Full wwPDB EM Validation Report ⓘ

Nov 17, 2022 – 02:16 AM EST

PDB ID	:	7LAB
EMDB ID	:	EMD-23248
Title	:	Structure of SARS-CoV-2 S protein in complex with N-terminal domain antibody DH1052
Authors	:	Manne, K.; Acharya, P.
Deposited on	:	2021-01-06
Resolution	:	2.97 Å(reported)
Based on initial model	:	6VXX

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:

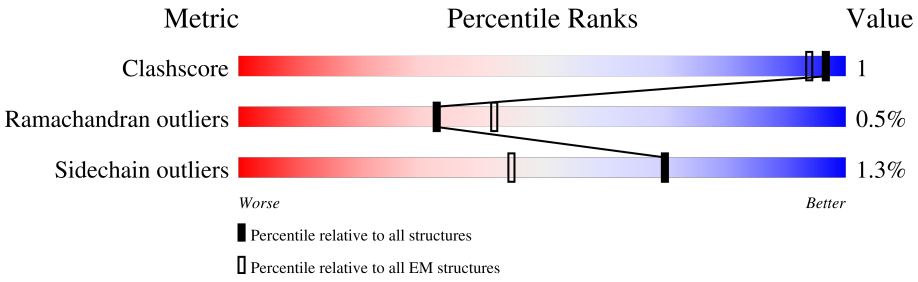
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	L	199	53% 98%
1	S	199	50% 94% 5%
1	X	199	51% 95% 5%
2	H	227	52% 96%
2	T	227	52% 95% 5%
2	Y	227	49% 96%
3	A	1121	82% 13%
3	B	1121	5% 84% 13%

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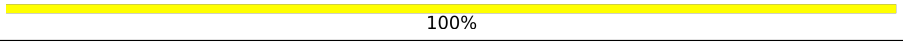
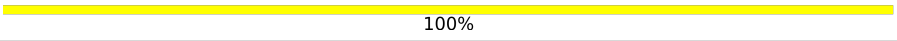
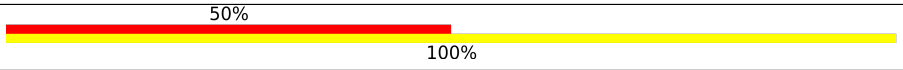
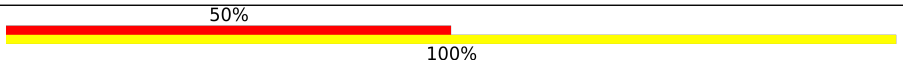
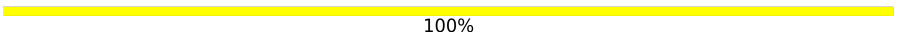
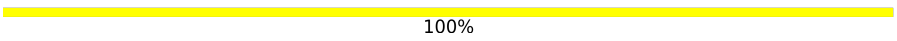
Mol	Chain	Length	Quality of chain
3	C	1121	
4	D	2	
4	E	2	
4	F	2	
4	G	2	
4	I	2	
4	J	2	
4	K	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	U	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	N	1	-	-	X	-
4	NAG	O	2	X	-	-	-
4	NAG	P	2	X	-	-	-
4	NAG	Q	2	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 65538 atoms, of which 32243 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 DH1052 light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	X	199	Total	C	H	N	O	S	0	0
			3002	955	1474	258	311	4		
1	S	199	Total	C	H	N	O	S	0	0
			3002	955	1474	258	311	4		
1	L	199	Total	C	H	N	O	S	0	0
			3002	955	1474	258	311	4		

- Molecule 2 is a protein called DH1052 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Y	227	Total	C	H	N	O	S	0	0
			3323	1064	1632	272	346	9		
2	T	227	Total	C	H	N	O	S	0	0
			3323	1064	1632	272	346	9		
2	H	227	Total	C	H	N	O	S	0	0
			3324	1064	1633	272	346	9		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	972	Total	C	H	N	O	S	0	0
			15033	4861	7429	1262	1448	33		
3	B	972	Total	C	H	N	O	S	0	0
			15035	4861	7431	1262	1448	33		
3	C	972	Total	C	H	N	O	S	0	0
			15032	4861	7428	1262	1448	33		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2

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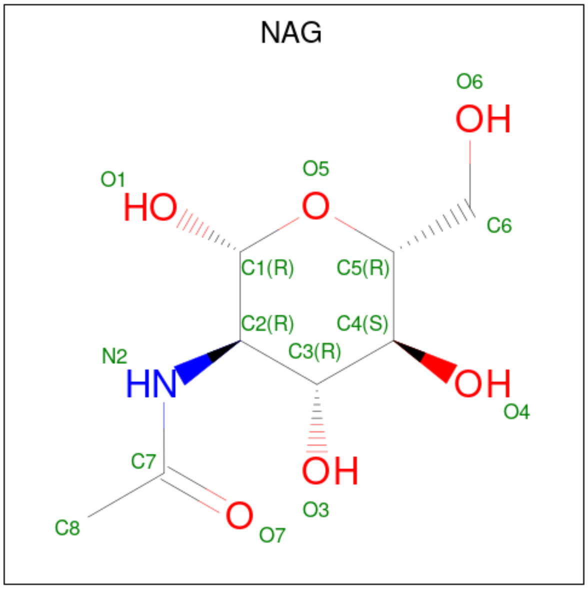
Chain	Residue	Modelled	Actual	Comment	Reference
B	987	PRO	VAL	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- 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	D	2	Total C H N O 55 16 27 2 10	0	0
4	E	2	Total C H N O 55 16 27 2 10	0	0
4	F	2	Total C H N O 55 16 27 2 10	0	0
4	G	2	Total C N O 28 16 2 10	0	0
4	I	2	Total C N O 28 16 2 10	0	0
4	J	2	Total C N O 28 16 2 10	0	0
4	K	2	Total C N O 28 16 2 10	0	0
4	M	2	Total C N O 28 16 2 10	0	0
4	N	2	Total C N O 28 16 2 10	0	0
4	O	2	Total C H N O 55 16 27 2 10	0	0
4	P	2	Total C H N O 55 16 27 2 10	0	0
4	Q	2	Total C H N O 55 16 27 2 10	0	0
4	R	2	Total C H N O 41 16 13 2 10	0	0
4	U	2	Total C H N O 55 16 27 2 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	A	1	Total 308	C 88	H 154	N 11	O 55	0
5	B	1	Total 252	C 72	H 126	N 9	O 45	0
5	B	1	Total 252	C 72	H 126	N 9	O 45	0

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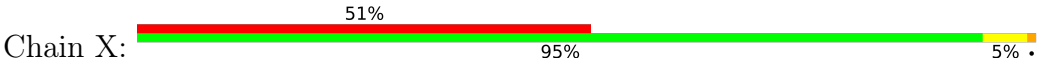
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total 252	C 72	H 126	N 9	O 45	0
5	B	1	Total 252	C 72	H 126	N 9	O 45	0
5	B	1	Total 252	C 72	H 126	N 9	O 45	0
5	B	1	Total 252	C 72	H 126	N 9	O 45	0
5	B	1	Total 252	C 72	H 126	N 9	O 45	0
5	B	1	Total 252	C 72	H 126	N 9	O 45	0
5	B	1	Total 252	C 72	H 126	N 9	O 45	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0
5	C	1	Total 308	C 88	H 154	N 11	O 55	0

