Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:22 AM UTC

PDB ID	:	6CS2 / pdb_00006cs2
EMDB ID	:	EMD-7582
Title	:	SARS Spike Glycoprotein - human ACE2 complex, Stabilized variant, all ACE2-bound particles
Authors	:	Kirchdoerfer, R.N.; Wang, N.; Pallesen, J.; Turner, H.L.; Cottrell, C.A.; McLellan, J.S.; Ward, A.B.
Deposited on	:	2018-03-19
Resolution	:	4.40 Å(reported)
Based on initial models	:	5X4S, 5I08, 2AJF

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:

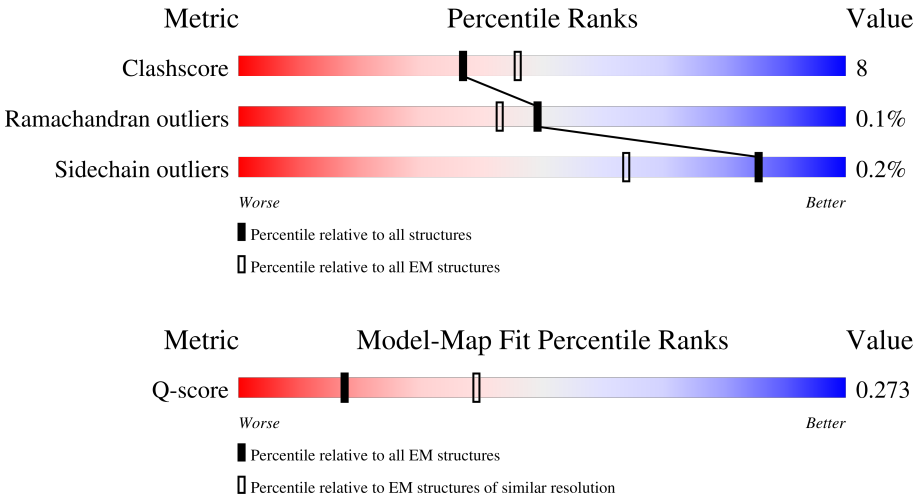
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
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 4.40 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	3132 (3.91 - 4.90)

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	1215	6% 61% 12% 27%
1	B	1215	8% 69% 19% 11%
1	C	1215	5% 58% 15% 27%
2	D	605	57% 72% 17% • 10%

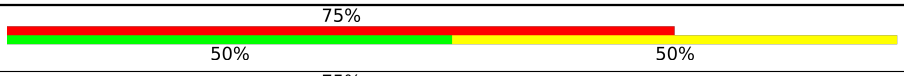
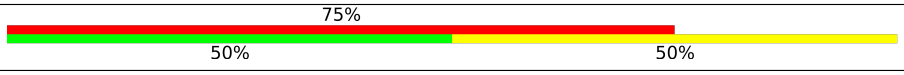
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	3	33% 33% 33% 33%
3	F	3	67% 67% 33%
3	M	3	67% 67% 33%
3	O	3	33% 67% 33%
3	Q	3	67% 33% 67%
3	T	3	67% 33% 67%
3	V	3	67% 67% 33%
3	W	3	100% 100%
3	X	3	67% 100%
4	G	2	50% 100%
4	J	2	50% 50% 50%
4	N	2	100% 100%
4	R	2	50% 50% 50%
4	Y	2	50% 100%
4	Z	2	100% 50% 50%
4	c	2	50% 100%
5	H	4	75% 75% 25%
5	I	4	50% 25% 75%
5	K	4	75% 25% 50% 25%
5	L	4	75% 25% 75%
5	P	4	75% 25% 75%
5	S	4	50% 25% 75%
5	a	4	75% 50% 25% 25%
5	b	4	50% 50% 50%
5	d	4	50% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	e	4	
6	U	4	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 27858 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 Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	891	Total	C	N	O	S	0	0
			6914	4403	1146	1328	37		
1	B	1076	Total	C	N	O	S	0	0
			8405	5371	1389	1599	46		
1	C	893	Total	C	N	O	S	0	0
			6927	4409	1149	1332	37		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	577	ALA	SER	conflict	UNP P59594
A	968	PRO	LYS	engineered mutation	UNP P59594
A	969	PRO	VAL	engineered mutation	UNP P59594
A	1191	GLY	-	linker	UNP P59594
A	1192	SER	ALA	linker	UNP D9IEJ2
A	1220	GLY	-	expression tag	UNP D9IEJ2
A	1221	ARG	-	expression tag	UNP D9IEJ2
A	1222	SER	-	expression tag	UNP D9IEJ2
A	1223	LEU	-	expression tag	UNP D9IEJ2
A	1224	GLU	-	expression tag	UNP D9IEJ2
A	1225	VAL	-	expression tag	UNP D9IEJ2
A	1226	LEU	-	expression tag	UNP D9IEJ2
A	1227	PHE	-	expression tag	UNP D9IEJ2
A	1228	GLN	-	expression tag	UNP D9IEJ2
B	577	ALA	SER	conflict	UNP P59594
B	968	PRO	LYS	engineered mutation	UNP P59594
B	969	PRO	VAL	engineered mutation	UNP P59594
B	1191	GLY	-	linker	UNP P59594
B	1192	SER	ALA	linker	UNP D9IEJ2
B	1220	GLY	-	expression tag	UNP D9IEJ2
B	1221	ARG	-	expression tag	UNP D9IEJ2
B	1222	SER	-	expression tag	UNP D9IEJ2
B	1223	LEU	-	expression tag	UNP D9IEJ2
B	1224	GLU	-	expression tag	UNP D9IEJ2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1225	VAL	-	expression tag	UNP D9IEJ2
B	1226	LEU	-	expression tag	UNP D9IEJ2
B	1227	PHE	-	expression tag	UNP D9IEJ2
B	1228	GLN	-	expression tag	UNP D9IEJ2
C	577	ALA	SER	conflict	UNP P59594
C	968	PRO	LYS	engineered mutation	UNP P59594
C	969	PRO	VAL	engineered mutation	UNP P59594
C	1191	GLY	-	linker	UNP P59594
C	1192	SER	ALA	linker	UNP D9IEJ2
C	1220	GLY	-	expression tag	UNP D9IEJ2
C	1221	ARG	-	expression tag	UNP D9IEJ2
C	1222	SER	-	expression tag	UNP D9IEJ2
C	1223	LEU	-	expression tag	UNP D9IEJ2
C	1224	GLU	-	expression tag	UNP D9IEJ2
C	1225	VAL	-	expression tag	UNP D9IEJ2
C	1226	LEU	-	expression tag	UNP D9IEJ2
C	1227	PHE	-	expression tag	UNP D9IEJ2
C	1228	GLN	-	expression tag	UNP D9IEJ2

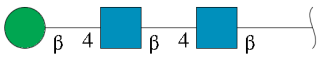
- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	544	4431	2828	736	839	28	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	GLY	-	expression tag	UNP Q9BYF1
D	617	SER	-	expression tag	UNP Q9BYF1
D	618	LEU	-	expression tag	UNP Q9BYF1
D	619	GLU	-	expression tag	UNP Q9BYF1
D	620	VAL	-	expression tag	UNP Q9BYF1
D	621	LEU	-	expression tag	UNP Q9BYF1
D	622	PHE	-	expression tag	UNP Q9BYF1
D	623	GLN	-	expression tag	UNP Q9BYF1

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		
3	T	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	W	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
4	c	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



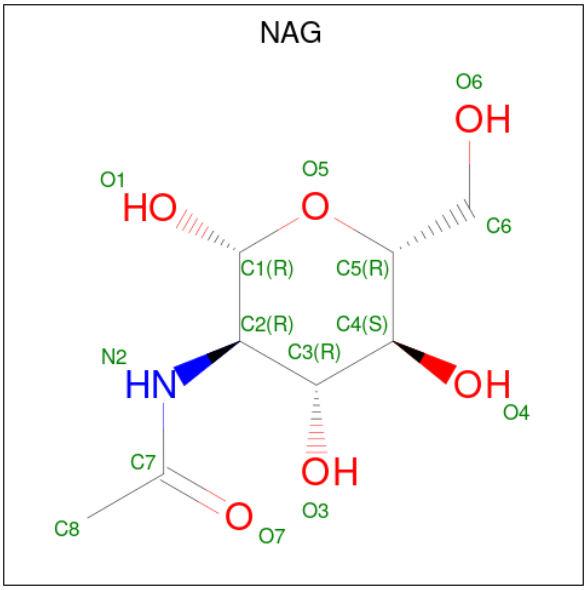
Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	4	Total 50	C 28	N 2	O 20	0	0
5	I	4	Total 50	C 28	N 2	O 20	0	0
5	K	4	Total 50	C 28	N 2	O 20	0	0
5	L	4	Total 50	C 28	N 2	O 20	0	0
5	P	4	Total 50	C 28	N 2	O 20	0	0
5	S	4	Total 50	C 28	N 2	O 20	0	0
5	a	4	Total 50	C 28	N 2	O 20	0	0
5	b	4	Total 50	C 28	N 2	O 20	0	0
5	d	4	Total 50	C 28	N 2	O 20	0	0
5	e	4	Total 50	C 28	N 2	O 20	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	U	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

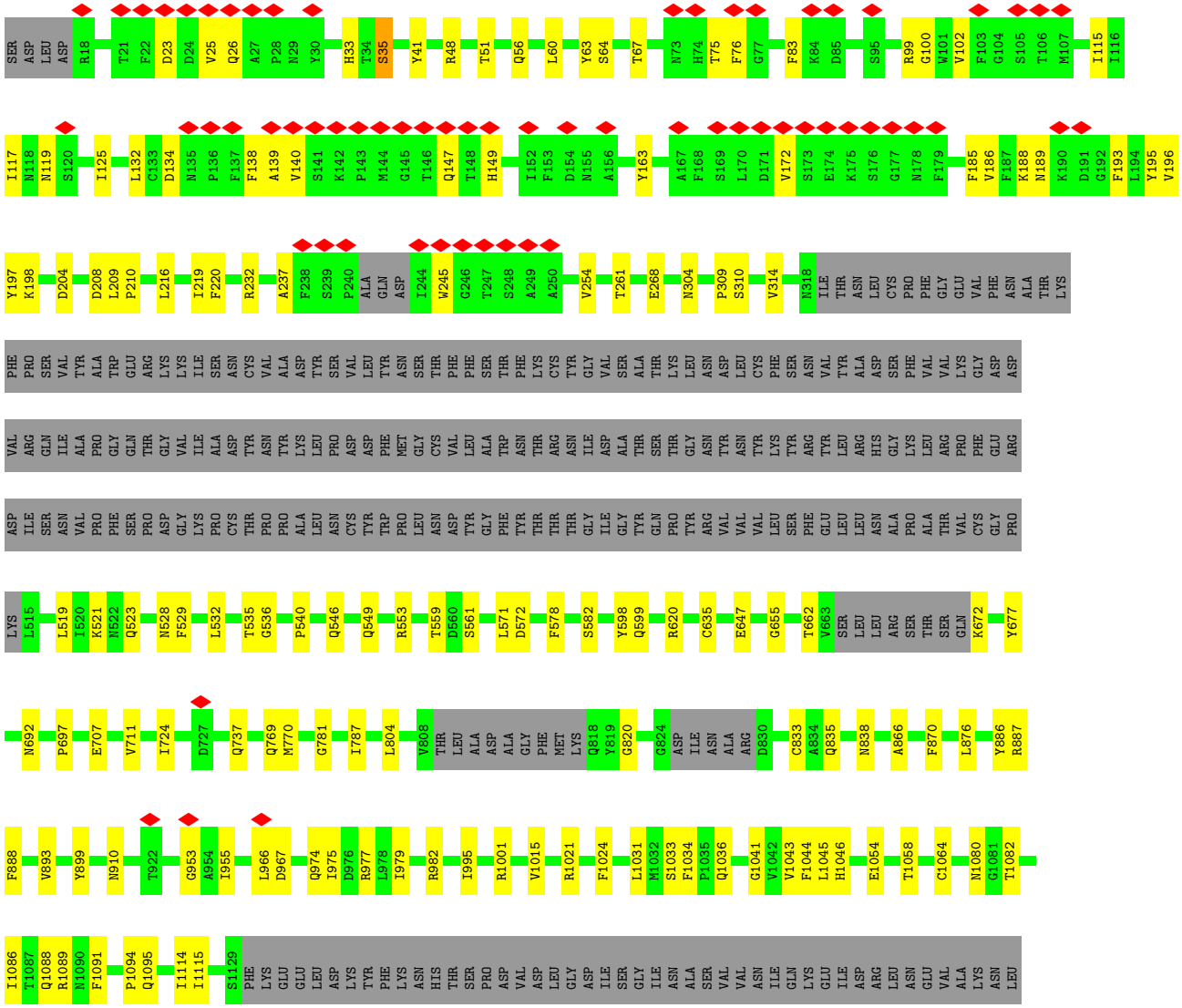
3 Residue-property plots (i)

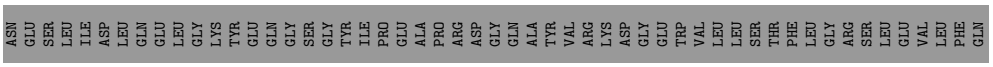
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein,Fibritin

Chain A:



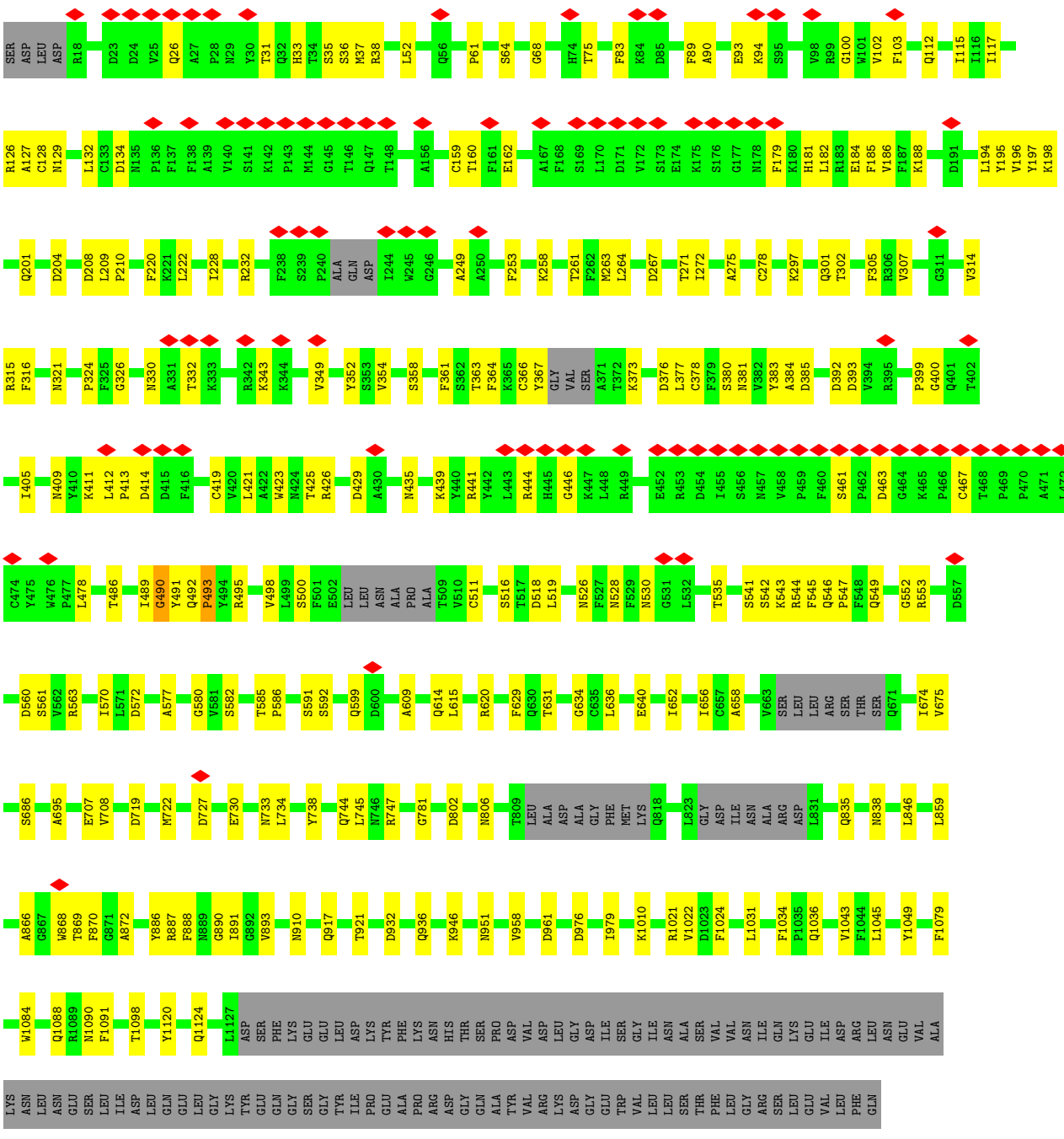




• Molecule 1: Spike glycoprotein,Fibritin

Chain B:

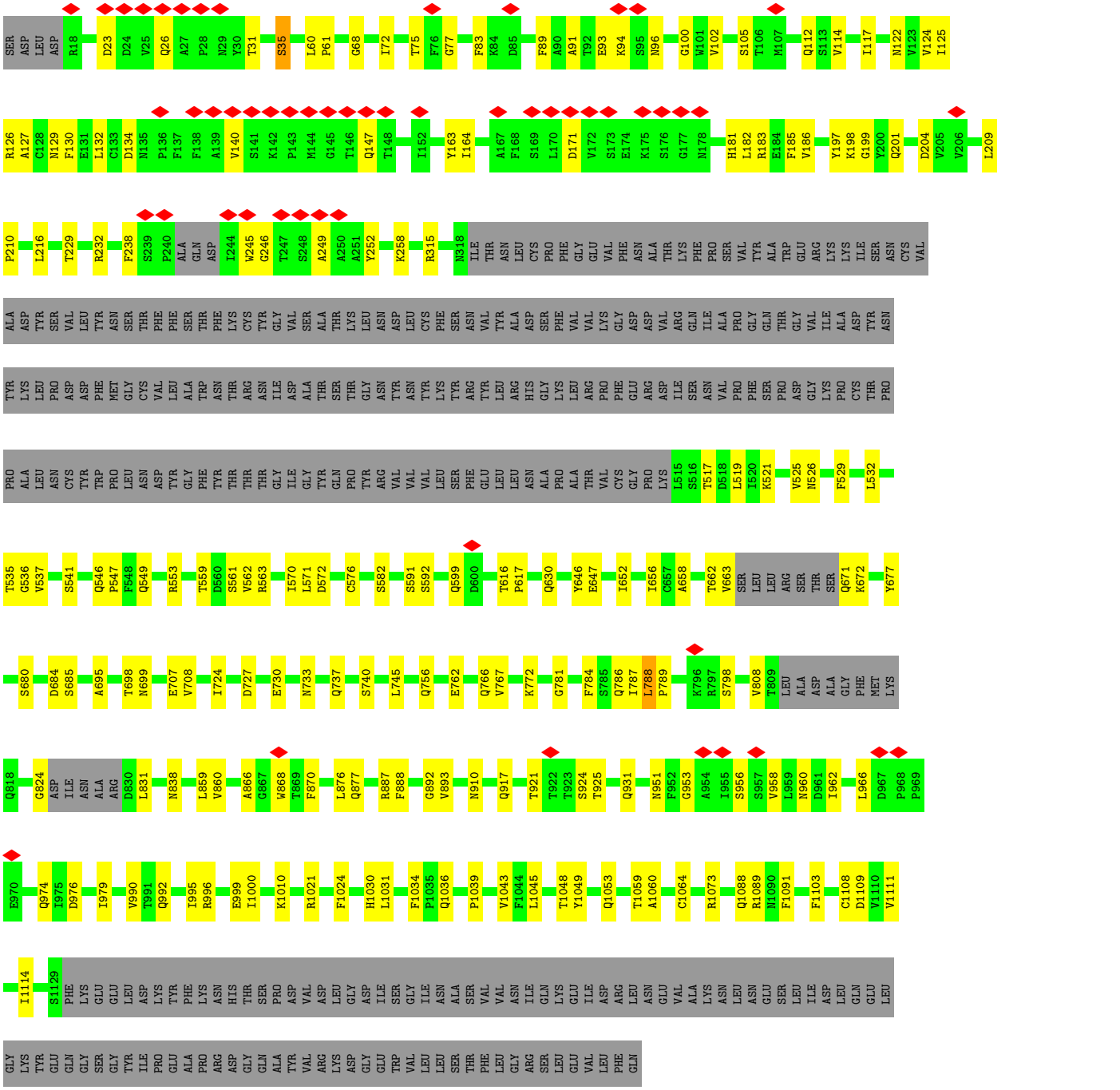




• Molecule 1: Spike glycoprotein,Fibritin

Chain C:

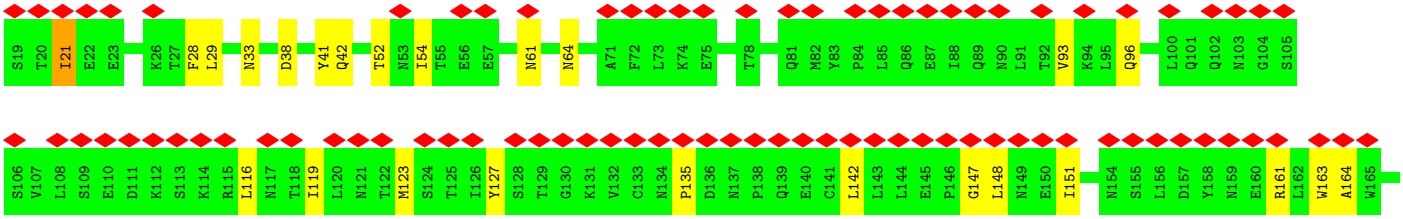


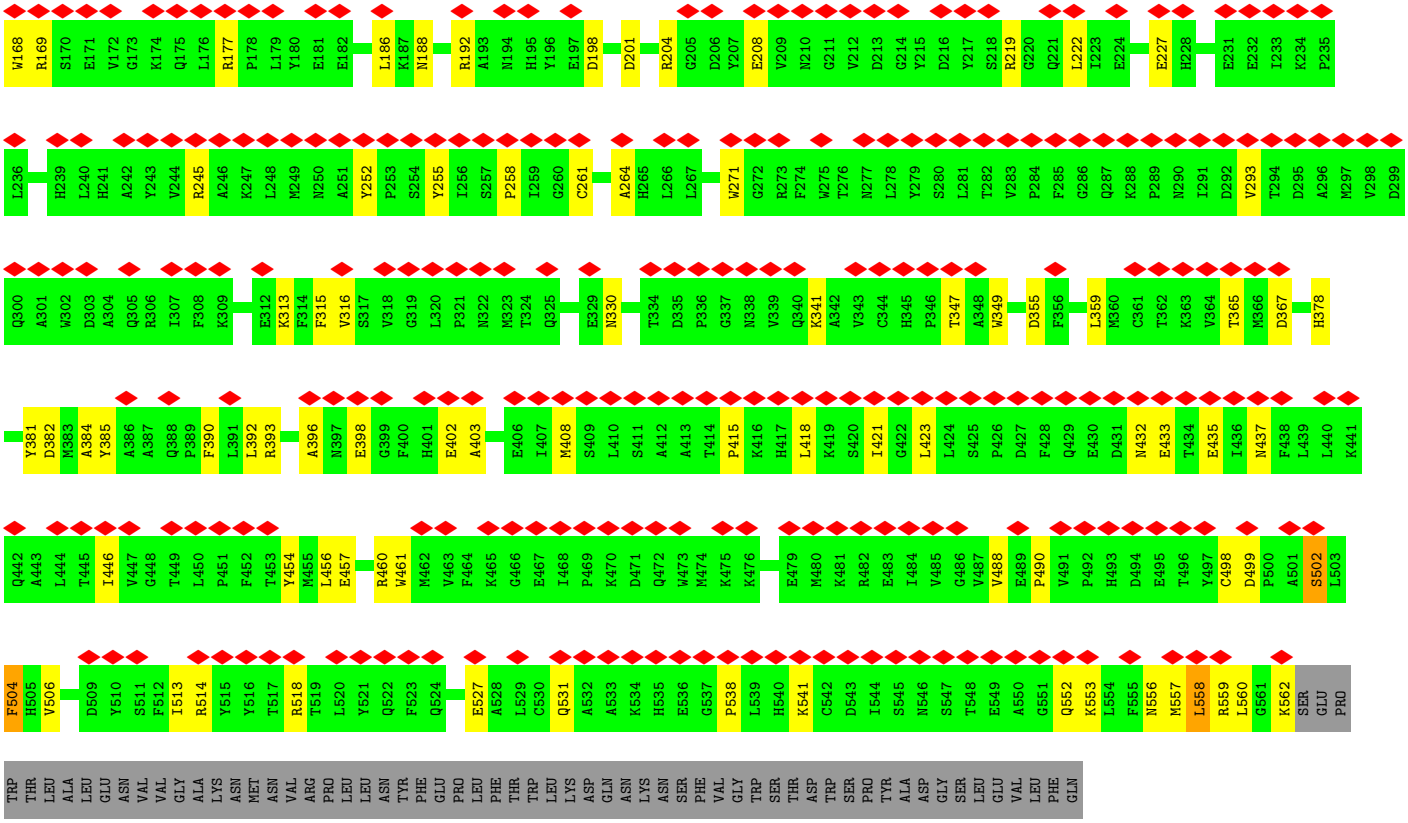


• Molecule 2: Angiotensin-converting enzyme 2

Chain D:

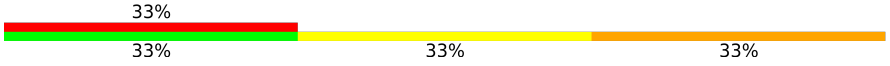






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:





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

Chain F:





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

Chain M:





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

Chain O:





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

Chain Q:





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

Chain T:





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

Chain V:





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

Chain W:





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

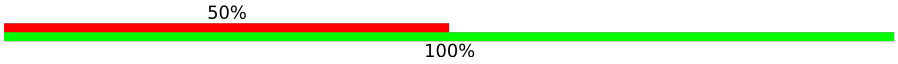
Chain X:





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

Chain G:





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

Chain J:





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

Chain N:





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

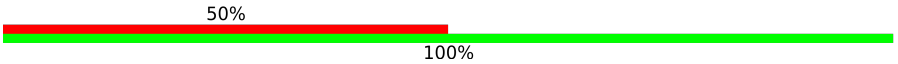
Chain R:





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

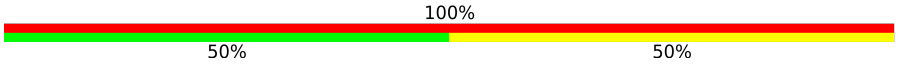
Chain Y:





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

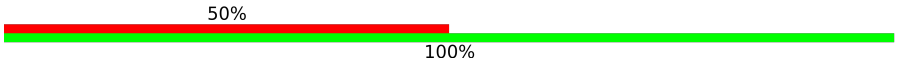
Chain Z:





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

Chain c:





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

Chain H:





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

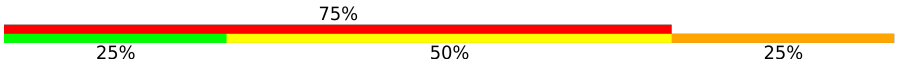
Chain I:





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

Chain K:





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

Chain L:





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

Chain P:





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

Chain S:





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

Chain a:





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

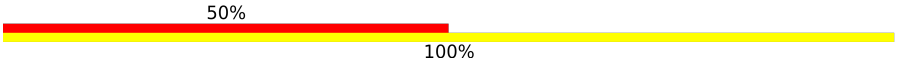
Chain b:





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

Chain d:





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

Chain e:





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

Chain U:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	370.8, 370.8, 370.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/7067	0.53	0/9612
1	B	0.30	1/8606 (0.0%)	0.53	2/11712 (0.0%)
1	C	0.31	0/7080	0.53	0/9630
2	D	0.19	0/4551	0.51	2/6176 (0.0%)
All	All	0.29	1/27304 (0.0%)	0.53	4/37130 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1124	GLN	C-N	5.41	1.39	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	502	SER	N-CA-C	-9.48	100.82	111.82
2	D	504	PHE	N-CA-C	5.94	119.63	112.38
1	B	1022	VAL	CA-C-N	5.12	131.32	121.54
1	B	1022	VAL	C-N-CA	5.12	131.32	121.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	SER	Peptide
1	A	83	PHE	Peptide
1	B	35	SER	Peptide
1	B	83	PHE	Peptide
1	C	35	SER	Peptide
1	C	83	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6914	0	6723	90	0
1	B	8405	0	8145	147	0
1	C	6927	0	6729	124	0
2	D	4431	0	4231	73	0
3	E	39	0	34	1	0
3	F	39	0	34	0	0
3	M	39	0	34	0	0
3	O	39	0	34	0	0
3	Q	39	0	34	0	0
3	T	39	0	34	0	0
3	V	39	0	34	0	0
3	W	39	0	34	0	0
3	X	39	0	34	0	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
4	N	28	0	25	0	0
4	R	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	0	0
4	c	28	0	25	0	0
5	H	50	0	43	0	0
5	I	50	0	43	0	0
5	K	50	0	43	1	0
5	L	50	0	43	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	50	0	43	0	0
5	S	50	0	43	0	0
5	a	50	0	43	1	0
5	b	50	0	43	0	0
5	d	50	0	43	2	0
5	e	50	0	43	0	0
6	U	50	0	43	0	0
7	A	28	0	26	0	0
7	B	28	0	26	0	0
7	C	28	0	26	0	0
All	All	27858	0	26860	415	0

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

All (415) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:THR:OG1	1:B:493:PRO:O	1.97	0.81
2:D:381:TYR:HD1	2:D:558:LEU:CD1	1.94	0.81
1:A:966:LEU:O	1:A:967:ASP:OD1	2.02	0.77
1:A:955:ILE:H	1:A:974:GLN:HE22	1.33	0.76
1:C:727:ASP:O	1:C:727:ASP:OD1	2.03	0.76
2:D:127:TYR:CE2	2:D:504:PHE:HD1	2.05	0.74
2:D:381:TYR:HD1	2:D:558:LEU:HD12	1.52	0.74
1:A:309:PRO:HB3	1:A:535:THR:HG21	1.71	0.71
1:B:383:TYR:HB2	1:B:500:SER:HB2	1.74	0.70
2:D:384:ALA:CB	2:D:558:LEU:HD23	2.21	0.70
1:A:188:LYS:HB3	1:A:195:TYR:HB2	1.74	0.69
1:C:535:THR:HG22	1:C:536:GLY:N	2.06	0.69
1:B:64:SER:HA	1:B:620:ARG:HH22	1.58	0.69
2:D:384:ALA:HB2	2:D:558:LEU:HD23	1.75	0.68
1:B:378:CYS:HA	1:B:511:CYS:HA	1.76	0.67
1:A:125:ILE:HB	1:A:163:TYR:HB3	1.77	0.66
1:B:1034:PHE:HB2	1:B:1045:LEU:HB2	1.78	0.65
1:C:529:PHE:HB2	1:C:532:LEU:HB2	1.78	0.65
2:D:499:ASP:O	2:D:502:SER:OG	2.08	0.65
1:C:788:LEU:HB3	1:C:789:PRO:HD2	1.79	0.65
2:D:33:ASN:HD22	2:D:390:PHE:HB3	1.62	0.64
1:C:887:ARG:NH1	1:C:1031:LEU:O	2.32	0.63
1:B:489:ILE:C	1:B:491:TYR:H	2.07	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:TYR:HE2	2:D:504:PHE:HD1	1.48	0.61
1:B:126:ARG:HG3	1:B:162:GLU:HG2	1.81	0.61
1:C:788:LEU:HD23	1:C:860:VAL:HG12	1.82	0.61
1:A:737:GLN:NE2	1:C:951:ASN:O	2.33	0.61
1:C:525:VAL:O	1:C:535:THR:HG23	2.00	0.61
2:D:559:ARG:O	2:D:559:ARG:HG2	1.98	0.61
1:A:995:ILE:HG22	1:C:995:ILE:HD12	1.83	0.61
2:D:381:TYR:CD1	2:D:558:LEU:HD12	2.36	0.61
1:A:887:ARG:NH1	1:A:1031:LEU:O	2.34	0.60
1:B:90:ALA:HB3	1:B:253:PHE:HB2	1.83	0.60
1:B:314:VAL:HG22	1:B:528:ASN:HB3	1.82	0.60
1:B:629:PHE:HB3	1:B:636:LEU:HB3	1.83	0.60
1:B:1088:GLN:HE21	1:B:1091:PHE:HB3	1.67	0.60
2:D:421:ILE:HG23	2:D:423:LEU:H	1.67	0.60
1:A:1034:PHE:HB2	1:A:1045:LEU:HB2	1.84	0.60
1:A:100:GLY:HA3	1:A:117:ILE:HG22	1.84	0.60
2:D:264:ALA:H	2:D:490:PRO:HD3	1.67	0.60
1:B:707:GLU:OE2	1:B:1010:LYS:NZ	2.34	0.60
1:B:326:GLY:HA2	1:B:330:ASN:HD22	1.65	0.60
2:D:261:CYS:HB2	2:D:488:VAL:HG23	1.84	0.60
1:B:324:PRO:O	1:B:343:LYS:NZ	2.35	0.59
1:C:699:ASN:H	1:C:1053:GLN:HB3	1.67	0.59
1:A:189:ASN:ND2	1:A:193:PHE:O	2.35	0.59
1:B:547:PRO:HA	1:B:563:ARG:HH22	1.66	0.59
1:B:744:GLN:HA	1:B:747:ARG:HG2	1.84	0.59
1:A:578:PHE:H	1:B:835:GLN:HE22	1.49	0.59
1:B:640:GLU:HB2	1:B:675:VAL:HG12	1.85	0.59
1:C:808:VAL:O	1:C:931:GLN:NE2	2.36	0.59
2:D:252:TYR:HB3	2:D:255:TYR:HB2	1.85	0.59
1:C:868:TRP:HZ2	1:C:887:ARG:HE	1.51	0.58
1:A:546:GLN:HB2	1:A:549:GLN:HG2	1.84	0.58
1:C:547:PRO:HA	1:C:563:ARG:HH22	1.67	0.58
1:B:100:GLY:HA3	1:B:117:ILE:HG22	1.84	0.58
1:A:535:THR:HG22	1:A:536:GLY:N	2.18	0.58
1:B:321:ASN:HB2	1:B:349:VAL:H	1.68	0.58
1:A:1089:ARG:HH22	1:B:886:TYR:HB2	1.68	0.58
1:A:314:VAL:HG22	1:A:528:ASN:HB3	1.86	0.58
1:A:102:VAL:HG11	1:A:132:LEU:HD11	1.86	0.58
1:A:561:SER:HA	1:A:572:ASP:HA	1.84	0.58
1:B:425:THR:O	1:B:493:PRO:HG2	2.04	0.58
1:C:315:ARG:HA	1:C:517:THR:HG22	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:553:LYS:O	2:D:557:MET:HG3	2.04	0.58
1:C:35:SER:HB2	1:C:60:LEU:HD21	1.86	0.57
1:B:261:THR:HG23	1:B:278:CYS:HB2	1.87	0.57
1:B:546:GLN:HB2	1:B:549:GLN:HE21	1.70	0.57
1:C:94:LYS:NZ	1:C:249:ALA:O	2.37	0.57
2:D:204:ARG:HG2	2:D:222:LEU:HD23	1.86	0.57
2:D:245:ARG:NH2	2:D:258:PRO:O	2.37	0.57
1:C:1034:PHE:HB2	1:C:1045:LEU:HB2	1.87	0.57
1:B:392:ASP:OD1	1:B:490:GLY:HA3	2.04	0.57
1:A:886:TYR:HB2	1:C:1089:ARG:HH12	1.70	0.57
1:B:267:ASP:OD1	1:B:271:THR:N	2.38	0.56
1:C:866:ALA:HB3	1:C:870:PHE:HB2	1.87	0.56
2:D:347:THR:OG1	2:D:349:TRP:NE1	2.38	0.56
2:D:381:TYR:CD1	2:D:558:LEU:CD1	2.84	0.56
1:C:630:GLN:HE22	5:d:1:NAG:H82	1.71	0.56
1:C:186:VAL:HB	1:C:197:TYR:HB2	1.87	0.56
1:B:439:LYS:HB3	1:B:478:LEU:HB3	1.87	0.56
2:D:54:ILE:HB	2:D:341:LYS:HB2	1.88	0.56
1:B:367:TYR:O	1:B:373:LYS:NZ	2.38	0.56
1:A:134:ASP:O	1:A:232:ARG:NH1	2.39	0.56
1:A:268:GLU:HB2	3:E:1:NAG:H82	1.88	0.56
1:B:188:LYS:HE3	1:B:195:TYR:HD2	1.70	0.56
1:C:784:PHE:CD1	1:C:787:ILE:HD12	2.40	0.56
1:C:663:VAL:O	1:C:671:GLN:N	2.39	0.56
2:D:460:ARG:HE	2:D:506:VAL:HG22	1.70	0.56
1:B:264:LEU:HD13	1:B:272:ILE:HG12	1.88	0.56
1:C:89:PHE:HB3	1:C:185:PHE:HB2	1.88	0.56
2:D:457:GLU:OE2	2:D:460:ARG:NH1	2.39	0.56
1:B:802:ASP:O	1:B:806:ASN:ND2	2.39	0.56
2:D:169:ARG:HH12	2:D:271:TRP:HA	1.71	0.56
1:C:93:GLU:HB2	1:C:181:HIS:HB2	1.88	0.55
1:C:953:GLY:O	1:C:974:GLN:NE2	2.39	0.55
1:A:309:PRO:HB3	1:A:535:THR:CG2	2.35	0.55
1:A:35:SER:HB2	1:A:60:LEU:HD21	1.88	0.55
1:B:891:ILE:O	1:B:1090:ASN:ND2	2.39	0.55
1:C:185:PHE:HE1	1:C:198:LYS:HG3	1.72	0.55
1:B:134:ASP:O	1:B:232:ARG:NH1	2.40	0.55
2:D:127:TYR:HE2	2:D:504:PHE:CD1	2.25	0.55
1:B:38:ARG:NH1	1:B:184:GLU:OE2	2.40	0.55
1:B:89:PHE:HB3	1:B:185:PHE:HB2	1.88	0.55
1:B:354:VAL:O	1:B:358:SER:OG	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ILE:HB	1:C:163:TYR:HB3	1.88	0.55
1:C:992:GLN:HE22	1:C:996:ARG:HH22	1.55	0.55
1:C:824:GLY:HA3	1:C:831:LEU:HA	1.89	0.54
1:A:1001:ARG:NH1	1:C:999:GLU:OE2	2.40	0.54
1:A:1088:GLN:HE21	1:A:1091:PHE:HB3	1.72	0.54
1:A:67:THR:HB	1:A:254:VAL:HB	1.90	0.54
1:C:537:VAL:HG23	1:C:576:CYS:HA	1.90	0.54
2:D:52:THR:HG22	2:D:359:LEU:HD13	1.90	0.54
1:A:553:ARG:HA	1:A:559:THR:HA	1.89	0.54
1:B:94:LYS:NZ	1:B:249:ALA:O	2.41	0.54
1:B:734:LEU:HD23	1:B:979:ILE:HD12	1.90	0.54
1:B:426:ARG:HA	1:B:493:PRO:CD	2.38	0.53
1:B:553:ARG:HA	1:B:560:ASP:H	1.73	0.53
1:B:61:PRO:HG2	1:B:258:LYS:HD2	1.89	0.53
1:B:400:GLY:O	1:B:411:LYS:NZ	2.40	0.53
1:C:784:PHE:HB3	1:C:788:LEU:HD11	1.91	0.53
1:C:784:PHE:HB3	1:C:788:LEU:CD1	2.38	0.53
1:B:343:LYS:HB3	1:B:384:ALA:HB3	1.90	0.53
1:B:526:ASN:HA	1:B:535:THR:HA	1.91	0.53
1:C:1108:CYS:SG	1:C:1109:ASP:N	2.81	0.53
2:D:151:ILE:O	2:D:161:ARG:NH1	2.42	0.53
1:B:544:ARG:NH1	1:B:545:PHE:O	2.42	0.53
2:D:365:THR:HG22	2:D:367:ASP:H	1.73	0.53
1:C:535:THR:CG2	1:C:536:GLY:N	2.70	0.53
2:D:499:ASP:HA	2:D:502:SER:HB3	1.90	0.53
1:B:385:ASP:HB2	1:B:498:VAL:HB	1.89	0.52
1:C:724:ILE:HD12	1:C:979:ILE:HD11	1.91	0.52
1:C:1073:ARG:HE	1:C:1103:PHE:HB3	1.74	0.52
1:A:707:GLU:HB3	1:A:1044:PHE:HB2	1.91	0.52
1:A:1064:CYS:N	1:A:1115:ILE:O	2.40	0.52
1:C:561:SER:HA	1:C:572:ASP:HA	1.91	0.52
1:A:64:SER:OG	1:A:620:ARG:NH1	2.43	0.52
1:A:707:GLU:OE1	1:A:1046:HIS:NE2	2.35	0.52
1:B:781:GLY:O	1:B:910:ASN:ND2	2.41	0.52
1:C:140:VAL:HG22	1:C:147:GLN:HA	1.92	0.52
1:B:580:GLY:H	1:B:599:GLN:HB2	1.74	0.52
1:B:695:ALA:HB3	1:C:877:GLN:H	1.74	0.52
1:B:951:ASN:HD22	1:C:737:GLN:HG2	1.73	0.52
2:D:433:GLU:O	2:D:437:ASN:ND2	2.43	0.52
1:B:182:LEU:HD23	1:B:201:GLN:HE21	1.75	0.52
1:B:708:VAL:HG22	1:B:1043:VAL:HG22	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:VAL:HG22	1:C:1043:VAL:HG22	1.91	0.52
1:A:833:CYS:H	5:d:1:NAG:H81	1.73	0.52
1:B:185:PHE:HE1	1:B:198:LYS:HG3	1.75	0.52
1:C:546:GLN:HB2	1:C:549:GLN:HG2	1.92	0.52
1:B:441:ARG:HD3	1:B:444:ARG:HB2	1.91	0.52
1:B:887:ARG:NH1	1:B:1031:LEU:O	2.42	0.52
2:D:293:VAL:HB	2:D:423:LEU:HB3	1.91	0.52
1:C:767:VAL:HG12	1:C:859:LEU:HD21	1.91	0.52
1:B:102:VAL:HG22	1:B:115:ILE:HG12	1.91	0.52
1:B:444:ARG:NH1	1:B:446:GLY:O	2.41	0.52
1:C:1088:GLN:HE21	1:C:1091:PHE:HB3	1.75	0.52
1:B:209:LEU:HD12	1:B:210:PRO:HD2	1.93	0.51
1:C:647:GLU:O	1:C:677:TYR:OH	2.28	0.51
1:C:730:GLU:HA	1:C:733:ASN:HB2	1.92	0.51
1:A:26:GLN:OE1	1:A:75:THR:OG1	2.28	0.51
1:A:662:THR:HA	1:A:672:LYS:HA	1.93	0.51
1:B:366:CYS:HA	1:B:419:CYS:HA	1.92	0.51
1:C:582:SER:OG	1:C:599:GLN:NE2	2.44	0.51
1:B:332:THR:O	1:B:495:ARG:NH2	2.44	0.51
1:B:102:VAL:HG11	1:B:132:LEU:HD11	1.93	0.51
1:A:1094:PRO:HG2	5:K:1:NAG:H81	1.93	0.51
1:C:553:ARG:HG2	1:C:559:THR:HA	1.92	0.51
1:A:140:VAL:HG22	1:A:147:GLN:HA	1.92	0.51
1:C:209:LEU:HD12	1:C:210:PRO:HD2	1.92	0.51
1:A:899:TYR:HB3	1:C:1111:VAL:HG11	1.93	0.50
2:D:119:ILE:HG22	2:D:123:MET:HE2	1.93	0.50
1:C:519:LEU:HD21	1:C:521:LYS:HE3	1.92	0.50
1:C:788:LEU:CB	1:C:789:PRO:HD2	2.41	0.50
2:D:432:ASN:HA	2:D:435:GLU:HB2	1.93	0.50
1:B:1098:THR:HG22	1:B:1120:TYR:HB3	1.94	0.50
1:A:186:VAL:HB	1:A:197:TYR:HB2	1.94	0.50
1:C:112:GLN:NE2	1:C:129:ASN:OD1	2.45	0.50
1:B:361:PHE:HA	1:B:423:TRP:HB3	1.94	0.50
1:C:958:VAL:HG12	1:C:960:ASN:H	1.76	0.50
1:A:521:LYS:HD3	1:A:540:PRO:HD3	1.94	0.49
1:A:804:LEU:HD11	1:A:1043:VAL:HG21	1.93	0.49
1:B:315:ARG:HH22	1:B:519:LEU:HB2	1.77	0.49
1:B:958:VAL:HG12	1:B:961:ASP:H	1.77	0.49
2:D:457:GLU:HG3	2:D:513:ILE:HB	1.94	0.49
1:B:516:SER:OG	1:B:518:ASP:OD2	2.30	0.49
2:D:116:LEU:HD13	2:D:186:LEU:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:O	1:A:620:ARG:NH2	2.44	0.49
1:B:543:LYS:H	1:B:570:ILE:HG21	1.77	0.49
1:A:33:HIS:ND1	1:A:208:ASP:OD1	2.46	0.49
1:A:198:LYS:HD2	1:A:219:ILE:HD13	1.95	0.49
1:A:598:TYR:HB2	1:A:635:CYS:HB2	1.94	0.49
1:B:429:ASP:O	1:B:435:ASN:ND2	2.37	0.49
1:A:102:VAL:HG22	1:A:115:ILE:HG12	1.95	0.49
1:A:1080:ASN:HB3	1:A:1082:THR:H	1.77	0.49
1:A:41:TYR:HA	1:A:216:LEU:H	1.78	0.49
1:A:953:GLY:O	1:A:977:ARG:NH1	2.45	0.49
1:B:301:GLN:NE2	1:B:302:THR:O	2.42	0.49
1:B:461:SER:OG	1:B:463:ASP:OD1	2.29	0.49
2:D:398:GLU:OE1	2:D:514:ARG:NH2	2.45	0.48
1:B:609:ALA:HB1	1:B:614:GLN:HB2	1.95	0.48
1:C:591:SER:OG	1:C:592:SER:N	2.46	0.48
1:B:917:GLN:O	1:B:921:THR:OG1	2.26	0.48
2:D:148:LEU:HD21	2:D:168:TRP:HB2	1.94	0.48
1:C:652:ILE:HD11	1:C:658:ALA:HB2	1.96	0.48
1:A:99:ARG:HH22	1:A:172:VAL:HA	1.78	0.48
1:B:946:LYS:NZ	1:C:740:SER:OG	2.45	0.48
1:C:31:THR:O	1:C:68:GLY:N	2.37	0.48
1:C:124:VAL:HG22	1:C:164:ILE:HG12	1.94	0.48
1:C:182:LEU:HD23	1:C:201:GLN:HE21	1.76	0.48
2:D:127:TYR:CE2	2:D:504:PHE:CD1	2.95	0.48
1:A:25:VAL:HG13	1:A:76:PHE:H	1.79	0.48
1:B:489:ILE:O	1:B:491:TYR:N	2.47	0.48
1:C:204:ASP:OD1	1:C:204:ASP:N	2.46	0.48
1:A:1036:GLN:HB2	1:A:1043:VAL:HB	1.94	0.48
1:C:745:LEU:HD22	1:C:990:VAL:HG21	1.95	0.48
2:D:330:ASN:ND2	2:D:355:ASP:OD1	2.43	0.48
1:A:304:ASN:ND2	1:B:719:ASP:OD1	2.47	0.47
1:B:486:THR:HG1	2:D:41:TYR:HH	1.62	0.47
1:B:868:TRP:O	1:B:872:ALA:N	2.46	0.47
1:B:373:LYS:HA	1:B:376:ASP:HB3	1.96	0.47
1:A:820:GLY:HA2	1:A:835:GLN:HA	1.96	0.47
1:C:26:GLN:OE1	1:C:75:THR:OG1	2.32	0.47
1:C:838:ASN:N	1:C:838:ASN:OD1	2.46	0.47
2:D:382:ASP:OD1	2:D:385:TYR:OH	2.31	0.47
2:D:415:PRO:HA	2:D:418:LEU:HB2	1.96	0.47
1:B:886:TYR:O	1:B:890:GLY:N	2.47	0.47
1:C:727:ASP:O	1:C:727:ASP:CG	2.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:TYR:OH	1:B:976:ASP:OD1	2.33	0.47
1:B:380:SER:OG	1:B:381:ASN:N	2.46	0.47
1:C:662:THR:HA	1:C:672:LYS:HA	1.96	0.47
1:A:697:PRO:HA	1:A:1054:GLU:HA	1.96	0.47
1:B:127:ALA:O	1:B:160:THR:N	2.47	0.47
1:B:489:ILE:C	1:B:491:TYR:N	2.73	0.47
1:C:61:PRO:HG2	1:C:258:LYS:HD2	1.97	0.47
1:C:549:GLN:O	1:C:563:ARG:NH1	2.48	0.47
1:C:562:VAL:N	1:C:571:LEU:O	2.42	0.47
2:D:403:ALA:HB2	2:D:518:ARG:HG2	1.97	0.47
1:A:781:GLY:O	1:A:910:ASN:ND2	2.33	0.46
1:B:316:PHE:HA	1:B:530:ASN:HD21	1.79	0.46
1:A:529:PHE:HB2	1:A:532:LEU:HB2	1.97	0.46
1:B:305:PHE:HB2	1:B:615:LEU:HD11	1.98	0.46
1:B:591:SER:OG	1:B:592:SER:N	2.48	0.46
1:C:956:SER:HB2	1:C:962:ILE:HD12	1.97	0.46
1:B:297:LYS:HA	1:B:585:THR:HG23	1.97	0.46
1:B:489:ILE:O	1:B:492:GLN:HG3	2.15	0.46
1:C:91:ALA:N	1:C:183:ARG:O	2.46	0.46
1:C:526:ASN:HA	1:C:535:THR:HA	1.98	0.46
1:A:866:ALA:HB3	1:A:870:PHE:HB2	1.98	0.46
1:C:199:GLY:HA3	1:C:216:LEU:HD22	1.96	0.46
2:D:538:PRO:HD2	2:D:541:LYS:HD3	1.97	0.46
2:D:227:GLU:HA	2:D:454:TYR:HE1	1.80	0.46
1:A:56:GLN:OE1	1:A:261:THR:OG1	2.31	0.46
1:B:363:THR:HB	1:B:421:LEU:HA	1.98	0.46
2:D:396:ALA:HA	2:D:562:LYS:HA	1.97	0.46
1:A:770:MET:HB2	1:C:684:ASP:HA	1.97	0.46
1:C:646:TYR:O	1:C:680:SER:N	2.49	0.46
1:C:652:ILE:HD12	1:C:656:ILE:HG22	1.98	0.46
1:A:582:SER:OG	1:A:599:GLN:NE2	2.49	0.46
1:C:976:ASP:HA	1:C:979:ILE:HG22	1.97	0.46
1:A:1086:ILE:O	1:A:1095:GLN:N	2.49	0.46
1:B:552:GLY:O	1:B:560:ASP:N	2.48	0.46
1:C:917:GLN:O	1:C:921:THR:OG1	2.26	0.46
1:C:962:ILE:HG13	1:C:966:LEU:HD12	1.97	0.46
1:C:1031:LEU:HD11	1:C:1049:TYR:HB2	1.97	0.46
2:D:390:PHE:HA	2:D:393:ARG:HD2	1.97	0.46
1:C:808:VAL:HG21	1:C:1039:PRO:HG2	1.97	0.45
1:B:932:ASP:O	1:B:936:GLN:N	2.47	0.45
1:B:727:ASP:OD1	1:B:727:ASP:O	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:THR:HG22	1:C:536:GLY:H	1.77	0.45
1:B:31:THR:O	1:B:68:GLY:N	2.42	0.45
2:D:378:HIS:HE1	2:D:402:GLU:HA	1.81	0.45
1:A:535:THR:CG2	1:A:536:GLY:N	2.79	0.45
1:C:788:LEU:CD2	1:C:860:VAL:HG12	2.46	0.45
1:C:546:GLN:O	1:C:563:ARG:NH1	2.49	0.45
1:B:33:HIS:ND1	1:B:208:ASP:OD1	2.50	0.45
1:B:204:ASP:N	1:B:204:ASP:OD1	2.48	0.45
1:A:185:PHE:HE1	1:A:198:LYS:HG3	1.82	0.45
1:B:888:PHE:HB3	1:B:893:VAL:HB	1.98	0.45
1:B:869:THR:HA	1:B:872:ALA:HB3	1.98	0.45
1:C:72:ILE:H	1:C:75:THR:HB	1.82	0.45
1:A:647:GLU:O	1:A:677:TYR:OH	2.32	0.45
2:D:177:ARG:HB2	2:D:498:CYS:HB2	1.98	0.45
1:A:769:GLN:HB3	1:C:685:SER:HB3	1.98	0.44
1:B:26:GLN:OE1	1:B:75:THR:OG1	2.35	0.44
1:C:114:VAL:HA	1:C:127:ALA:HA	1.99	0.44
2:D:408:MET:SD	2:D:408:MET:N	2.89	0.44
1:A:204:ASP:OD1	1:A:204:ASP:N	2.47	0.44
1:A:692:ASN:HB2	1:A:1058:THR:HG23	2.00	0.44
1:B:461:SER:HB2	1:B:467:CYS:HB2	2.00	0.44
1:B:652:ILE:HD11	1:B:658:ALA:HB2	1.98	0.44
1:A:23:ASP:H	1:A:245:TRP:HE1	1.65	0.44
1:B:103:PHE:HB3	1:B:228:ILE:HG21	2.00	0.44
1:B:631:THR:OG1	1:B:634:GLY:N	2.50	0.44
1:A:138:PHE:O	1:A:237:ALA:N	2.48	0.44
1:B:264:LEU:HA	1:B:275:ALA:HA	1.99	0.44
1:A:975:ILE:O	1:A:979:ILE:N	2.45	0.44
1:B:686:SER:HB2	1:C:772:LYS:HD2	2.00	0.44
5:a:3:BMA:O6	5:a:3:BMA:O4	2.32	0.44
1:A:578:PHE:CG	1:B:722:MET:HG3	2.53	0.44
1:B:541:SER:HB3	1:B:570:ILE:HG22	2.00	0.44
1:C:91:ALA:HB3	1:C:183:ARG:HB2	1.99	0.44
1:C:924:SER:OG	1:C:925:THR:N	2.51	0.44
1:A:1021:ARG:HG3	1:A:1024:PHE:HB3	2.00	0.44
1:B:52:LEU:HD22	1:B:263:MET:HG2	2.00	0.44
1:B:951:ASN:HB2	1:C:737:GLN:HB3	1.99	0.44
1:A:724:ILE:HG22	1:A:982:ARG:HB3	2.00	0.43
1:B:196:VAL:HB	1:B:220:PHE:HB2	1.99	0.43
1:B:393:ASP:HB3	1:B:405:ILE:HG13	2.00	0.43
1:B:838:ASN:OD1	1:B:838:ASN:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:313:LYS:HA	2:D:316:VAL:HG12	2.00	0.43
1:A:655:GLY:N	1:B:846:LEU:O	2.51	0.43
1:B:572:ASP:N	1:B:572:ASP:OD1	2.51	0.43
1:C:762:GLU:O	1:C:766:GLN:NE2	2.46	0.43
1:C:781:GLY:O	1:C:910:ASN:ND2	2.50	0.43
2:D:93:VAL:HA	2:D:96:GLN:HB2	2.00	0.43
2:D:382:ASP:HA	2:D:385:TYR:CZ	2.53	0.43
2:D:527:GLU:O	2:D:531:GLN:N	2.45	0.43
1:B:186:VAL:HB	1:B:197:TYR:HB2	1.99	0.43
1:C:134:ASP:O	1:C:232:ARG:NH1	2.51	0.43
2:D:38:ASP:OD2	2:D:42:GLN:NE2	2.51	0.43
2:D:61:ASN:HA	2:D:64:ASN:HB2	2.00	0.43
2:D:208:GLU:OE1	2:D:219:ARG:NH1	2.51	0.43
1:A:540:PRO:HA	1:A:571:LEU:HG	1.99	0.43
1:B:582:SER:OG	1:B:599:GLN:NE2	2.44	0.43
1:B:586:PRO:HG2	1:B:591:SER:HB3	2.00	0.43
1:B:1021:ARG:H	1:B:1021:ARG:HG2	1.63	0.43
1:C:102:VAL:HG11	1:C:132:LEU:HD11	2.00	0.43
1:A:838:ASN:OD1	1:A:838:ASN:N	2.46	0.43
1:B:36:SER:OG	1:B:37:MET:N	2.52	0.43
1:B:112:GLN:NE2	1:B:129:ASN:OD1	2.52	0.43
1:B:561:SER:HA	1:B:572:ASP:HA	2.00	0.43
1:C:541:SER:HB3	1:C:570:ILE:HG22	1.99	0.43
2:D:21:ILE:H	2:D:21:ILE:HG13	1.53	0.43
1:A:310:SER:O	1:A:523:GLN:NE2	2.52	0.43
1:B:1031:LEU:HD11	1:B:1049:TYR:HB2	2.01	0.43
2:D:28:PHE:HD2	2:D:29:LEU:HD22	1.83	0.43
1:B:364:PHE:HA	1:B:421:LEU:HG	2.01	0.43
1:C:535:THR:CG2	1:C:536:GLY:H	2.31	0.43
1:C:888:PHE:O	1:C:892:GLY:N	2.51	0.43
2:D:552:GLN:O	2:D:556:ASN:HB2	2.19	0.43
1:A:711:VAL:HG22	1:A:1041:GLY:HA2	2.01	0.42
1:B:409:ASN:OD1	1:B:441:ARG:N	2.42	0.42
1:B:486:THR:O	2:D:330:ASN:ND2	2.52	0.42
1:C:23:ASP:H	1:C:245:TRP:HE1	1.66	0.42
1:C:707:GLU:OE2	1:C:1010:LYS:NZ	2.37	0.42
2:D:198:ASP:OD1	2:D:201:ASP:N	2.52	0.42
1:A:35:SER:OG	1:A:64:SER:N	2.45	0.42
1:B:541:SER:OG	1:B:542:SER:N	2.52	0.42
1:B:1036:GLN:HB2	1:B:1043:VAL:HB	2.00	0.42
1:B:352:TYR:CZ	1:B:377:LEU:HD22	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:PHE:O	1:C:893:VAL:N	2.51	0.42
1:C:1021:ARG:HG3	1:C:1024:PHE:HB3	2.01	0.42
1:C:1036:GLN:HB2	1:C:1043:VAL:HB	2.02	0.42
2:D:127:TYR:CE1	2:D:502:SER:O	2.73	0.42
2:D:457:GLU:O	2:D:461:TRP:N	2.44	0.42
1:A:876:LEU:HB3	1:C:695:ALA:HB3	2.01	0.42
1:C:77:GLY:O	1:C:252:TYR:OH	2.29	0.42
1:B:652:ILE:HD12	1:B:656:ILE:HG22	2.02	0.42
1:C:1030:HIS:HA	1:C:1048:THR:HG22	2.01	0.42
2:D:135:PRO:HD3	2:D:163:TRP:CZ3	2.55	0.42
1:A:209:LEU:HD12	1:A:210:PRO:HD2	2.01	0.42
1:A:888:PHE:HB3	1:A:893:VAL:HB	2.02	0.42
1:C:100:GLY:HA3	1:C:117:ILE:HG22	2.02	0.42
1:C:1059:THR:OG1	1:C:1060:ALA:N	2.52	0.42
1:C:1064:CYS:HB2	1:C:1114:ILE:HG22	2.02	0.42
1:B:194:LEU:HB3	1:B:222:LEU:HB2	2.02	0.42
1:B:412:LEU:HD12	1:B:413:PRO:HD2	2.01	0.42
1:C:126:ARG:HG2	1:C:130:PHE:HZ	1.84	0.42
1:B:392:ASP:CG	1:B:490:GLY:HA3	2.45	0.42
1:A:139:ALA:HB3	1:A:149:HIS:HB2	2.02	0.42
2:D:96:GLN:HE21	2:D:392:LEU:HD13	1.85	0.42
2:D:142:LEU:HD22	2:D:147:GLY:HA3	2.01	0.42
1:A:787:ILE:HG23	1:A:1036:GLN:HE22	1.84	0.41
1:A:1015:VAL:HA	1:A:1033:SER:HB3	2.00	0.41
1:A:125:ILE:O	1:A:163:TYR:N	2.43	0.41
1:B:730:GLU:HA	1:B:733:ASN:HD22	1.84	0.41
1:C:786:GLN:O	1:C:798:SER:HB2	2.20	0.41
1:A:119:ASN:HA	1:A:138:PHE:HE2	1.84	0.41
1:C:788:LEU:HD23	1:C:860:VAL:CG1	2.48	0.41
2:D:148:LEU:HD11	2:D:164:ALA:HB1	2.02	0.41
1:B:546:GLN:HB2	1:B:549:GLN:HG2	2.01	0.41
1:B:859:LEU:HA	1:B:870:PHE:HZ	1.85	0.41
1:C:756:GLN:HE22	1:C:1000:ILE:HD11	1.85	0.41
1:C:866:ALA:HB2	1:C:876:LEU:H	1.84	0.41
1:B:94:LYS:HB3	1:B:179:PHE:HA	2.03	0.41
1:B:727:ASP:O	1:B:727:ASP:CG	2.64	0.41
1:B:1079:PHE:HB2	1:B:1084:TRP:CZ3	2.56	0.41
1:A:519:LEU:HD21	1:A:521:LYS:HE3	2.02	0.41
1:B:745:LEU:HD23	1:B:745:LEU:HA	1.92	0.41
1:B:932:ASP:OD1	1:B:932:ASP:N	2.52	0.41
1:C:238:PHE:N	1:C:246:GLY:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:PHE:CE1	2:D:408:MET:HG2	2.56	0.41
1:B:93:GLU:HB2	1:B:181:HIS:HB2	2.03	0.41
1:B:399:PRO:HB3	1:B:414:ASP:HA	2.02	0.41
1:B:1010:LYS:HG2	1:B:1024:PHE:CZ	2.56	0.41
1:C:698:THR:N	1:C:1053:GLN:O	2.54	0.41
2:D:558:LEU:HG	2:D:558:LEU:O	2.20	0.41
1:A:196:VAL:HB	1:A:220:PHE:HB2	2.02	0.41
1:C:96:ASN:ND2	1:C:171:ASP:O	2.40	0.41
2:D:188:ASN:HB3	2:D:192:ARG:NH2	2.36	0.41
2:D:384:ALA:CB	2:D:558:LEU:CD2	2.96	0.41
2:D:418:LEU:HD13	2:D:418:LEU:HA	1.90	0.41
1:B:128:CYS:HA	1:B:159:CYS:HA	2.03	0.41
1:C:72:ILE:HD12	1:C:72:ILE:HA	1.97	0.41
1:C:105:SER:HA	1:C:229:THR:HG22	2.03	0.41
1:B:586:PRO:HD3	1:B:674:ILE:HD11	2.03	0.40
2:D:402:GLU:HB3	2:D:518:ARG:HG3	2.03	0.40
1:B:866:ALA:HB3	1:B:870:PHE:HB2	2.04	0.40
1:A:48:ARG:HB3	1:A:51:THR:HG21	2.04	0.40
1:B:307:VAL:HB	1:B:577:ALA:HB3	2.04	0.40
1:B:426:ARG:HA	1:B:493:PRO:HD2	2.02	0.40
1:C:616:THR:HA	1:C:617:PRO:HA	1.85	0.40
1:C:122:ASN:HB3	1:C:164:ILE:HG23	2.04	0.40
1:C:888:PHE:HB3	1:C:893:VAL:HB	2.03	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	
1	A	879/1215 (72%)	821 (93%)	58 (7%)	0	100	100
1	B	1062/1215 (87%)	973 (92%)	87 (8%)	2 (0%)	43	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	881/1215 (72%)	811 (92%)	70 (8%)	0	100 100
2	D	542/605 (90%)	521 (96%)	21 (4%)	0	100 100
All	All	3364/4250 (79%)	3126 (93%)	236 (7%)	2 (0%)	49 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	490	GLY
1	B	493	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	771/1053 (73%)	770 (100%)	1 (0%)	88 88
1	B	934/1053 (89%)	934 (100%)	0	100 100
1	C	772/1053 (73%)	771 (100%)	1 (0%)	88 88
2	D	479/534 (90%)	474 (99%)	5 (1%)	68 76
All	All	2956/3693 (80%)	2949 (100%)	7 (0%)	85 85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1114	ILE
1	C	788	LEU
2	D	21	ILE
2	D	446	ILE
2	D	456	LEU
2	D	558	LEU
2	D	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	112	GLN
1	A	189	ASN
1	A	201	GLN
1	A	523	GLN
1	A	549	GLN
1	A	599	GLN
1	A	733	ASN
1	A	974	GLN
1	A	1088	GLN
1	B	112	GLN
1	B	189	ASN
1	B	201	GLN
1	B	330	ASN
1	B	445	HIS
1	B	473	ASN
1	B	549	GLN
1	B	733	ASN
1	B	806	ASN
1	B	835	GLN
1	B	883	GLN
1	B	951	ASN
1	B	987	GLN
1	B	1088	GLN
1	C	112	GLN
1	C	189	ASN
1	C	201	GLN
1	C	301	GLN
1	C	523	GLN
1	C	599	GLN
1	C	630	GLN
1	C	786	GLN
1	C	835	GLN
1	C	877	GLN
1	C	908	GLN
1	C	935	ASN
1	C	939	GLN
1	C	1018	GLN
1	C	1046	HIS
1	C	1088	GLN
2	D	33	ASN
2	D	49	ASN
2	D	60	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	63	ASN
2	D	64	ASN
2	D	154	ASN
2	D	239	HIS
2	D	322	ASN
2	D	388	GLN
2	D	437	ASN
2	D	526	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)

