	4:D:445:ASN:HB3	1.97	0.47
4:D:219:ALA:O	4:D:246:GLN:NE2	2.45	0.46
4:M:185(C):ARG:NH2	9:M:601:NAG:HN2	2.14	0.46
6:O:534:LEU:HD12	6:O:534:LEU:C	2.40	0.46
4:M:236:THR:HB	9:M:608:NAG:O7	2.16	0.46
6:O:648:ASN:HD21	6:P:536:VAL:HG22	1.81	0.46
6:Q:526:THR:CG2	6:Q:527:MET:H	2.29	0.46
4:D:295:VAL:HG22	4:D:443:LYS:HG2	1.98	0.46
6:Q:617:ASP:OD1	6:Q:618:GLU:N	2.48	0.46
4:D:257:THR:O	4:D:259:LEU:N	2.49	0.46
6:O:600:ILE:HG13	6:O:600:ILE:O	2.16	0.46
4:M:185(D):LYS:NZ	1:N:30:UNK:O	2.31	0.45
4:M:185(C):ARG:HB3	4:M:187:ASN:HB2	1.99	0.45
4:I:257:THR:O	4:I:259:LEU:N	2.50	0.45
4:M:164:GLU:HG2	4:M:165:LEU:N	2.31	0.45
4:M:185(C):ARG:HH22	9:M:601:NAG:HN2	1.64	0.45
4:M:296:CYS:SG	4:M:373:PHE:HZ	2.37	0.45
4:M:50:THR:O	4:M:103:GLN:NE2	2.47	0.45
6:O:526:THR:HG22	6:O:527:MET:N	2.32	0.45
6:Q:618:GLU:O	6:Q:623:MET:N	2.44	0.44
6:O:532:ILE:HG23	6:Q:652:GLN:NE2	2.32	0.44
6:Q:538:ALA:HB1	6:Q:599:LEU:HD13	1.99	0.44
6:P:533:THR:O	6:P:537:GLN:HG2	2.17	0.44
4:D:54:CYS:SG	4:D:215:ILE:HG23	2.58	0.44
4:D:347:LEU:O	4:D:351:PHE:N	2.51	0.44
4:D:50:THR:O	4:D:103:GLN:NE2	2.45	0.44
4:D:378:GLU:HB2	4:D:380:PHE:CE1	2.52	0.43
4:M:267:GLU:OE1	4:M:267:GLU:N	2.52	0.43
6:P:617:ASP:OD1	6:P:618:GLU:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:610:NAG:H81	8:a:1:NAG:H62	2.00	0.43
6:O:589:LEU:HB3	6:O:593:TRP:CZ3	2.54	0.43
4:D:304:VAL:H	4:D:437:GLU:CD	2.27	0.42
4:M:102:GLU:HG2	4:M:473:ARG:HH12	1.84	0.42
6:O:529:ALA:O	6:O:533:THR:HG23	2.19	0.42
6:O:589:LEU:HB3	6:O:593:TRP:CH2	2.53	0.42
6:O:539:ARG:HE	6:Q:648:ASN:HB2	1.84	0.42
6:P:534:LEU:O	6:P:538:ALA:CB	2.68	0.42
7:h:1:NAG:H82	7:h:1:NAG:H3	2.00	0.42
4:I:45:TRP:H	6:Q:626:MET:HE1	1.85	0.42
4:I:194:ILE:O	4:I:195:ASN:HB2	2.18	0.42
4:M:259:LEU:HB3	4:M:446:ILE:HG23	2.02	0.42
6:O:531:SER:HA	6:O:534:LEU:CD2	2.50	0.42
4:M:185:GLU:HG2	4:M:185(A):GLU:N	2.35	0.41
6:O:647:GLN:NE2	6:O:651:GLU:OE2	2.53	0.41
4:D:267:GLU:OE1	4:D:267:GLU:N	2.51	0.41
4:I:291:SER:HB2	4:I:445:ASN:HB3	2.02	0.41
4:I:54:CYS:SG	4:I:215:ILE:HG23	2.60	0.41
6:O:540:GLN:O	6:O:542:LEU:HG	2.19	0.41
4:D:464:ILE:HD11	7:X:1:NAG:H81	2.02	0.41
9:I:610:NAG:C8	8:a:1:NAG:H62	2.51	0.41
4:M:72:HIS:HB3	4:M:111:LEU:HD21	2.02	0.41
4:I:347:LEU:O	4:I:351:PHE:N	2.53	0.41
4:I:464:ILE:HD11	7:c:1:NAG:H81	2.03	0.41
4:M:185(C):ARG:HH22	9:M:601:NAG:C8	2.34	0.41
4:M:360:GLN:HE22	7:h:2:NAG:C1	2.34	0.41
6:O:542:LEU:HD22	6:Q:592:ILE:CD1	2.50	0.41
6:O:600:ILE:HD11	6:Q:651:GLU:HB3	2.03	0.41
6:O:628:TRP:CH2	6:O:632:ILE:CG2	3.04	0.41
4:M:257:THR:O	4:M:259:LEU:N	2.50	0.41
6:O:628:TRP:CE2	6:O:632:ILE:HD13	2.55	0.41
6:P:592:ILE:HD13	6:Q:599:LEU:HD11	2.03	0.41
6:Q:539:ARG:NH1	6:Q:599:LEU:HD12	2.36	0.40
4:D:302:ASN:O	4:D:437:GLU:HG3	2.21	0.40
6:Q:594:GLY:HA3	6:Q:647:GLN:OE1	2.21	0.40
9:D:602:NAG:H83	9:D:608:NAG:H4	2.04	0.40

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	
4	D	421/514 (82%)	406 (96%)	15 (4%)	0	100	100
4	I	421/514 (82%)	408 (97%)	13 (3%)	0	100	100
4	M	421/514 (82%)	407 (97%)	14 (3%)	0	100	100
6	O	123/155 (79%)	121 (98%)	2 (2%)	0	100	100
6	P	124/155 (80%)	118 (95%)	6 (5%)	0	100	100
6	Q	124/155 (80%)	118 (95%)	6 (5%)	0	100	100
All	All	1634/2007 (81%)	1578 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	390/460 (85%)	385 (99%)	5 (1%)	61	71
4	I	390/460 (85%)	385 (99%)	5 (1%)	61	71
4	M	390/460 (85%)	390 (100%)	0	100	100
6	O	109/131 (83%)	109 (100%)	0	100	100
6	P	110/131 (84%)	110 (100%)	0	100	100
6	Q	110/131 (84%)	110 (100%)	0	100	100
All	All	1499/1773 (84%)	1489 (99%)	10 (1%)	73	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	185	GLU
4	D	185(A)	GLU
4	D	185(B)	GLU
4	D	185(C)	ARG
4	D	185(D)	LYS
4	I	185	GLU
4	I	185(A)	GLU
4	I	185(B)	GLU
4	I	185(C)	ARG
4	I	185(D)	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	195	ASN
4	D	350	HIS
4	D	422	ASN
4	D	429	GLN
4	I	195	ASN
4	I	313	GLN
4	I	350	HIS
4	I	422	ASN
4	I	429	GLN
4	M	195	ASN
4	M	422	ASN
4	M	429	GLN
6	Q	537	GLN
6	Q	648	ASN
6	Q	652	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

43 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	$\#\|Z\| > 2$
7	NAG	S	1	4,7	14,14,15	0.15	0	17,19,21	0.60	0
7	NAG	S	2	7	14,14,15	0.22	0	17,19,21	0.47	0
7	NAG	T	1	4,7	14,14,15	0.53	0	17,19,21	0.70	0
7	NAG	T	2	7	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	U	1	4,7	14,14,15	0.24	0	17,19,21	0.41	0
7	NAG	U	2	7	14,14,15	0.50	0	17,19,21	0.50	0
8	NAG	V	1	4,8	14,14,15	0.31	0	17,19,21	0.76	1 (5%)
8	NAG	V	2	8	14,14,15	0.34	0	17,19,21	0.75	1 (5%)
8	BMA	V	3	8	11,11,12	0.61	0	15,15,17	0.82	0
8	MAN	V	4	8	11,11,12	0.57	0	15,15,17	0.90	1 (6%)
8	MAN	V	5	8	11,11,12	0.62	0	15,15,17	0.92	2 (13%)
7	NAG	W	1	4,7	14,14,15	0.26	0	17,19,21	0.43	0
7	NAG	W	2	7	14,14,15	0.24	0	17,19,21	0.50	0
7	NAG	X	1	4,7	14,14,15	0.26	0	17,19,21	0.46	0
7	NAG	X	2	7	14,14,15	0.23	0	17,19,21	0.45	0
7	NAG	Y	1	4,7	14,14,15	0.53	0	17,19,21	1.09	1 (5%)
7	NAG	Y	2	7	14,14,15	0.20	0	17,19,21	0.55	0
7	NAG	Z	1	4,7	14,14,15	0.34	0	17,19,21	0.41	0
7	NAG	Z	2	7	14,14,15	0.49	0	17,19,21	0.52	0
8	NAG	a	1	4,8	14,14,15	0.44	0	17,19,21	0.54	0
8	NAG	a	2	8	14,14,15	0.39	0	17,19,21	0.76	0
8	BMA	a	3	8	11,11,12	1.04	1 (9%)	15,15,17	1.48	2 (13%)
8	MAN	a	4	8	11,11,12	1.37	1 (9%)	15,15,17	1.19	3 (20%)
8	MAN	a	5	8	11,11,12	0.62	0	15,15,17	1.00	2 (13%)
7	NAG	b	1	4,7	14,14,15	0.26	0	17,19,21	0.50	0
7	NAG	b	2	7	14,14,15	0.24	0	17,19,21	0.48	0
7	NAG	c	1	4,7	14,14,15	0.26	0	17,19,21	0.47	0
7	NAG	c	2	7	14,14,15	0.22	0	17,19,21	0.45	0
7	NAG	d	1	4,7	14,14,15	0.45	0	17,19,21	1.08	1 (5%)
7	NAG	d	2	7	14,14,15	0.20	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	e	1	4,8	14,14,15	0.24	0	17,19,21	0.56	0
8	NAG	e	2	8	14,14,15	0.22	0	17,19,21	0.42	0
8	BMA	e	3	8	11,11,12	0.53	0	15,15,17	0.71	0
8	MAN	e	4	8	11,11,12	0.53	0	15,15,17	0.94	2 (13%)
8	MAN	e	5	8	11,11,12	0.59	0	15,15,17	0.90	1 (6%)
7	NAG	f	1	4,7	14,14,15	0.32	0	17,19,21	0.83	1 (5%)
7	NAG	f	2	7	14,14,15	0.25	0	17,19,21	0.51	0
7	NAG	g	1	4,7	14,14,15	0.33	0	17,19,21	0.54	0
7	NAG	g	2	7	14,14,15	0.29	0	17,19,21	0.55	0
7	NAG	h	1	4,7	14,14,15	0.38	0	17,19,21	1.21	3 (17%)
7	NAG	h	2	7	14,14,15	0.30	0	17,19,21	0.64	0
7	NAG	i	1	4,7	14,14,15	0.33	0	17,19,21	0.55	0
7	NAG	i	2	7	14,14,15	0.27	0	17,19,21	0.65	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	S	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	3/6/23/26	0/1/1/1
7	NAG	T	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	NAG	U	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	2/6/23/26	0/1/1/1
8	NAG	V	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
8	BMA	V	3	8	-	2/2/19/22	0/1/1/1
8	MAN	V	4	8	-	2/2/19/22	0/1/1/1
8	MAN	V	5	8	-	0/2/19/22	0/1/1/1
7	NAG	W	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	4/6/23/26	0/1/1/1
7	NAG	X	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	1/6/23/26	0/1/1/1
7	NAG	Y	1	4,7	-	4/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	0/6/23/26	0/1/1/1
7	NAG	Z	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	a	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	BMA	a	3	8	-	2/2/19/22	0/1/1/1
8	MAN	a	4	8	-	0/2/19/22	0/1/1/1
8	MAN	a	5	8	-	2/2/19/22	0/1/1/1
7	NAG	b	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	4/6/23/26	0/1/1/1
7	NAG	c	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	1/6/23/26	0/1/1/1
7	NAG	d	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
8	NAG	e	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	2/6/23/26	0/1/1/1
8	BMA	e	3	8	-	0/2/19/22	0/1/1/1
8	MAN	e	4	8	-	0/2/19/22	0/1/1/1
8	MAN	e	5	8	-	2/2/19/22	0/1/1/1
7	NAG	f	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	f	2	7	-	2/6/23/26	0/1/1/1
7	NAG	g	1	4,7	-	3/6/23/26	0/1/1/1
7	NAG	g	2	7	-	4/6/23/26	0/1/1/1
7	NAG	h	1	4,7	-	3/6/23/26	0/1/1/1
7	NAG	h	2	7	-	2/6/23/26	0/1/1/1
7	NAG	i	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	4	MAN	C1-C2	4.35	1.62	1.52
8	a	3	BMA	C1-C2	2.27	1.57	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	3	BMA	C1-C2-C3	-3.88	104.00	109.64
7	d	1	NAG	C2-N2-C7	3.20	127.18	122.90
7	Y	1	NAG	C2-N2-C7	3.17	127.15	122.90
7	h	1	NAG	C1-O5-C5	-2.94	108.24	112.19
7	f	1	NAG	C2-N2-C7	2.78	126.62	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	4	MAN	O2-C2-C3	-2.69	104.57	110.15
8	a	3	BMA	O3-C3-C2	2.43	115.01	110.05
8	e	4	MAN	C1-O5-C5	2.41	115.42	112.19
8	a	4	MAN	C1-C2-C3	2.37	113.10	109.64
7	h	1	NAG	C4-C3-C2	2.34	114.45	111.02
8	a	5	MAN	O2-C2-C3	-2.32	105.34	110.15
7	h	1	NAG	C3-C4-C5	2.27	114.34	110.23
8	V	2	NAG	C1-O5-C5	2.23	115.17	112.19
8	V	4	MAN	O2-C2-C3	-2.18	105.63	110.15
8	a	5	MAN	C1-O5-C5	2.14	115.06	112.19
8	e	4	MAN	O2-C2-C3	-2.12	105.77	110.15
8	V	1	NAG	C1-O5-C5	2.10	115.00	112.19
8	e	5	MAN	O2-C2-C3	-2.09	105.82	110.15
8	V	5	MAN	C1-O5-C5	2.08	114.98	112.19
8	a	4	MAN	C1-O5-C5	2.08	114.98	112.19
8	V	5	MAN	O2-C2-C3	-2.02	105.97	110.15

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	g	2	NAG	C3-C2-N2-C7
7	g	2	NAG	C8-C7-N2-C2
7	g	2	NAG	O7-C7-N2-C2
7	h	1	NAG	C1-C2-N2-C7
7	h	1	NAG	C8-C7-N2-C2
7	h	1	NAG	O7-C7-N2-C2
7	h	2	NAG	C8-C7-N2-C2
7	h	2	NAG	O7-C7-N2-C2
8	a	3	BMA	C4-C5-C6-O6
8	a	5	MAN	C4-C5-C6-O6
8	e	2	NAG	O5-C5-C6-O6
8	V	4	MAN	O5-C5-C6-O6
8	e	5	MAN	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
8	V	3	BMA	O5-C5-C6-O6
8	a	3	BMA	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	Y	1	NAG	O5-C5-C6-O6
8	a	5	MAN	O5-C5-C6-O6
7	Y	1	NAG	C4-C5-C6-O6
8	e	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	Y	1	NAG	C8-C7-N2-C2
7	Y	1	NAG	O7-C7-N2-C2
7	d	1	NAG	C8-C7-N2-C2
7	d	1	NAG	O7-C7-N2-C2
7	f	1	NAG	C8-C7-N2-C2
7	f	1	NAG	O7-C7-N2-C2
7	b	2	NAG	C4-C5-C6-O6
8	V	4	MAN	C4-C5-C6-O6
8	e	5	MAN	C4-C5-C6-O6
7	g	1	NAG	C8-C7-N2-C2
7	b	2	NAG	O5-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
7	g	1	NAG	O7-C7-N2-C2
7	Z	2	NAG	O5-C5-C6-O6
7	U	2	NAG	C4-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	W	2	NAG	C1-C2-N2-C7
7	b	2	NAG	C1-C2-N2-C7
7	f	2	NAG	C1-C2-N2-C7
8	V	2	NAG	C1-C2-N2-C7
8	V	3	BMA	C4-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
7	T	1	NAG	C3-C2-N2-C7
7	i	2	NAG	C3-C2-N2-C7
8	a	2	NAG	C3-C2-N2-C7
7	c	1	NAG	O5-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
7	S	2	NAG	C1-C2-N2-C7
7	T	1	NAG	C1-C2-N2-C7
7	i	2	NAG	C1-C2-N2-C7
8	a	2	NAG	C1-C2-N2-C7
7	g	1	NAG	O5-C5-C6-O6
7	W	2	NAG	C3-C2-N2-C7
7	b	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	f	2	NAG	C3-C2-N2-C7
8	V	2	NAG	C3-C2-N2-C7
7	X	1	NAG	O5-C5-C6-O6

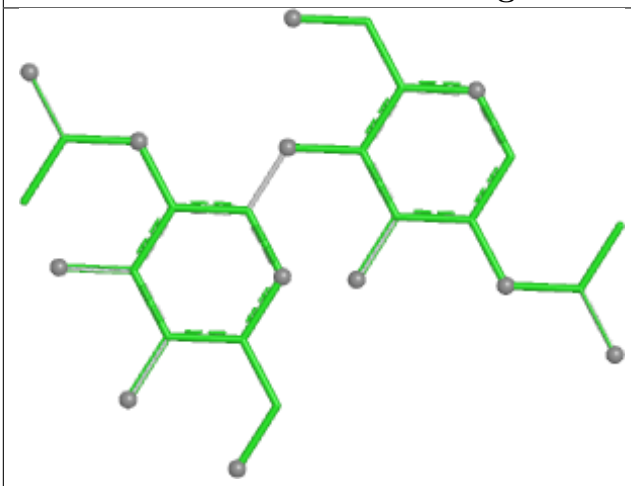
There are no ring outliers.