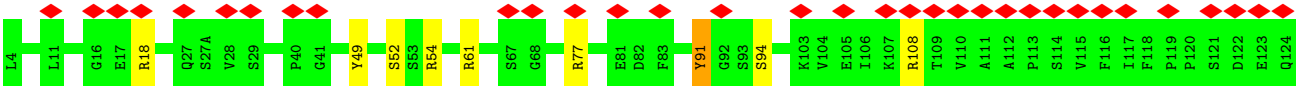
3 Residue-property plots (i)

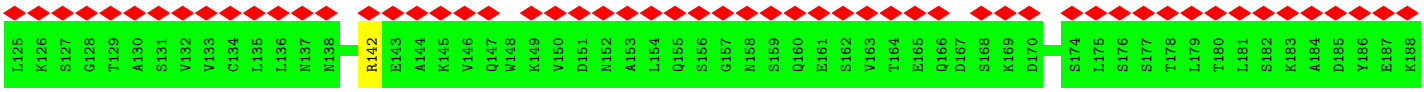
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

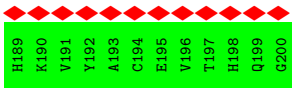
• Molecule 1: DH1052 light chain

Chain X:



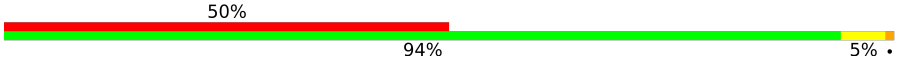


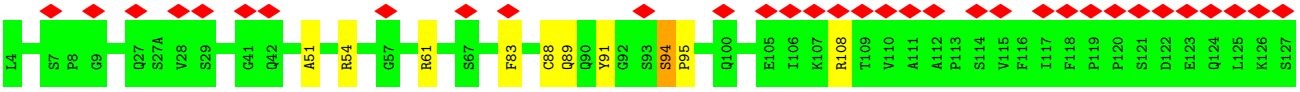


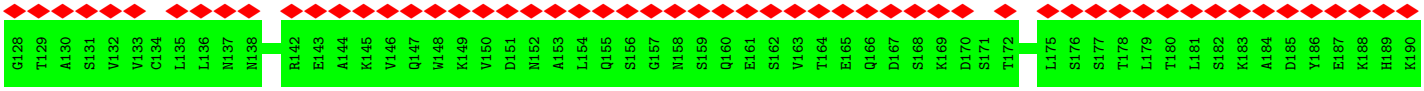


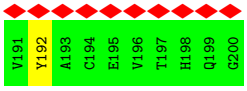
• Molecule 1: DH1052 light chain

Chain S:



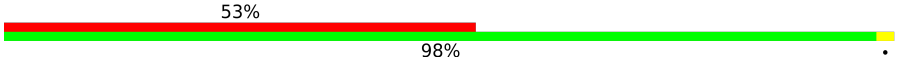


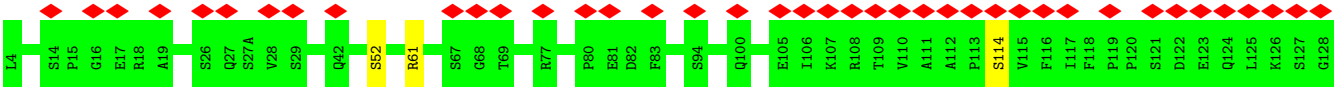


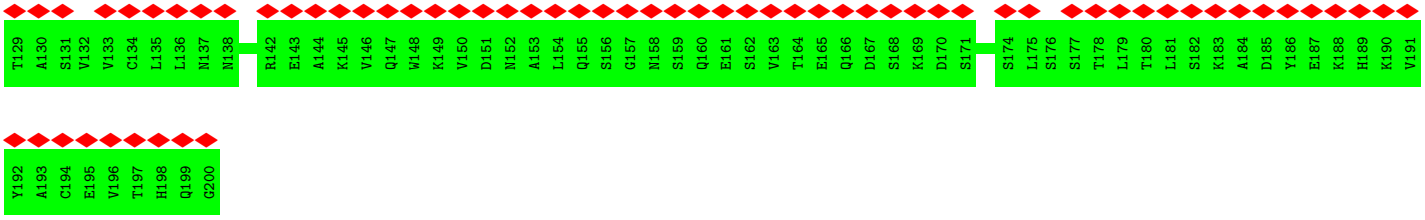


• Molecule 1: DH1052 light chain

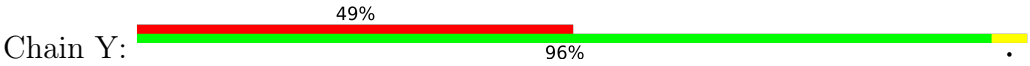
Chain L:

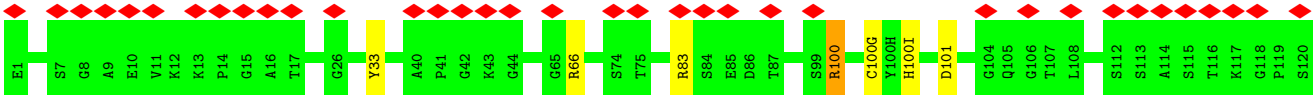




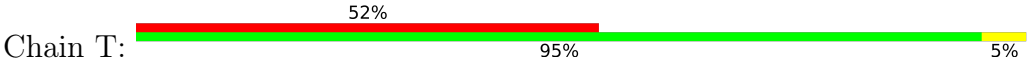


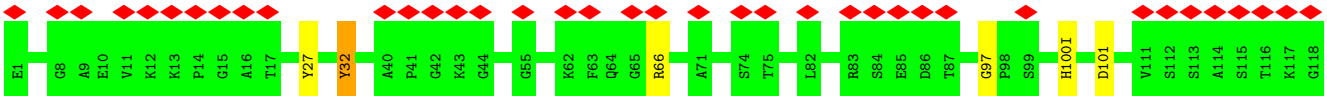
• Molecule 2: DH1052 heavy chain



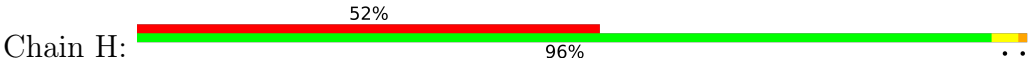


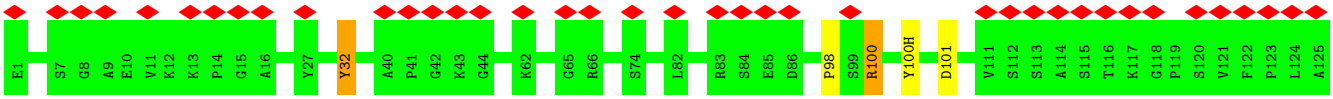
• Molecule 2: DH1052 heavy chain

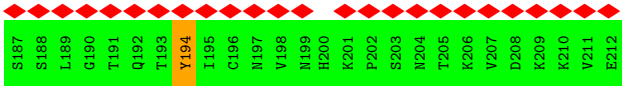




• Molecule 2: DH1052 heavy chain

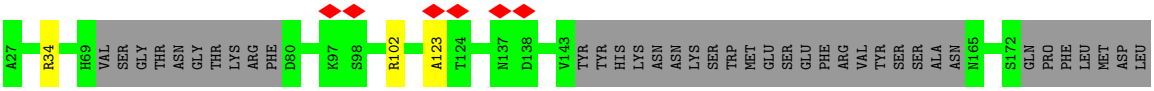






• Molecule 3: Spike glycoprotein

Chain A:

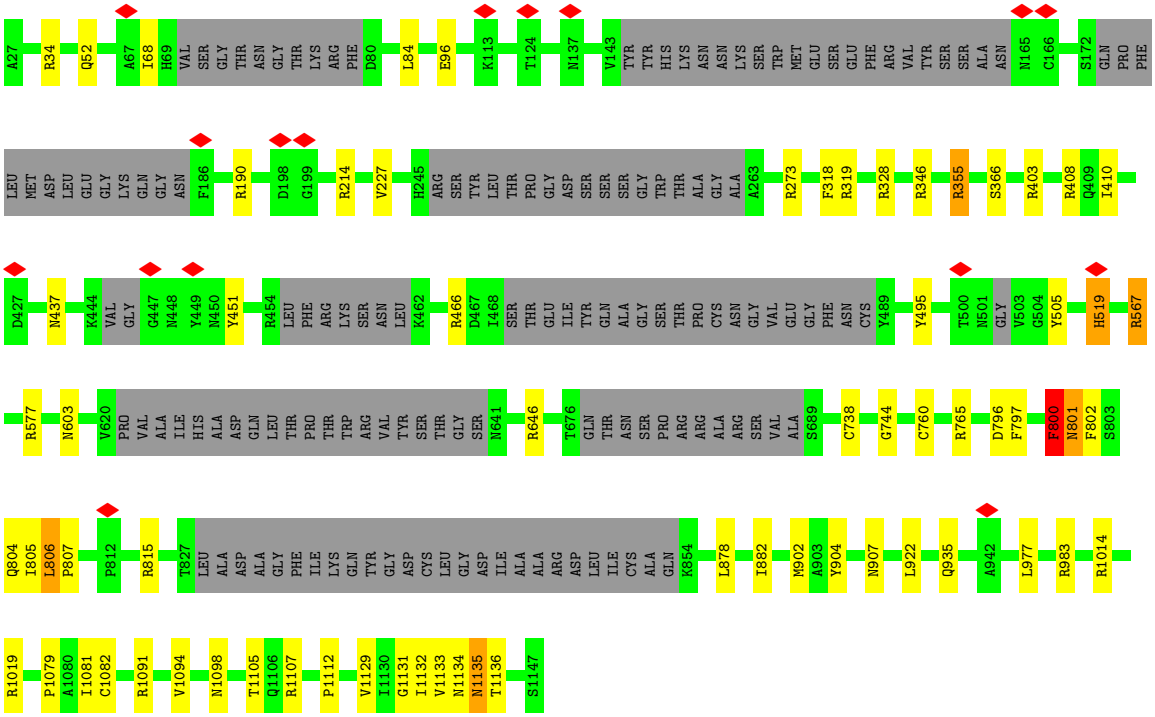


• Molecule 3: Spike glycoprotein

Chain B:

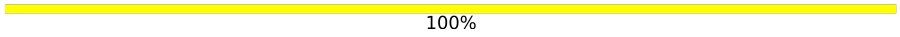
• Molecule 3: Spike glycoprotein

Chain C:



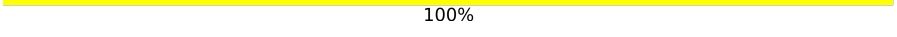
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



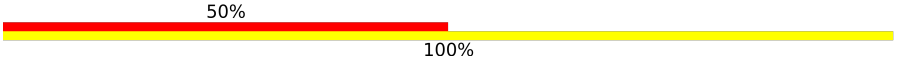
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain F:



• 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 I:

• 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 K:

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

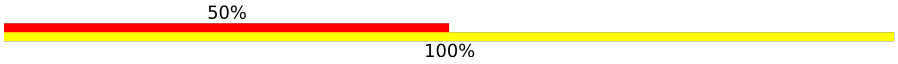
Chain M:

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

Chain N:

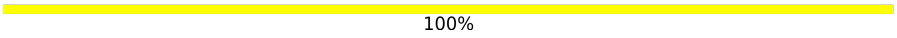
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



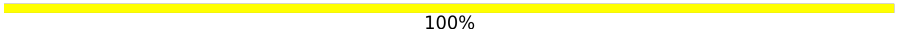
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



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

Chain Q:



• 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 U:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143411	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 ($e^-/Å^2$)	66.71	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.934	Depositor
Minimum map value	-1.673	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.274	Depositor
Map size (Å)	338.56, 338.56, 338.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	L	0.68	0/1563	0.99	1/2123 (0.0%)
1	S	0.69	0/1563	1.03	3/2123 (0.1%)
1	X	0.70	0/1563	1.06	7/2123 (0.3%)
2	H	0.65	0/1732	1.02	4/2360 (0.2%)
2	T	0.65	0/1732	0.98	1/2360 (0.0%)
2	Y	0.65	0/1732	1.01	4/2360 (0.2%)
3	A	0.65	0/7772	0.99	23/10572 (0.2%)
3	B	0.65	0/7772	0.99	20/10572 (0.2%)
3	C	0.75	4/7771 (0.1%)	1.02	32/10569 (0.3%)
All	All	0.68	4/33200 (0.0%)	1.01	95/45162 (0.2%)

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	S	0	2
1	X	0	1
2	H	0	4
2	Y	0	1
3	A	0	4
3	B	0	3
3	C	0	5
All	All	0	20

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	ASN	C-N	-20.13	0.87	1.34
3	C	806	LEU	C-N	19.64	1.71	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1129	VAL	C-N	-15.93	0.97	1.34
3	C	800	PHE	C-N	-8.52	1.14	1.34