85 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.46	0
3	BMA	E	3	3	11,11,12	0.79	0	15,15,17	0.94	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.33	0	17,19,21	0.45	0
3	NAG	F	2	3	14,14,15	0.19	0	17,19,21	0.58	0
3	BMA	F	3	3	11,11,12	0.81	0	15,15,17	1.25	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.39	0	17,19,21	0.59	0
4	NAG	G	2	4	14,14,15	0.24	0	17,19,21	0.57	0
5	NAG	H	1	1,5	14,14,15	0.37	0	17,19,21	0.43	0
5	NAG	H	2	5	14,14,15	0.42	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	H	3	5	11,11,12	0.81	0	15,15,17	0.78	0
5	MAN	H	4	5	11,11,12	0.78	0	15,15,17	1.00	2 (13%)
5	NAG	I	1	1,5	14,14,15	0.59	1 (7%)	17,19,21	0.77	0
5	NAG	I	2	5	14,14,15	0.22	0	17,19,21	0.52	0
5	BMA	I	3	5	11,11,12	0.45	0	15,15,17	1.12	1 (6%)
5	MAN	I	4	5	11,11,12	0.93	1 (9%)	15,15,17	1.45	2 (13%)
4	NAG	J	1	1,4	14,14,15	0.32	0	17,19,21	0.63	0
4	NAG	J	2	4	14,14,15	0.36	0	17,19,21	0.64	1 (5%)
5	NAG	K	1	1,5	14,14,15	0.64	1 (7%)	17,19,21	0.86	1 (5%)
5	NAG	K	2	5	14,14,15	0.22	0	17,19,21	0.49	0
5	BMA	K	3	5	11,11,12	0.74	0	15,15,17	0.88	1 (6%)
5	MAN	K	4	5	11,11,12	0.83	0	15,15,17	1.06	2 (13%)
5	NAG	L	1	1,5	14,14,15	0.73	1 (7%)	17,19,21	0.70	0
5	NAG	L	2	5	14,14,15	0.18	0	17,19,21	0.54	0
5	BMA	L	3	5	11,11,12	0.75	0	15,15,17	0.95	1 (6%)
5	MAN	L	4	5	11,11,12	0.92	0	15,15,17	1.03	2 (13%)
3	NAG	M	1	1,3	14,14,15	0.53	0	17,19,21	0.69	0
3	NAG	M	2	3	14,14,15	0.24	0	17,19,21	0.58	0
3	BMA	M	3	3	11,11,12	0.72	0	15,15,17	0.90	1 (6%)
4	NAG	N	1	1,4	14,14,15	0.44	0	17,19,21	0.60	0
4	NAG	N	2	4	14,14,15	0.42	0	17,19,21	0.57	0
3	NAG	O	1	1,3	14,14,15	0.32	0	17,19,21	0.50	0
3	NAG	O	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	BMA	O	3	3	11,11,12	0.70	0	15,15,17	0.88	1 (6%)
5	NAG	P	1	1,5	14,14,15	0.53	0	17,19,21	0.68	0
5	NAG	P	2	5	14,14,15	0.40	0	17,19,21	0.90	1 (5%)
5	BMA	P	3	5	11,11,12	0.58	0	15,15,17	1.09	2 (13%)
5	MAN	P	4	5	11,11,12	0.68	0	15,15,17	0.99	2 (13%)
3	NAG	Q	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.77	0
3	NAG	Q	2	3	14,14,15	0.18	0	17,19,21	0.61	0
3	BMA	Q	3	3	11,11,12	0.77	0	15,15,17	1.26	1 (6%)
4	NAG	R	1	1,4	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	R	2	4	14,14,15	0.26	0	17,19,21	0.60	1 (5%)
5	NAG	S	1	1,5	14,14,15	0.90	1 (7%)	17,19,21	0.78	0
5	NAG	S	2	5	14,14,15	0.28	0	17,19,21	0.50	0
5	BMA	S	3	5	11,11,12	0.56	0	15,15,17	1.05	1 (6%)
5	MAN	S	4	5	11,11,12	0.84	0	15,15,17	1.00	1 (6%)
3	NAG	T	1	1,3	14,14,15	0.66	1 (7%)	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	T	2	3	14,14,15	0.23	0	17,19,21	0.46	0
3	BMA	T	3	3	11,11,12	0.60	0	15,15,17	0.87	1 (6%)
6	NAG	U	1	1,6	14,14,15	0.32	0	17,19,21	0.55	0
6	NAG	U	2	6	14,14,15	0.26	0	17,19,21	0.66	0
6	BMA	U	3	6	11,11,12	0.86	0	15,15,17	1.19	2 (13%)
6	MAN	U	4	6	11,11,12	1.06	1 (9%)	15,15,17	1.37	3 (20%)
3	NAG	V	1	1,3	14,14,15	0.34	0	17,19,21	0.58	0
3	NAG	V	2	3	14,14,15	0.24	0	17,19,21	0.54	0
3	BMA	V	3	3	11,11,12	0.60	0	15,15,17	1.10	1 (6%)
3	NAG	W	1	1,3	14,14,15	0.21	0	17,19,21	0.62	0
3	NAG	W	2	3	14,14,15	0.30	0	17,19,21	0.61	0
3	BMA	W	3	3	11,11,12	0.62	0	15,15,17	0.75	0
3	NAG	X	1	1,3	14,14,15	0.25	0	17,19,21	0.61	0
3	NAG	X	2	3	14,14,15	0.27	0	17,19,21	0.56	0
3	BMA	X	3	3	11,11,12	0.85	0	15,15,17	0.75	0
4	NAG	Y	1	1,4	14,14,15	0.29	0	17,19,21	0.62	0
4	NAG	Y	2	4	14,14,15	0.23	0	17,19,21	0.55	0
4	NAG	Z	1	1,4	14,14,15	0.51	0	17,19,21	0.56	0
4	NAG	Z	2	4	14,14,15	0.37	0	17,19,21	0.65	1 (5%)
5	NAG	a	1	1,5	14,14,15	0.38	0	17,19,21	0.47	0
5	NAG	a	2	5	14,14,15	0.25	0	17,19,21	0.56	0
5	BMA	a	3	5	11,11,12	0.76	0	15,15,17	1.20	2 (13%)
5	MAN	a	4	5	11,11,12	0.89	0	15,15,17	0.89	1 (6%)
5	NAG	b	1	1,5	14,14,15	0.44	0	17,19,21	0.48	0
5	NAG	b	2	5	14,14,15	0.23	0	17,19,21	0.47	0
5	BMA	b	3	5	11,11,12	0.84	1 (9%)	15,15,17	1.13	1 (6%)
5	MAN	b	4	5	11,11,12	0.82	0	15,15,17	0.95	2 (13%)
4	NAG	c	1	1,4	14,14,15	0.51	0	17,19,21	0.73	0
4	NAG	c	2	4	14,14,15	0.46	0	17,19,21	0.42	0
5	NAG	d	1	1,5	14,14,15	0.25	0	17,19,21	0.54	0
5	NAG	d	2	5	14,14,15	0.20	0	17,19,21	0.68	1 (5%)
5	BMA	d	3	5	11,11,12	0.54	0	15,15,17	0.91	2 (13%)
5	MAN	d	4	5	11,11,12	0.71	0	15,15,17	1.25	2 (13%)
5	NAG	e	1	1,5	14,14,15	0.46	0	17,19,21	0.55	0
5	NAG	e	2	5	14,14,15	0.20	0	17,19,21	0.45	0
5	BMA	e	3	5	11,11,12	0.70	0	15,15,17	0.79	1 (6%)
5	MAN	e	4	5	11,11,12	0.87	1 (9%)	15,15,17	1.18	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	MAN	K	4	5	-	2/2/19/22	0/1/1/1
5	NAG	L	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	0/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	P	3	5	-	2/2/19/22	0/1/1/1
5	MAN	P	4	5	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	3/6/23/26	0/1/1/1
5	NAG	S	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	BMA	S	3	5	-	2/2/19/22	0/1/1/1
5	MAN	S	4	5	-	0/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
6	NAG	U	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
6	BMA	U	3	6	-	0/2/19/22	0/1/1/1
6	MAN	U	4	6	-	0/2/19/22	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	BMA	V	3	3	-	2/2/19/22	0/1/1/1
3	NAG	W	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
4	NAG	Y	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
5	NAG	a	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	1/6/23/26	0/1/1/1
5	BMA	a	3	5	-	2/2/19/22	0/1/1/1
5	MAN	a	4	5	-	0/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	1	NAG	O5-C1	-3.28	1.38	1.43
6	U	4	MAN	C1-C2	2.94	1.59	1.52
5	I	4	MAN	O5-C5	2.73	1.48	1.43
3	Q	1	NAG	O5-C1	-2.44	1.39	1.43
5	L	1	NAG	O5-C1	-2.44	1.39	1.43
5	K	1	NAG	O5-C1	-2.26	1.39	1.43
3	T	1	NAG	O5-C1	-2.22	1.40	1.43
5	e	4	MAN	O5-C5	2.21	1.47	1.43
5	I	1	NAG	O5-C1	-2.11	1.40	1.43
5	b	3	BMA	C2-C3	2.02	1.55	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	4	MAN	C1-O5-C5	4.69	118.47	112.19
5	d	4	MAN	C1-O5-C5	3.82	117.31	112.19
5	e	4	MAN	C1-O5-C5	3.73	117.18	112.19
3	Q	3	BMA	C1-O5-C5	3.46	116.82	112.19
3	F	3	BMA	C1-O5-C5	3.24	116.52	112.19
3	V	3	BMA	C1-O5-C5	3.19	116.47	112.19
5	I	3	BMA	C1-O5-C5	3.12	116.37	112.19
6	U	4	MAN	C1-O5-C5	3.10	116.34	112.19
5	S	3	BMA	C1-O5-C5	3.05	116.27	112.19
5	a	3	BMA	C1-O5-C5	2.72	115.83	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	3	BMA	C1-O5-C5	2.68	115.78	112.19
5	L	4	MAN	C1-O5-C5	2.57	115.63	112.19
5	d	3	BMA	C1-O5-C5	2.45	115.47	112.19
3	E	3	BMA	C1-O5-C5	2.43	115.45	112.19
3	E	1	NAG	C1-O5-C5	2.42	115.43	112.19
6	U	3	BMA	C1-O5-C5	2.38	115.37	112.19
5	b	3	BMA	C1-C2-C3	2.37	113.09	109.64
3	T	3	BMA	C1-O5-C5	2.37	115.36	112.19
5	K	4	MAN	C1-O5-C5	2.37	115.36	112.19
5	b	4	MAN	O2-C2-C3	-2.35	105.29	110.15
3	M	3	BMA	C1-O5-C5	2.34	115.32	112.19
5	S	4	MAN	C1-O5-C5	2.33	115.31	112.19
5	d	4	MAN	O2-C2-C3	-2.33	105.33	110.15
5	P	4	MAN	O2-C2-C3	-2.31	105.36	110.15
5	b	4	MAN	C1-O5-C5	2.31	115.28	112.19
5	d	2	NAG	C1-O5-C5	2.28	115.24	112.19
6	U	3	BMA	C1-C2-C3	2.27	112.95	109.64
6	U	4	MAN	C1-C2-C3	2.26	112.94	109.64
5	P	4	MAN	C1-O5-C5	2.25	115.20	112.19
3	O	3	BMA	C1-O5-C5	2.22	115.16	112.19
4	Z	2	NAG	C1-O5-C5	2.21	115.15	112.19
5	H	4	MAN	O2-C2-C3	-2.19	105.61	110.15
5	H	4	MAN	C1-O5-C5	2.19	115.12	112.19
5	K	4	MAN	O2-C2-C3	-2.18	105.63	110.15
6	U	4	MAN	O2-C2-C3	-2.17	105.66	110.15
5	L	4	MAN	O2-C2-C3	-2.16	105.68	110.15
5	L	3	BMA	C1-O5-C5	2.13	115.05	112.19
5	K	3	BMA	C1-O5-C5	2.12	115.03	112.19
5	a	3	BMA	C1-C2-C3	2.11	112.72	109.64
4	J	2	NAG	C1-O5-C5	2.11	115.01	112.19
5	K	1	NAG	O4-C4-C3	-2.08	105.47	110.38
5	e	3	BMA	O2-C2-C3	-2.07	105.86	110.15
4	R	2	NAG	C1-O5-C5	2.05	114.93	112.19
5	P	2	NAG	C3-C4-C5	2.05	113.94	110.23
5	a	4	MAN	C1-O5-C5	2.04	114.92	112.19
5	P	3	BMA	O2-C2-C3	-2.04	105.93	110.15
5	d	3	BMA	O2-C2-C3	-2.03	105.94	110.15
5	I	4	MAN	O2-C2-C3	-2.03	105.95	110.15
5	e	4	MAN	O2-C2-C3	-2.01	105.99	110.15

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	2	NAG	O5-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
5	e	4	MAN	C4-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	a	3	BMA	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
5	d	4	MAN	O5-C5-C6-O6
3	V	3	BMA	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	e	3	BMA	O5-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
5	e	4	MAN	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
5	S	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	O	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
5	S	3	BMA	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
5	I	4	MAN	C4-C5-C6-O6
5	P	3	BMA	C4-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
5	d	4	MAN	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	K	4	MAN	O5-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
5	e	3	BMA	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
5	K	4	MAN	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	V	3	BMA	C4-C5-C6-O6
5	a	3	BMA	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	b	3	BMA	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
5	e	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
5	e	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C1-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
5	H	1	NAG	C1-C2-N2-C7
5	I	2	NAG	C1-C2-N2-C7
5	d	2	NAG	C1-C2-N2-C7
4	J	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6

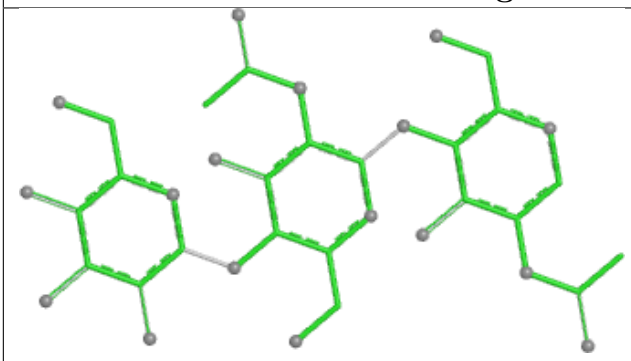
There are no ring outliers.