6 monomers are involved in 7 short contacts:

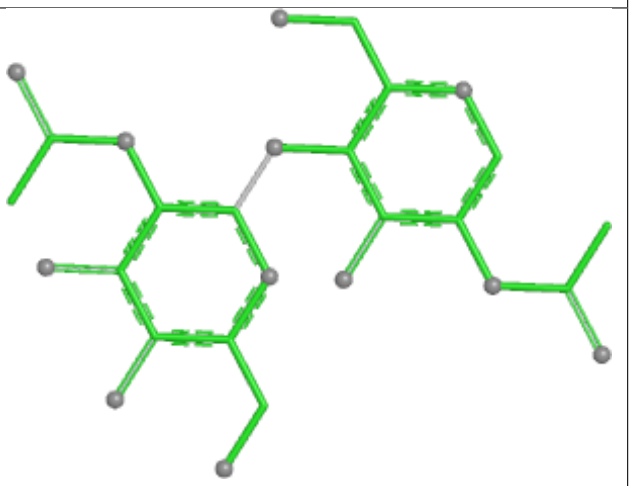
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	1	NAG	1	0
7	X	1	NAG	1	0
7	h	2	NAG	1	0
8	a	1	NAG	2	0
7	h	1	NAG	1	0
7	c	1	NAG	1	0