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	800	PHE	O-C-N	-16.86	95.73	122.70
1	S	61	ARG	NE-CZ-NH1	9.60	125.10	120.30
2	H	100	ARG	NE-CZ-NH2	8.77	124.69	120.30
2	Y	100	ARG	NE-CZ-NH2	8.70	124.65	120.30
3	A	904	TYR	CB-CG-CD2	-8.69	115.79	121.00
3	B	904	TYR	CB-CG-CD2	-8.58	115.85	121.00
3	C	1129	VAL	O-C-N	-8.26	109.49	122.70
3	B	1019	ARG	NE-CZ-NH1	8.20	124.40	120.30
3	A	1014	ARG	NE-CZ-NH1	8.19	124.40	120.30
3	B	273	ARG	NE-CZ-NH1	8.09	124.35	120.30
3	C	1129	VAL	C-N-CA	8.06	141.85	121.70
3	C	1019	ARG	NE-CZ-NH1	8.02	124.31	120.30
3	A	1019	ARG	NE-CZ-NH1	8.01	124.30	120.30
3	A	408	ARG	NE-CZ-NH1	7.99	124.30	120.30
3	A	273	ARG	NE-CZ-NH1	7.81	124.20	120.30
3	C	904	TYR	CB-CG-CD2	-7.77	116.34	121.00
3	A	905	ARG	NE-CZ-NH1	7.75	124.18	120.30
3	C	408	ARG	NE-CZ-NH1	7.70	124.15	120.30
3	A	995	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	X	61	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	C	346	ARG	NE-CZ-NH1	7.49	124.04	120.30
3	B	815	ARG	NE-CZ-NH1	7.47	124.04	120.30
3	C	214	ARG	NE-CZ-NH1	7.46	124.03	120.30
3	C	328	ARG	NE-CZ-NH1	6.98	123.79	120.30
3	B	403	ARG	NE-CZ-NH1	6.92	123.76	120.30
3	A	577	ARG	NE-CZ-NH1	6.82	123.71	120.30
3	B	1014	ARG	NE-CZ-NH1	6.79	123.70	120.30
3	B	346	ARG	NE-CZ-NH1	6.76	123.68	120.30
3	A	346	ARG	NE-CZ-NH1	6.74	123.67	120.30
3	A	319	ARG	NE-CZ-NH1	6.71	123.65	120.30
3	C	34	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	T	66	ARG	NE-CZ-NH1	6.65	123.63	120.30
3	B	214	ARG	NE-CZ-NH1	6.64	123.62	120.30
3	A	815	ARG	NE-CZ-NH1	6.62	123.61	120.30
3	B	454	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	L	61	ARG	NE-CZ-NH1	6.55	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	214	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	S	108	ARG	NE-CZ-NH2	6.52	123.56	120.30
3	B	319	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	X	108	ARG	NE-CZ-NH2	6.48	123.54	120.30
3	C	646	ARG	NE-CZ-NH1	6.46	123.53	120.30
3	C	273	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	X	54	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	S	54	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	C	800	PHE	CA-C-N	6.35	131.18	117.20
3	C	815	ARG	NE-CZ-NH1	6.34	123.47	120.30
3	C	1091	ARG	NE-CZ-NH1	6.30	123.45	120.30
3	C	577	ARG	NE-CZ-NH1	6.27	123.44	120.30
3	C	765	ARG	NE-CZ-NH1	6.24	123.42	120.30
3	C	319	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	A	190	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	C	1014	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	H	32	TYR	CB-CG-CD2	-6.12	117.33	121.00
3	B	760	CYS	CA-CB-SG	-6.09	103.03	114.00
3	C	403	ARG	NE-CZ-NH1	6.09	123.35	120.30
3	C	355	ARG	NE-CZ-NH1	6.08	123.34	120.30
3	C	760	CYS	CA-CB-SG	-6.07	103.07	114.00
3	B	815	ARG	NE-CZ-NH2	-6.00	117.30	120.30
3	A	765	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	X	77	ARG	NE-CZ-NH2	5.99	123.30	120.30
3	A	328	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	A	466	ARG	NE-CZ-NH1	5.94	123.27	120.30
3	C	190	ARG	NE-CZ-NH1	5.91	123.26	120.30
3	B	282	ASN	CB-CG-ND2	5.90	130.85	116.70
2	Y	66	ARG	NE-CZ-NH1	5.89	123.24	120.30
3	A	403	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	X	142	ARG	NE-CZ-NH2	5.84	123.22	120.30
3	B	408	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	X	91	TYR	CB-CG-CD1	-5.73	117.56	121.00
3	B	237	ARG	NE-CZ-NH1	5.67	123.14	120.30
3	C	815	ARG	NE-CZ-NH2	-5.67	117.46	120.30
3	C	983	ARG	NE-CZ-NH1	5.60	123.10	120.30
3	C	806	LEU	O-C-N	-5.59	110.47	121.10
3	A	355	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	H	32	TYR	CB-CG-CD1	5.52	124.31	121.00
3	A	454	ARG	NE-CZ-NH1	5.51	123.06	120.30
3	B	355	ARG	NE-CZ-NH1	5.45	123.03	120.30
3	A	34	ARG	NE-CZ-NH1	5.43	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	357	ARG	NE-CZ-NH1	5.41	123.01	120.30
2	Y	83	ARG	NE-CZ-NH1	5.38	122.99	120.30
3	C	466	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	B	995	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	Y	33	TYR	CB-CG-CD2	-5.29	117.83	121.00
3	C	567	ARG	NE-CZ-NH1	5.22	122.91	120.30
3	C	451	TYR	CB-CG-CD1	-5.22	117.87	121.00
3	B	466	ARG	NE-CZ-NH1	5.20	122.90	120.30
3	C	800	PHE	C-N-CA	5.15	134.57	121.70
3	A	102	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	C	1107	ARG	NE-CZ-NH1	5.12	122.86	120.30
3	C	1129	VAL	CA-C-N	5.11	128.44	117.20
3	B	577	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	X	18	ARG	NE-CZ-NH2	5.03	122.81	120.30
3	A	237	ARG	NE-CZ-NH1	5.02	122.81	120.30
3	B	567	ARG	NE-CZ-NH2	-5.01	117.79	120.30
2	H	32	TYR	CA-CB-CG	5.00	122.91	113.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	279	TYR	Sidechain
3	A	355	ARG	Sidechain
3	A	495	TYR	Sidechain
3	A	983	ARG	Sidechain
3	B	269	TYR	Sidechain
3	B	34	ARG	Sidechain
3	B	355	ARG	Sidechain
3	C	1135	ASN	Mainchain
3	C	355	ARG	Sidechain
3	C	495	TYR	Sidechain
3	C	800	PHE	Mainchain
3	C	801	ASN	Mainchain
2	H	100	ARG	Sidechain
2	H	100(H)	TYR	Sidechain
2	H	194	TYR	Sidechain
2	H	98	PRO	Peptide
1	S	192	TYR	Sidechain
1	S	91	TYR	Sidechain
1	X	49	TYR	Sidechain
2	Y	100	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1528	1474	1471	0	0
1	S	1528	1474	1471	1	0
1	X	1528	1474	1471	0	0
2	H	1691	1633	1632	1	0
2	T	1691	1632	1632	3	0
2	Y	1691	1632	1632	1	0
3	A	7604	7429	7415	4	0
3	B	7604	7431	7415	2	0
3	C	7604	7428	7411	30	0
4	D	28	27	25	0	0
4	E	28	27	25	0	0
4	F	28	27	25	0	0
4	G	28	0	25	1	0
4	I	28	0	25	1	0
4	J	28	0	25	1	0
4	K	28	0	25	1	0
4	M	28	0	25	2	0
4	N	28	0	25	7	0
4	O	28	27	25	0	0
4	P	28	27	25	0	0
4	Q	28	27	25	0	0
4	R	28	13	25	1	0
4	U	28	27	25	2	0
5	A	154	154	143	0	0
5	B	126	126	117	0	0
5	C	154	154	143	1	0
All	All	33295	32243	32303	47	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 1.