4 monomers are involved in 5 short contacts:

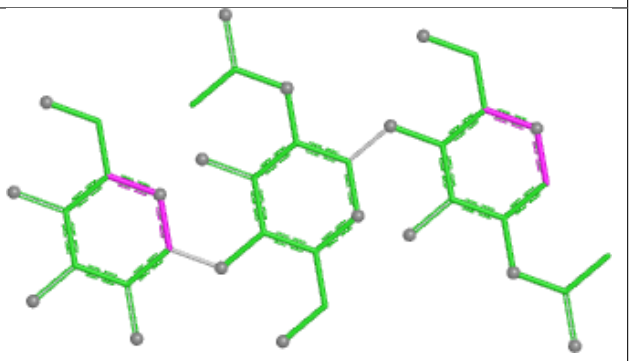
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	a	3	BMA	1	0
5	K	1	NAG	1	0
5	d	1	NAG	2	0
3	E	1	NAG	1	0

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

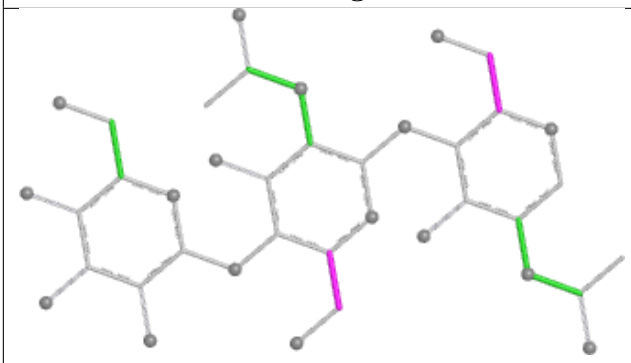
Oligosaccharide Chain E



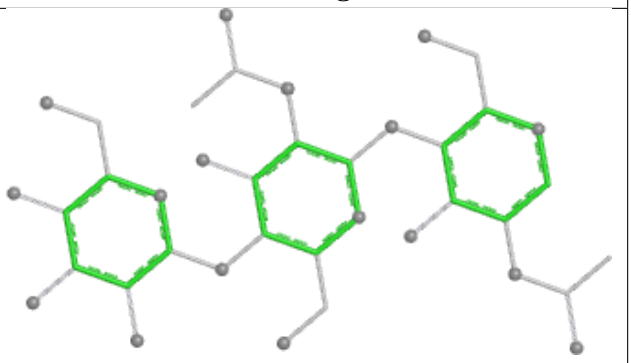
Bond lengths



Bond angles

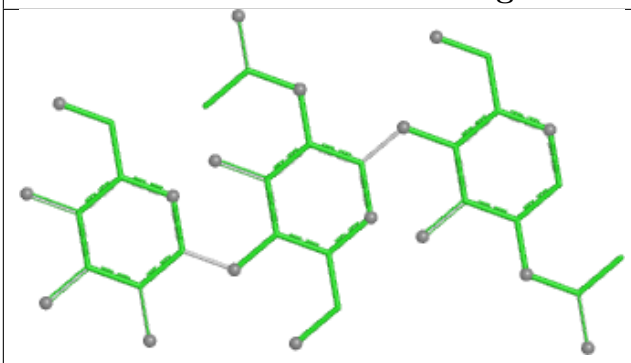


Torsions

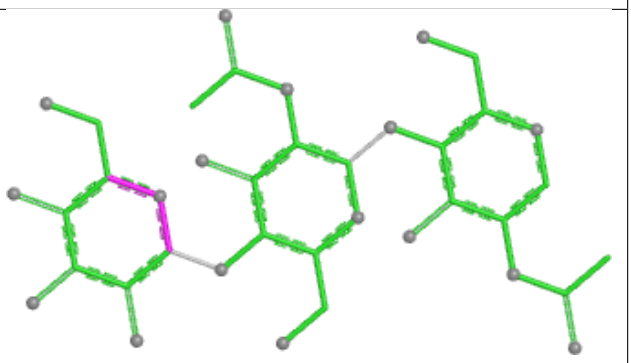


Rings

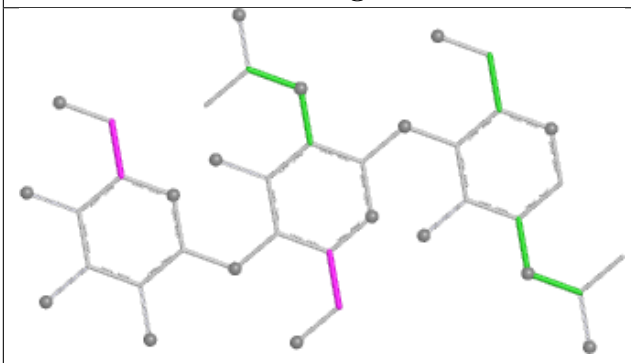
Oligosaccharide Chain F



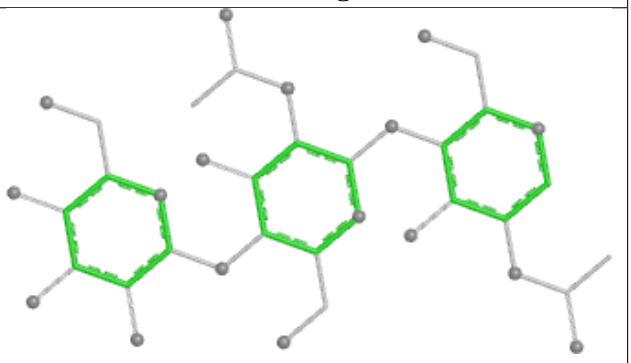
Bond lengths



Bond angles

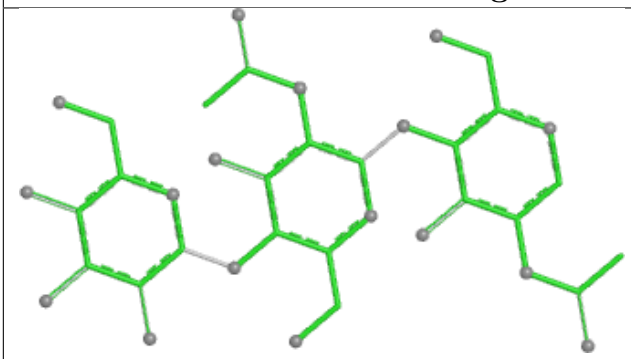


Torsions

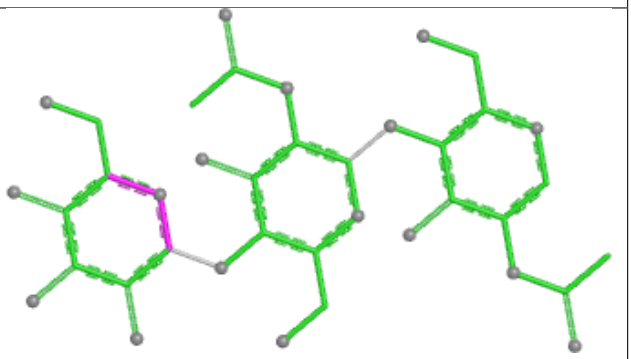


Rings

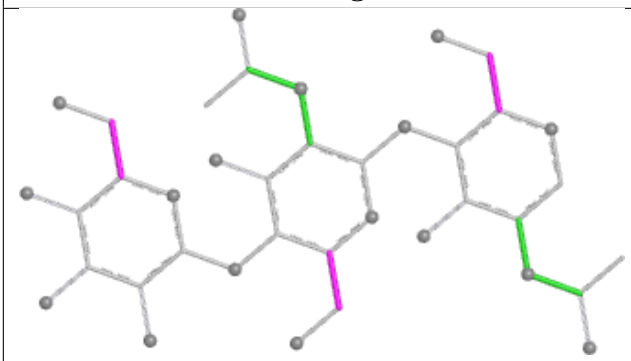
Oligosaccharide Chain M



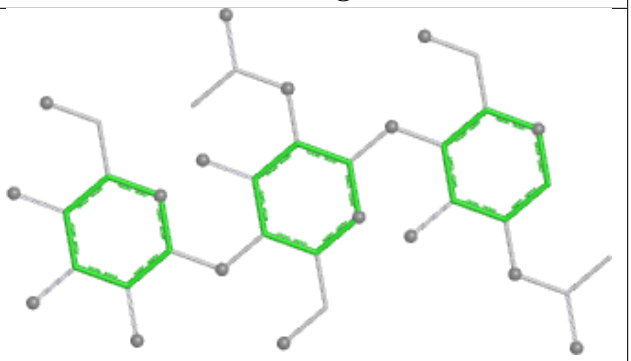
Bond lengths



Bond angles

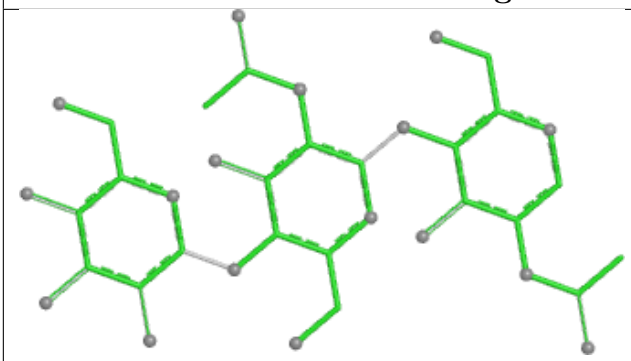


Torsions

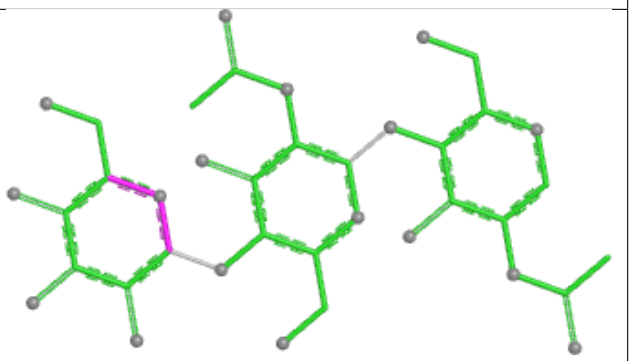


Rings

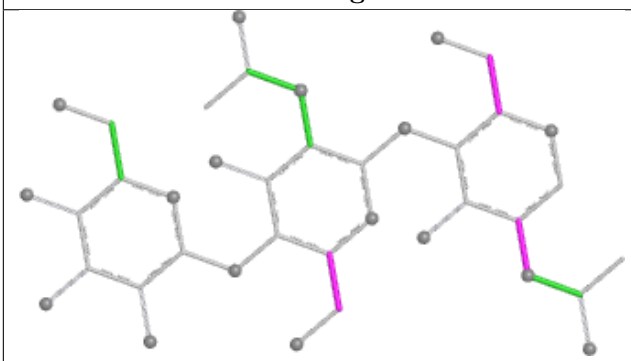
Oligosaccharide Chain O



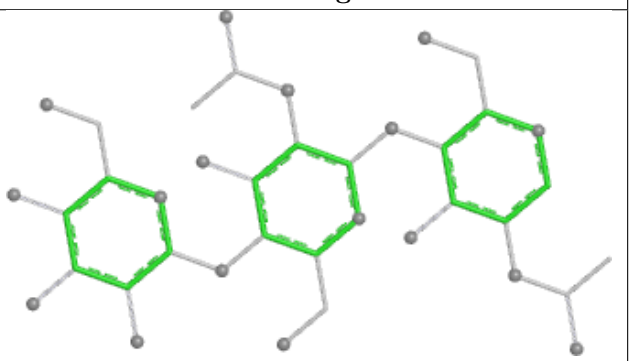
Bond lengths



Bond angles

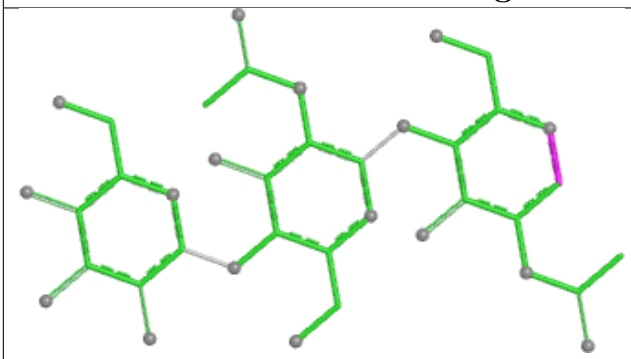


Torsions

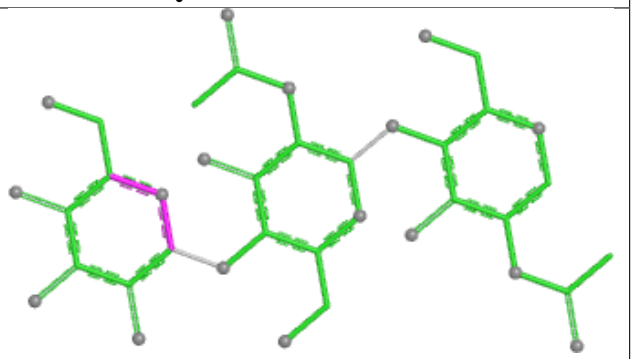


Rings

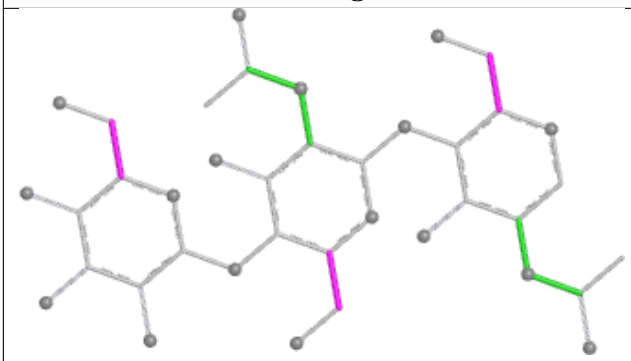
Oligosaccharide Chain Q



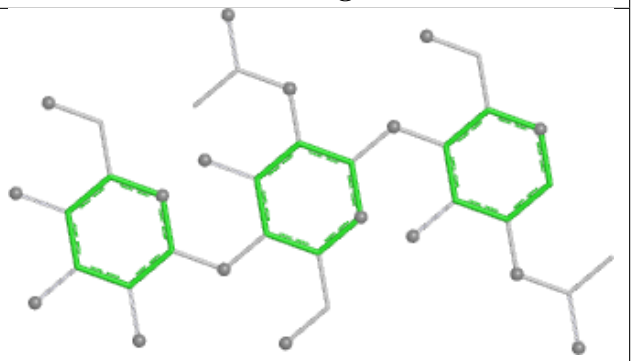
Bond lengths



Bond angles

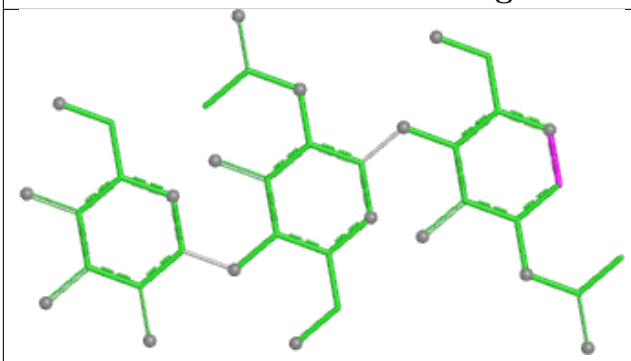


Torsions

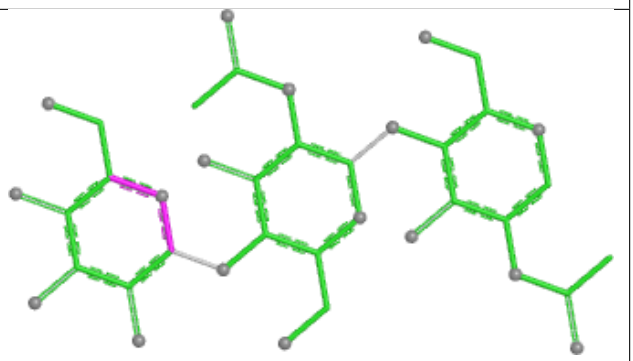


Rings

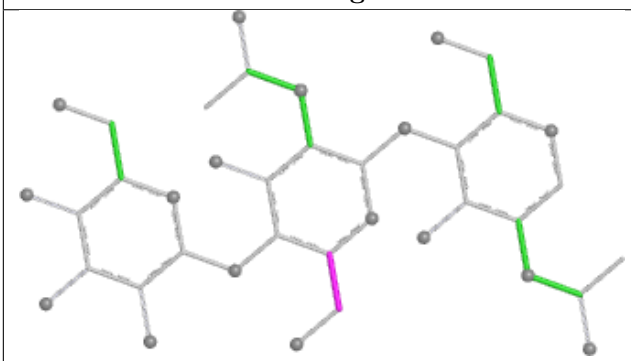
Oligosaccharide Chain T



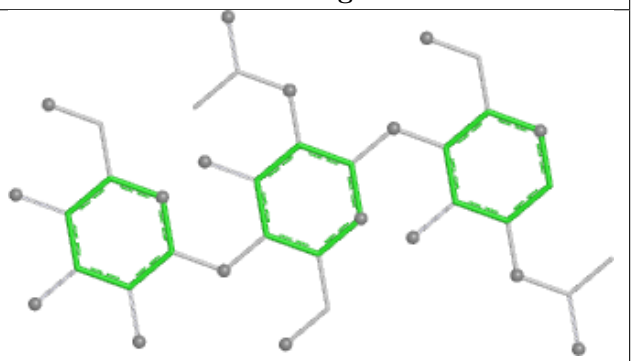
Bond lengths



Bond angles

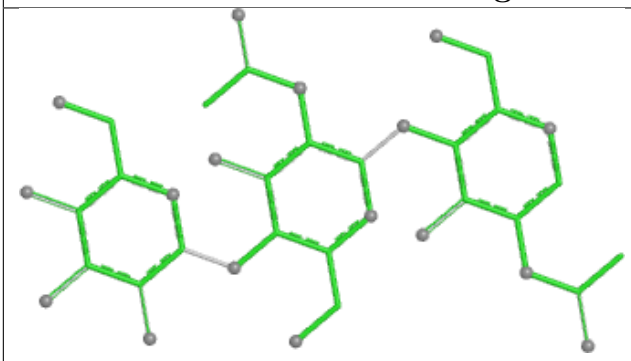


Torsions