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

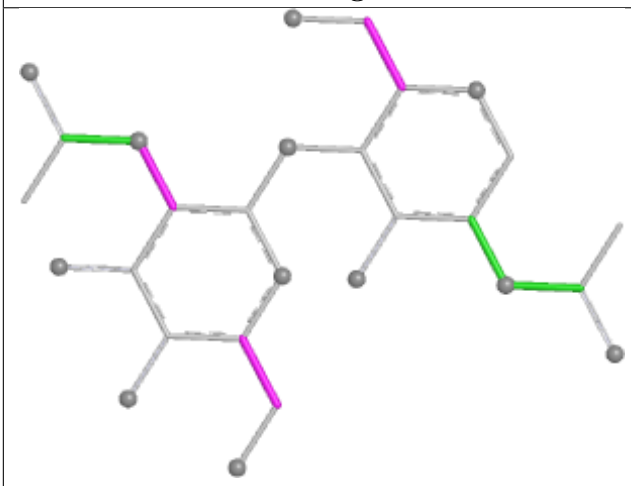
Oligosaccharide Chain S



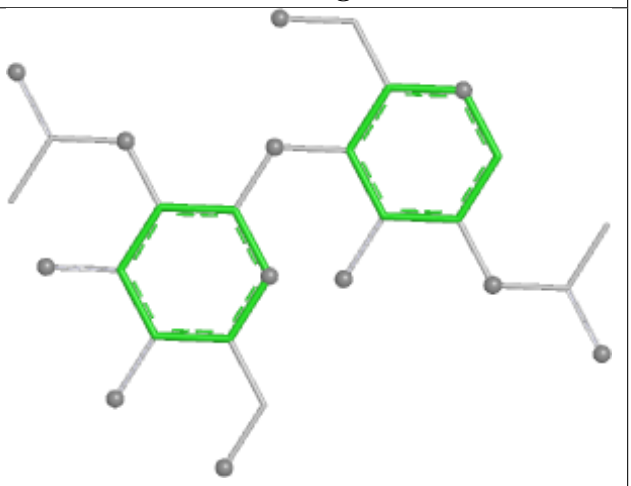
Bond lengths



Bond angles

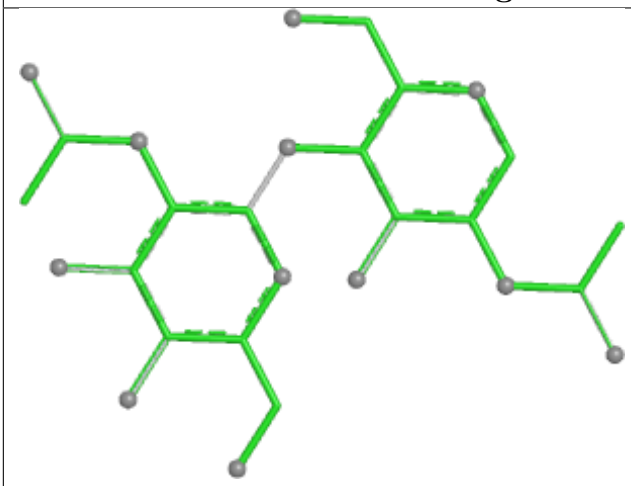


Torsions

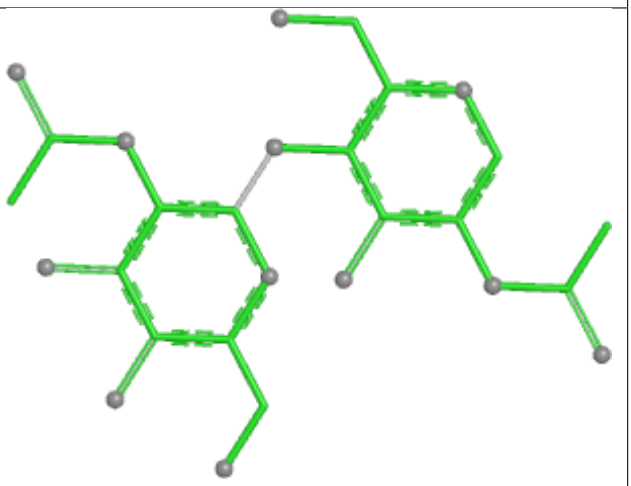


Rings

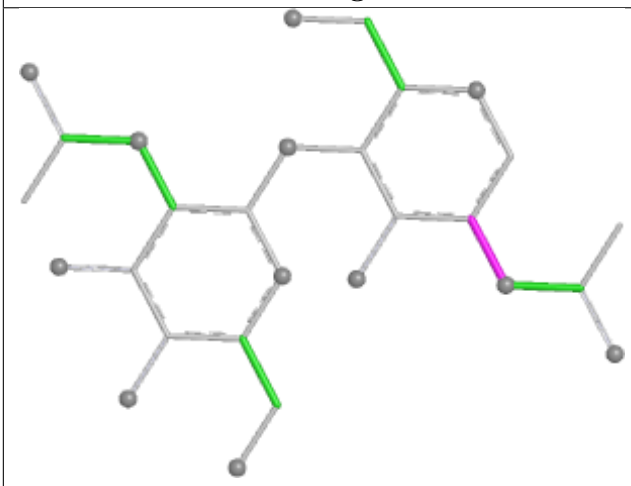
Oligosaccharide Chain T



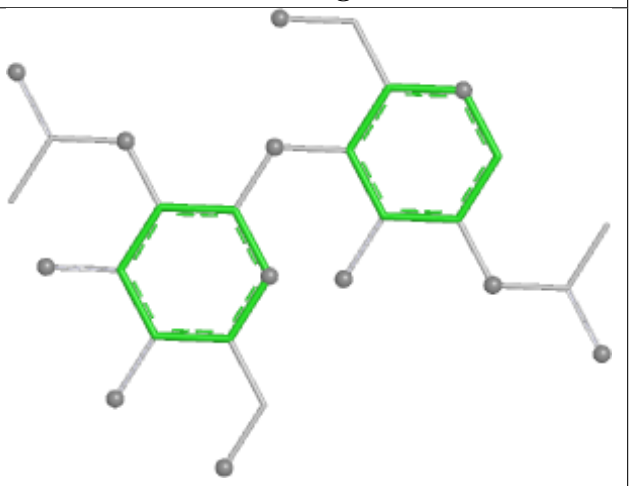
Bond lengths



Bond angles

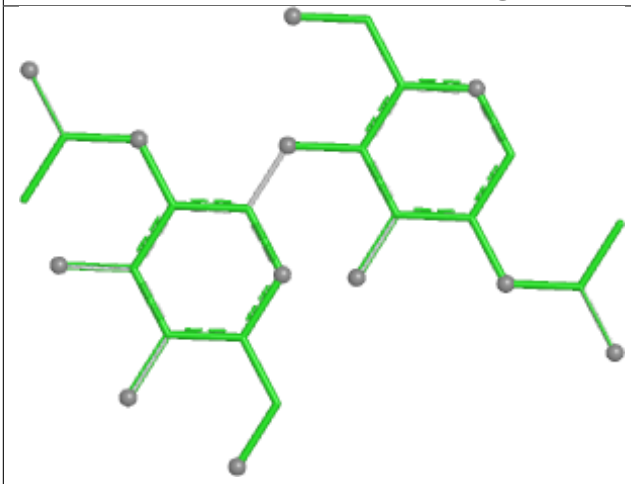


Torsions

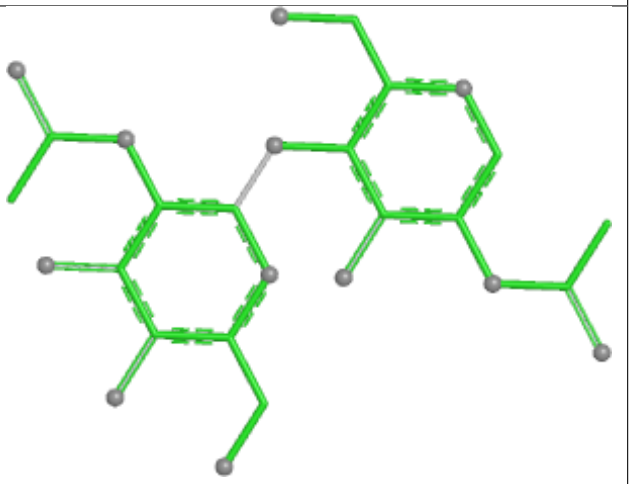


Rings

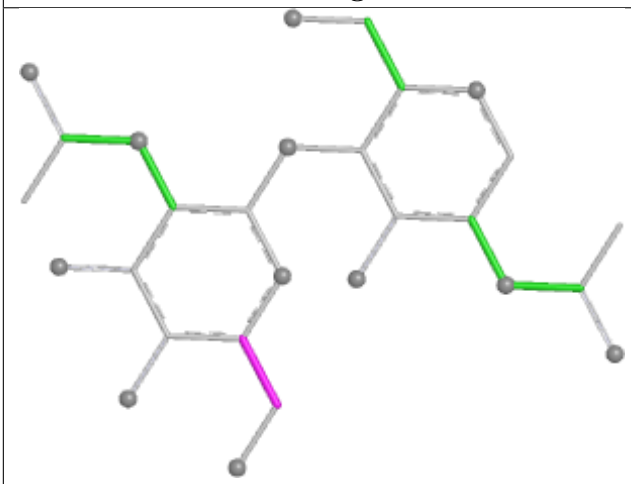
Oligosaccharide Chain U



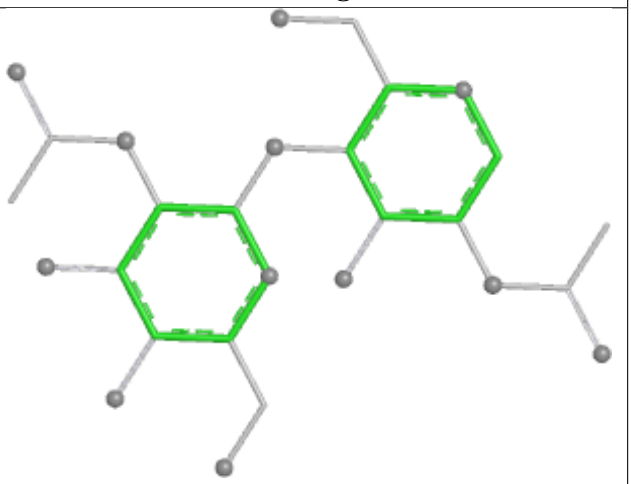
Bond lengths



Bond angles

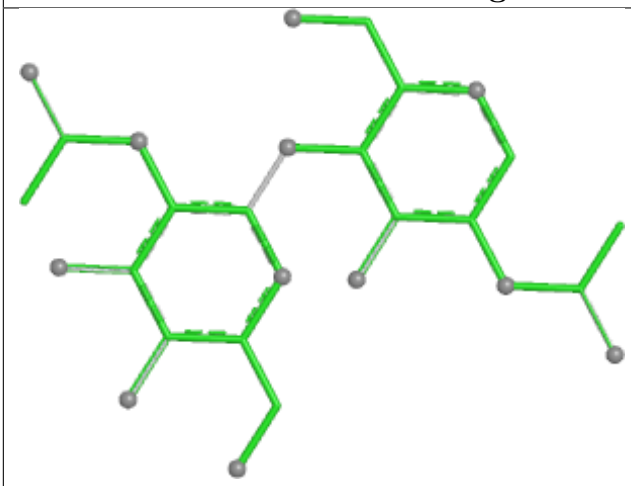


Torsions

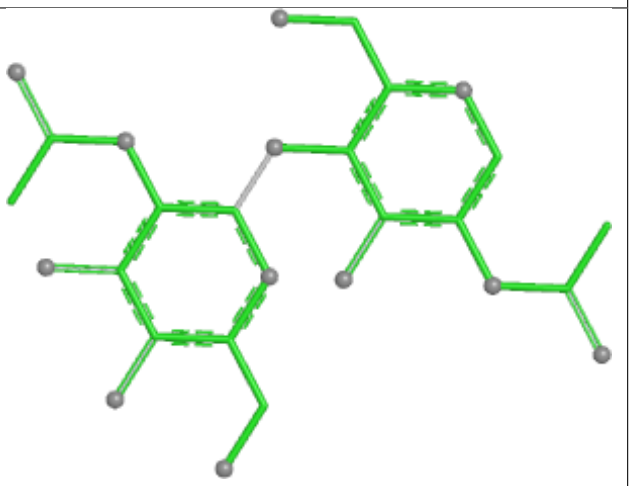


Rings

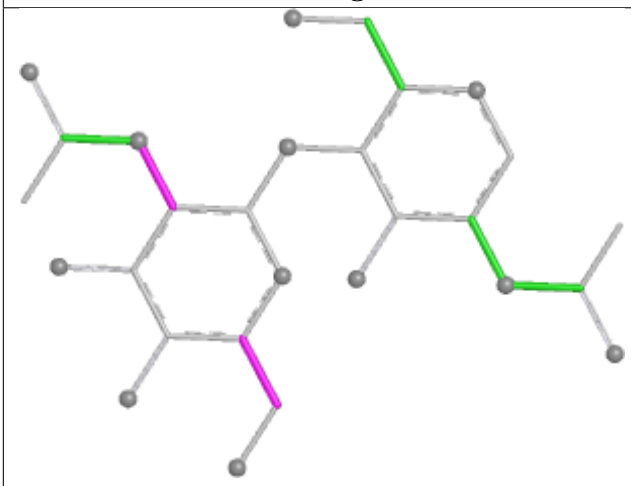
Oligosaccharide Chain W



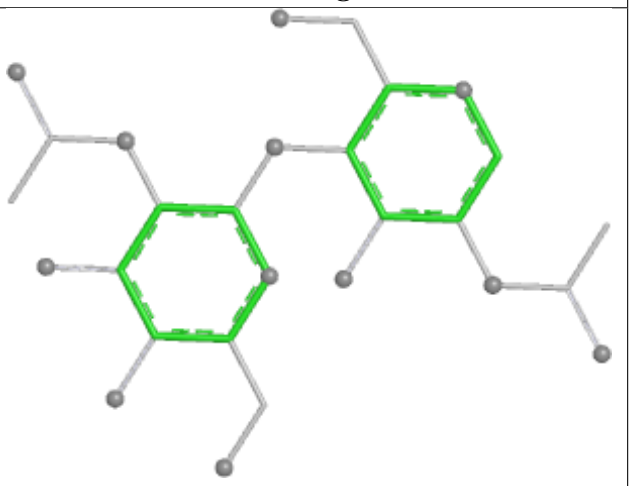
Bond lengths



Bond angles

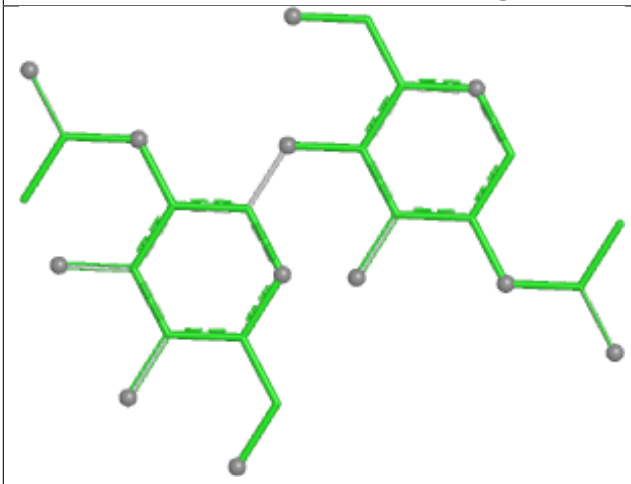


Torsions

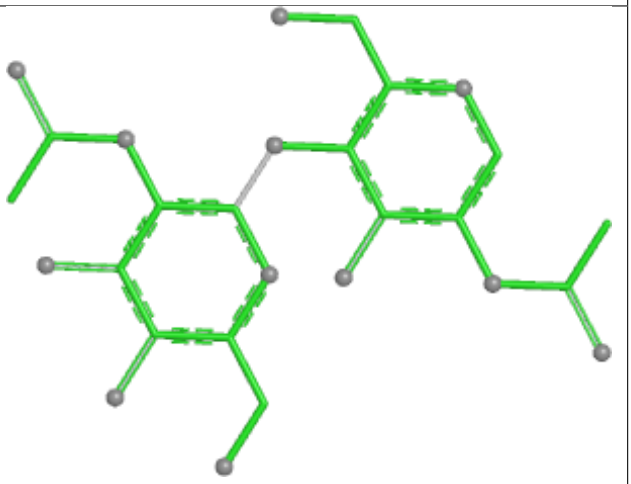


Rings

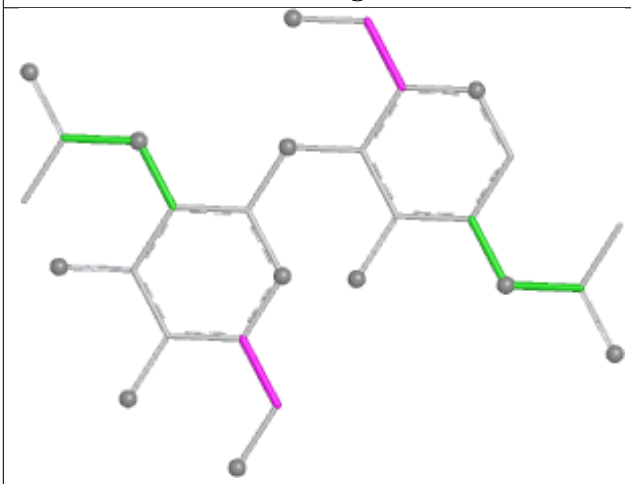
Oligosaccharide Chain X



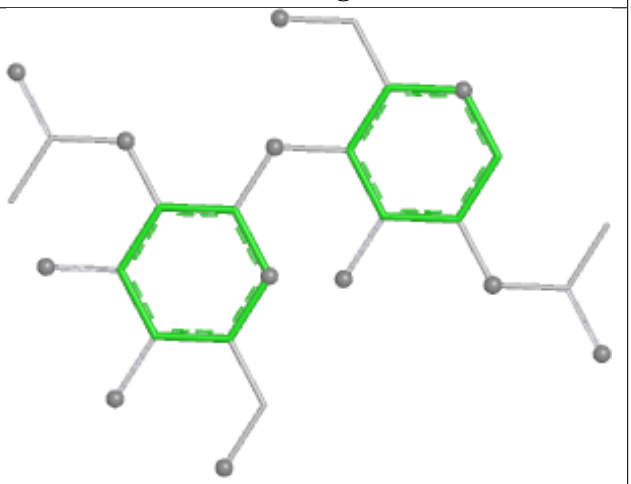
Bond lengths



Bond angles

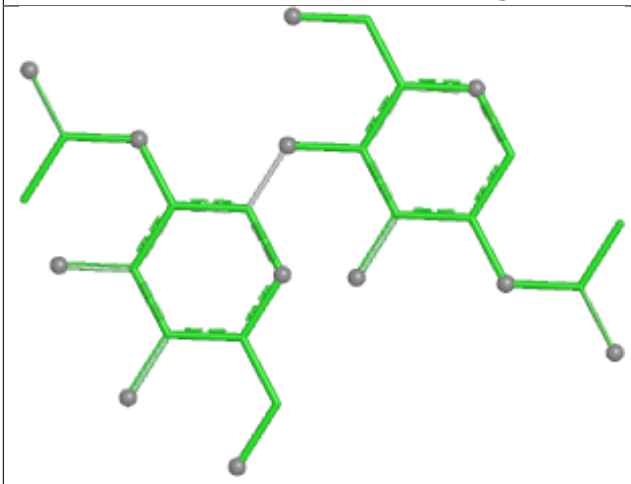


Torsions

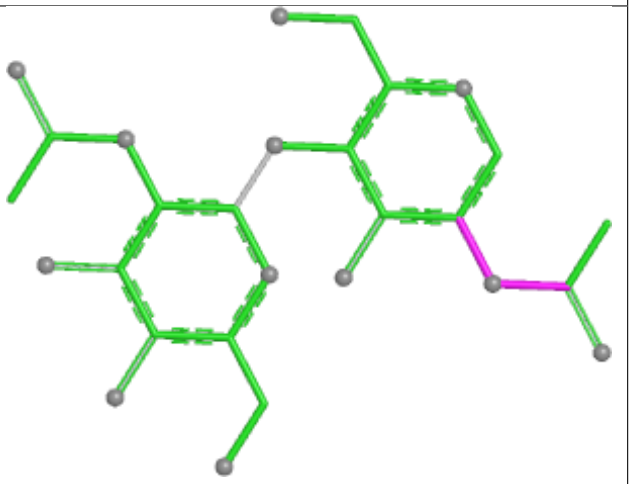


Rings

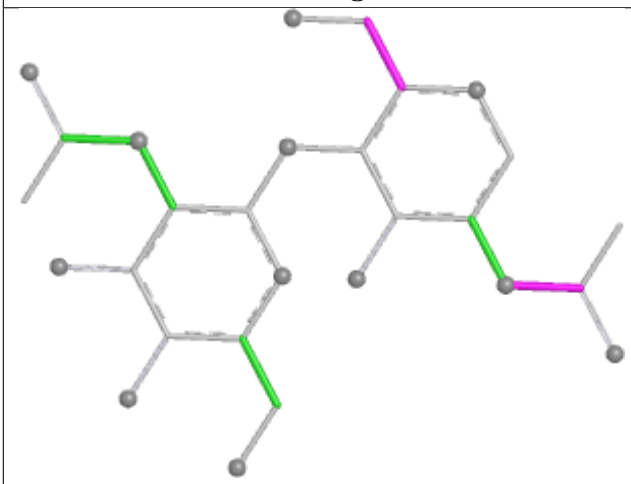
Oligosaccharide Chain Y



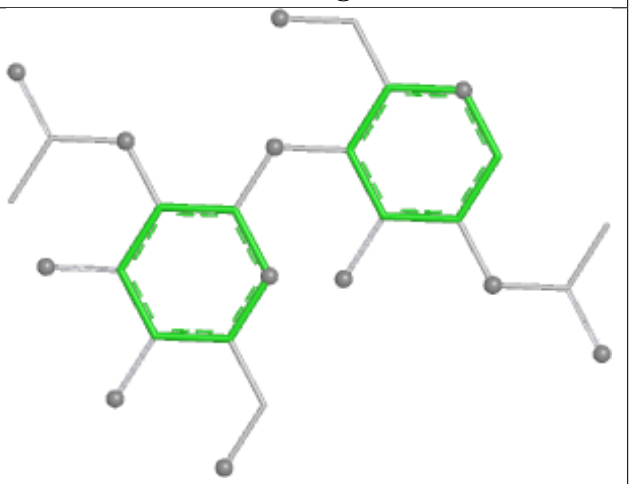
Bond lengths



Bond angles

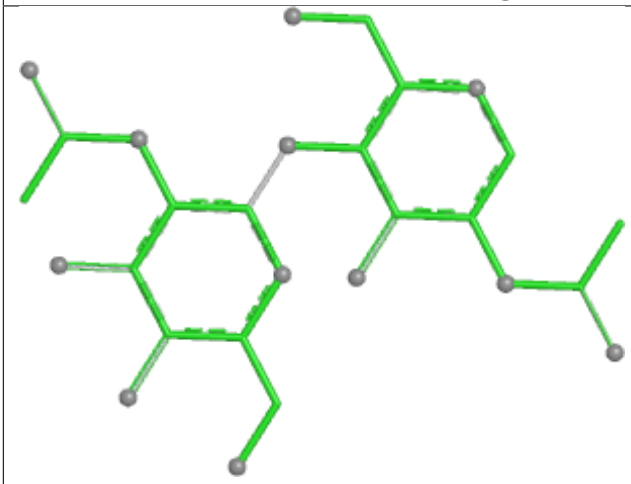


Torsions

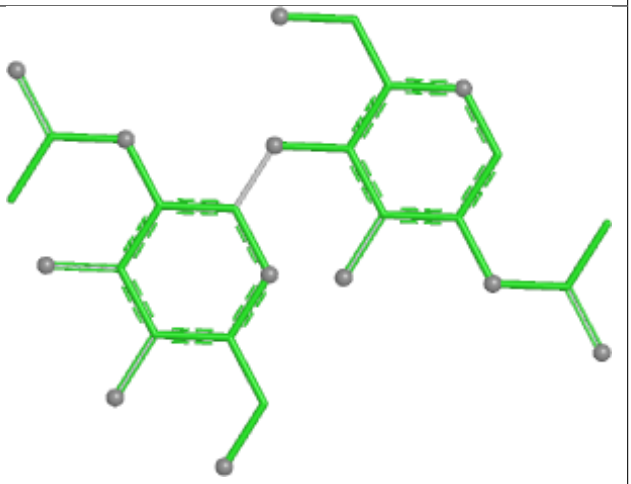


Rings

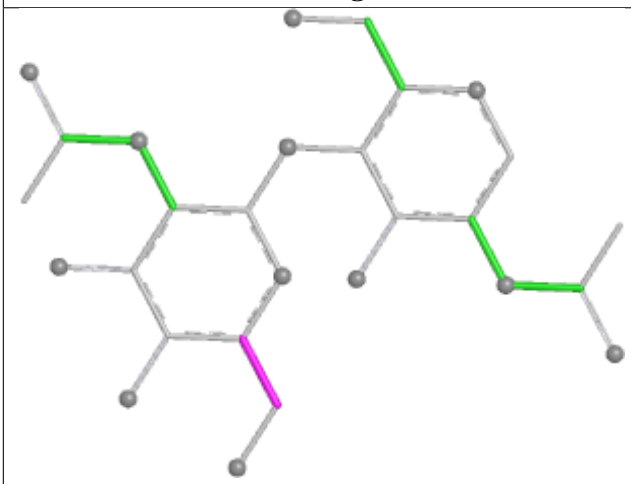
Oligosaccharide Chain Z



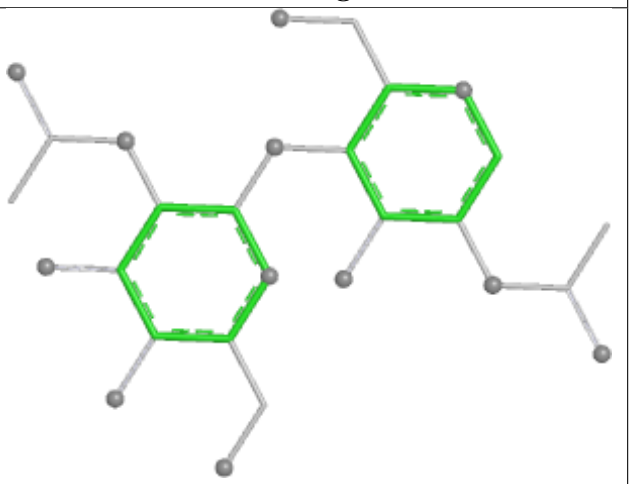
Bond lengths



Bond angles

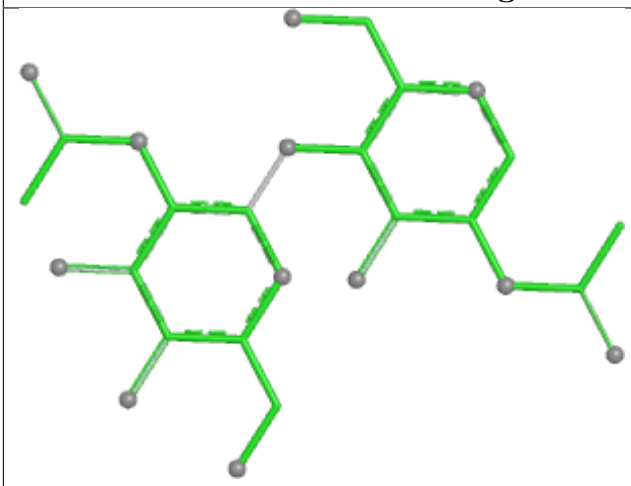


Torsions

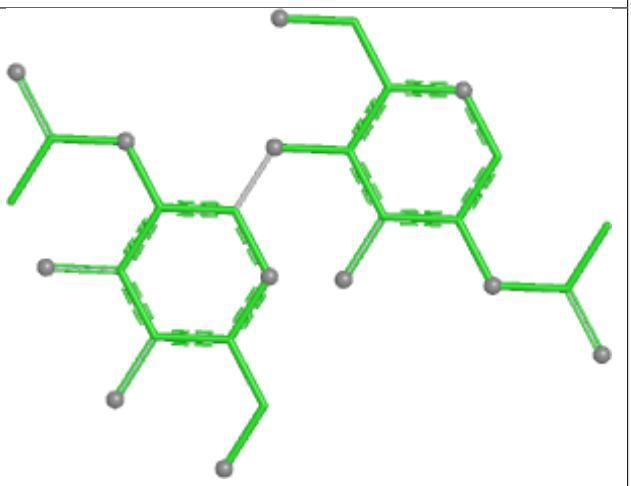


Rings

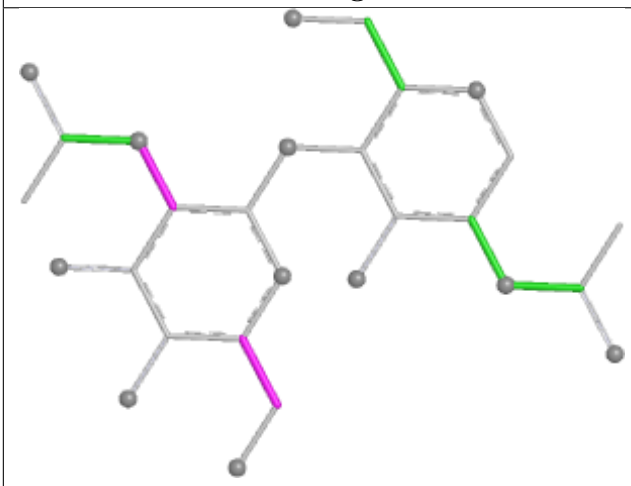
Oligosaccharide Chain b



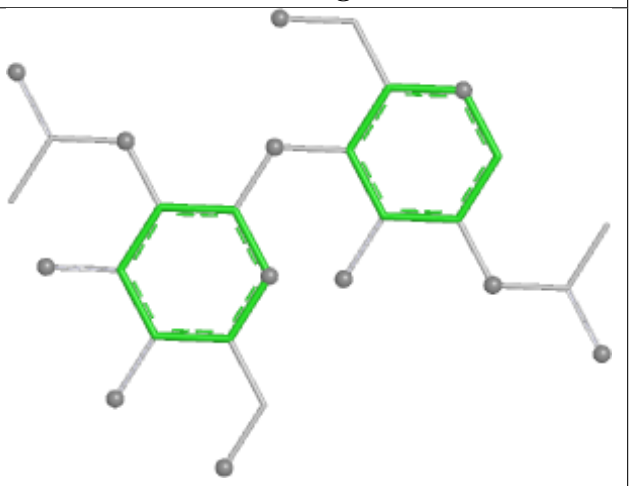
Bond lengths



Bond angles

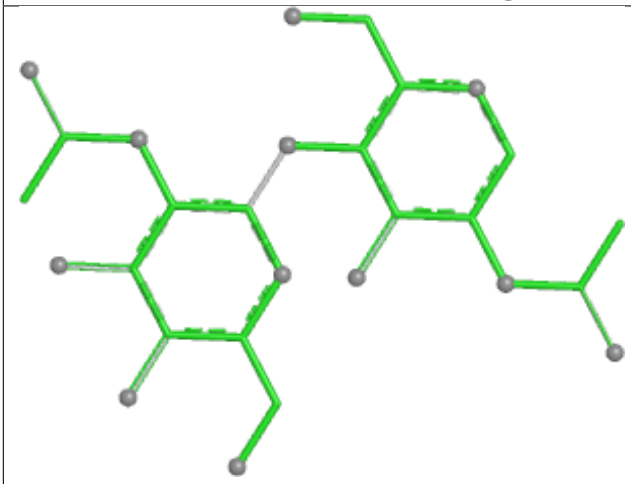


Torsions

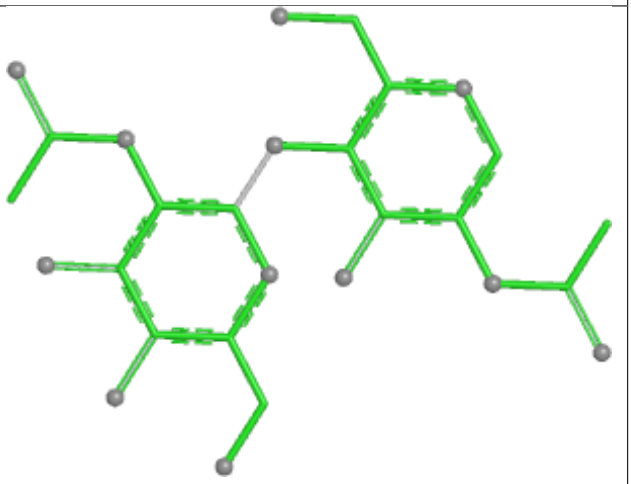


Rings

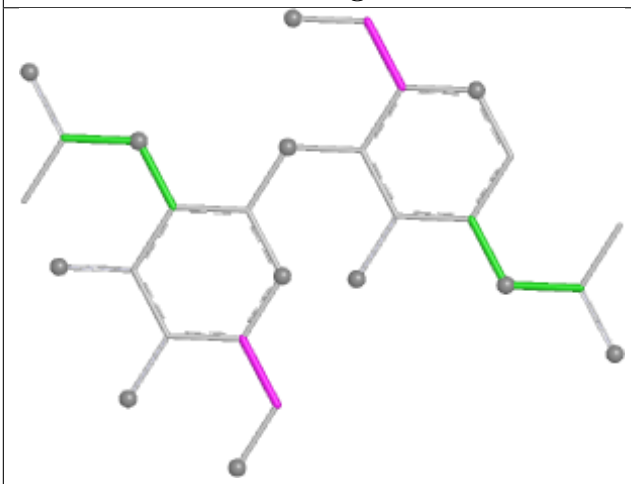
Oligosaccharide Chain c



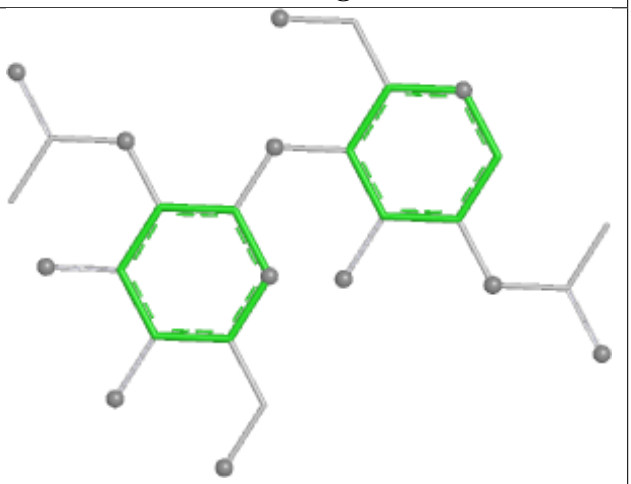
Bond lengths



Bond angles

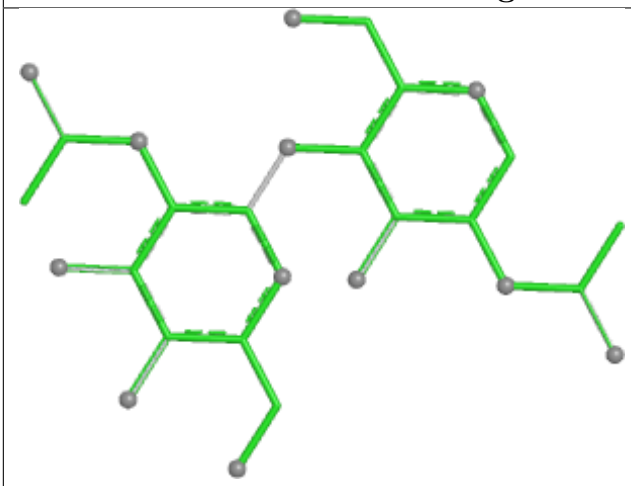


Torsions

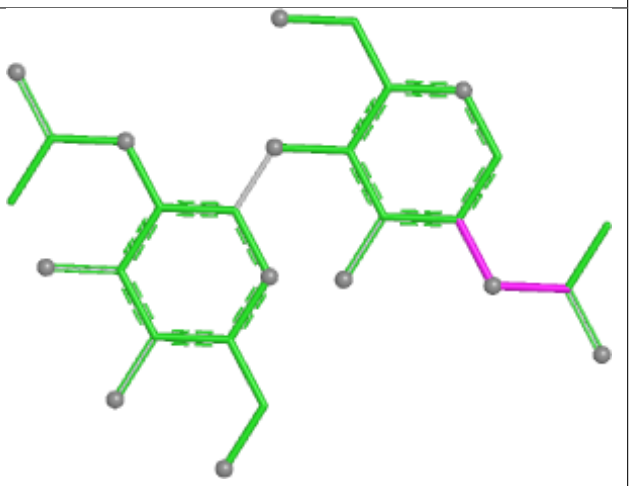


Rings

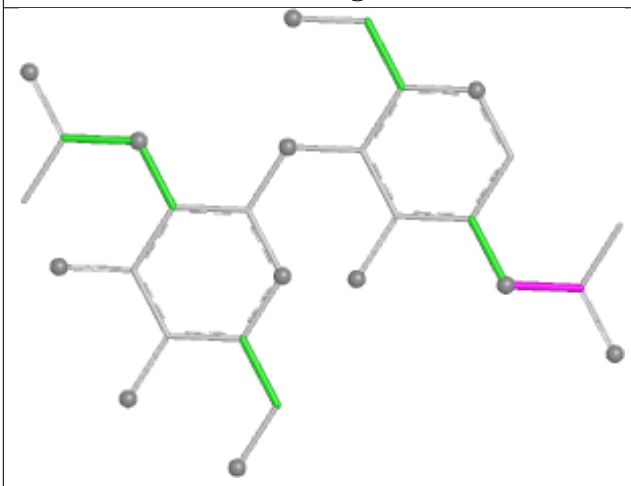
Oligosaccharide Chain d



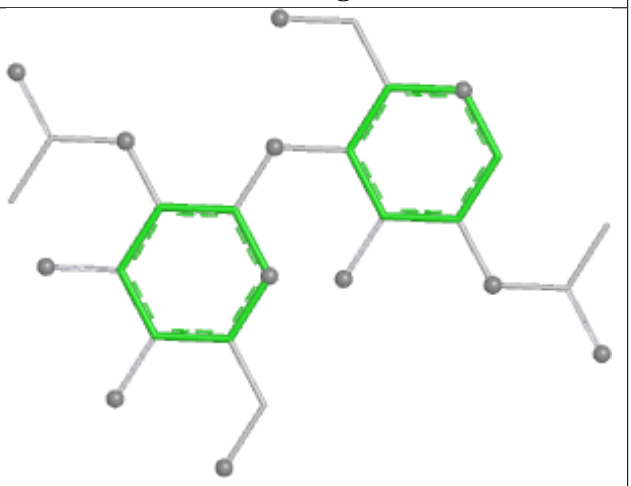