All (47) 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)
3:C:1134:ASN:CG	4:N:1:NAG:C1	1.76	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:806:LEU:C	3:C:807:PRO:N	1.71	1.39
3:C:1134:ASN:ND2	4:N:1:NAG:O5	1.56	1.33
3:C:1134:ASN:ND2	4:N:1:NAG:C2	2.05	1.17
3:C:805:ILE:HD12	3:C:878:LEU:HD11	1.33	1.07
3:C:796:ASP:C	3:C:797:PHE:N	2.12	1.01
3:C:1134:ASN:ND2	4:N:1:NAG:C1	0.84	0.99
3:C:804:GLN:NE2	3:C:935:GLN:OE1	2.03	0.92
3:C:1135:ASN:ND2	3:C:1136:THR:O	2.02	0.91
3:C:1134:ASN:OD1	4:N:1:NAG:C1	2.25	0.85
3:C:805:ILE:HD12	3:C:878:LEU:CD1	2.08	0.81
3:C:1082:CYS:SG	3:C:1132:ILE:HD13	2.24	0.77
3:C:1098:ASN:HD21	4:U:1:NAG:C1	2.00	0.74
4:G:1:NAG:H61	4:G:2:NAG:O5	1.90	0.71
3:C:1098:ASN:ND2	4:U:1:NAG:C1	2.60	0.64
3:C:806:LEU:CA	3:C:807:PRO:N	2.61	0.64
3:C:1082:CYS:SG	3:C:1132:ILE:CD1	2.86	0.64
3:B:922:LEU:HD11	4:I:1:NAG:H5	1.83	0.60
3:C:1081:ILE:CG2	3:C:1135:ASN:HB3	2.31	0.60
3:C:1079:PRO:HD2	3:C:1131:GLY:O	2.07	0.54
3:B:804:GLN:OE1	4:J:1:NAG:H62	2.08	0.53
3:C:1081:ILE:HG23	3:C:1135:ASN:HB3	1.90	0.52
2:Y:135:THR:HA	2:Y:138:LEU:HD13	1.92	0.50
1:S:94:SER:H	1:S:95:PRO:HD2	1.75	0.50
3:A:1098:ASN:HD21	4:R:1:NAG:C1	2.25	0.50
3:C:800:PHE:HB3	3:C:802:PHE:CZ	2.48	0.49
2:T:32:TYR:CD2	2:T:97:GLY:HA2	2.48	0.49
2:T:135:THR:HA	2:T:138:LEU:HD13	1.95	0.48
3:C:797:PHE:CE1	3:C:882:ILE:CG2	2.98	0.47
3:C:922:LEU:HD11	4:K:1:NAG:H5	1.95	0.47
3:C:1131:GLY:HA2	5:C:1309:NAG:H83	1.97	0.47
3:C:805:ILE:CD1	3:C:878:LEU:HD11	2.23	0.46
2:H:138:LEU:HD13	2:H:194:TYR:CE1	2.50	0.46
3:C:519:HIS:CD2	3:C:567:ARG:HH21	2.35	0.45
3:C:1081:ILE:HD13	3:C:1133:VAL:CG2	2.46	0.44
3:C:806:LEU:C	3:C:807:PRO:CA	2.75	0.44
3:A:193:VAL:HG23	3:A:223:LEU:HD22	1.99	0.44
4:M:1:NAG:H61	4:M:2:NAG:O5	2.18	0.44
4:M:1:NAG:H4	4:M:2:NAG:H2	1.59	0.43
3:A:726:ILE:HG22	3:A:948:LEU:HD13	2.01	0.42
3:C:1105:THR:HG22	3:C:1112:PRO:HA	2.00	0.42
3:C:796:ASP:C	3:C:797:PHE:CA	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:1:NAG:H61	4:N:2:NAG:C7	2.50	0.42
3:C:410:ILE:HD12	3:C:410:ILE:N	2.34	0.41
3:A:391:CYS:HB3	3:A:522:ALA:HB1	2.03	0.41
2:T:154:TRP:CD2	2:T:182:VAL:HG23	2.56	0.40
4:N:1:NAG:H3	4:N:1:NAG:H82	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	L	197/199 (99%)	178 (90%)	18 (9%)	1 (0%)	29	66
1	S	197/199 (99%)	181 (92%)	14 (7%)	2 (1%)	15	50
1	X	197/199 (99%)	175 (89%)	20 (10%)	2 (1%)	15	50
2	H	225/227 (99%)	207 (92%)	16 (7%)	2 (1%)	17	53
2	T	225/227 (99%)	207 (92%)	15 (7%)	3 (1%)	12	43
2	Y	225/227 (99%)	207 (92%)	16 (7%)	2 (1%)	17	53
3	A	948/1121 (85%)	888 (94%)	55 (6%)	5 (0%)	29	66
3	B	948/1121 (85%)	885 (93%)	61 (6%)	2 (0%)	47	80
3	C	946/1121 (84%)	894 (94%)	51 (5%)	1 (0%)	51	83
All	All	4108/4641 (88%)	3822 (93%)	266 (6%)	20 (0%)	32	66

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	94	SER
1	S	94	SER
2	T	186	SER

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Mol	Chain	Res	Type
3	A	123	ALA
3	B	215	ASP
3	C	744	GLY
1	X	52	SER
2	Y	100(I)	HIS
2	Y	129	LYS
2	T	100(I)	HIS
2	T	129	LYS
3	B	123	ALA
2	H	129	LYS
3	A	614	ASP
2	H	135	THR
1	L	52	SER
1	S	51	ALA
3	A	216	LEU
3	A	744	GLY
3	A	213	VAL

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	L	171/171 (100%)	170 (99%)	1 (1%)	86 94
1	S	171/171 (100%)	168 (98%)	3 (2%)	59 83
1	X	171/171 (100%)	170 (99%)	1 (1%)	86 94
2	H	191/191 (100%)	188 (98%)	3 (2%)	62 85
2	T	191/191 (100%)	188 (98%)	3 (2%)	62 85
2	Y	191/191 (100%)	189 (99%)	2 (1%)	76 91
3	A	852/972 (88%)	840 (99%)	12 (1%)	67 86
3	B	852/972 (88%)	844 (99%)	8 (1%)	78 91
3	C	852/972 (88%)	836 (98%)	16 (2%)	57 82
All	All	3642/4002 (91%)	3593 (99%)	49 (1%)	70 88

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	91	TYR
2	Y	100(G)	CYS
2	Y	101	ASP
1	S	83	PHE
1	S	88	CYS
1	S	89	GLN
2	T	27	TYR
2	T	32	TYR
2	T	101	ASP
3	A	215	ASP
3	A	216	LEU
3	A	238	PHE
3	A	328	ARG
3	A	422	ASN
3	A	578	ASP
3	A	619	GLU
3	A	760	CYS
3	A	854	LYS
3	A	1004	LEU
3	A	1094	VAL
3	A	1105	THR
3	B	84	LEU
3	B	125	ASN
3	B	645	THR
3	B	738	CYS
3	B	907	ASN
3	B	977	LEU
3	B	1004	LEU
3	B	1135	ASN
3	C	52	GLN
3	C	68	ILE
3	C	84	LEU
3	C	96	GLU
3	C	227	VAL
3	C	318	PHE
3	C	366	SER
3	C	437	ASN
3	C	505	TYR
3	C	519	HIS
3	C	603	ASN
3	C	738	CYS
3	C	902	MET

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Mol	Chain	Res	Type
3	C	907	ASN
3	C	977	LEU
3	C	1094	VAL
2	H	32	TYR
2	H	101	ASP
2	H	183	THR
1	L	114	SER