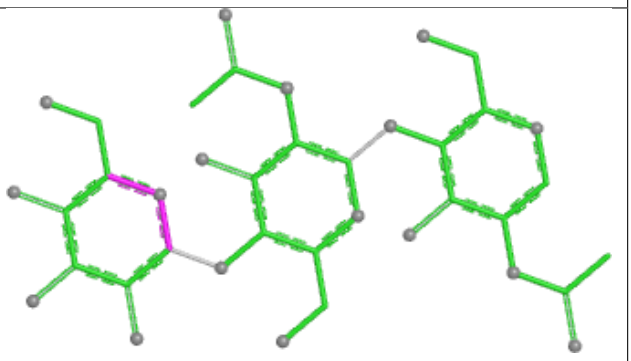


Rings

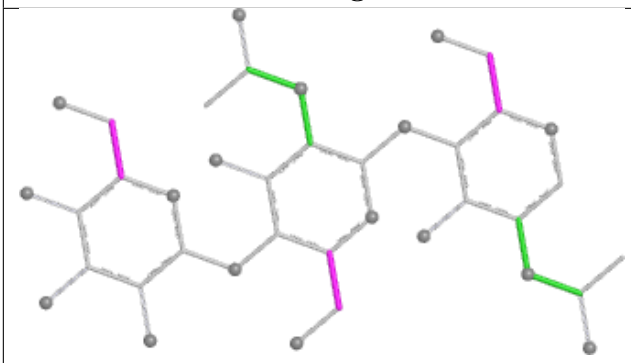
Oligosaccharide Chain V



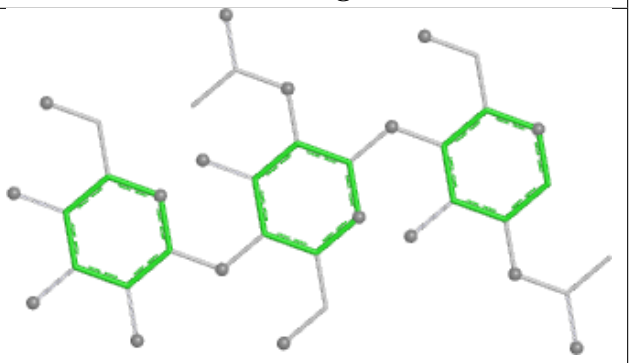
Bond lengths



Bond angles

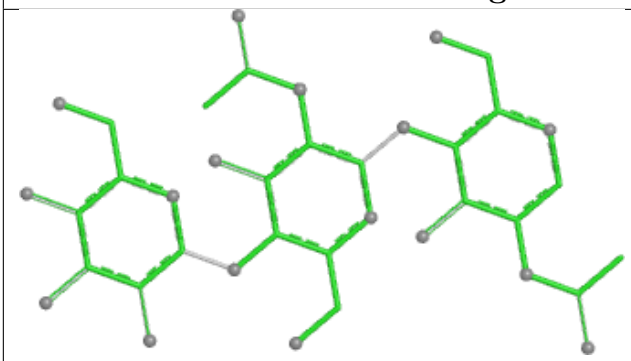


Torsions

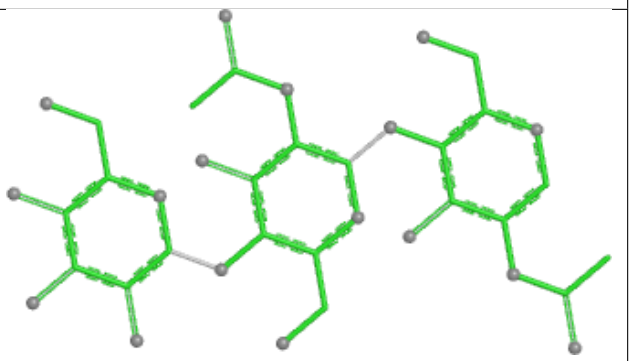


Rings

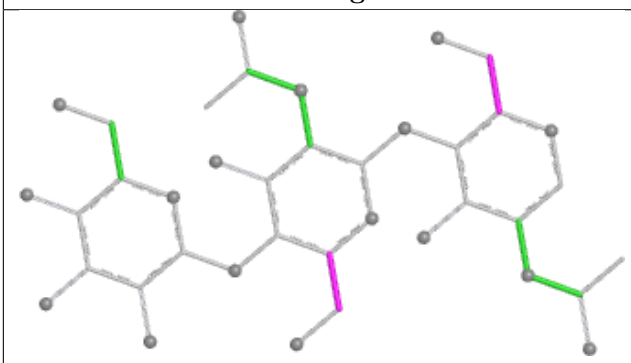
Oligosaccharide Chain W



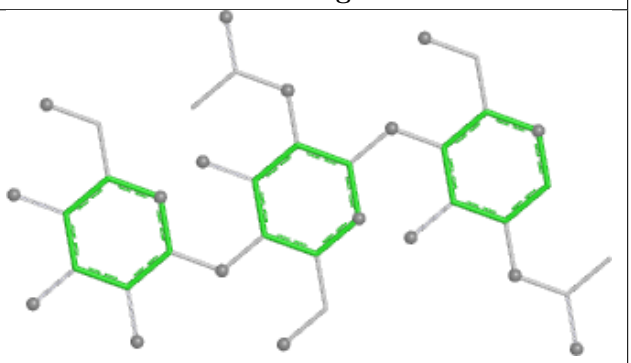
Bond lengths



Bond angles

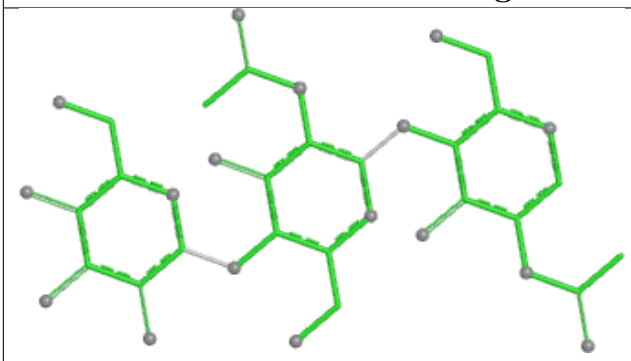


Torsions

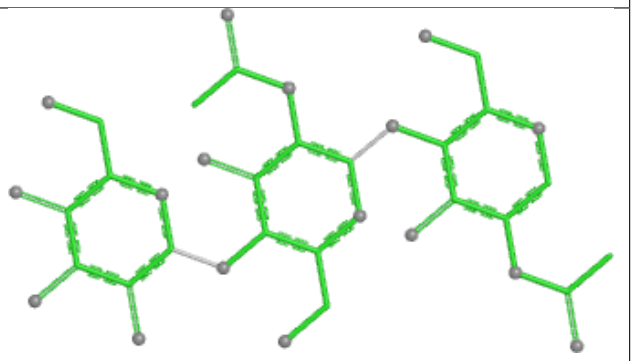


Rings

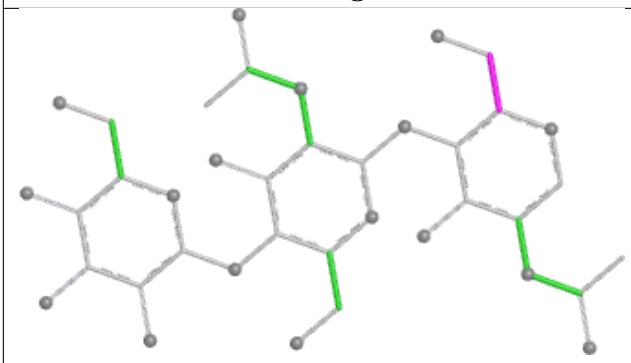
Oligosaccharide Chain X



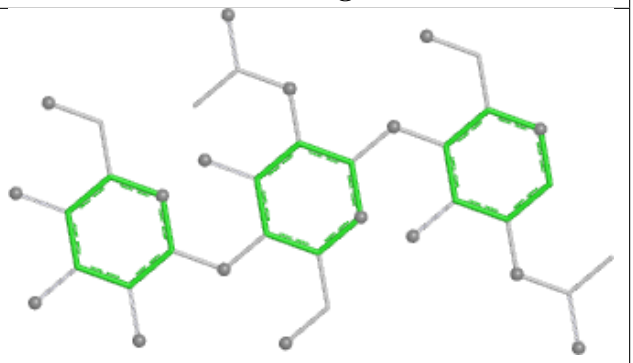
Bond lengths



Bond angles

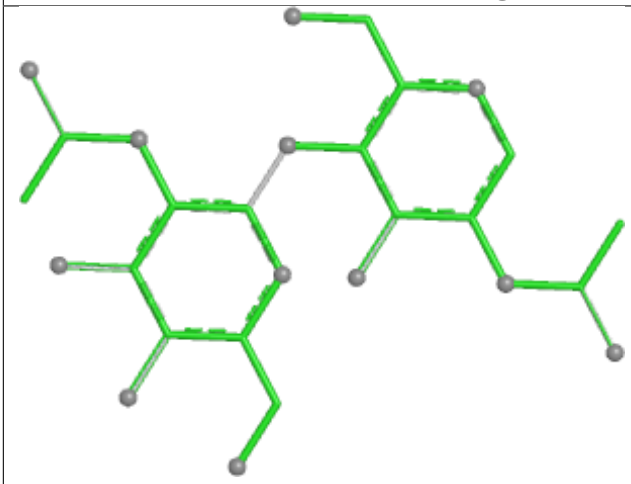


Torsions

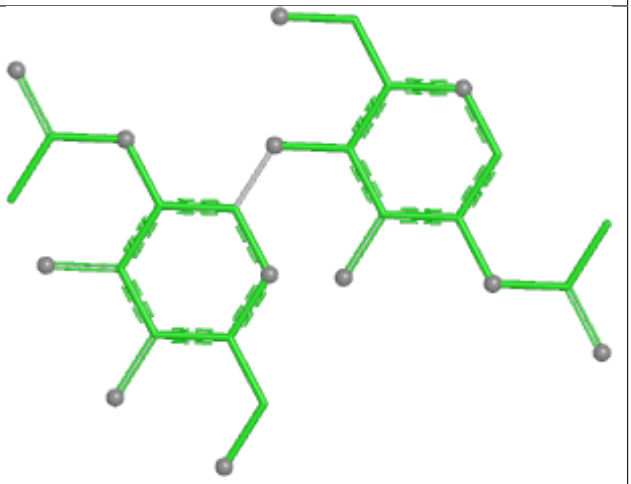


Rings

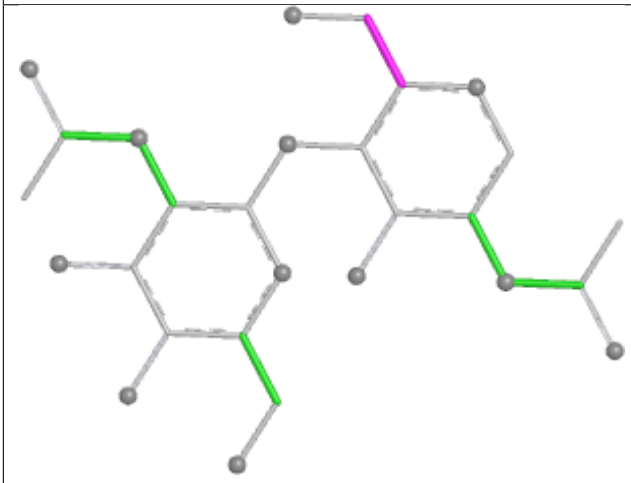
Oligosaccharide Chain G



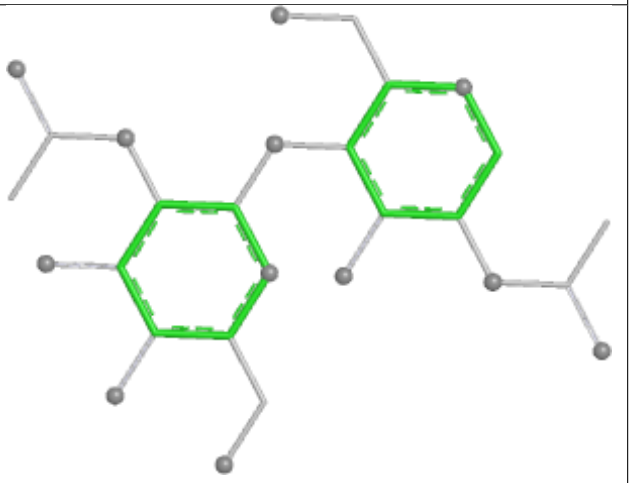
Bond lengths



Bond angles

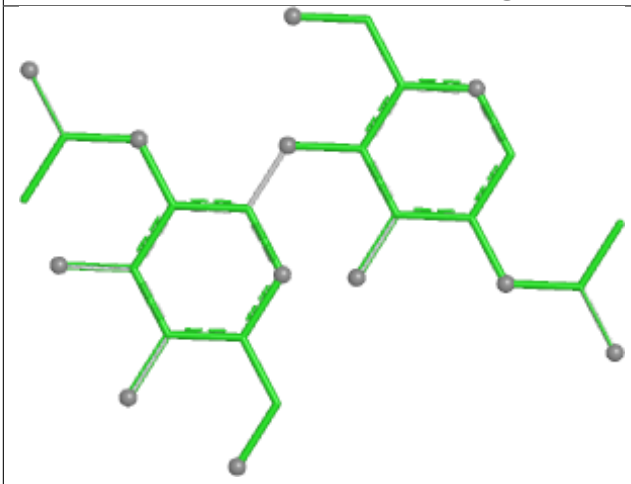


Torsions

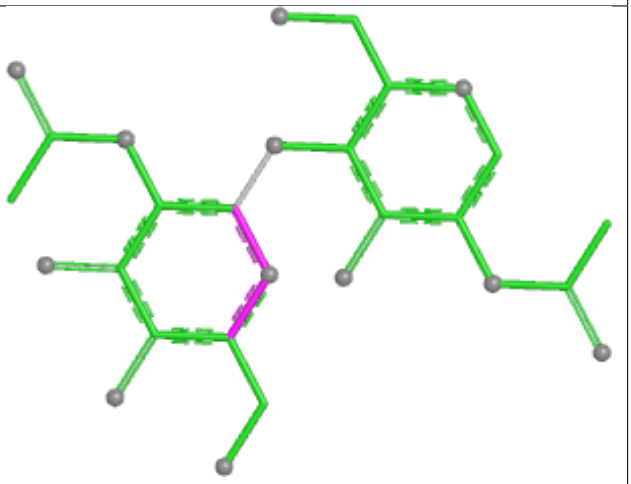


Rings

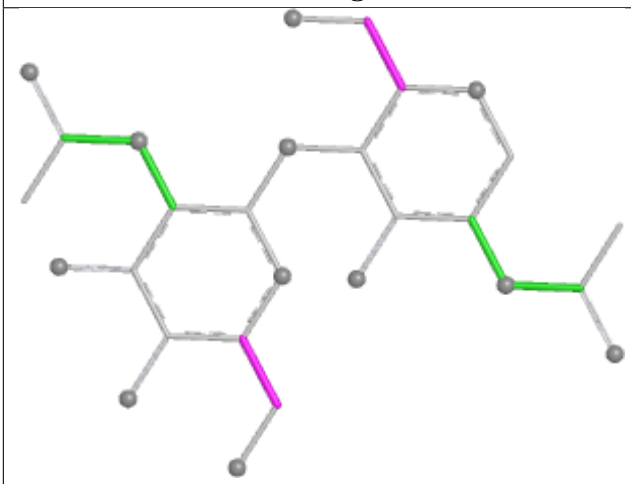
Oligosaccharide Chain J



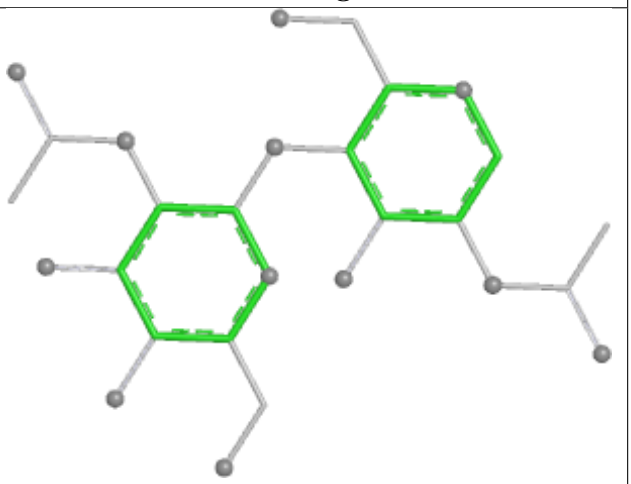
Bond lengths



Bond angles

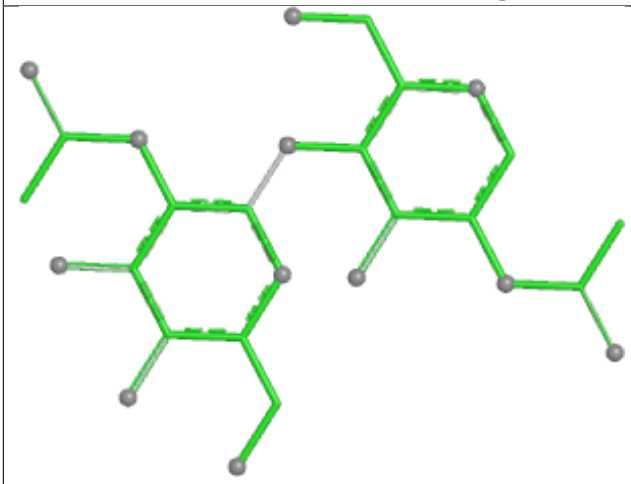


Torsions

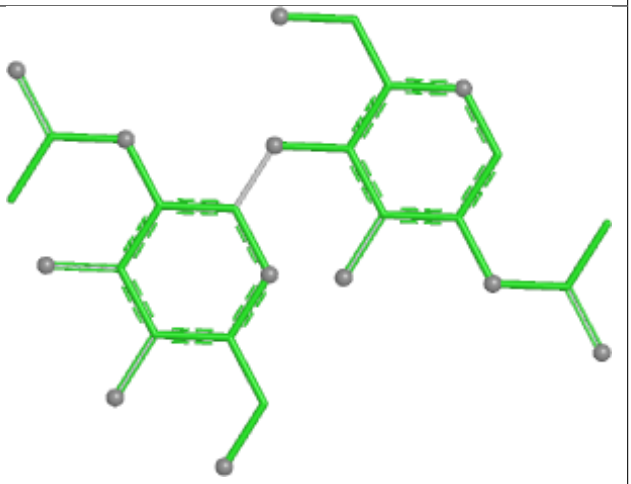


Rings

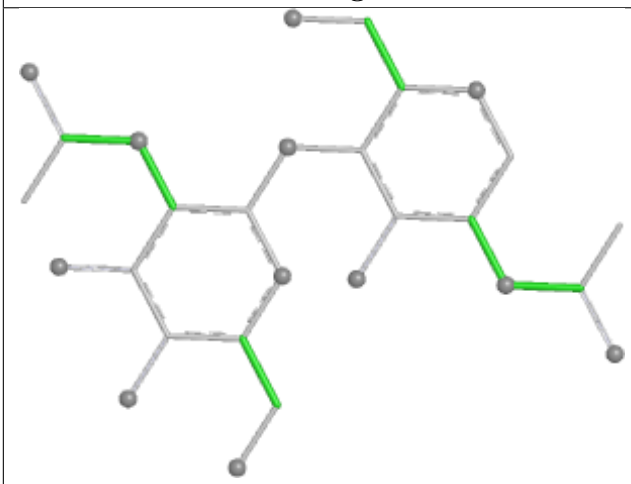
Oligosaccharide Chain N



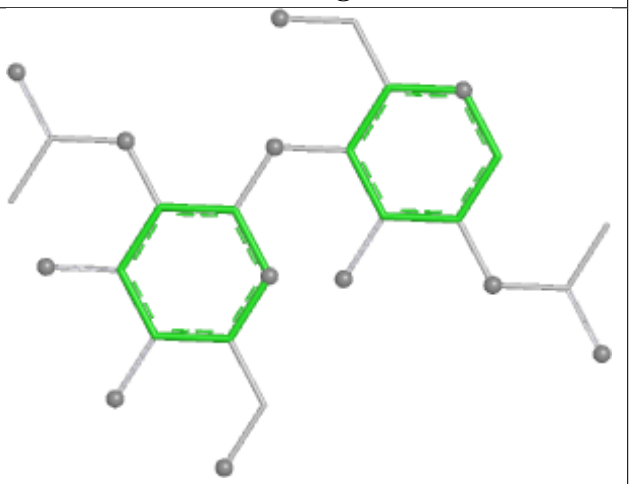
Bond lengths



Bond angles

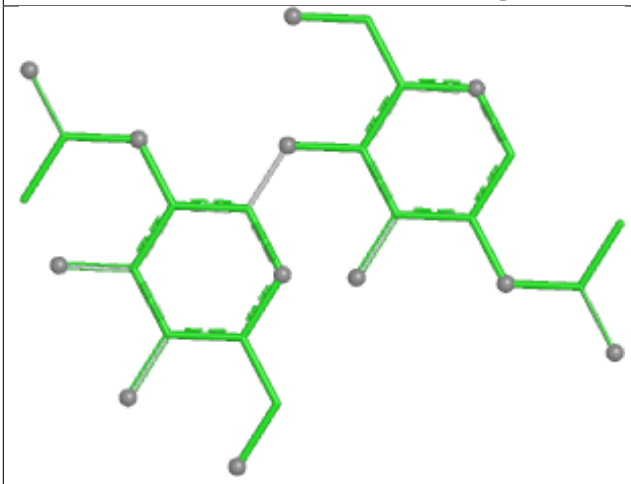


Torsions

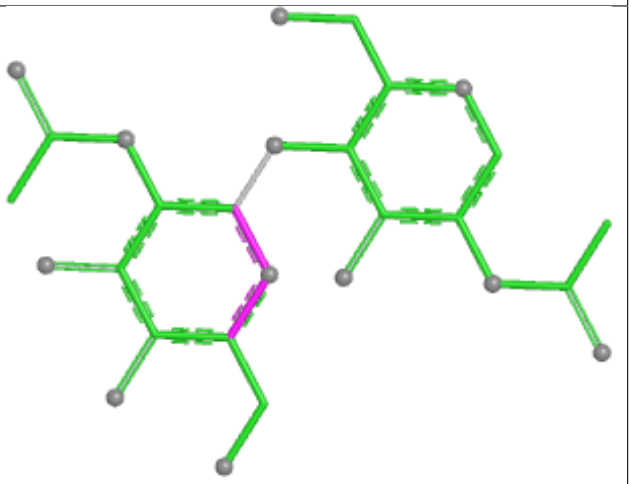


Rings

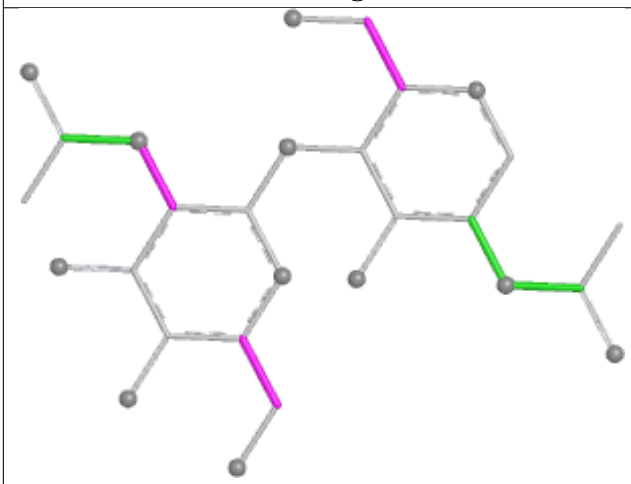
Oligosaccharide Chain R



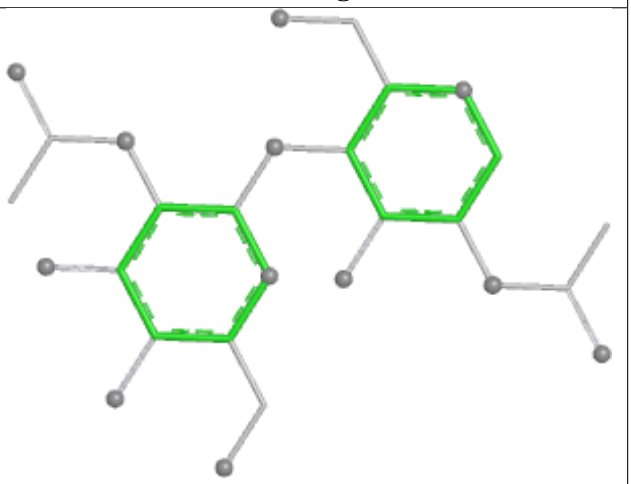
Bond lengths



Bond angles

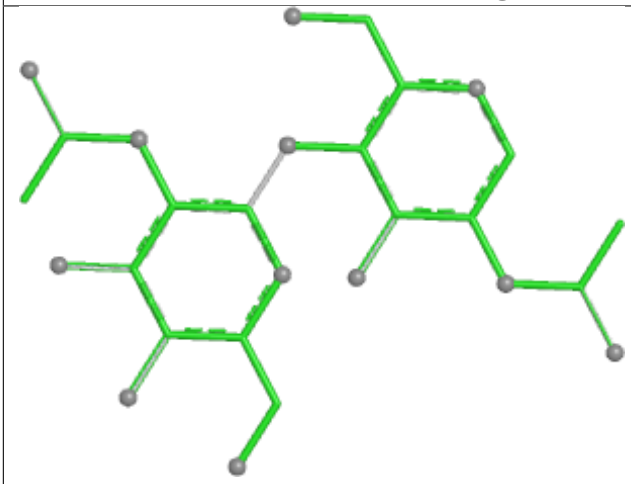