Bond lengths



Bond angles

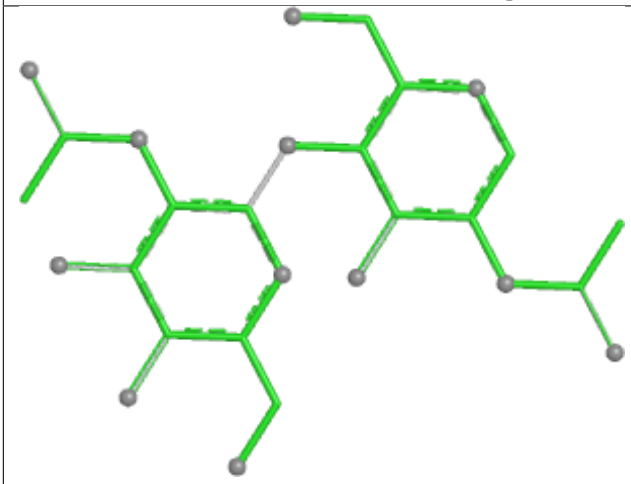


Torsions

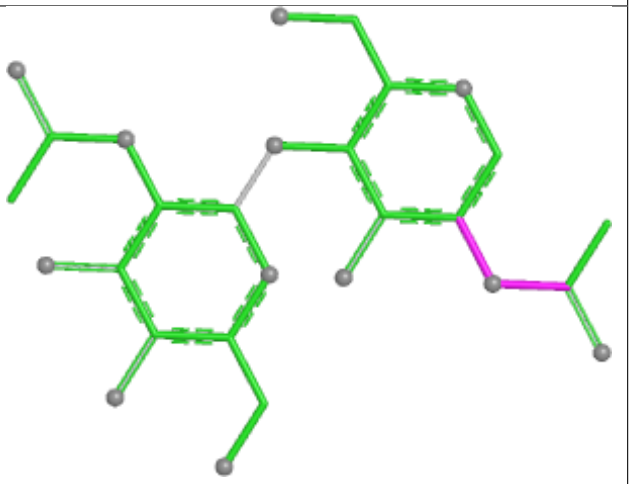


Rings

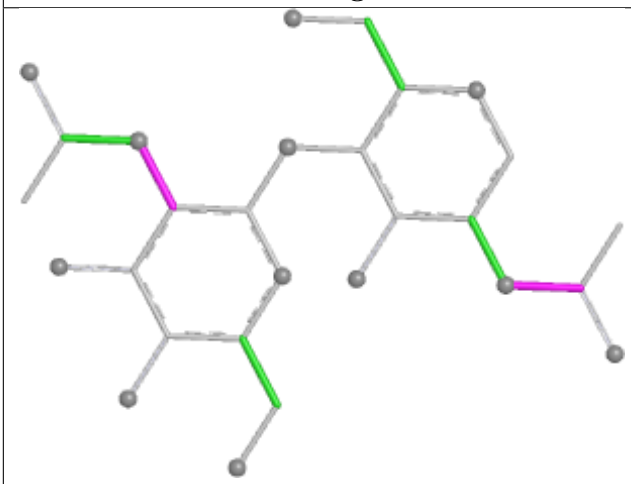
Oligosaccharide Chain f



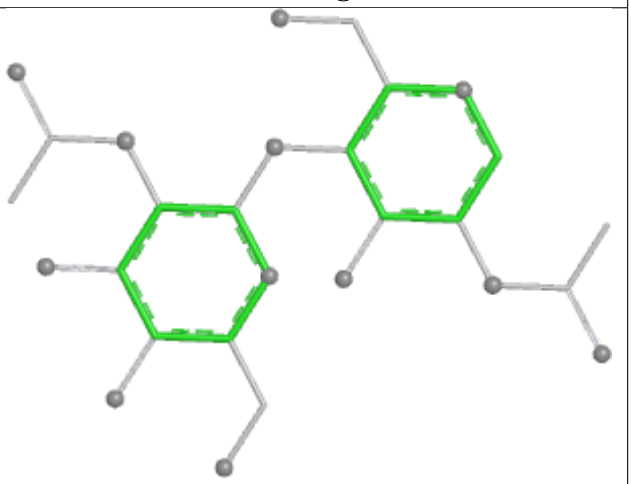
Bond lengths



Bond angles

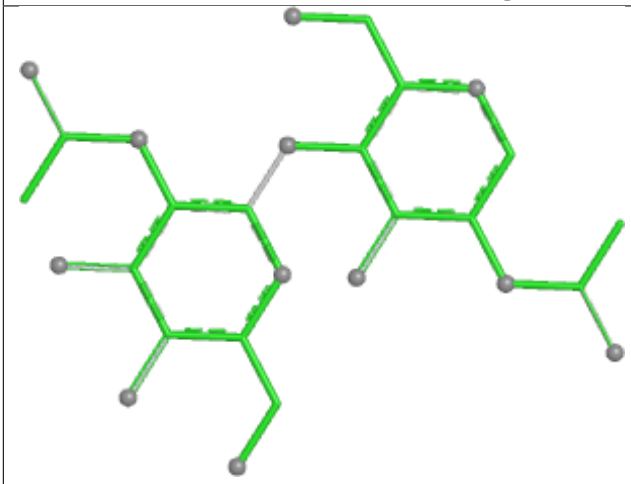


Torsions

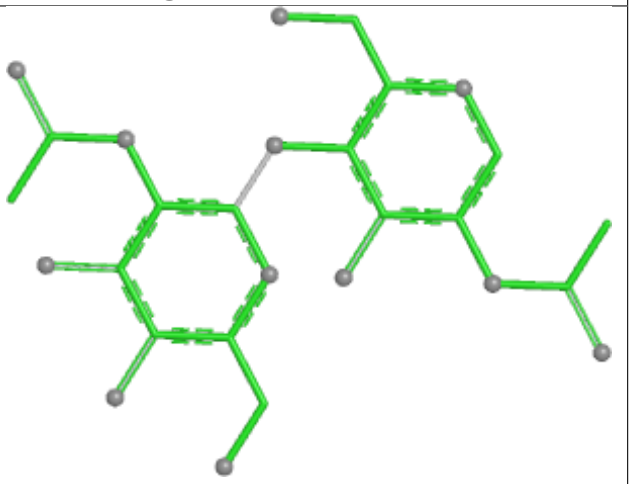


Rings

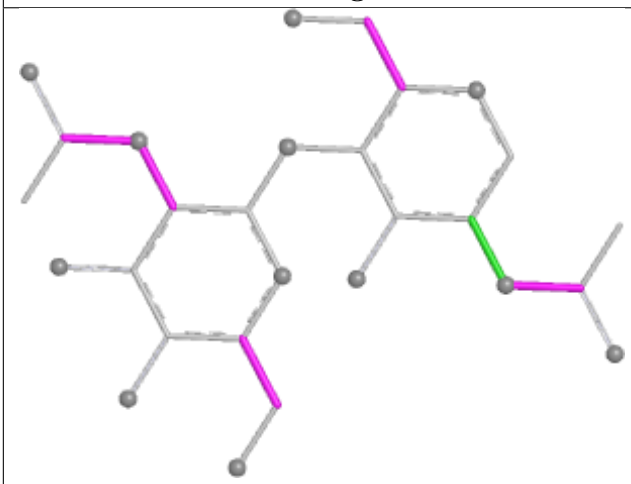
Oligosaccharide Chain g



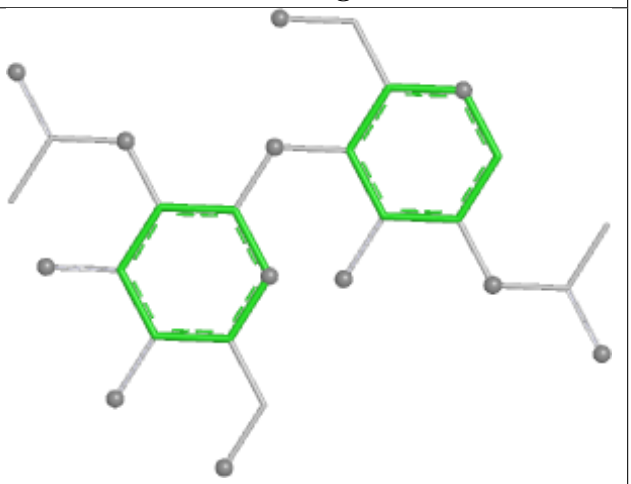
Bond lengths



Bond angles

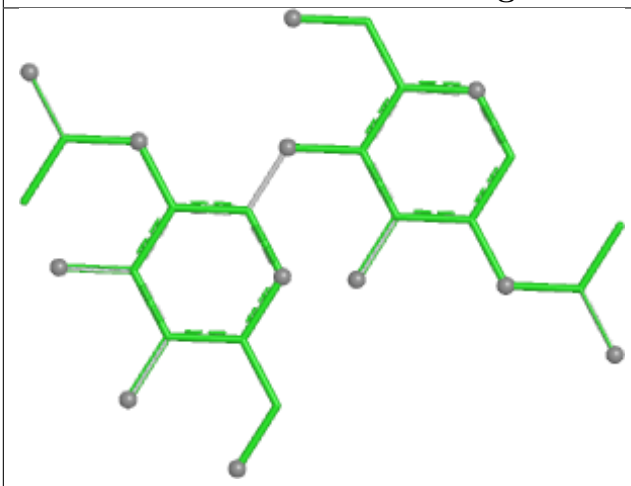


Torsions

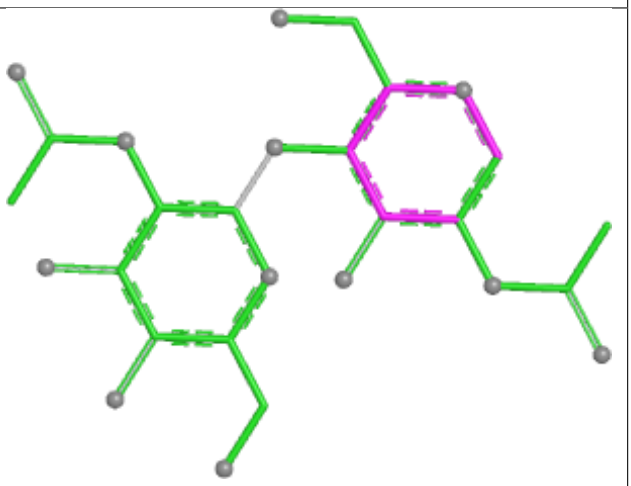


Rings

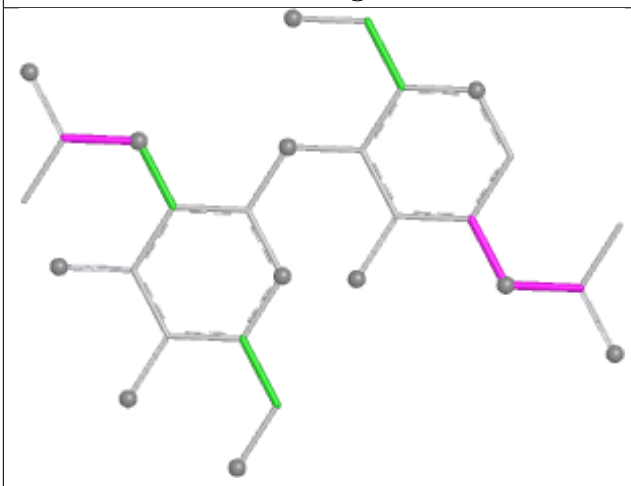
Oligosaccharide Chain h



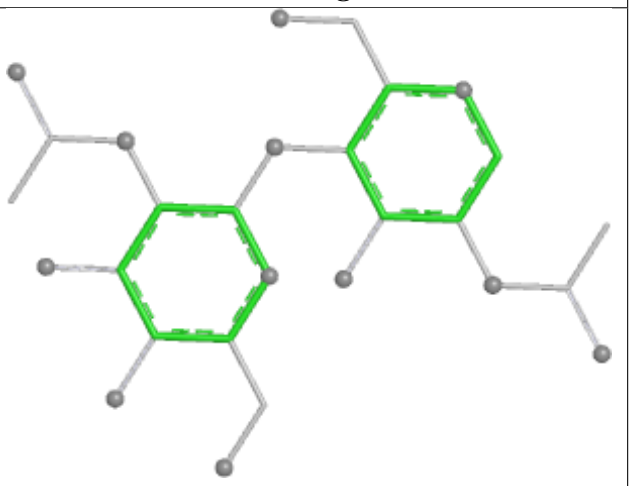
Bond lengths



Bond angles

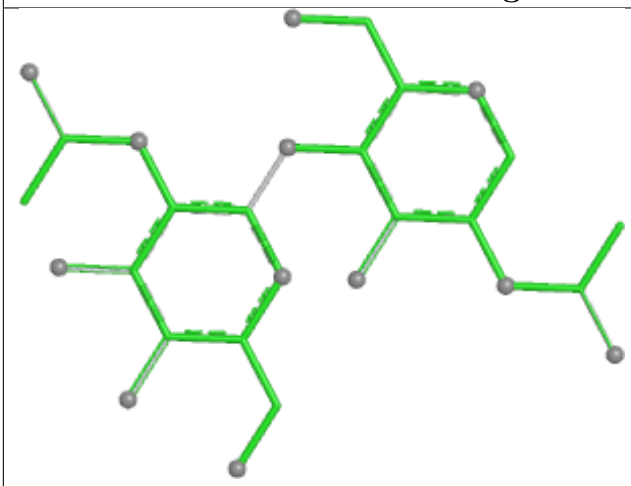


Torsions

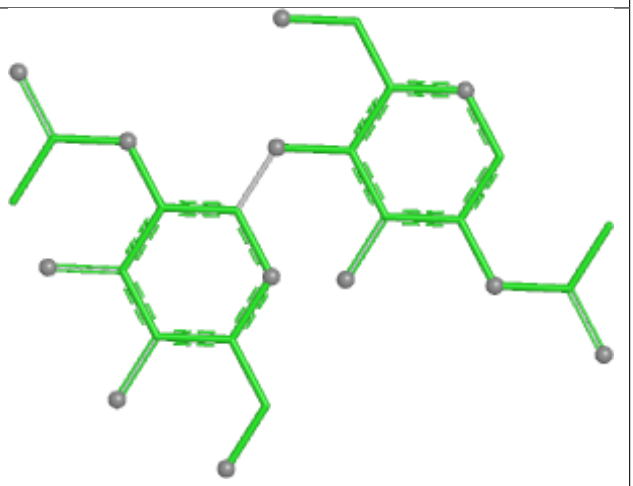


Rings

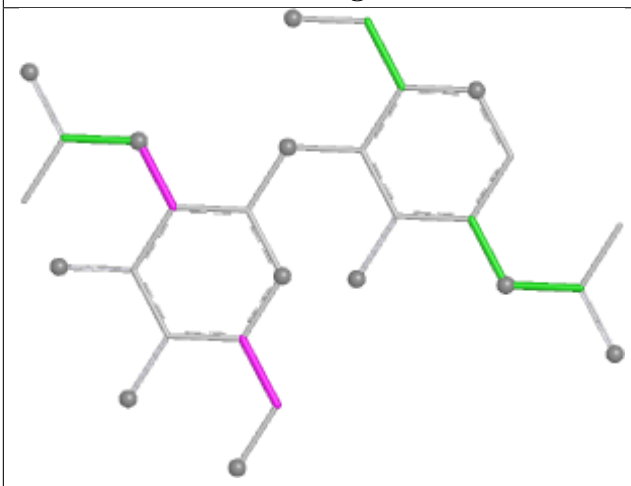
Oligosaccharide Chain i



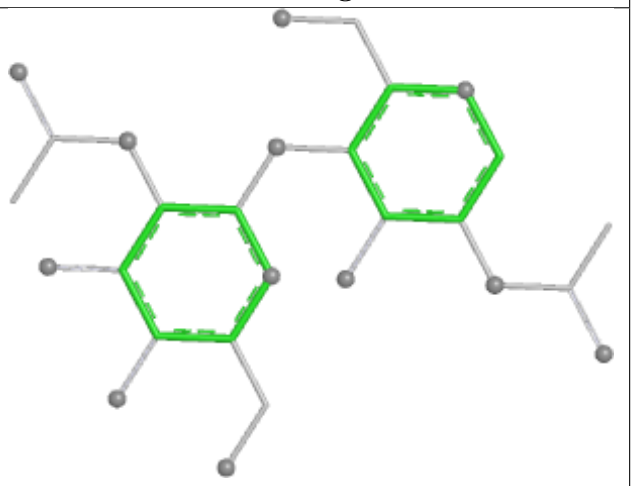
Bond lengths



Bond angles

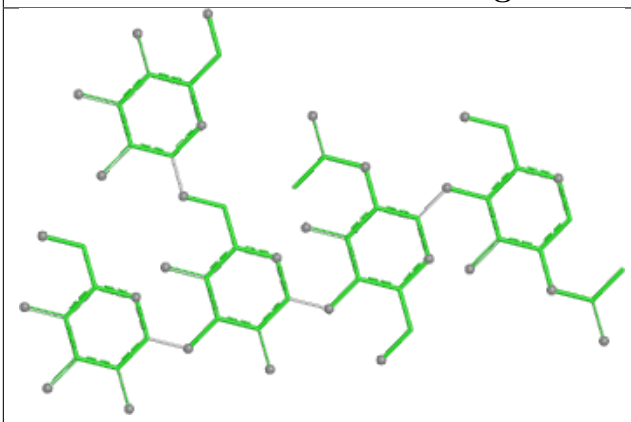


Torsions

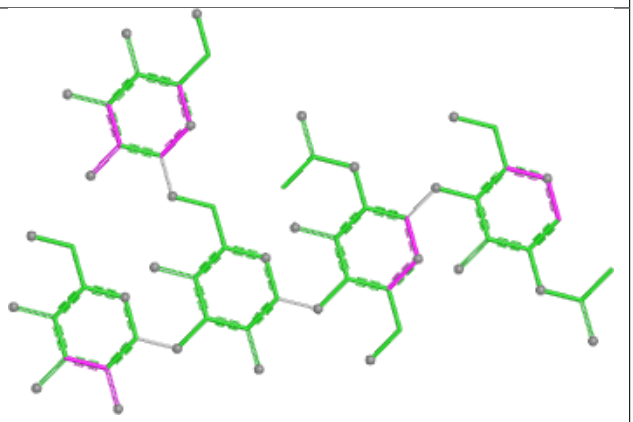


Rings

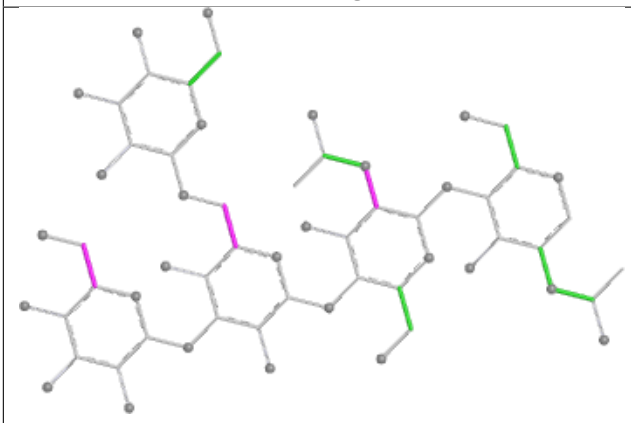
Oligosaccharide Chain V



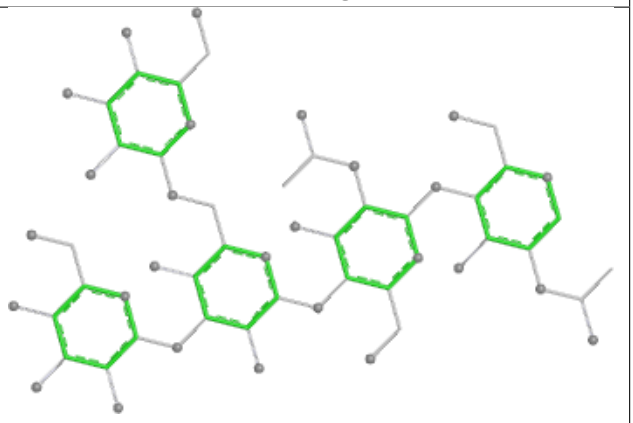
Bond lengths



Bond angles

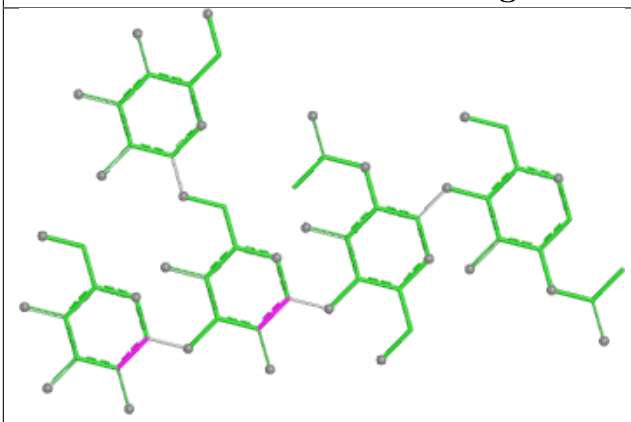


Torsions

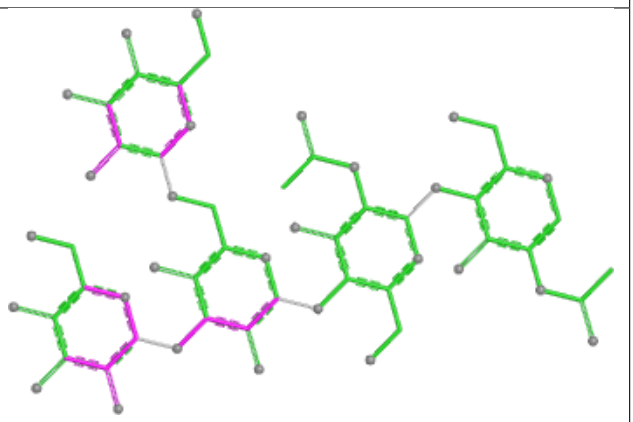


Rings

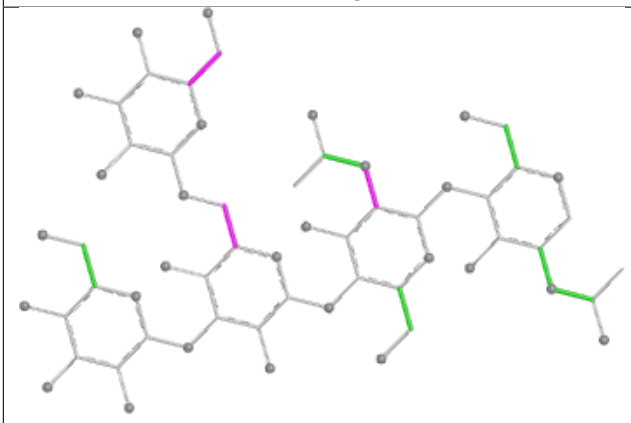
Oligosaccharide Chain a



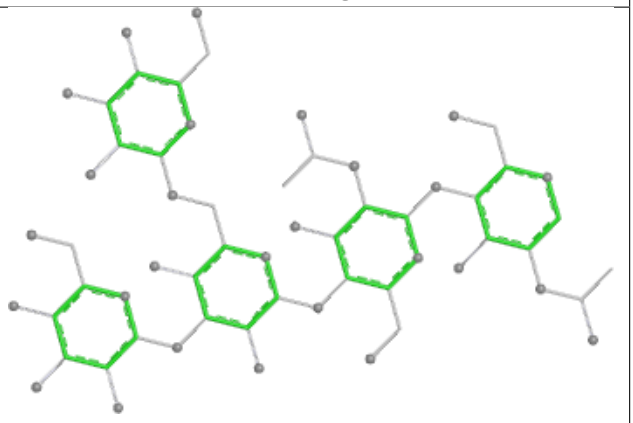
Bond lengths



Bond angles

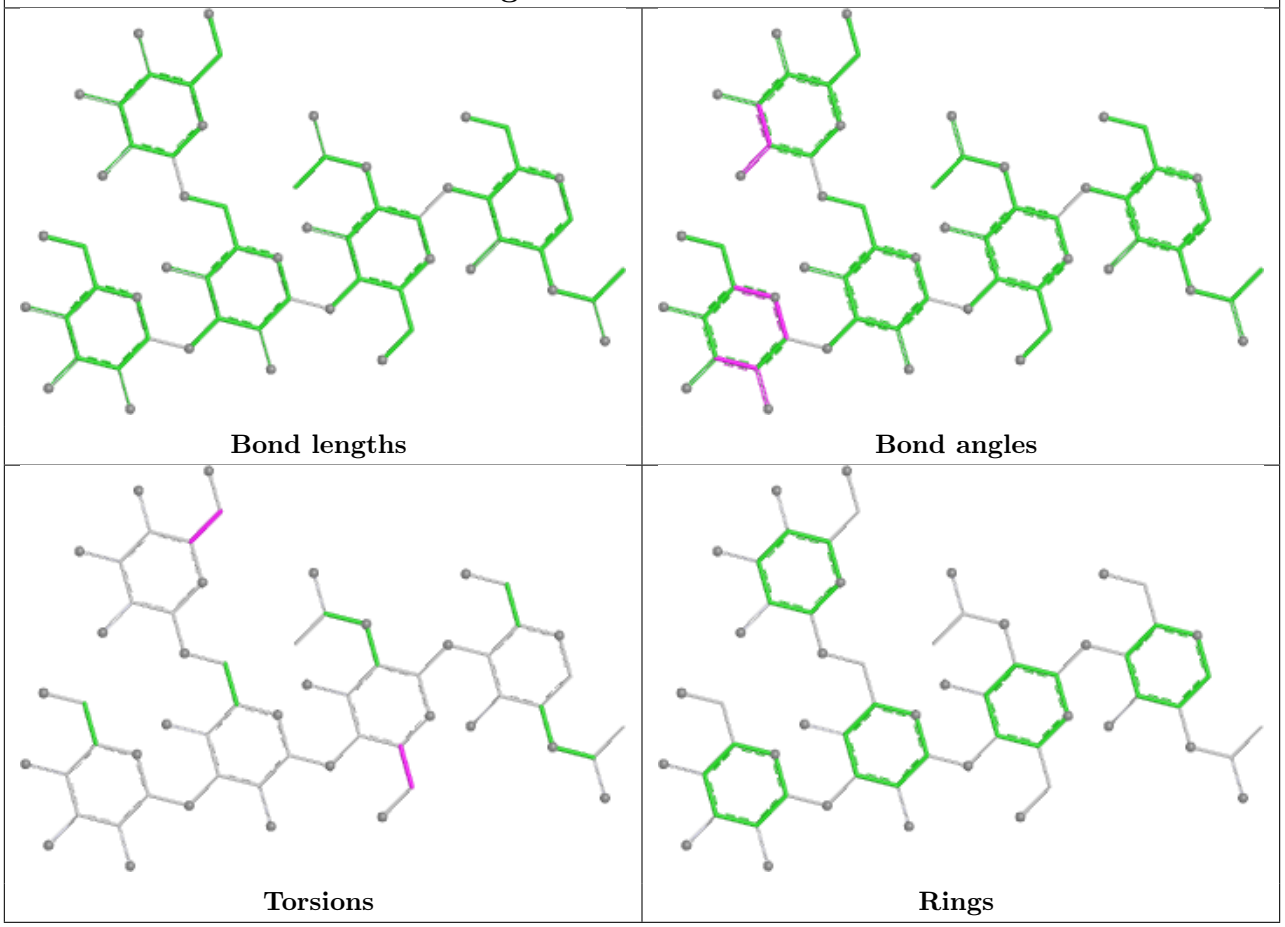


Torsions



Rings

Oligosaccharide Chain e



5.6 Ligand geometry (i)

29 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	$\#\|Z\| > 2$
9	NAG	D	606	4	14,14,15	0.28	0	17,19,21	0.45	0
9	NAG	I	604	4	14,14,15	0.20	0	17,19,21	0.53	0
9	NAG	D	607	4	14,14,15	0.18	0	17,19,21	0.41	0
9	NAG	M	607	4	14,14,15	0.28	0	17,19,21	0.53	0
9	NAG	D	605	4	14,14,15	0.16	0	17,19,21	0.47	0
9	NAG	M	602	4	14,14,15	0.23	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	I	605	4	14,14,15	0.26	0	17,19,21	0.45	0
9	NAG	I	601	4	14,14,15	0.37	0	17,19,21	0.42	0
9	NAG	M	604	4	14,14,15	0.27	0	17,19,21	0.44	0
9	NAG	D	604	4	14,14,15	0.31	0	17,19,21	0.54	0
9	NAG	I	610	4	14,14,15	0.40	0	17,19,21	0.75	0
9	NAG	D	609	4	14,14,15	0.24	0	17,19,21	0.64	0
9	NAG	M	608	4	14,14,15	0.31	0	17,19,21	0.73	1 (5%)