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

Mol	Chain	Res	Type
2	Y	38	GLN
3	C	519	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	3,4	14,14,15	1.28	2 (14%)	17,19,21	0.79	0
4	NAG	D	2	4	14,14,15	1.21	2 (14%)	17,19,21	0.85	0
4	NAG	E	1	3,4	14,14,15	1.19	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	E	2	4	14,14,15	1.24	1 (7%)	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	F	1	3,4	14,14,15	1.27	2 (14%)	17,19,21	0.90	1 (5%)
4	NAG	F	2	4	14,14,15	1.22	1 (7%)	17,19,21	0.76	0
4	NAG	G	1	3,4	14,14,15	0.60	0	17,19,21	1.75	3 (17%)
4	NAG	G	2	4	14,14,15	0.42	0	17,19,21	1.10	1 (5%)
4	NAG	I	1	3,4	14,14,15	0.31	0	17,19,21	1.01	1 (5%)
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	0.59	0
4	NAG	J	1	3,4	14,14,15	0.28	0	17,19,21	0.98	1 (5%)
4	NAG	J	2	4	14,14,15	0.25	0	17,19,21	0.66	0
4	NAG	K	1	3,4	14,14,15	0.35	0	17,19,21	0.96	1 (5%)
4	NAG	K	2	4	14,14,15	0.24	0	17,19,21	0.82	0
4	NAG	M	1	3,4	14,14,15	0.67	0	17,19,21	1.15	1 (5%)
4	NAG	M	2	4	14,14,15	0.33	0	17,19,21	1.36	3 (17%)
4	NAG	N	1	4	14,14,15	0.25	0	17,19,21	0.80	1 (5%)
4	NAG	N	2	4	14,14,15	0.31	0	17,19,21	0.70	0
4	NAG	O	1	3,4	14,14,15	1.48	4 (28%)	17,19,21	0.90	1 (5%)
4	NAG	O	2	4	14,14,15	1.27	3 (21%)	17,19,21	0.94	1 (5%)
4	NAG	P	1	3,4	14,14,15	1.20	2 (14%)	17,19,21	1.37	2 (11%)
4	NAG	P	2	4	14,14,15	1.24	2 (14%)	17,19,21	1.01	1 (5%)
4	NAG	Q	1	3,4	14,14,15	1.28	3 (21%)	17,19,21	1.10	1 (5%)
4	NAG	Q	2	4	14,14,15	1.22	2 (14%)	17,19,21	1.36	1 (5%)
4	NAG	R	1	4	14,14,15	0.50	0	17,19,21	1.37	3 (17%)
4	NAG	R	2	4	14,14,15	0.24	0	17,19,21	1.03	2 (11%)
4	NAG	U	1	4	14,14,15	0.23	0	17,19,21	0.56	0
4	NAG	U	2	4	14,14,15	0.23	0	17,19,21	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	NAG	G	1	3,4	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	NAG	K	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	3/6/23/26	0/1/1/1
4	NAG	N	1	4	-	3/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	1/1/7/7	1/6/23/26	0/1/1/1
4	NAG	P	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	1/1/7/7	1/6/23/26	0/1/1/1
4	NAG	Q	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	1/1/7/7	1/6/23/26	0/1/1/1
4	NAG	R	1	4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	3/6/23/26	0/1/1/1
4	NAG	U	1	4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	O5-C5	2.97	1.49	1.43
4	O	1	NAG	O4-C4	2.83	1.49	1.43
4	P	2	NAG	O5-C5	2.80	1.49	1.43
4	Q	2	NAG	O5-C5	2.78	1.49	1.43
4	O	1	NAG	O5-C5	2.73	1.49	1.43
4	D	1	NAG	O4-C4	2.71	1.49	1.43
4	D	2	NAG	O5-C5	2.60	1.48	1.43
4	Q	1	NAG	O5-C5	2.55	1.48	1.43
4	F	1	NAG	O5-C5	2.55	1.48	1.43
4	F	1	NAG	O4-C4	2.52	1.48	1.43
4	E	1	NAG	O5-C5	2.50	1.48	1.43
4	O	2	NAG	O5-C5	2.49	1.48	1.43
4	Q	1	NAG	O4-C4	2.46	1.48	1.43
4	Q	2	NAG	O5-C1	2.46	1.47	1.43
4	P	1	NAG	O4-C4	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C5	2.31	1.48	1.43
4	O	1	NAG	C1-C2	2.29	1.55	1.52
4	F	2	NAG	O5-C5	2.22	1.47	1.43
4	Q	1	NAG	O5-C1	2.15	1.47	1.43
4	P	1	NAG	O5-C5	2.06	1.47	1.43
4	D	2	NAG	C1-C2	2.05	1.55	1.52
4	O	2	NAG	O5-C1	2.03	1.47	1.43
4	O	2	NAG	C1-C2	2.01	1.55	1.52
4	P	2	NAG	O5-C1	2.01	1.46	1.43
4	O	1	NAG	O5-C1	2.00	1.46	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	1	NAG	C1-O5-C5	4.69	118.55	112.19
4	G	1	NAG	O4-C4-C3	-4.20	100.64	110.35
4	Q	2	NAG	C1-O5-C5	4.17	117.84	112.19
4	Q	1	NAG	C1-O5-C5	3.80	117.34	112.19
4	R	1	NAG	O4-C4-C3	-3.64	101.94	110.35
4	G	2	NAG	C1-O5-C5	3.61	117.08	112.19
4	E	2	NAG	C1-O5-C5	3.41	116.81	112.19
4	I	1	NAG	C1-O5-C5	3.25	116.60	112.19
4	J	1	NAG	C1-O5-C5	3.15	116.46	112.19
4	P	2	NAG	C1-O5-C5	3.14	116.44	112.19
4	M	1	NAG	O4-C4-C3	-3.05	103.29	110.35
4	K	1	NAG	C1-O5-C5	2.96	116.20	112.19
4	G	1	NAG	C1-C2-N2	-2.95	105.45	110.49
4	R	1	NAG	O5-C5-C6	-2.82	102.78	107.20
4	M	2	NAG	C1-C2-N2	-2.65	105.97	110.49
4	F	1	NAG	O5-C1-C2	-2.63	107.14	111.29
4	O	2	NAG	C1-O5-C5	2.62	115.75	112.19
4	O	1	NAG	C1-O5-C5	2.58	115.68	112.19
4	M	2	NAG	C1-O5-C5	2.51	115.60	112.19
4	G	1	NAG	C2-N2-C7	2.51	126.48	122.90
4	M	2	NAG	C2-N2-C7	2.36	126.27	122.90
4	R	1	NAG	O5-C1-C2	2.31	114.93	111.29
4	E	1	NAG	C1-O5-C5	2.18	115.15	112.19
4	R	2	NAG	C2-N2-C7	2.09	125.87	122.90
4	R	2	NAG	C4-C3-C2	-2.06	108.00	111.02
4	P	1	NAG	O4-C4-C3	2.01	114.98	110.35
4	N	1	NAG	C1-O5-C5	2.00	114.90	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	O	2	NAG	C1
4	P	2	NAG	C1
4	Q	2	NAG	C1

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	M	2	NAG	C3-C2-N2-C7
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	N	1	NAG	C1-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
4	J	2	NAG	C1-C2-N2-C7
4	I	1	NAG	C8-C7-N2-C2
4	J	1	NAG	C1-C2-N2-C7
4	P	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C1-C2-N2-C7
4	F	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7

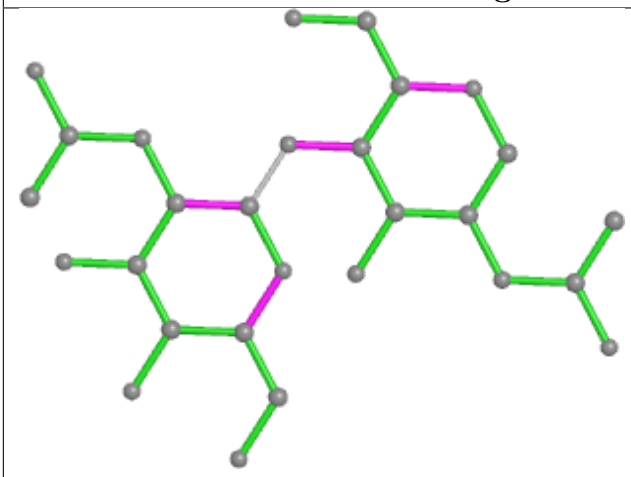
There are no ring outliers.