Torsions

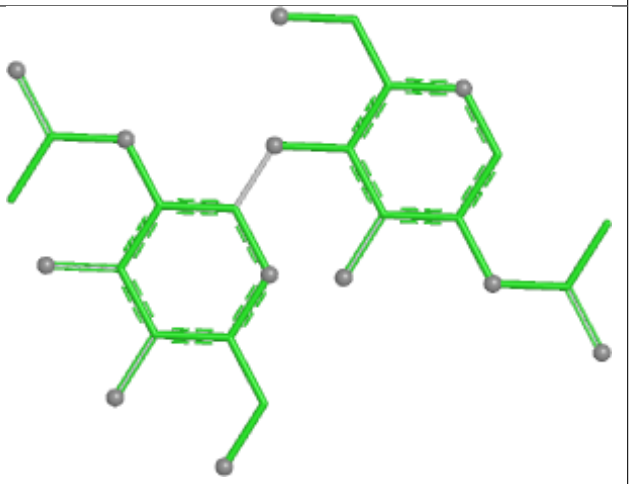


Rings

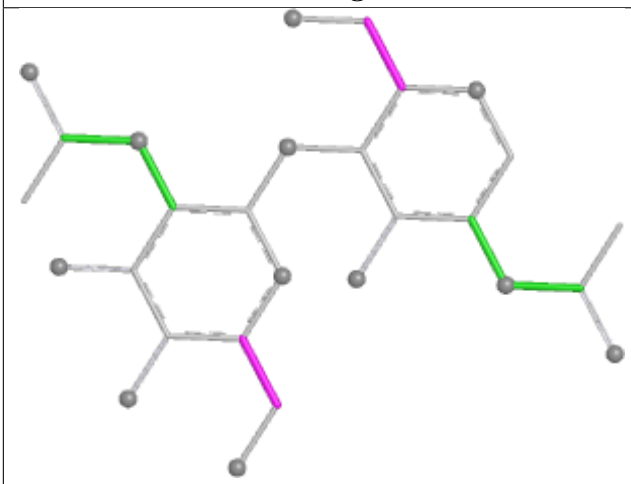
Oligosaccharide Chain Y



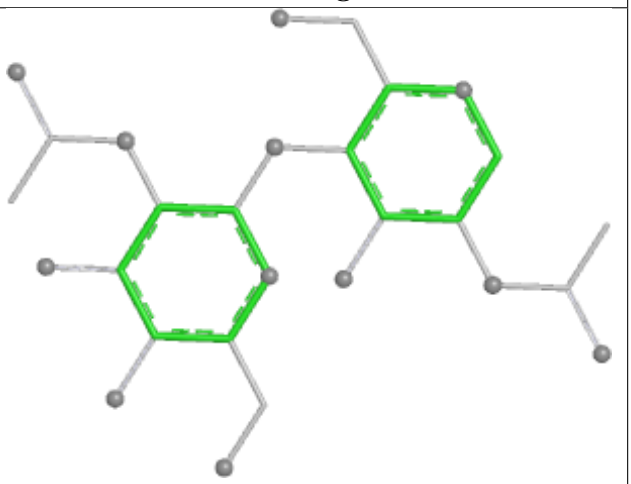
Bond lengths



Bond angles

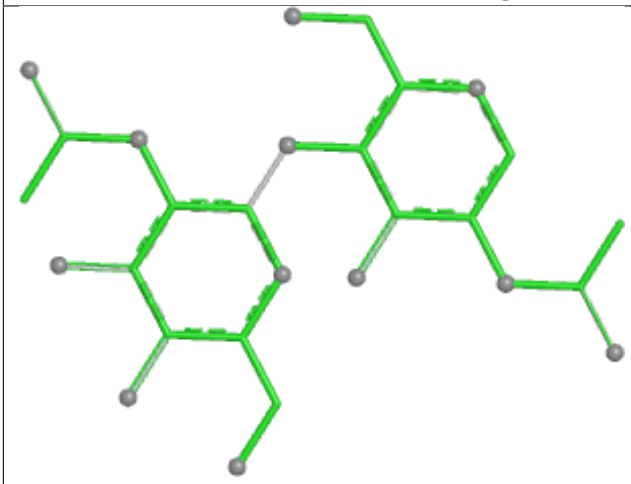


Torsions

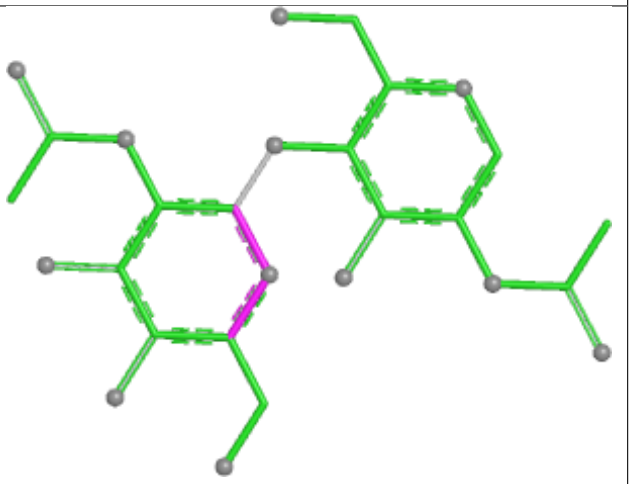


Rings

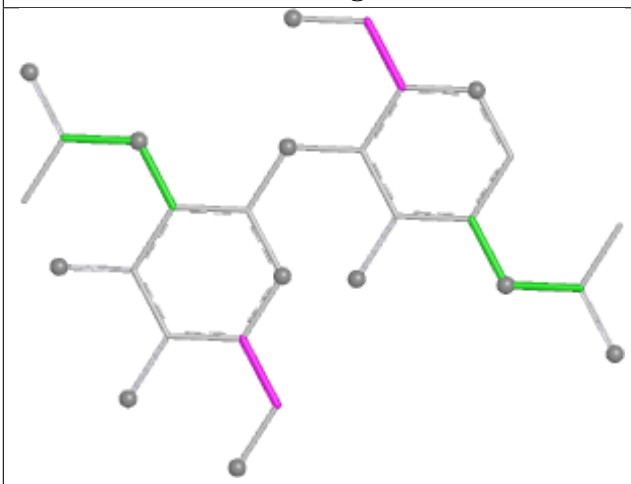
Oligosaccharide Chain Z



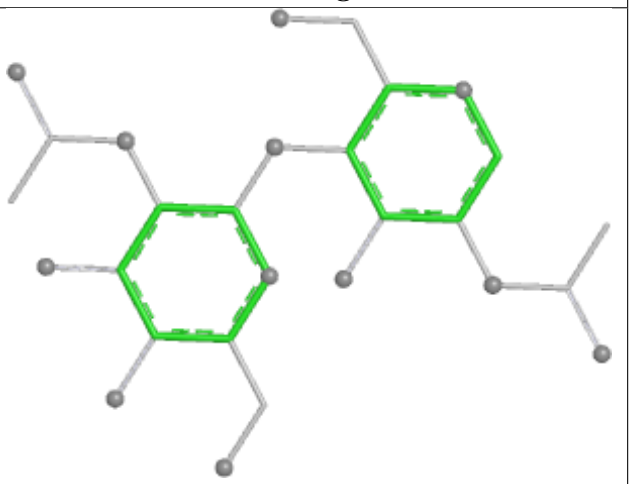
Bond lengths



Bond angles

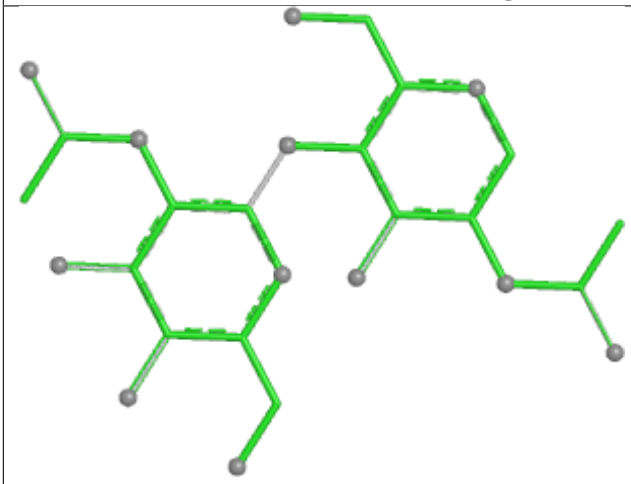


Torsions

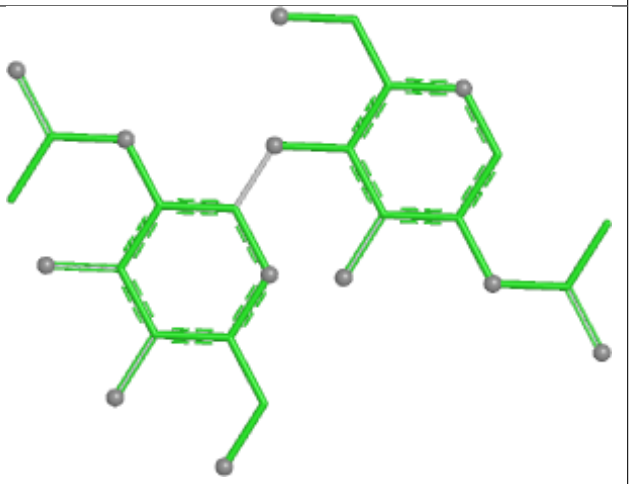


Rings

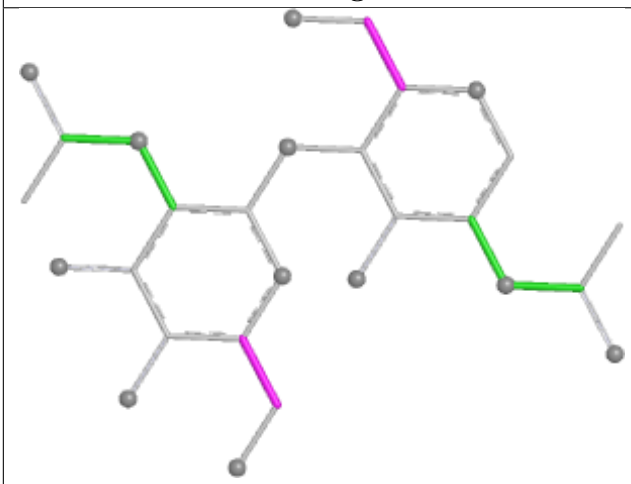
Oligosaccharide Chain c



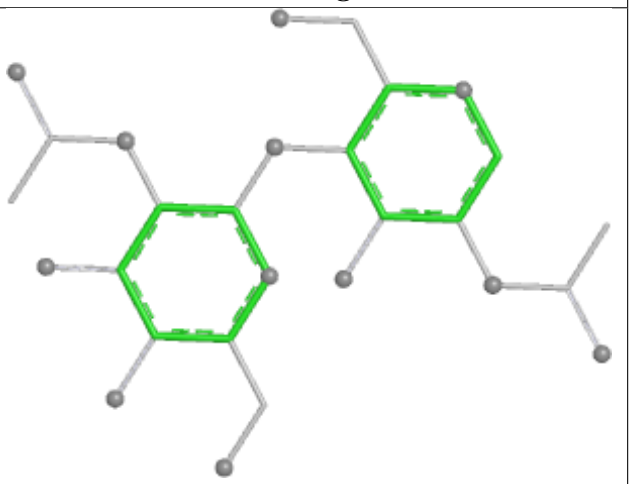
Bond lengths



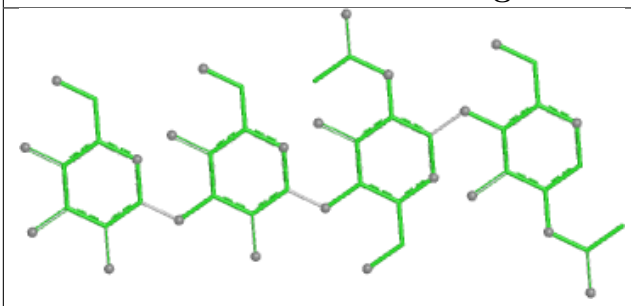
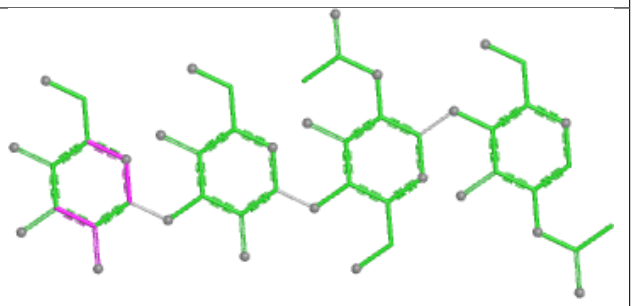
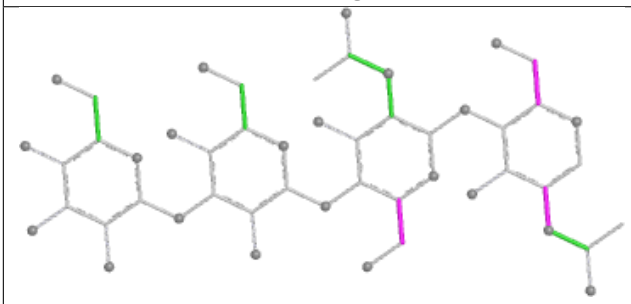
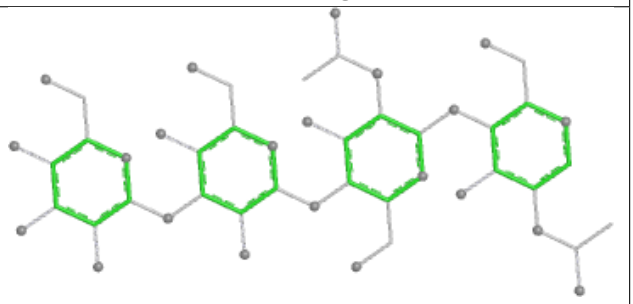
Bond angles

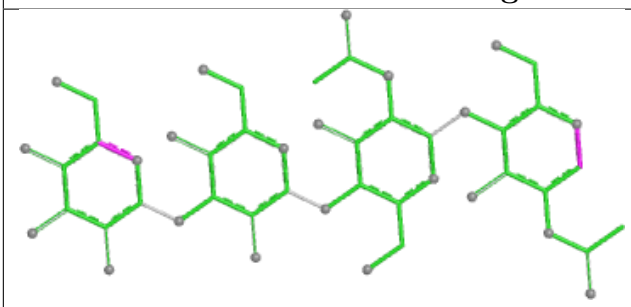
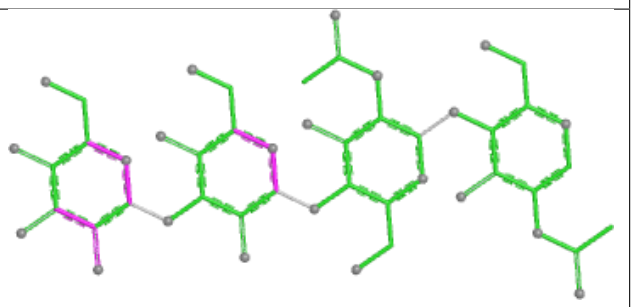
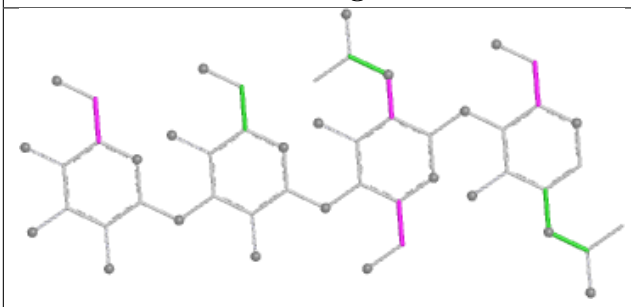
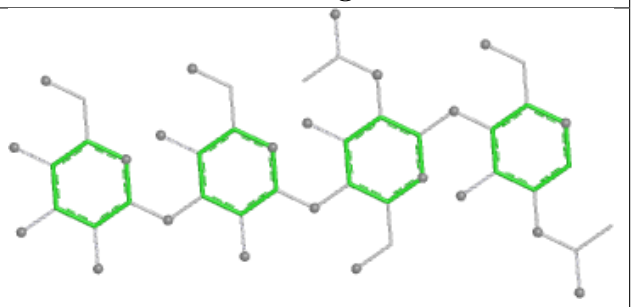


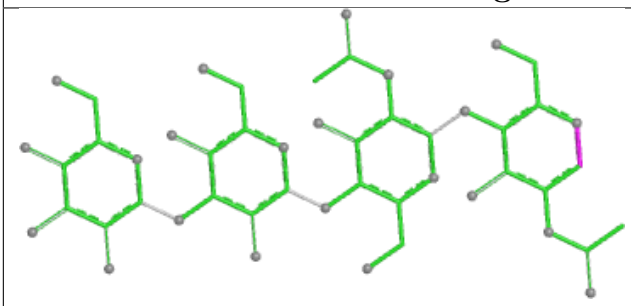
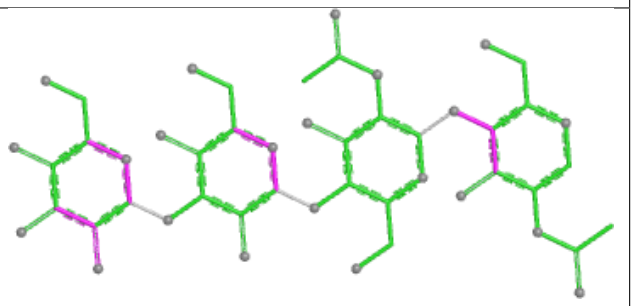
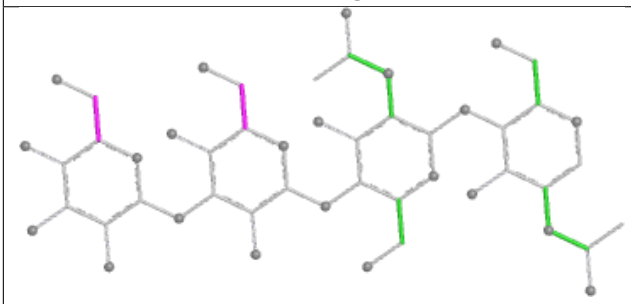
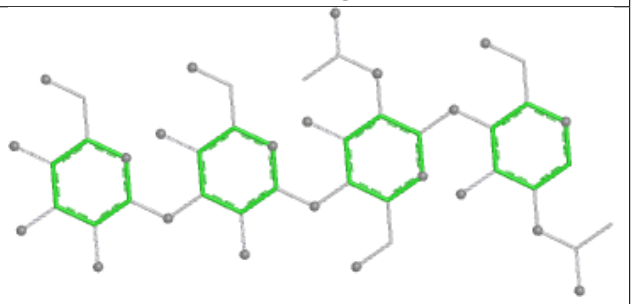
Torsions

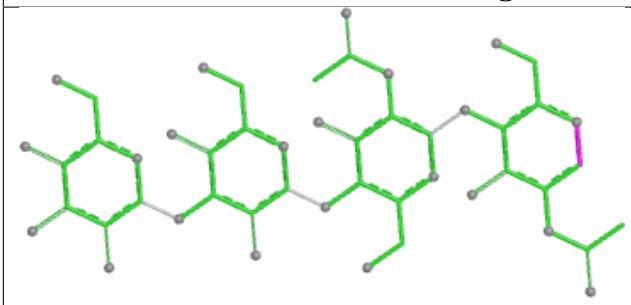
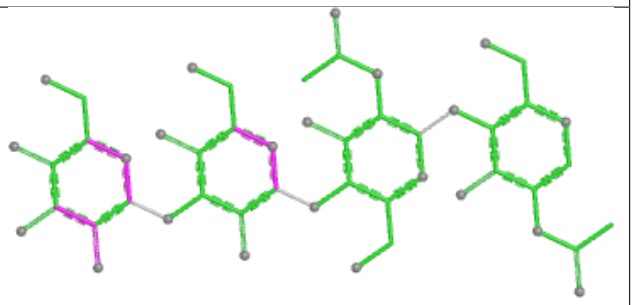
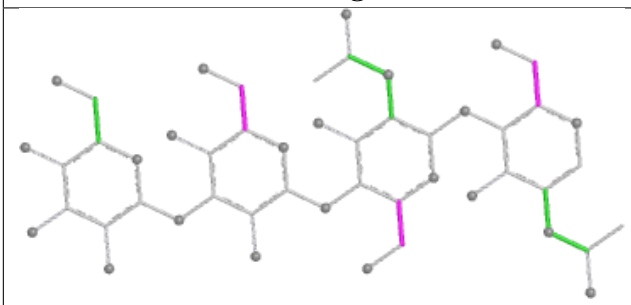
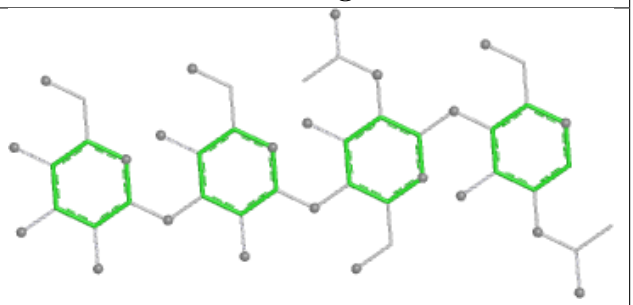


Rings

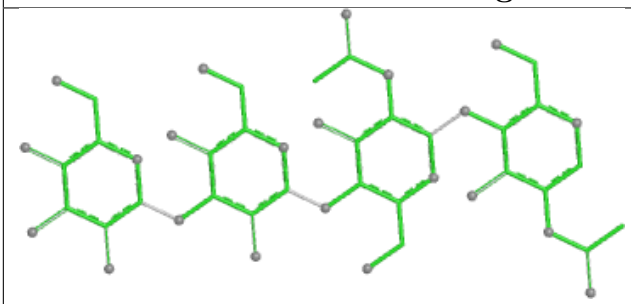
Oligosaccharide Chain H	
	
Bond lengths	Bond angles
	
Torsions	Rings

Oligosaccharide Chain I	
	
Bond lengths	Bond angles
	
Torsions	Rings

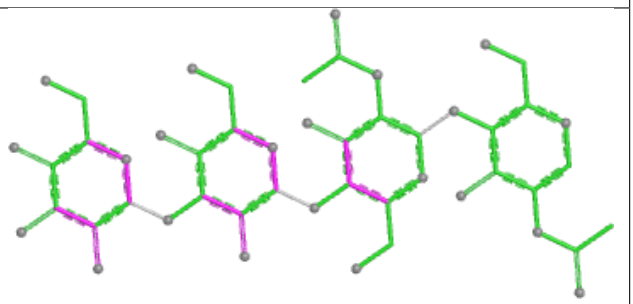
Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