9	NAG	D	601	4	14,14,15	0.46	0	17,19,21	0.80	1 (5%)
9	NAG	M	605	4	14,14,15	0.28	0	17,19,21	0.53	0
9	NAG	M	603	4	14,14,15	0.20	0	17,19,21	0.52	0
9	NAG	M	601	4	14,14,15	0.52	0	17,19,21	0.36	0
9	NAG	M	606	4	14,14,15	0.29	0	17,19,21	0.59	0
9	NAG	M	610	4	14,14,15	0.39	0	17,19,21	0.75	0
9	NAG	D	608	4	14,14,15	0.26	0	17,19,21	0.61	0
9	NAG	D	603	4	14,14,15	0.20	0	17,19,21	0.53	0
9	NAG	I	606	4	14,14,15	0.16	0	17,19,21	0.48	0
9	NAG	I	602	4	14,14,15	0.27	0	17,19,21	0.44	0
9	NAG	D	602	4	14,14,15	0.25	0	17,19,21	0.44	0
9	NAG	I	603	4	14,14,15	0.18	0	17,19,21	0.52	0
9	NAG	I	608	4	14,14,15	0.19	0	17,19,21	0.41	0
9	NAG	M	609	4	14,14,15	0.28	0	17,19,21	0.39	0
9	NAG	I	609	4	14,14,15	0.41	0	17,19,21	0.76	0
9	NAG	I	607	4	14,14,15	0.33	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
9	NAG	D	606	4	-	2/6/23/26	0/1/1/1
9	NAG	I	604	4	-	1/6/23/26	0/1/1/1
9	NAG	D	607	4	-	1/6/23/26	0/1/1/1
9	NAG	M	607	4	-	5/6/23/26	0/1/1/1
9	NAG	D	605	4	-	2/6/23/26	0/1/1/1
9	NAG	M	602	4	-	0/6/23/26	0/1/1/1
9	NAG	I	605	4	-	4/6/23/26	0/1/1/1
9	NAG	I	601	4	-	0/6/23/26	0/1/1/1
9	NAG	M	604	4	-	3/6/23/26	0/1/1/1
9	NAG	D	604	4	-	4/6/23/26	0/1/1/1
9	NAG	I	610	4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	D	609	4	-	3/6/23/26	0/1/1/1
9	NAG	M	608	4	-	3/6/23/26	0/1/1/1
9	NAG	D	601	4	-	2/6/23/26	0/1/1/1
9	NAG	M	605	4	-	3/6/23/26	0/1/1/1
9	NAG	M	603	4	-	0/6/23/26	0/1/1/1
9	NAG	M	601	4	-	0/6/23/26	0/1/1/1
9	NAG	M	606	4	-	1/6/23/26	0/1/1/1
9	NAG	M	610	4	-	3/6/23/26	0/1/1/1
9	NAG	D	608	4	-	3/6/23/26	0/1/1/1
9	NAG	D	603	4	-	0/6/23/26	0/1/1/1
9	NAG	I	606	4	-	2/6/23/26	0/1/1/1
9	NAG	I	602	4	-	1/6/23/26	0/1/1/1
9	NAG	D	602	4	-	1/6/23/26	0/1/1/1
9	NAG	I	603	4	-	1/6/23/26	0/1/1/1
9	NAG	I	608	4	-	1/6/23/26	0/1/1/1
9	NAG	M	609	4	-	0/6/23/26	0/1/1/1
9	NAG	I	609	4	-	3/6/23/26	0/1/1/1
9	NAG	I	607	4	-	2/6/23/26	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})
9	D	601	NAG	C2-N2-C7	2.80	126.65	122.90
9	M	608	NAG	C1-O5-C5	-2.12	109.34	112.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	609	NAG	C1-C2-N2-C7
9	I	609	NAG	C3-C2-N2-C7
9	I	610	NAG	C1-C2-N2-C7
9	M	607	NAG	C1-C2-N2-C7
9	M	607	NAG	C8-C7-N2-C2
9	M	607	NAG	O7-C7-N2-C2
9	M	608	NAG	C1-C2-N2-C7
9	M	608	NAG	C8-C7-N2-C2
9	M	608	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	M	610	NAG	C1-C2-N2-C7
9	D	604	NAG	O5-C5-C6-O6
9	D	608	NAG	C8-C7-N2-C2
9	D	608	NAG	O7-C7-N2-C2
9	I	605	NAG	O5-C5-C6-O6