11 monomers are involved in 16 short contacts:

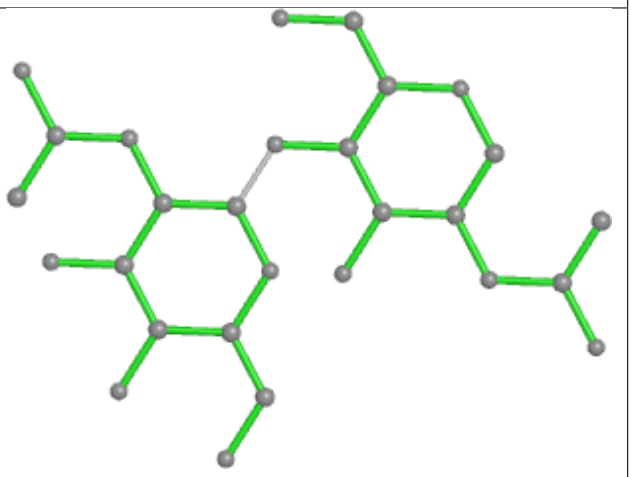
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	1	NAG	2	0
4	N	2	NAG	1	0
4	G	2	NAG	1	0
4	M	1	NAG	2	0
4	N	1	NAG	7	0
4	J	1	NAG	1	0
4	R	1	NAG	1	0
4	K	1	NAG	1	0
4	G	1	NAG	1	0
4	M	2	NAG	2	0
4	I	1	NAG	1	0