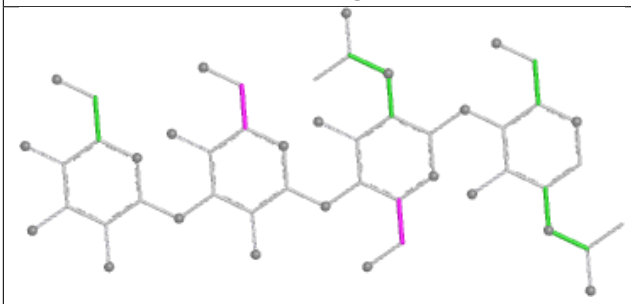
Oligosaccharide Chain P



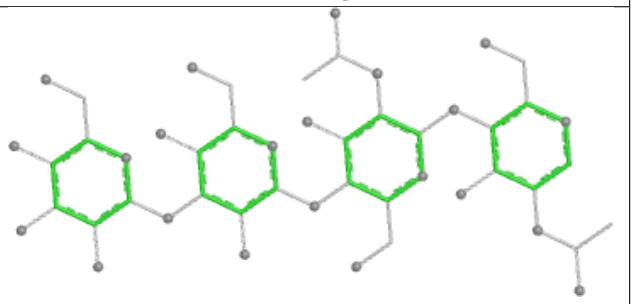
Bond lengths



Bond angles

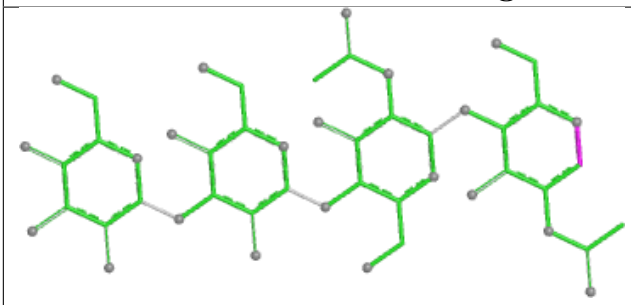


Torsions

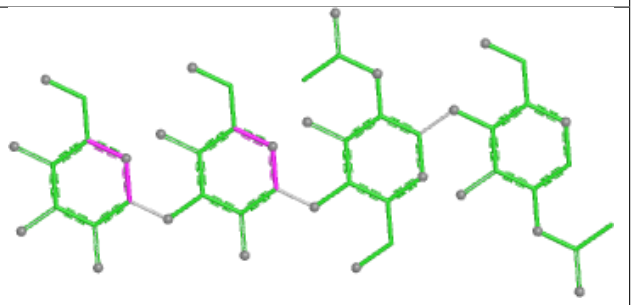


Rings

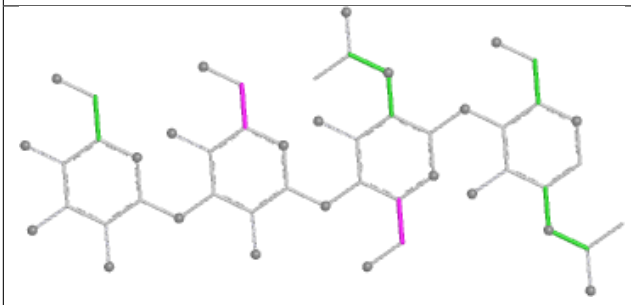
Oligosaccharide Chain S



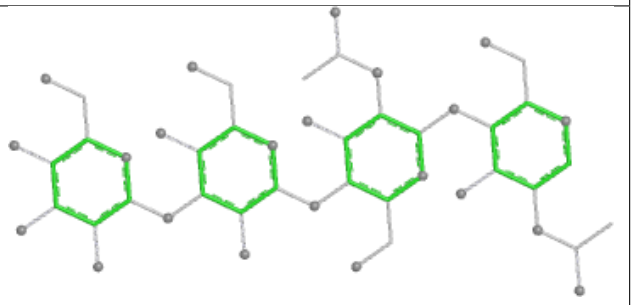
Bond lengths



Bond angles

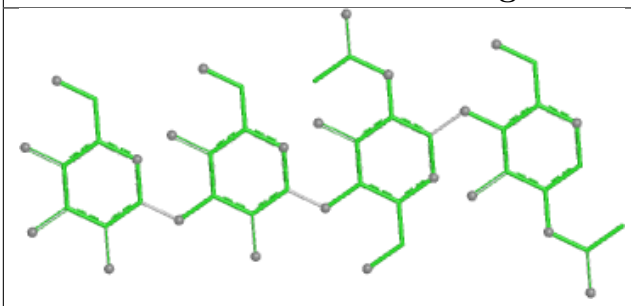


Torsions

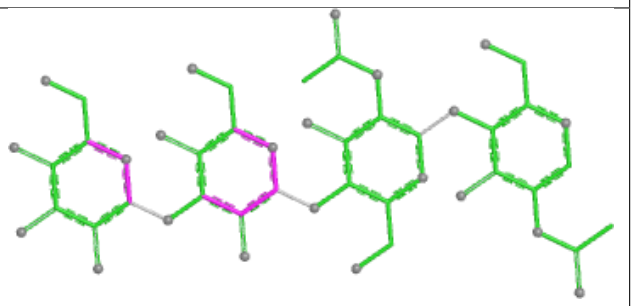


Rings

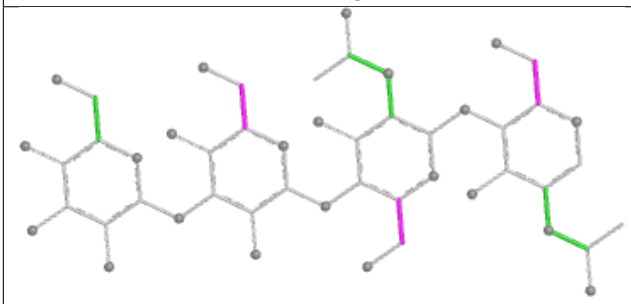
Oligosaccharide Chain a



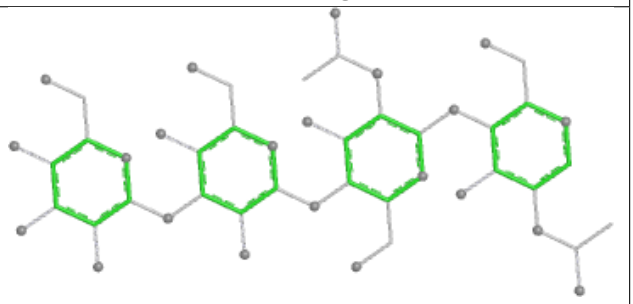
Bond lengths



Bond angles

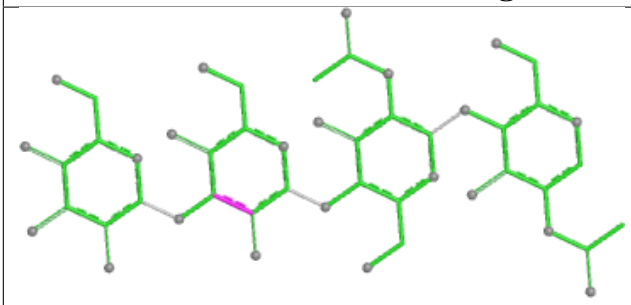


Torsions

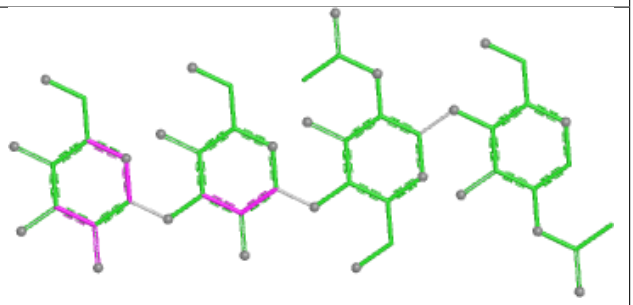


Rings

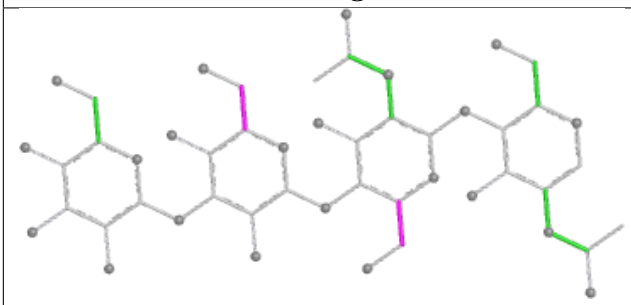
Oligosaccharide Chain b



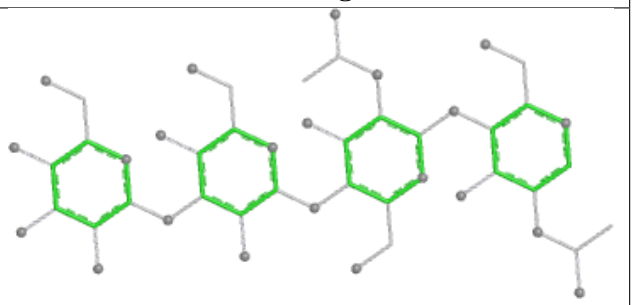
Bond lengths



Bond angles

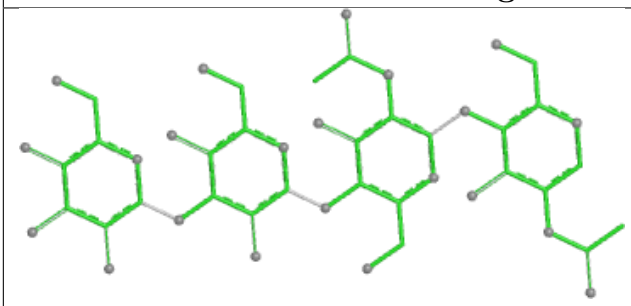


Torsions

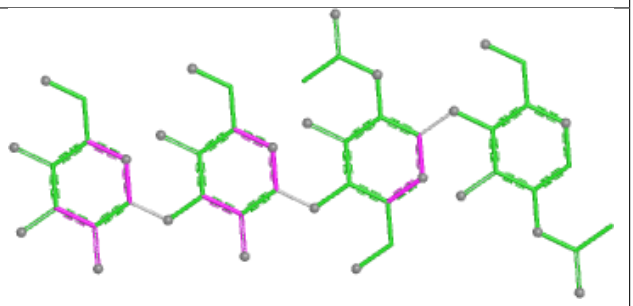


Rings

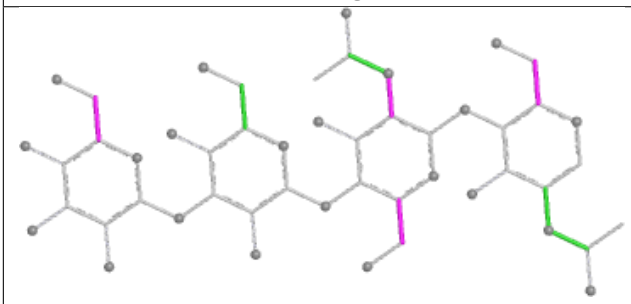
Oligosaccharide Chain d



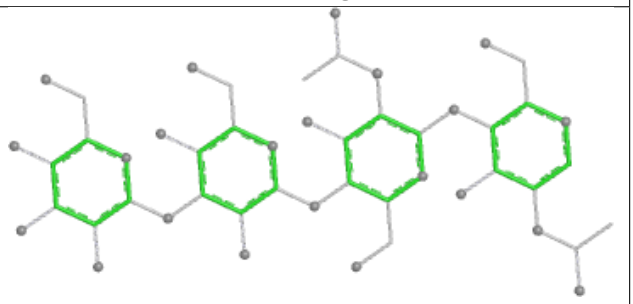
Bond lengths



Bond angles

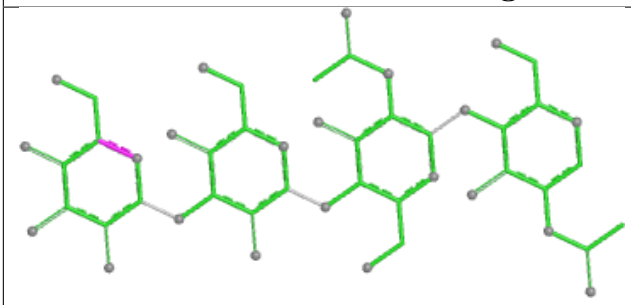


Torsions

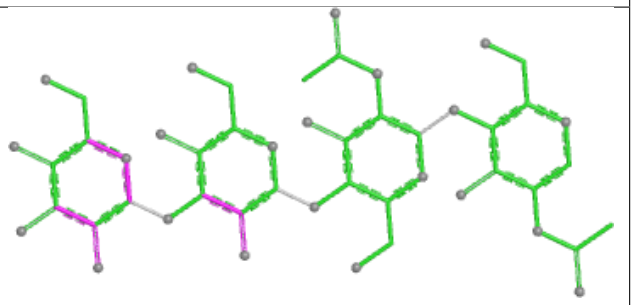


Rings

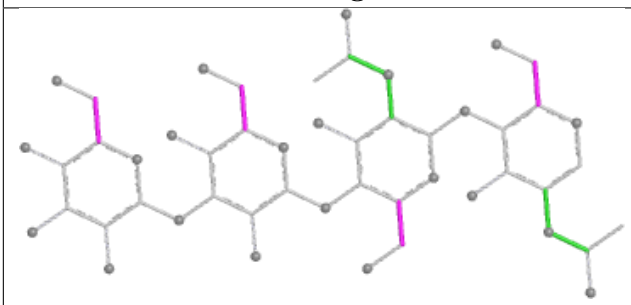
Oligosaccharide Chain e



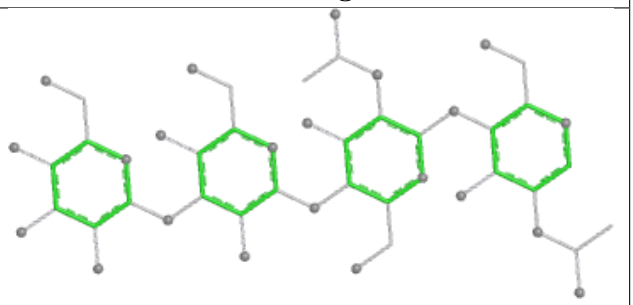
Bond lengths



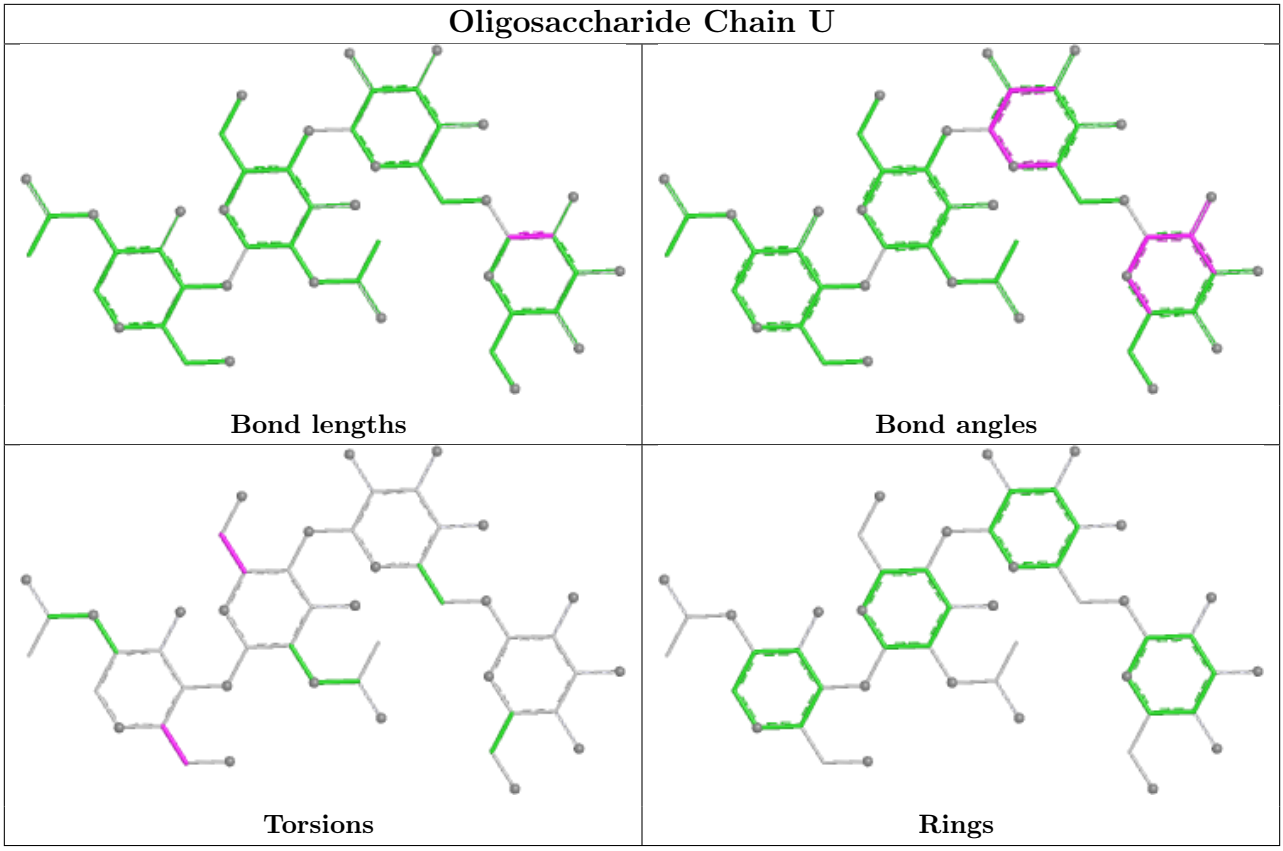
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
7	NAG	B	1310	1	14,14,15	0.25	0	17,19,21	0.59	1 (5%)
7	NAG	A	1301	1	14,14,15	0.39	0	17,19,21	0.54	0
7	NAG	A	1308	1	14,14,15	0.45	0	17,19,21	0.43	0
7	NAG	C	1309	1	14,14,15	0.27	0	17,19,21	0.46	0
7	NAG	B	1320	1	14,14,15	0.50	0	17,19,21	0.64	0
7	NAG	C	1320	1	14,14,15	0.35	0	17,19,21	0.46	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	B	1310	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1320	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1320	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1310	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1310	NAG	O5-C5-C6-O6
7	B	1310	NAG	C4-C5-C6-O6
7	C	1320	NAG	O5-C5-C6-O6
7	C	1320	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

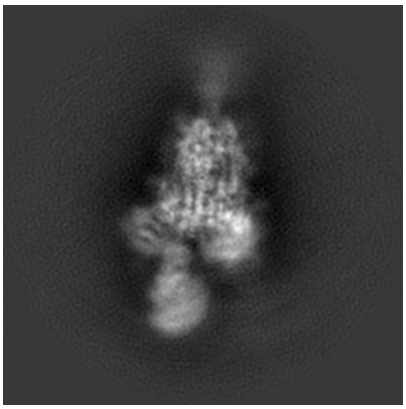
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7582. These allow visual inspection of the internal detail of the map and identification of artifacts.

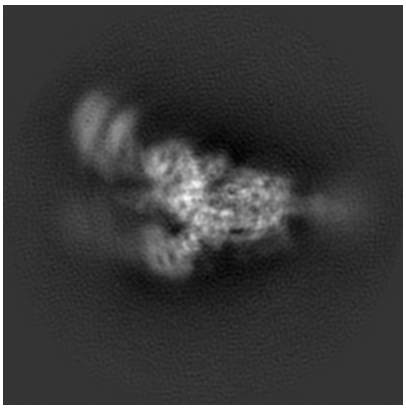
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

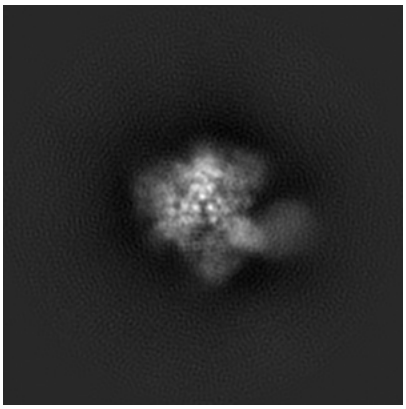
6.1.1 Primary map



X

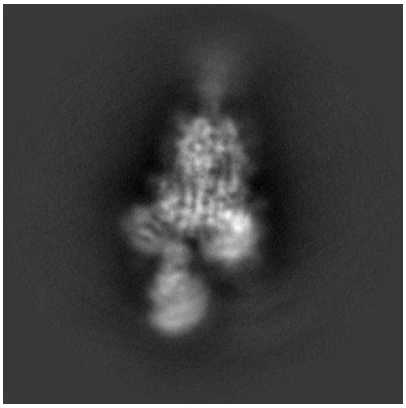


Y

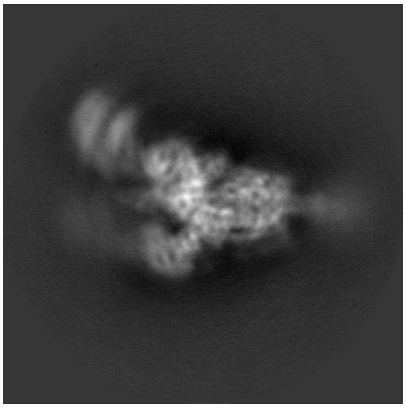


Z

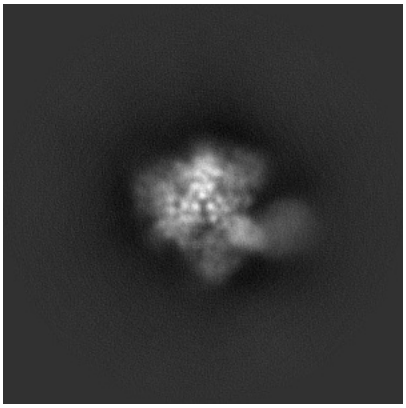
6.1.2 Raw map



X



Y

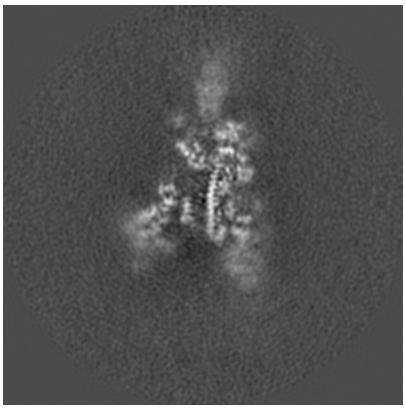


Z

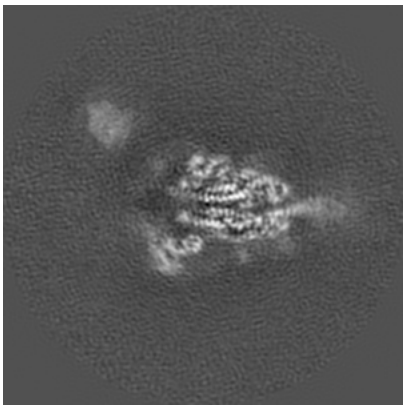
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

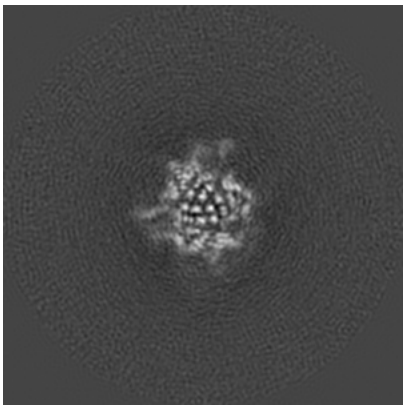
6.2.1 Primary map



X Index: 180

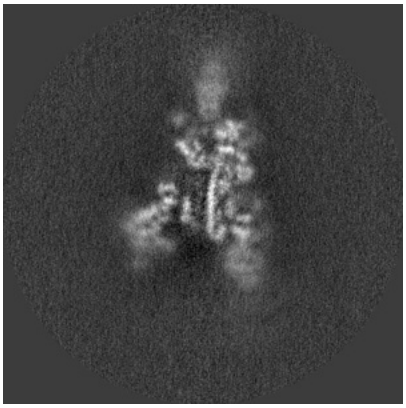


Y Index: 180

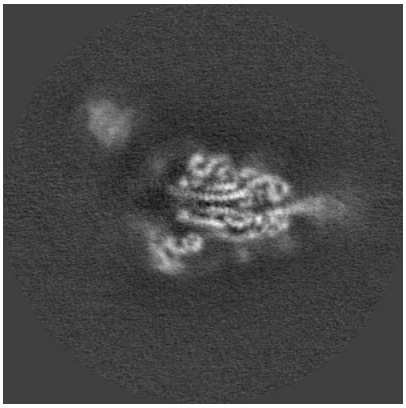


Z Index: 180

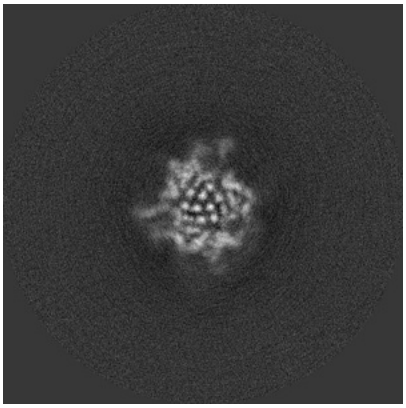
6.2.2 Raw map



X Index: 180



Y Index: 180

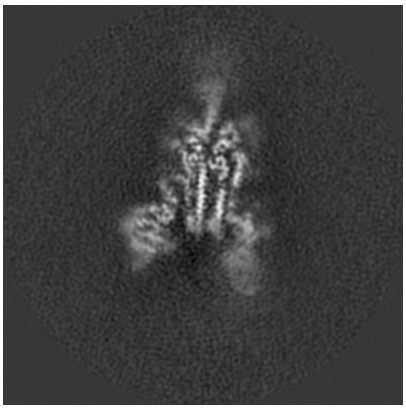


Z Index: 180

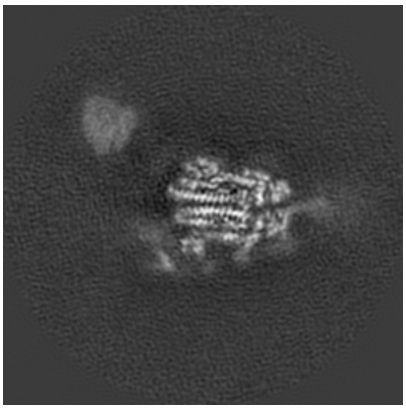
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

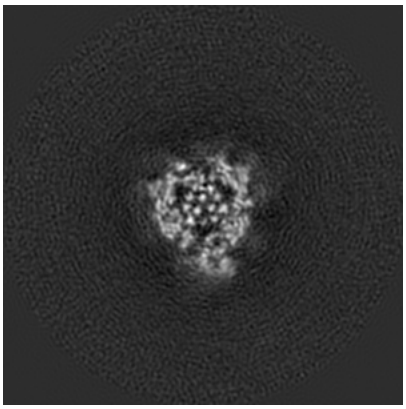
6.3.1 Primary map



X Index: 186



Y Index: 176

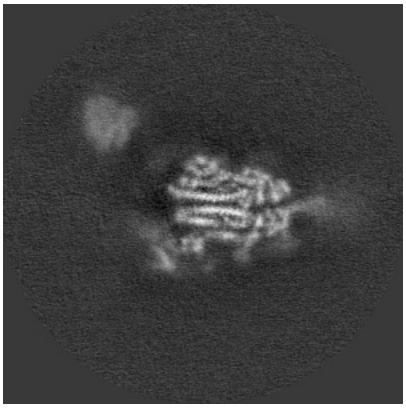


Z Index: 172

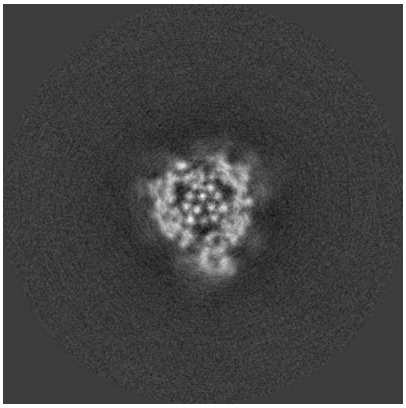
6.3.2 Raw map



X Index: 186



Y Index: 177

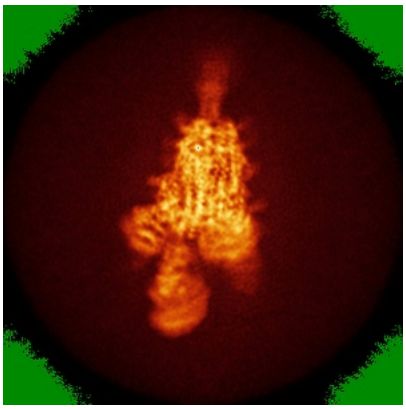


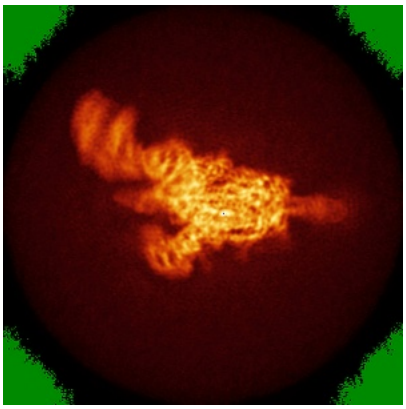
Z Index: 172

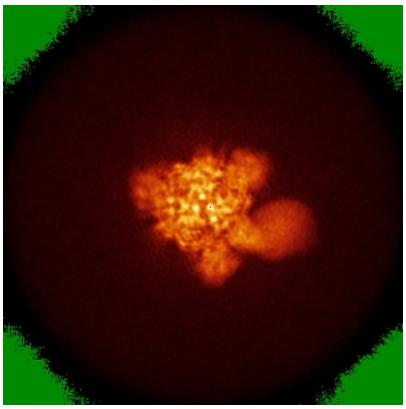
The images above show the largest variance slices of the map in three orthogonal directions.

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

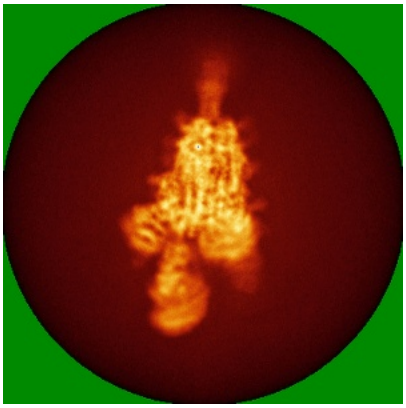
6.4.1 Primary map

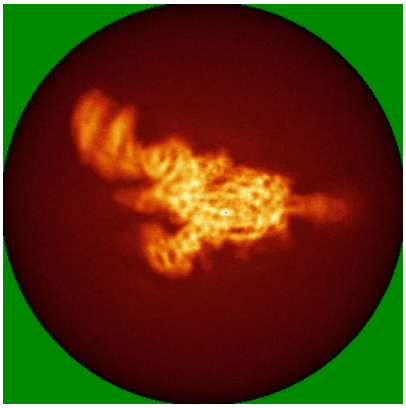

X

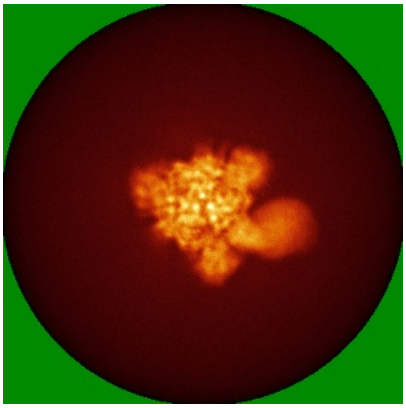

Y


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)

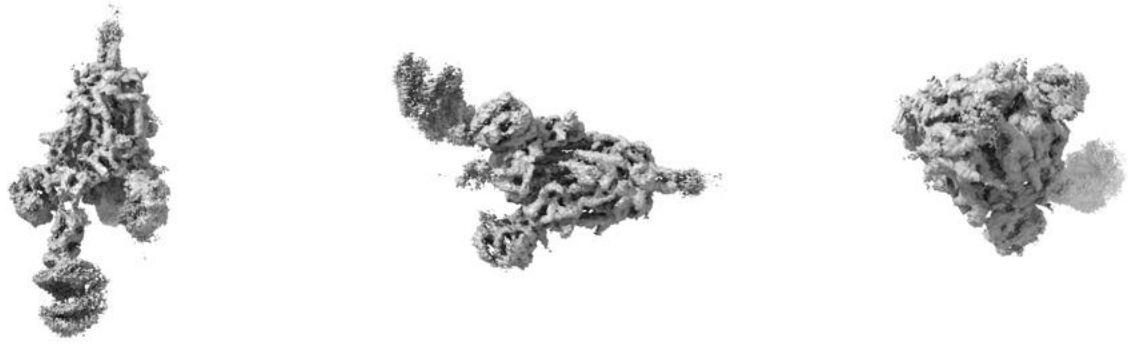
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. 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.