9	D	604	NAG	C4-C5-C6-O6
9	D	605	NAG	O5-C5-C6-O6
9	I	610	NAG	O5-C5-C6-O6
9	I	605	NAG	C4-C5-C6-O6
9	D	609	NAG	C8-C7-N2-C2
9	D	609	NAG	O7-C7-N2-C2
9	I	609	NAG	O5-C5-C6-O6
9	I	606	NAG	O5-C5-C6-O6
9	I	609	NAG	C4-C5-C6-O6
9	M	610	NAG	O5-C5-C6-O6
9	M	610	NAG	C4-C5-C6-O6
9	I	610	NAG	C4-C5-C6-O6
9	D	601	NAG	C8-C7-N2-C2
9	D	601	NAG	O7-C7-N2-C2
9	I	602	NAG	O5-C5-C6-O6
9	I	603	NAG	O5-C5-C6-O6
9	D	602	NAG	O5-C5-C6-O6
9	M	606	NAG	O5-C5-C6-O6
9	M	607	NAG	C4-C5-C6-O6
9	M	607	NAG	O5-C5-C6-O6
9	M	604	NAG	O5-C5-C6-O6
9	D	608	NAG	O5-C5-C6-O6
9	I	608	NAG	O5-C5-C6-O6
9	D	607	NAG	O5-C5-C6-O6
9	M	605	NAG	O5-C5-C6-O6
9	D	605	NAG	C4-C5-C6-O6
9	D	604	NAG	C1-C2-N2-C7
9	D	606	NAG	C1-C2-N2-C7
9	I	605	NAG	C1-C2-N2-C7
9	I	607	NAG	C1-C2-N2-C7
9	M	604	NAG	C1-C2-N2-C7
9	I	606	NAG	C4-C5-C6-O6
9	M	605	NAG	C8-C7-N2-C2
9	M	605	NAG	O7-C7-N2-C2
9	I	604	NAG	C1-C2-N2-C7
9	D	604	NAG	C3-C2-N2-C7
9	D	606	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	I	605	NAG	C3-C2-N2-C7
9	I	607	NAG	C3-C2-N2-C7
9	M	604	NAG	C3-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	604	NAG	1	0
9	I	610	NAG	3	0
9	D	609	NAG	1	0
9	M	608	NAG	1	0
9	M	601	NAG	4	0
9	M	606	NAG	1	0
9	M	610	NAG	1	0
9	D	608	NAG	1	0
9	D	602	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.

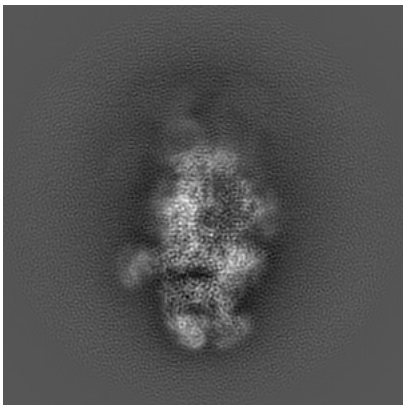
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43838. These allow visual inspection of the internal detail of the map and identification of artifacts.

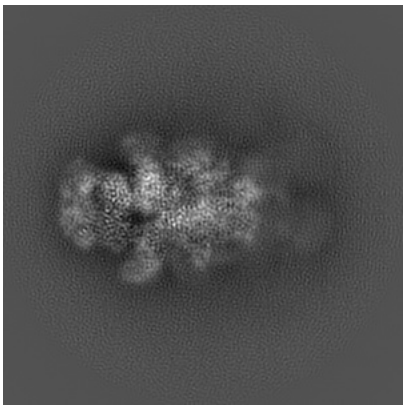
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

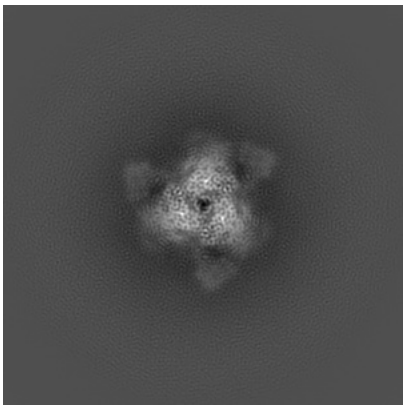
6.1.1 Primary map



X

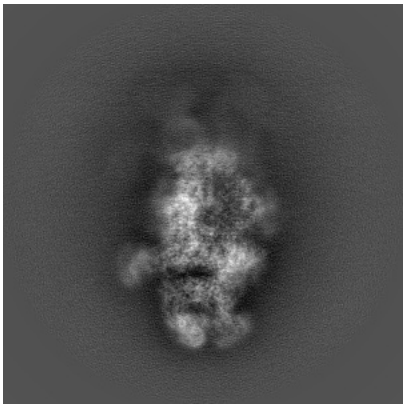


Y

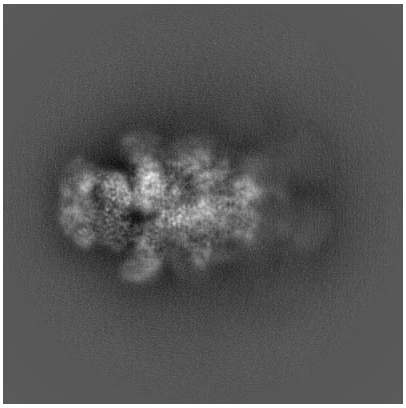


Z

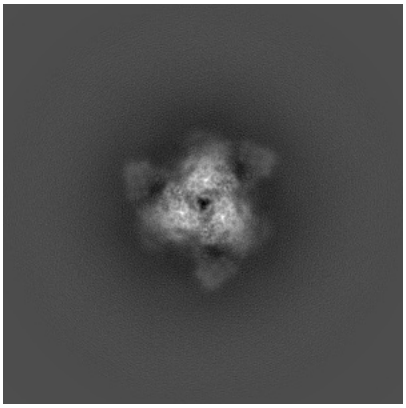
6.1.2 Raw map



X



Y

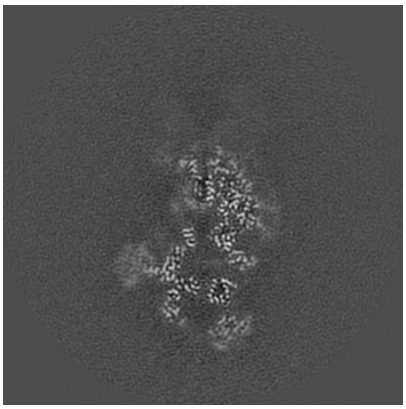


Z

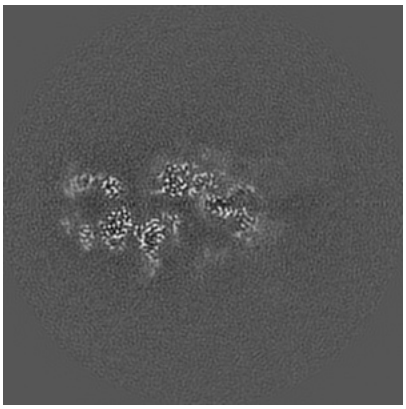
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

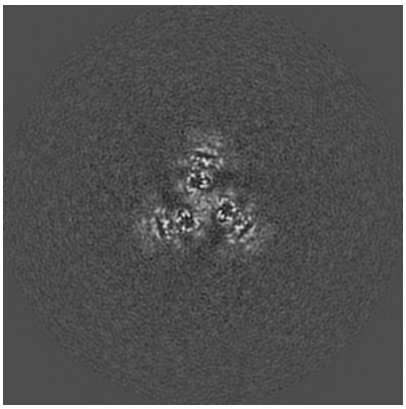
6.2.1 Primary map



X Index: 180

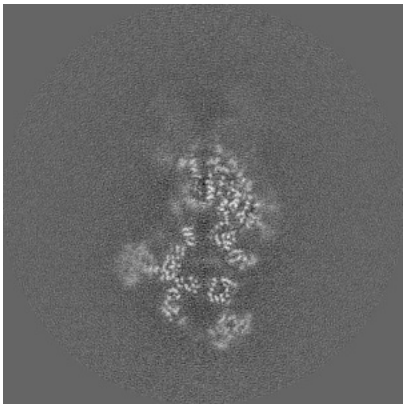


Y Index: 180

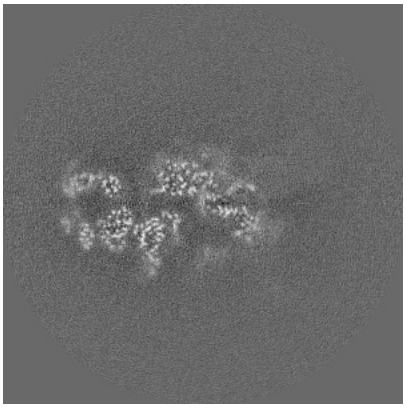


Z Index: 180

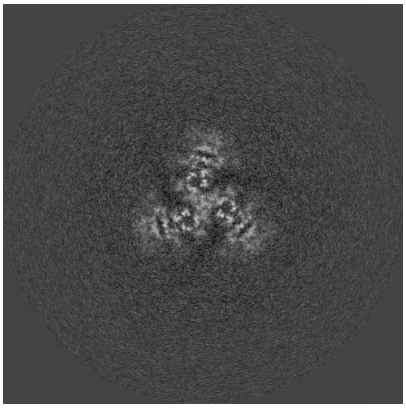
6.2.2 Raw map



X Index: 180



Y Index: 180

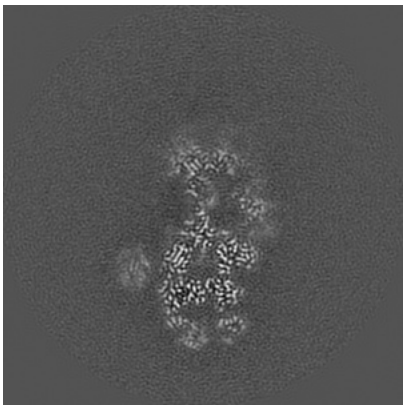


Z Index: 180

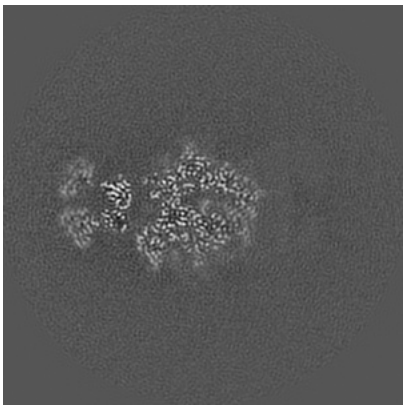
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

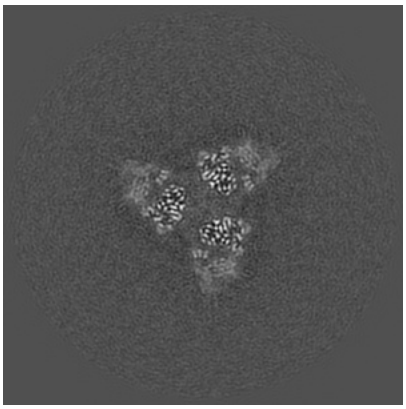
6.3.1 Primary map



X Index: 191

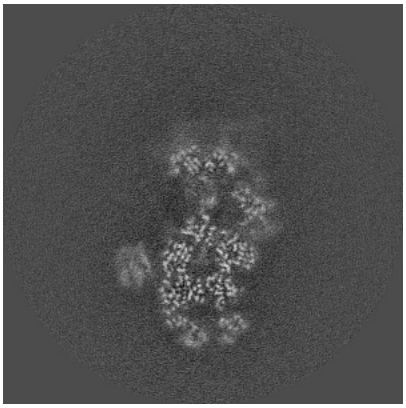


Y Index: 168

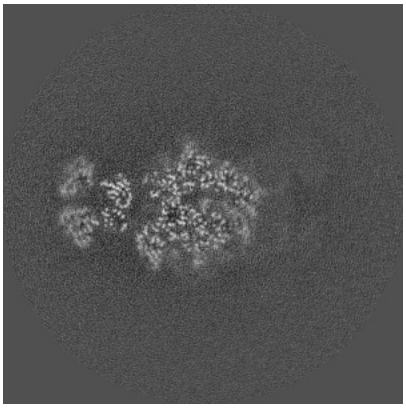


Z Index: 128

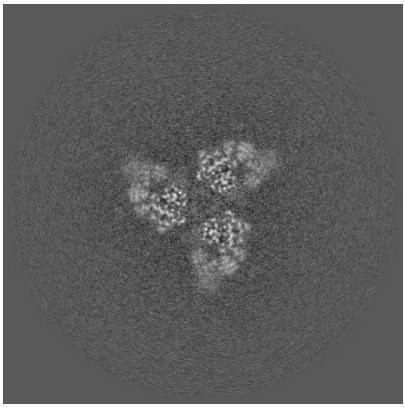
6.3.2 Raw map



X Index: 190



Y Index: 168

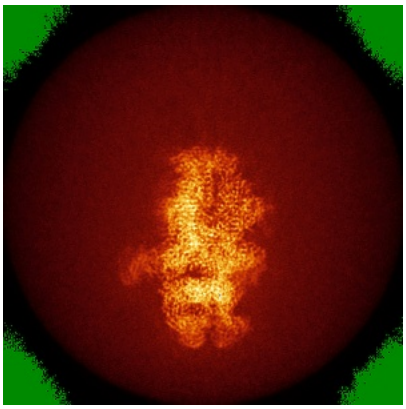


Z Index: 130

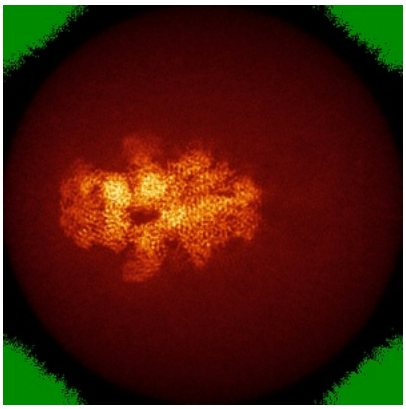
The images above show the largest variance slices of the map in three orthogonal directions.

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

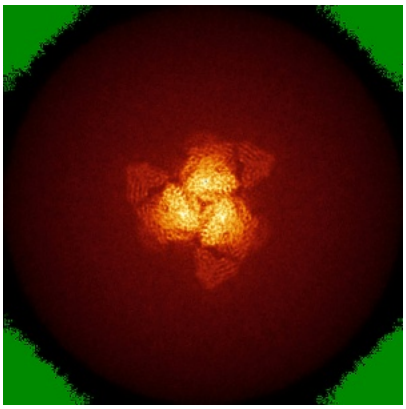
6.4.1 Primary map



X

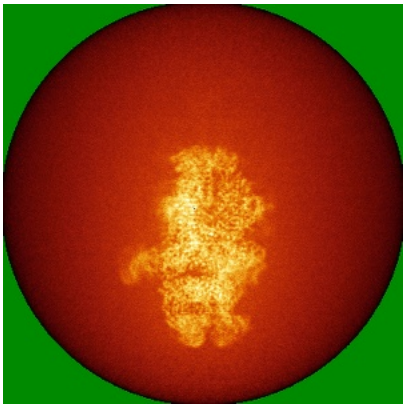


Y

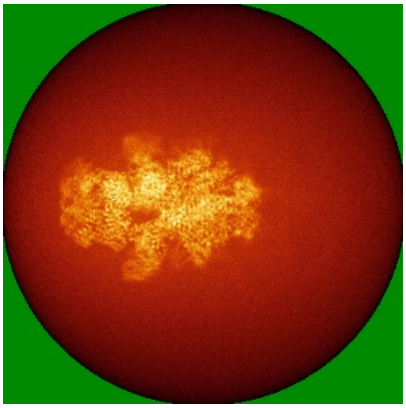


Z

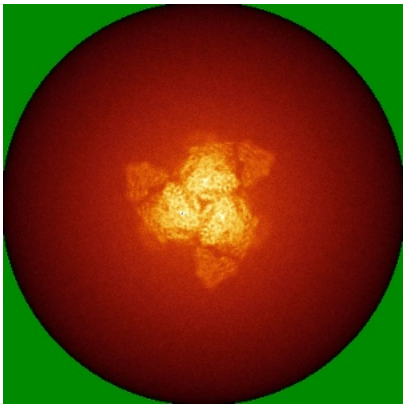
6.4.2 Raw map



X



Y

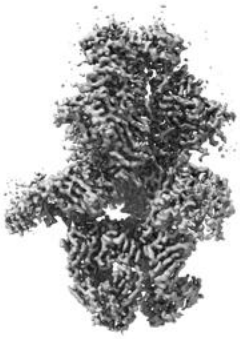


Z

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.

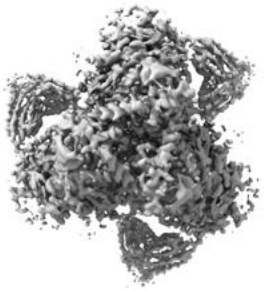
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

Y

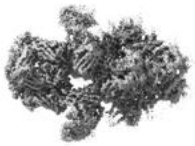


Z

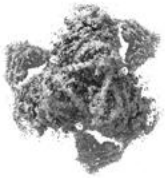
The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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.

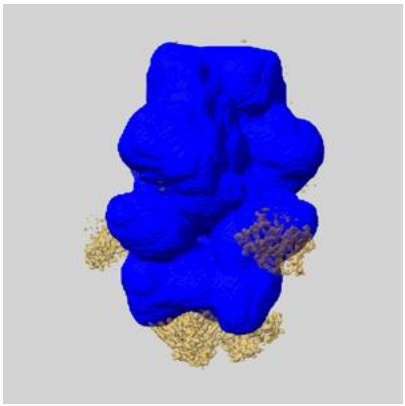
6.6 Mask visualisation (i)

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

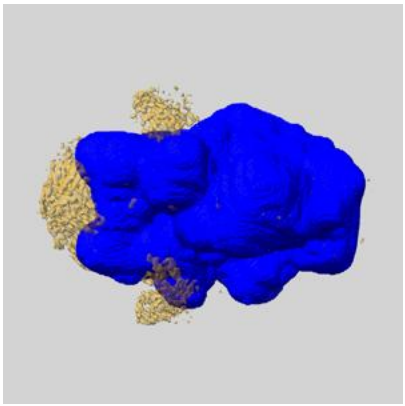
A mask typically either:

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

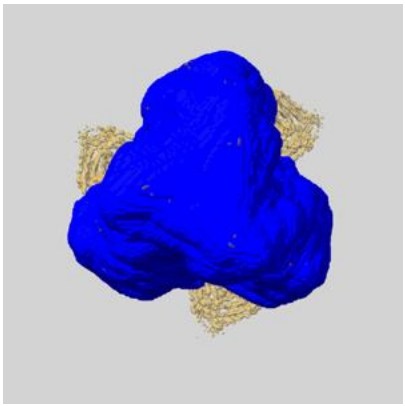
6.6.1 emd_43838_msk_1.map (i)



X



Y

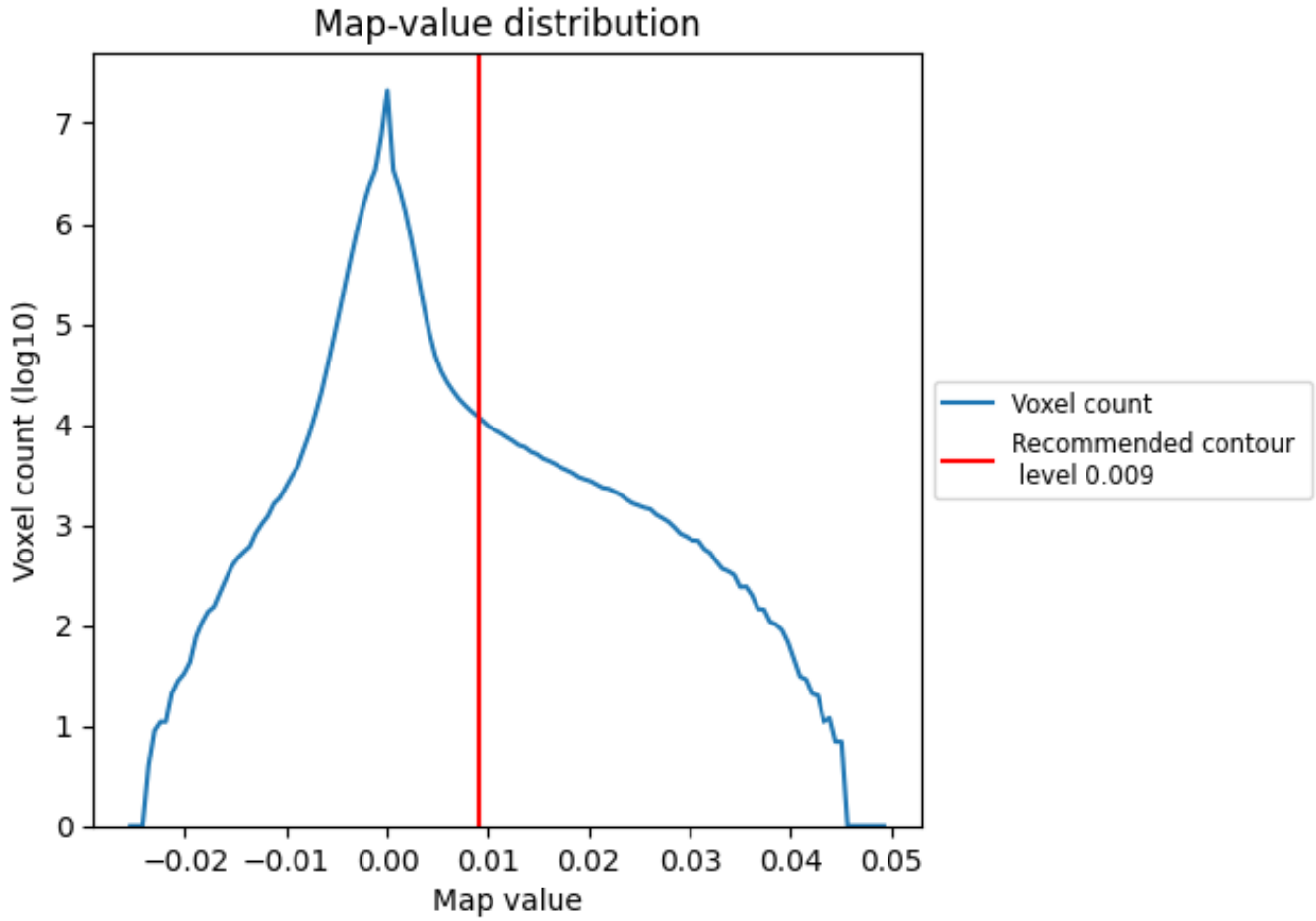


Z

7 Map analysis

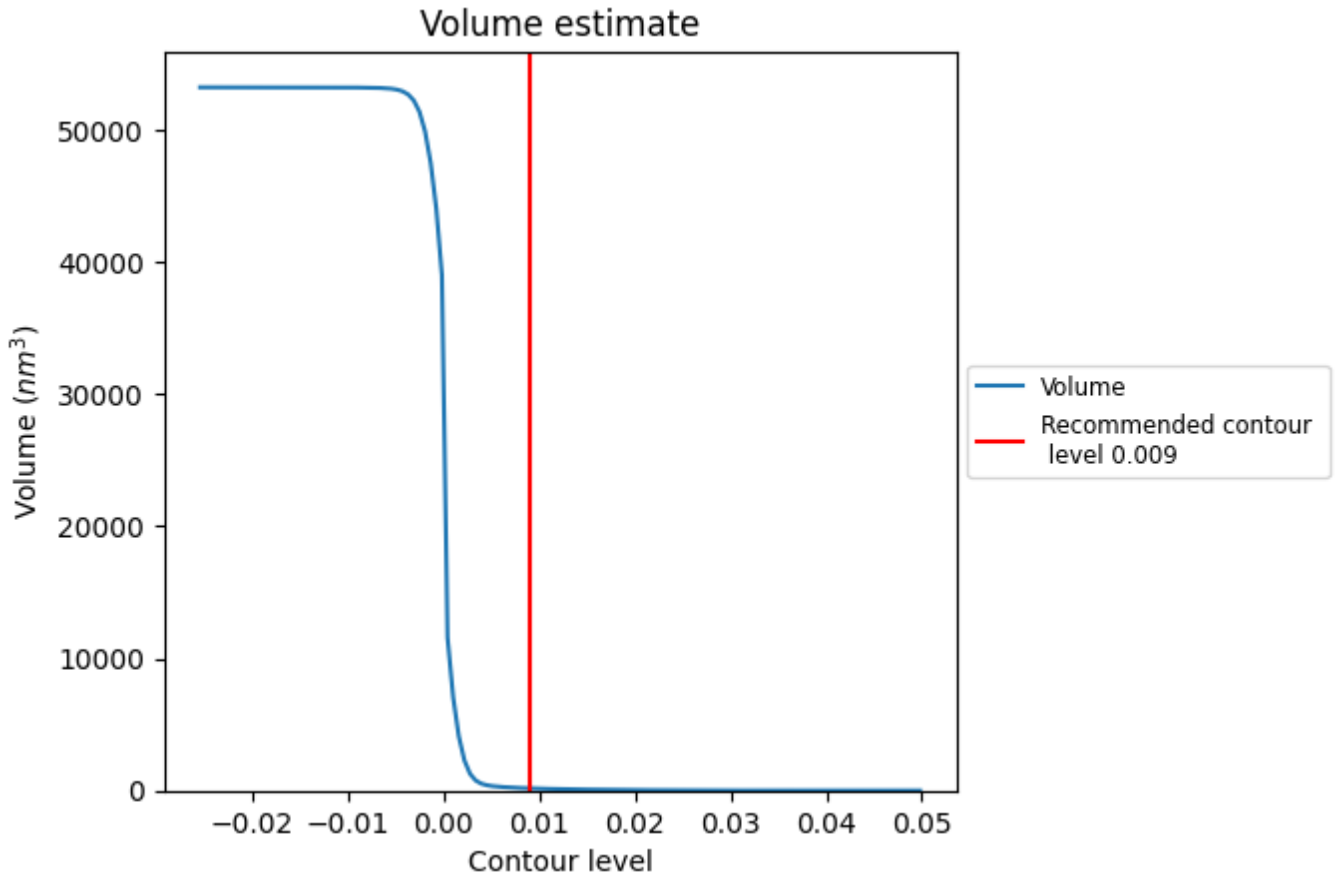
This section contains the results of statistical analysis of the map.

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.