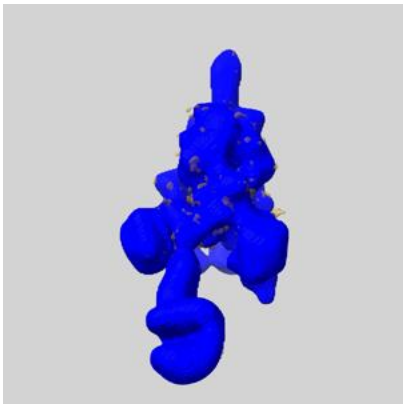
6.6 Mask visualisation

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

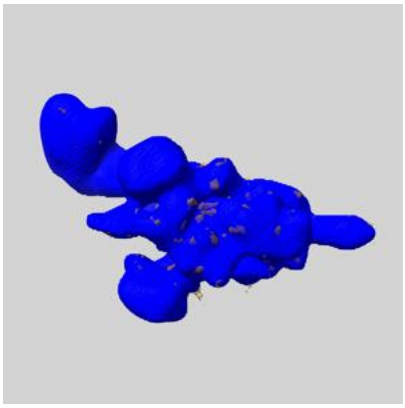
A mask typically either:

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

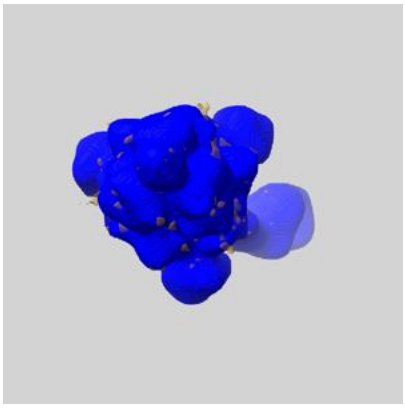
6.6.1 emd_7582_msk_1.map



X



Y

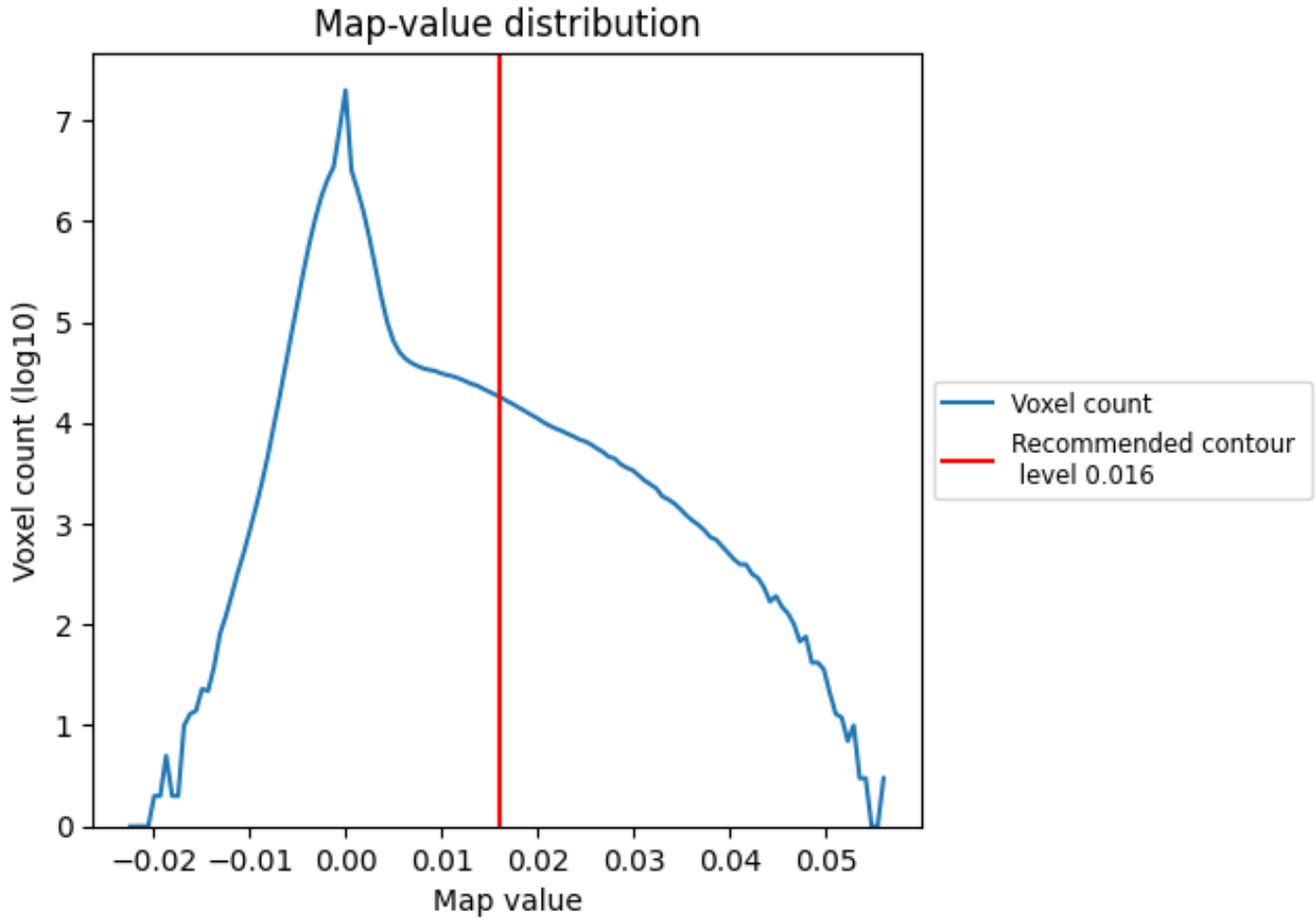


Z

7 Map analysis

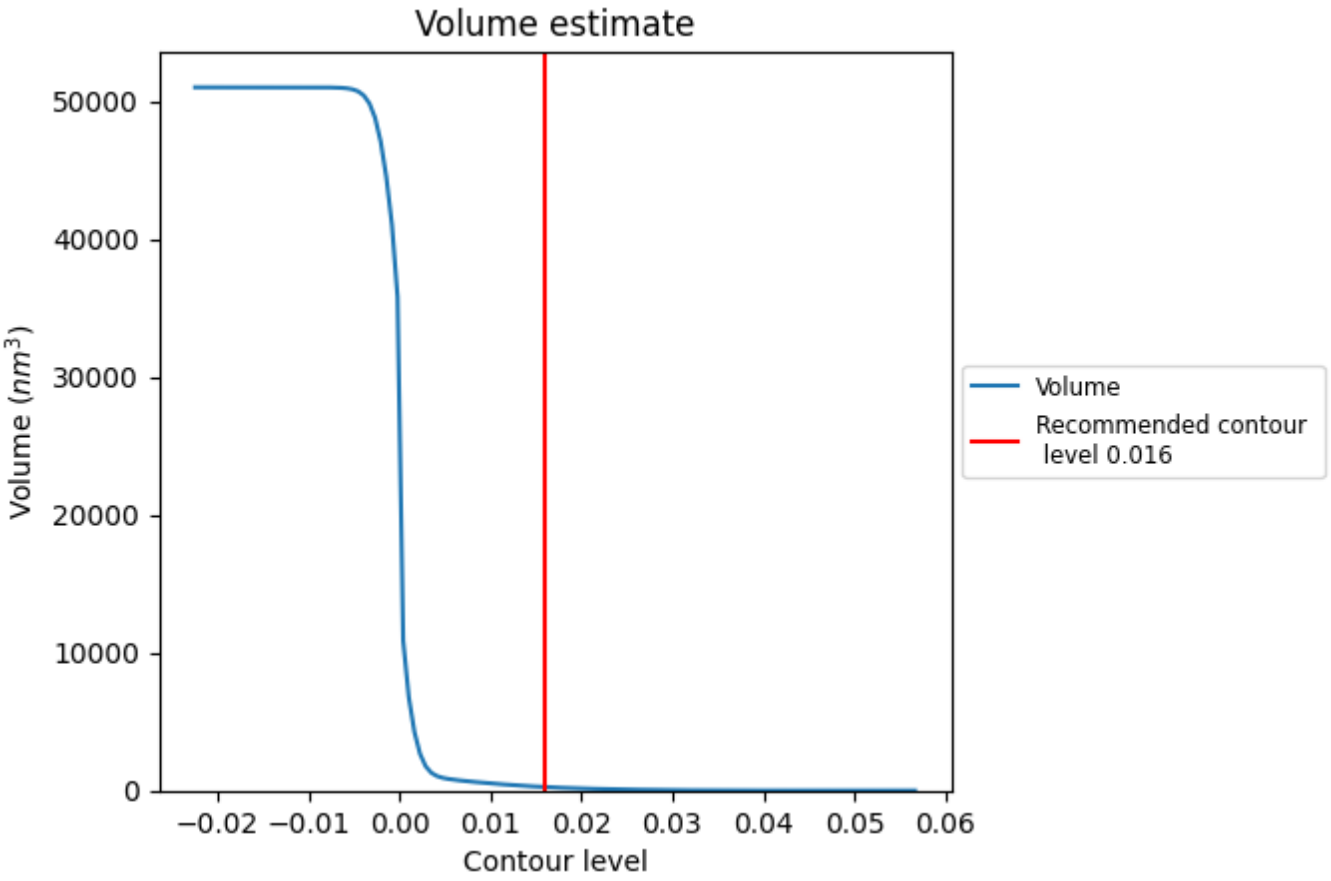
This section contains the results of statistical analysis of the map.

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.

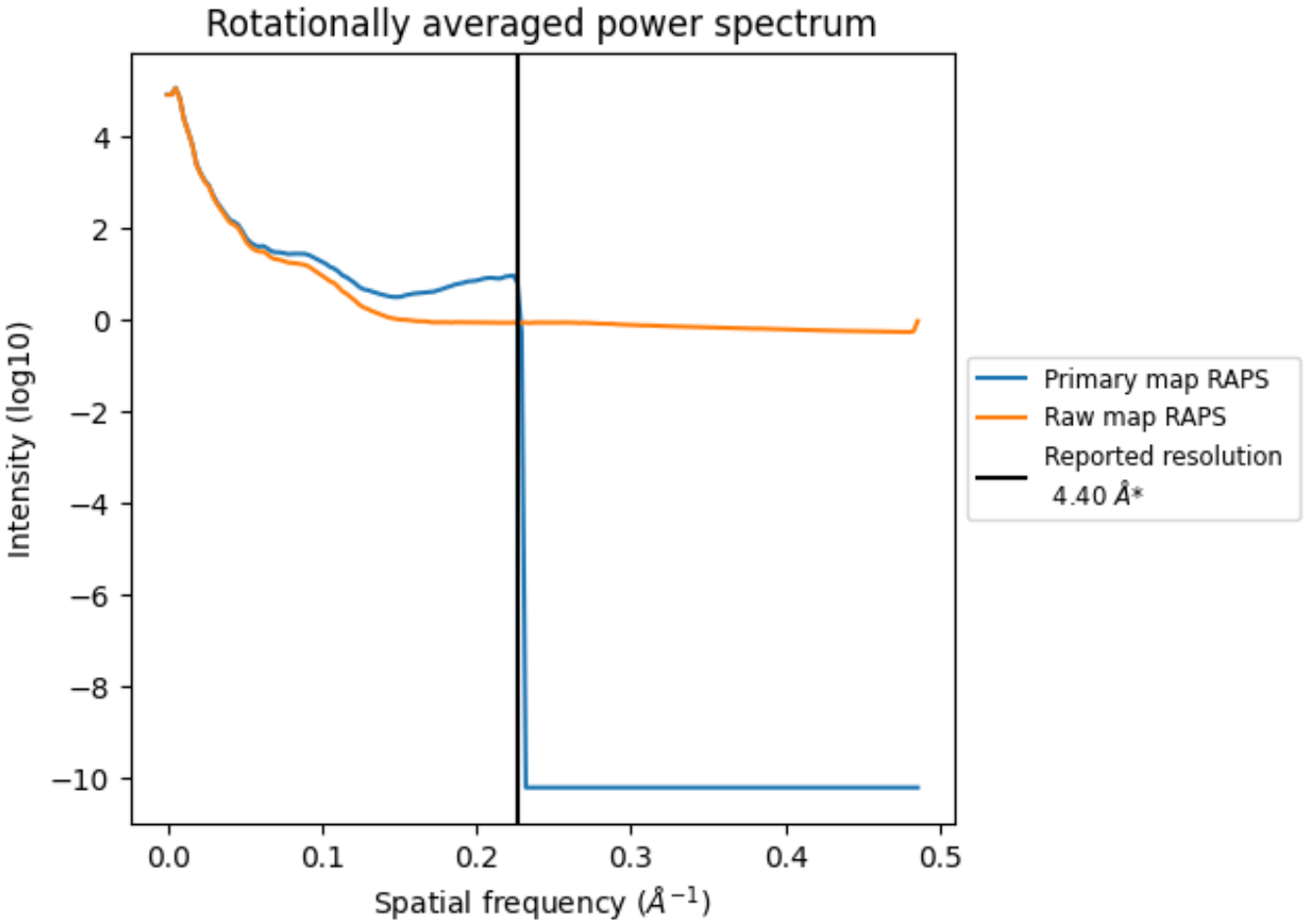
7.2 Volume estimate



The volume at the recommended contour level is 256 nm^3; this corresponds to an approximate mass of 232 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)

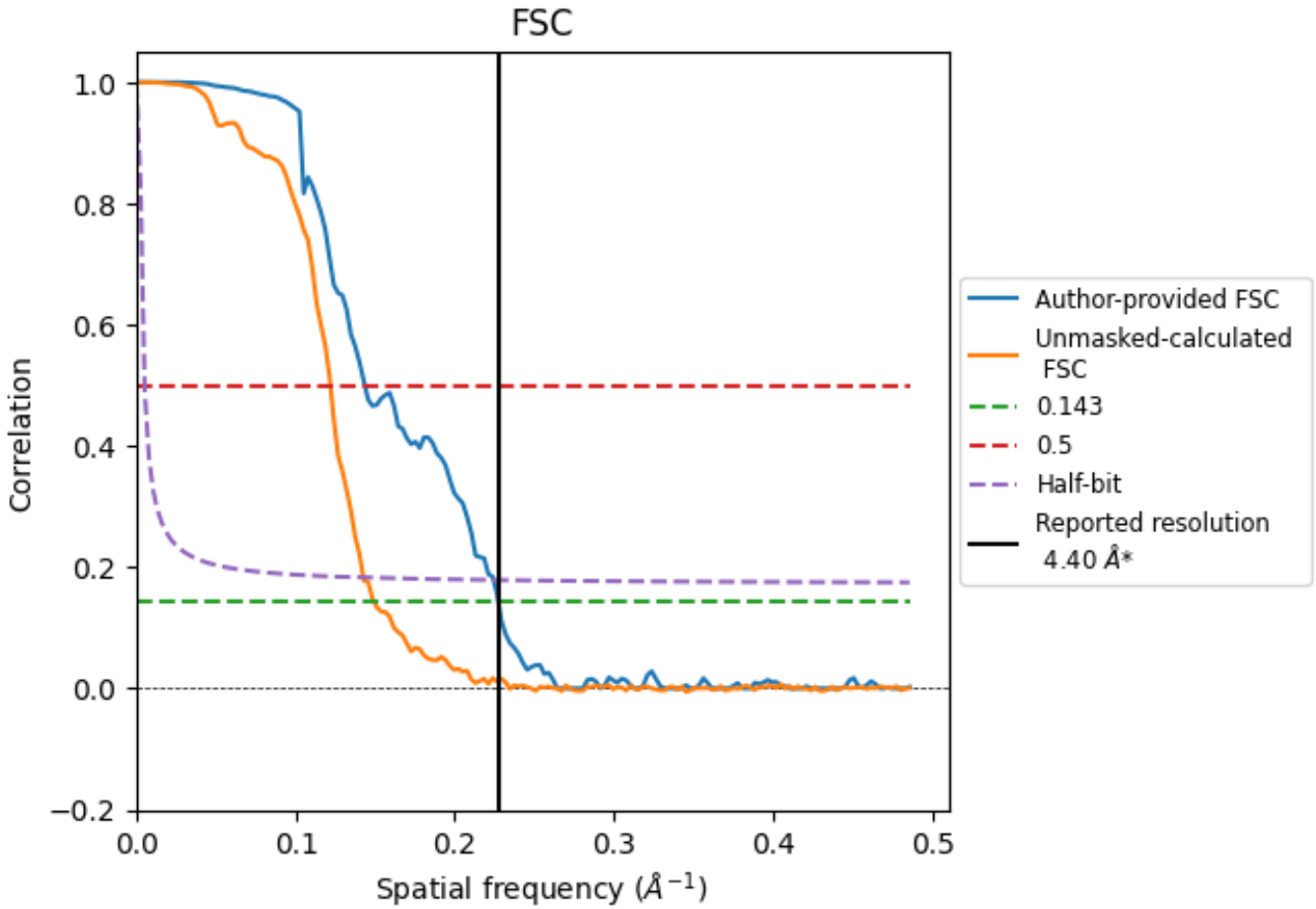


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

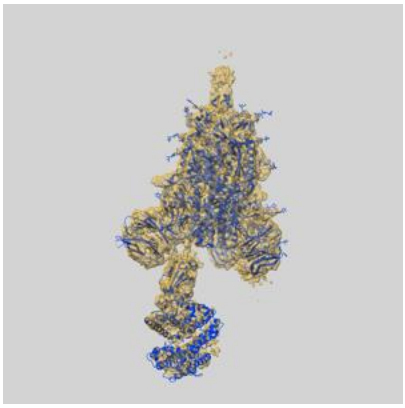
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	6.96	4.46
Unmasked-calculated*	6.70	8.20	7.01

*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 6.70 differs from the reported value 4.4 by more than 10 %

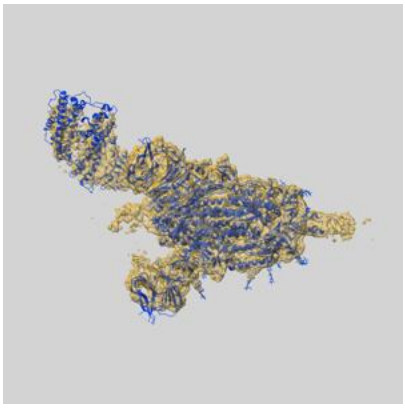
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7582 and PDB model 6CS2. Per-residue inclusion information can be found in section 3 on page 10.

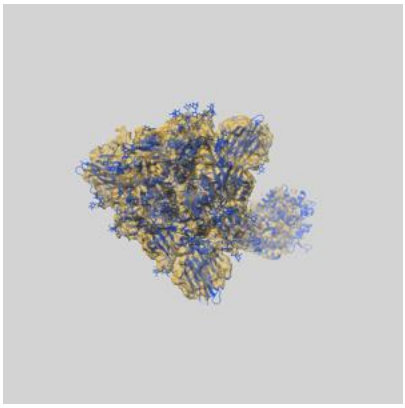
9.1 Map-model overlay



X



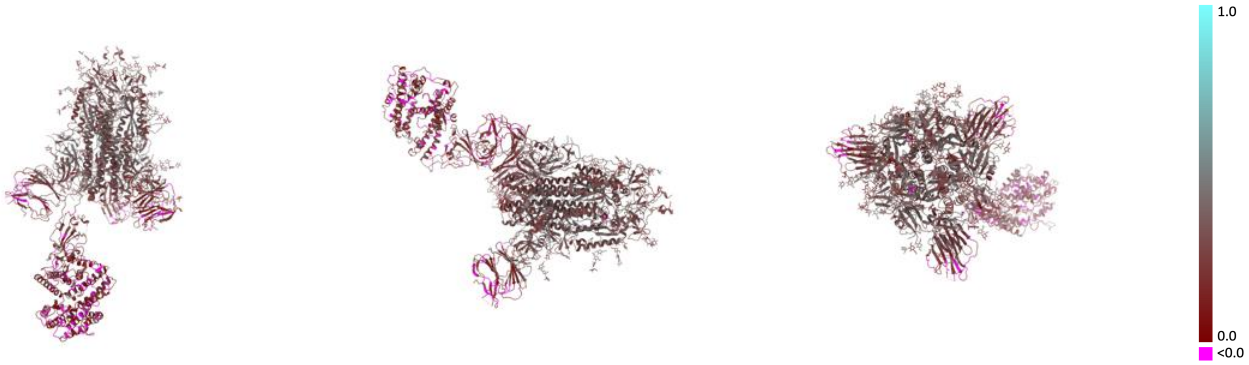
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

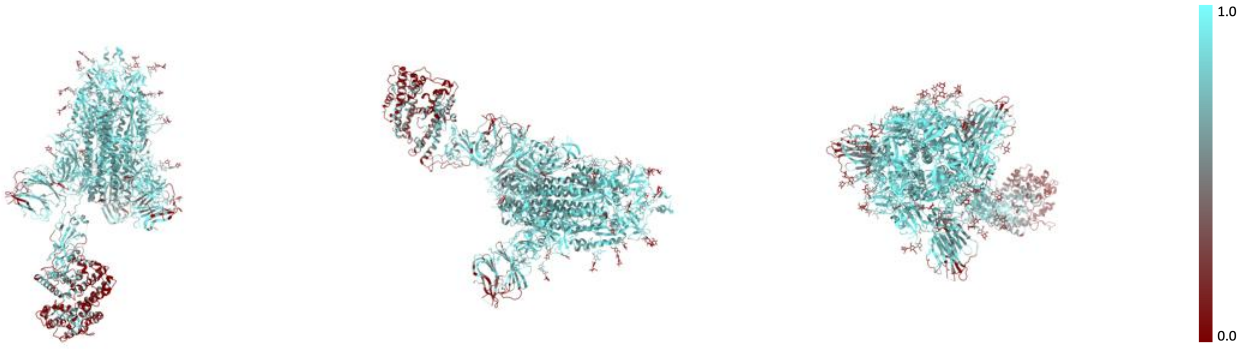
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

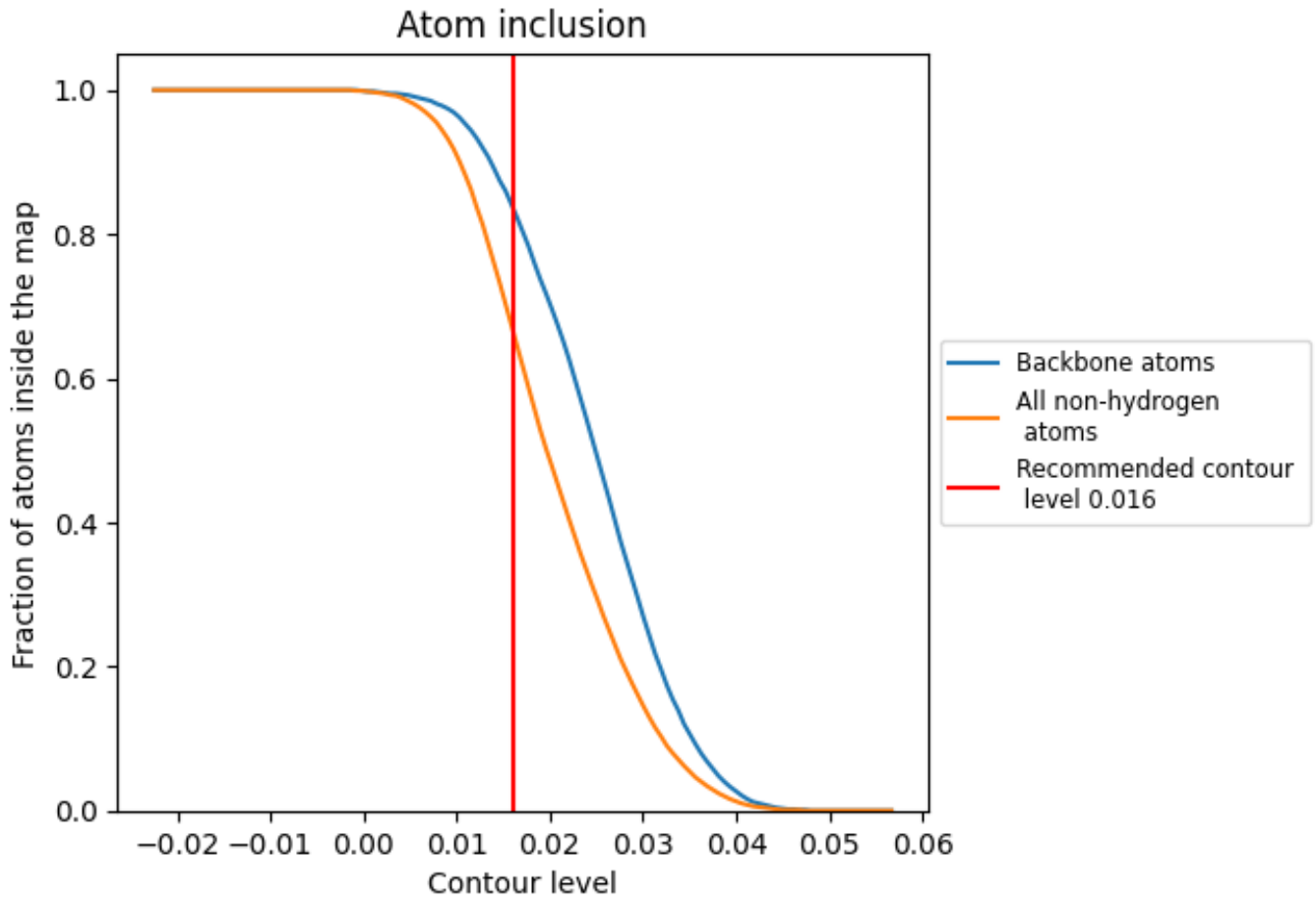
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 67% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6680	0.2730
A	0.7490	0.3050
B	0.7460	0.2850
C	0.7670	0.3080
D	0.3220	0.1330
E	0.4100	0.3530
F	0.3080	0.2470
G	0.3210	0.4030
H	0.2400	0.3410
I	0.4400	0.3450
J	0.3210	0.2870
K	0.2200	0.3130
L	0.2200	0.2520
M	0.4100	0.2790
N	0.1790	0.2210
O	0.3850	0.3880
P	0.2200	0.3170
Q	0.4100	0.3290
R	0.2140	0.3170
S	0.4600	0.2710
T	0.4360	0.2740
U	0.3400	0.3360
V	0.2310	0.3230
W	0.1030	0.2790
X	0.3590	0.3090
Y	0.3210	0.3010
Z	0.1790	0.2440
a	0.3000	0.2980
b	0.4000	0.3150
c	0.2500	0.3760
d	0.5000	0.3300
e	0.4200	0.3180