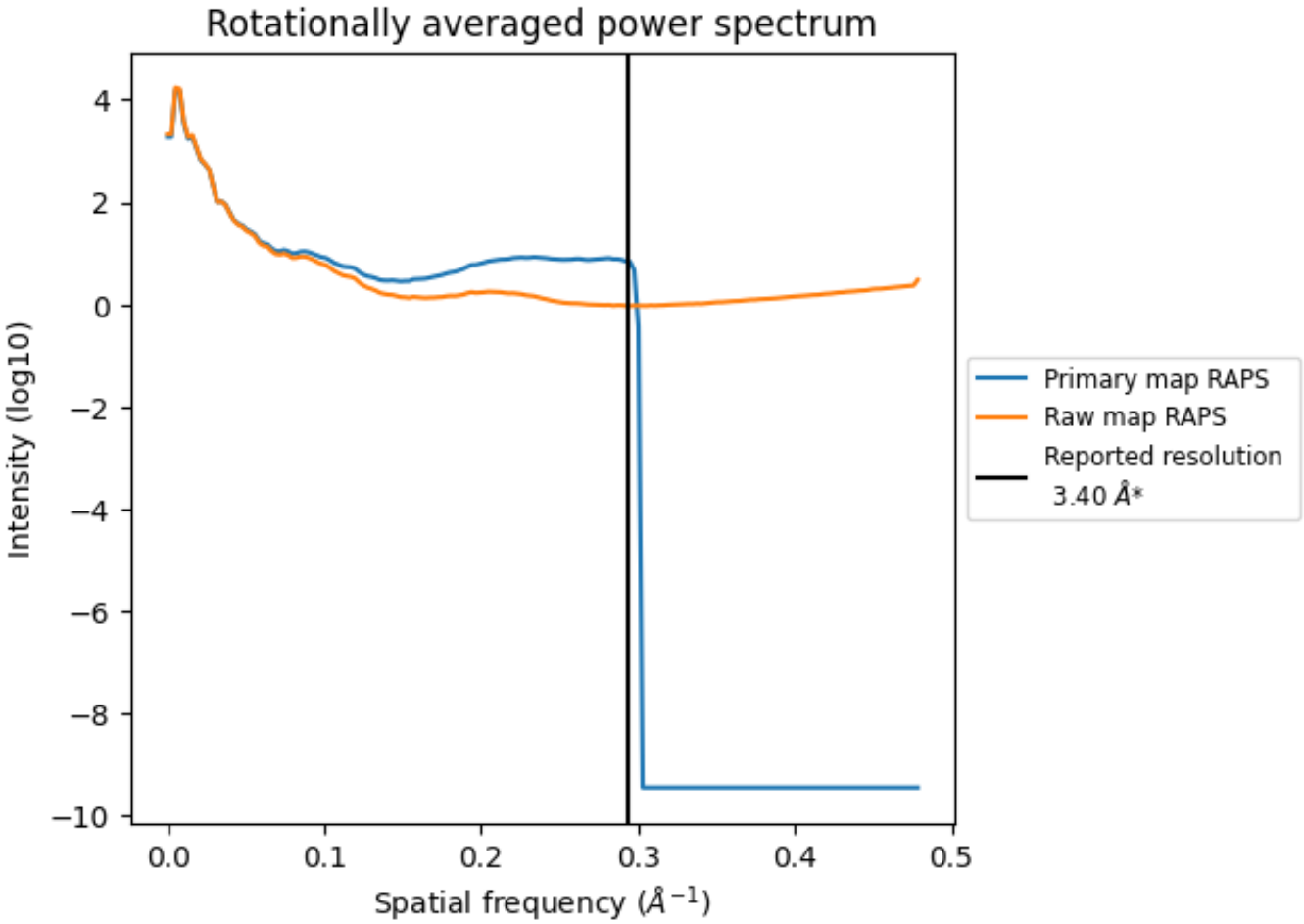
7.2 Volume estimate



The volume at the recommended contour level is 169 nm^3; this corresponds to an approximate mass of 152 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)

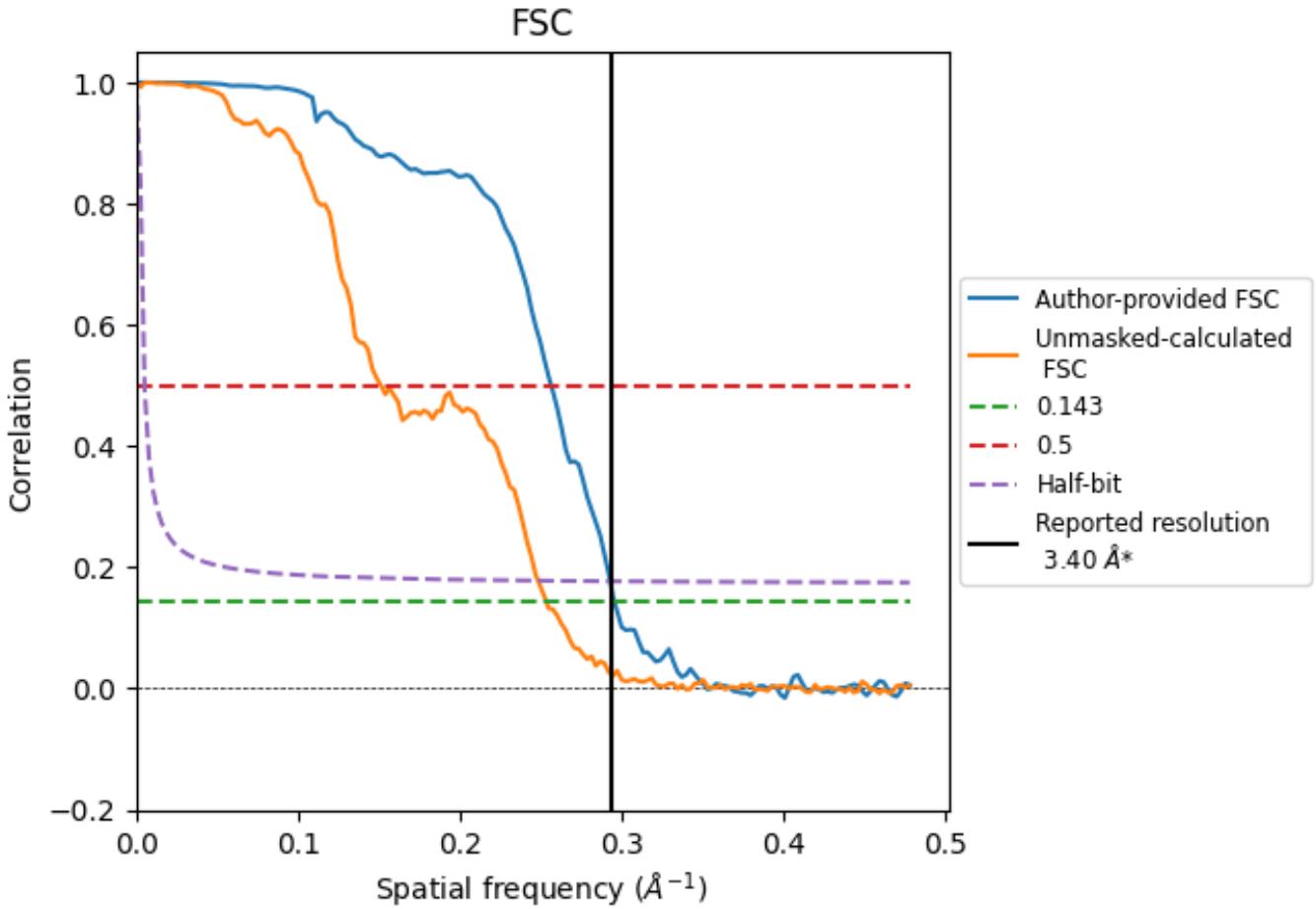


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

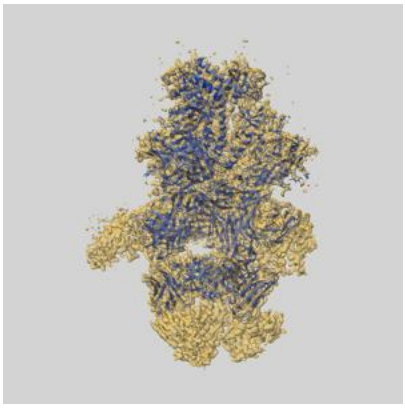
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	3.89	3.41
Unmasked-calculated*	3.94	6.60	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.4 by more than 10 %

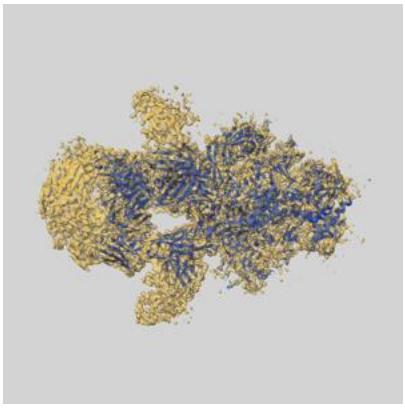
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43838 and PDB model 9ATZ. Per-residue inclusion information can be found in section 3 on page 15.

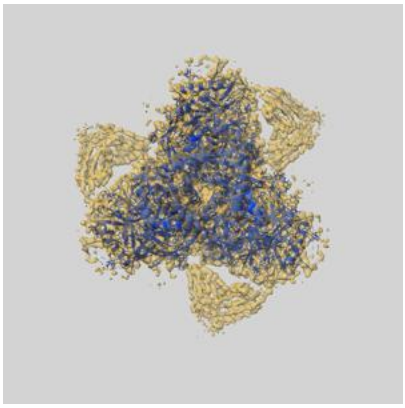
9.1 Map-model overlay



X



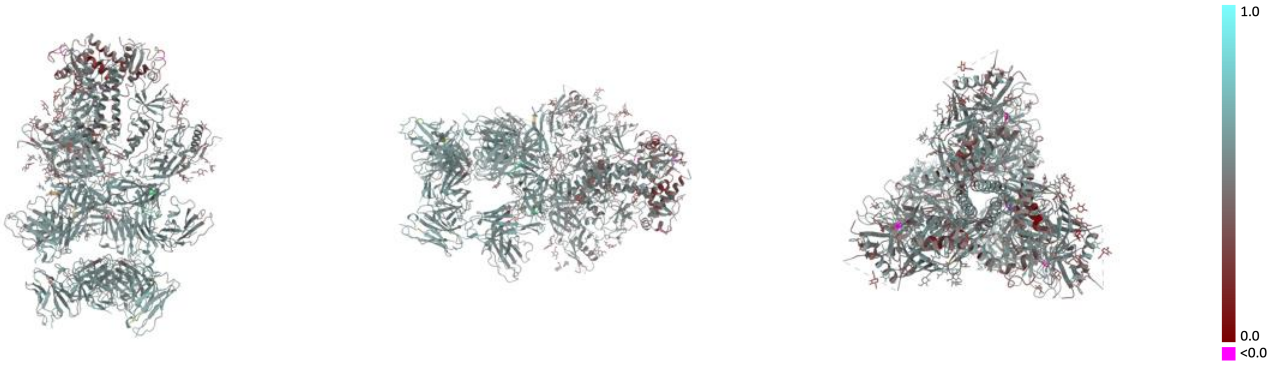
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

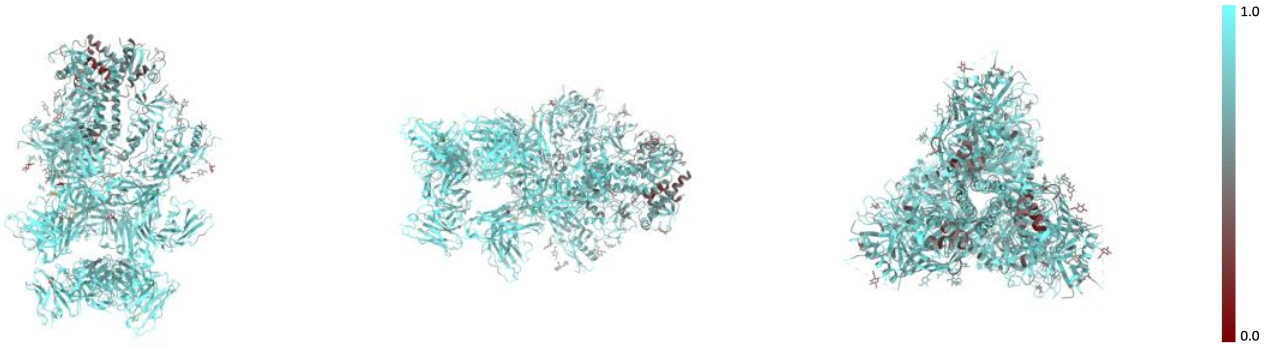
9.2 Q-score mapped to coordinate model



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.

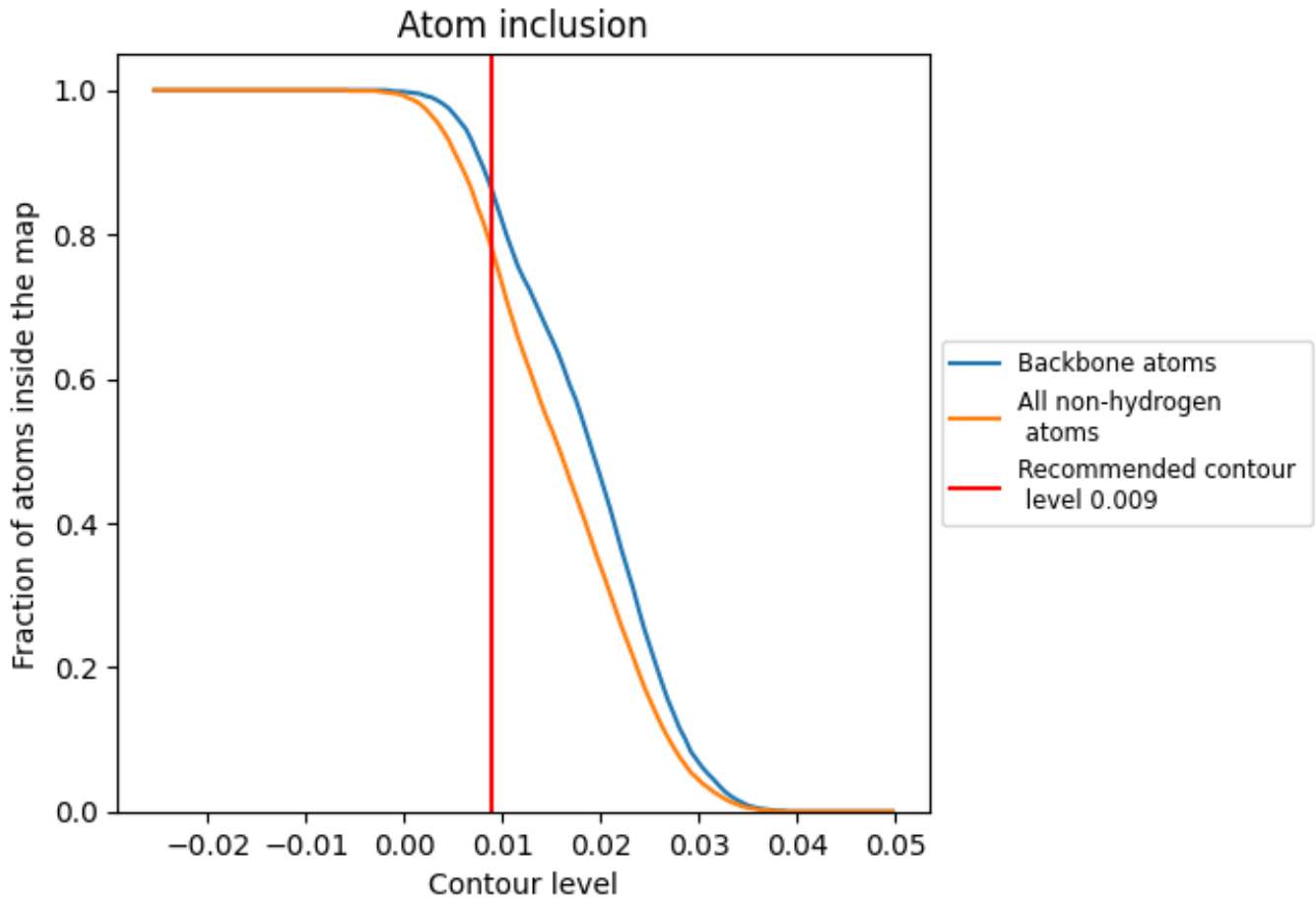
9.3 Atom inclusion mapped to coordinate model



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7780	0.5110
A	0.8550	0.5240
B	0.8750	0.5480
C	0.8680	0.5560
D	0.7740	0.5180
E	0.8560	0.5560
F	0.8500	0.5260
G	0.8800	0.5580
H	0.8680	0.5580
I	0.7800	0.5200
J	0.8490	0.5530
K	0.8730	0.5530
L	0.8730	0.5580
M	0.7790	0.5190
N	0.8570	0.5300
O	0.6050	0.4000
P	0.6360	0.4380
Q	0.6320	0.4240
R	0.8560	0.5540
S	0.4640	0.4170
T	0.3570	0.3620
U	0.4290	0.1960
V	0.6230	0.3850
W	0.5360	0.4080
X	0.4290	0.3940
Y	0.5000	0.3670
Z	0.4290	0.2610
a	0.8030	0.5020
b	0.5360	0.4150
c	0.4290	0.3790
d	0.5000	0.3680
e	0.7700	0.5250
f	0.6070	0.3990
g	0.4640	0.3980
h	0.5000	0.3580
i	0.5000	0.4310