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

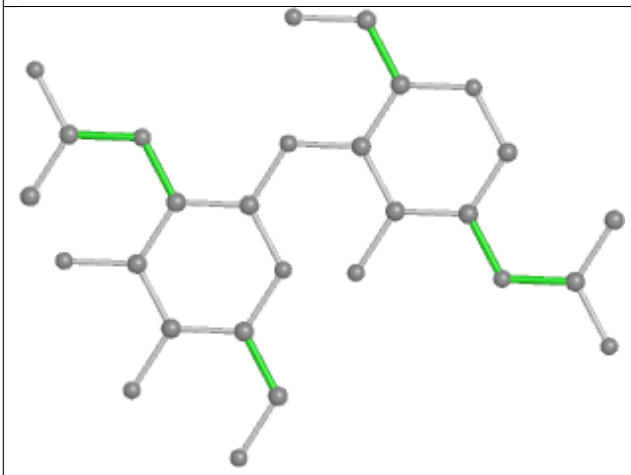
Oligosaccharide Chain D



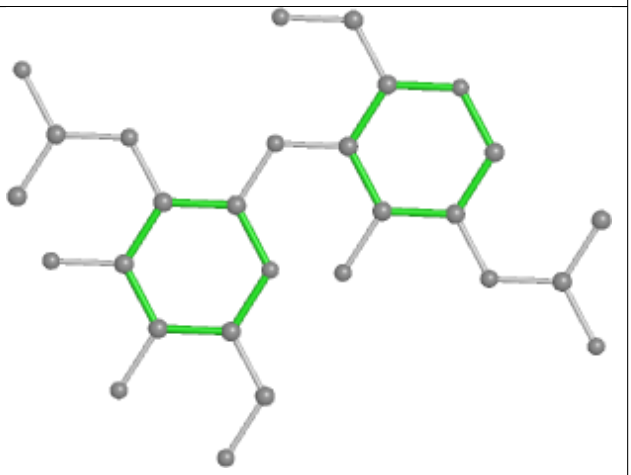
Bond lengths



Bond angles

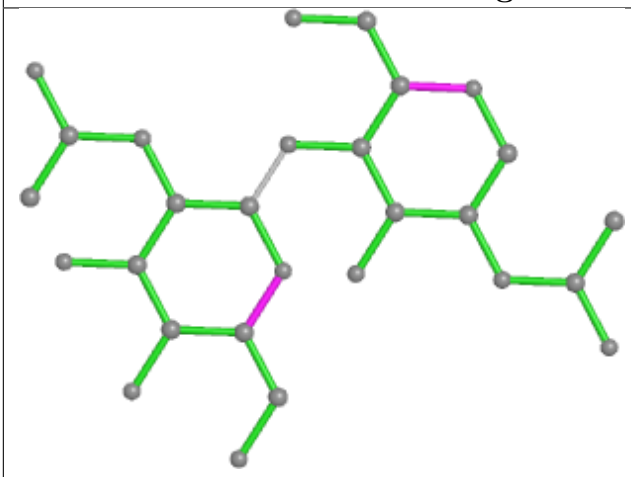


Torsions

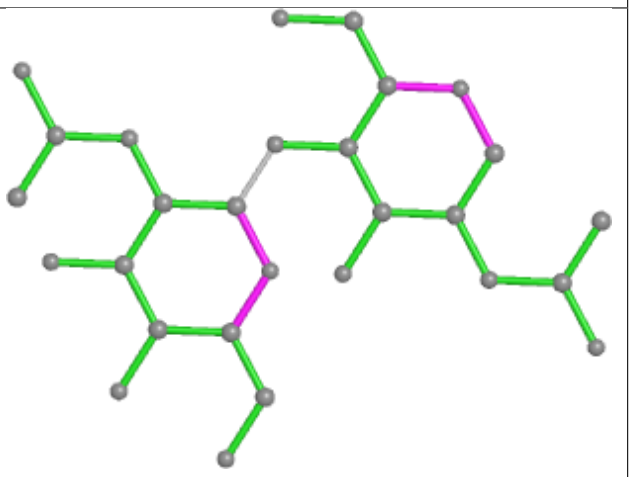


Rings

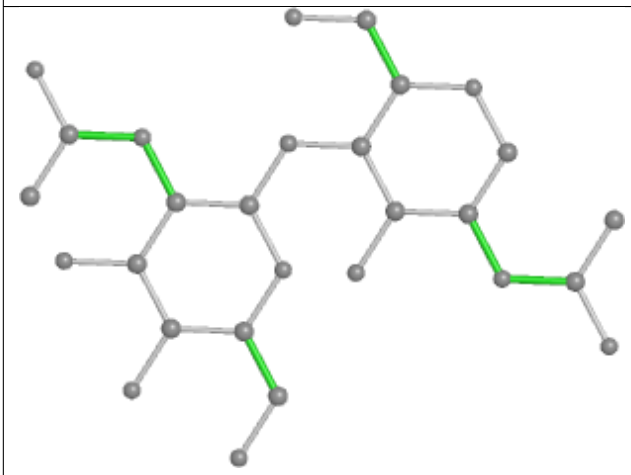
Oligosaccharide Chain E



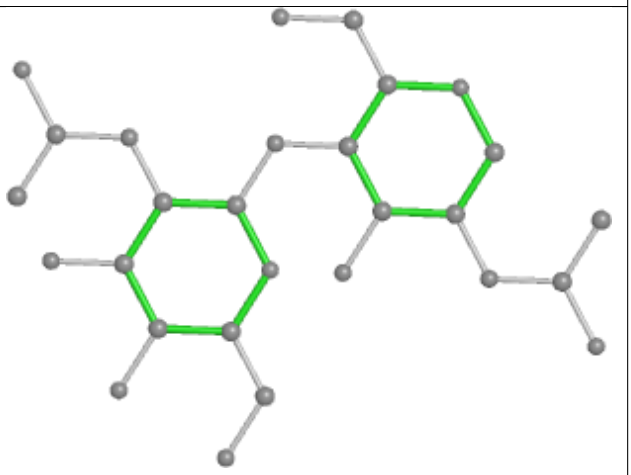
Bond lengths



Bond angles

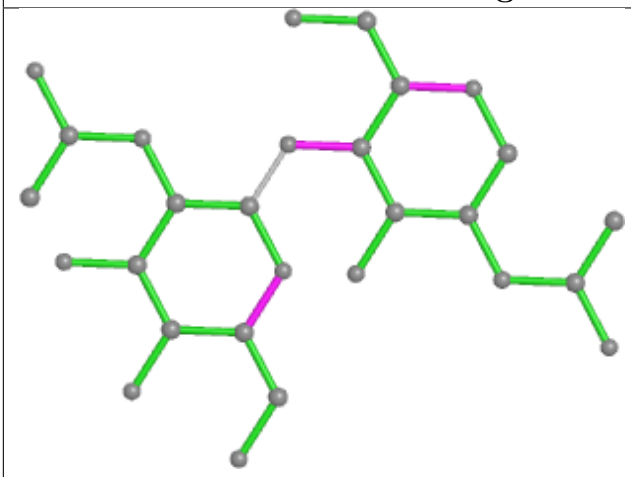


Torsions

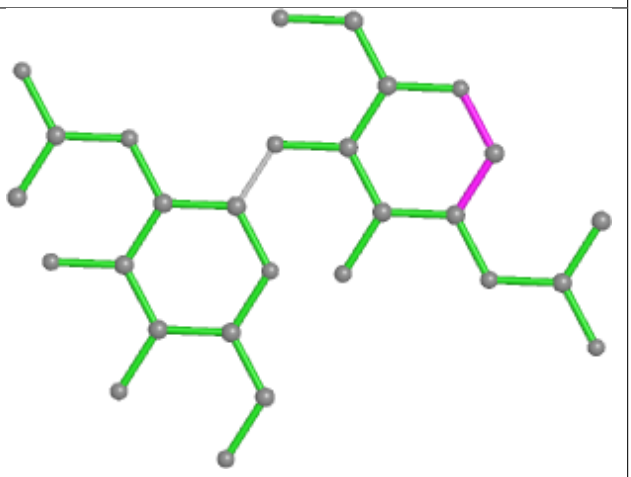


Rings

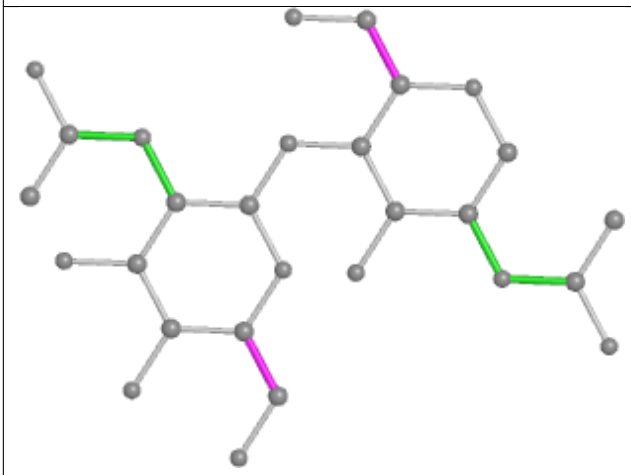
Oligosaccharide Chain F



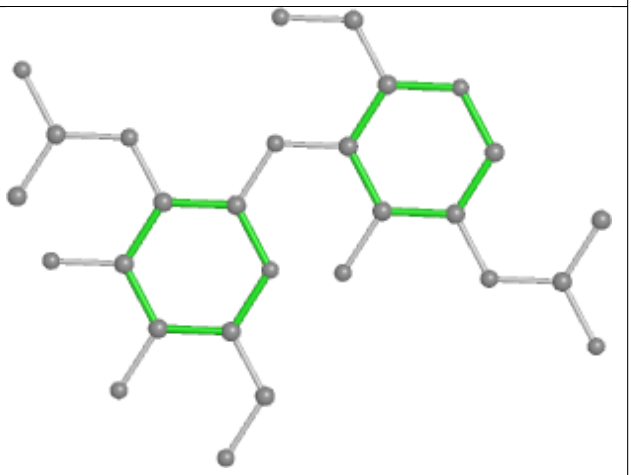
Bond lengths



Bond angles

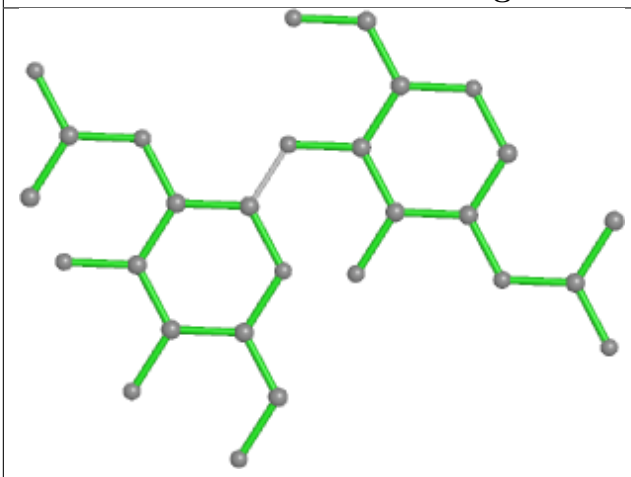


Torsions

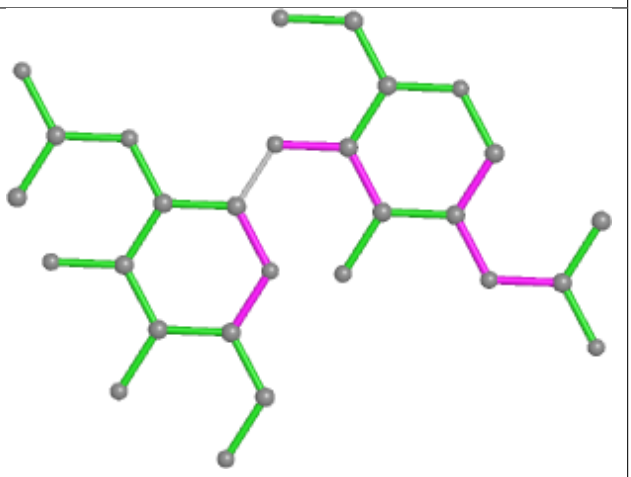


Rings

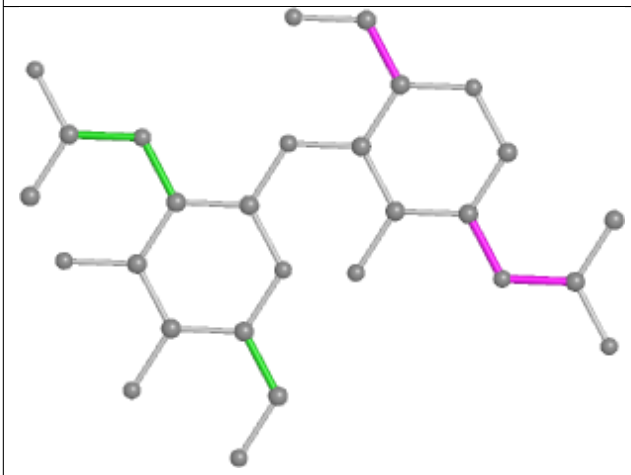
Oligosaccharide Chain G



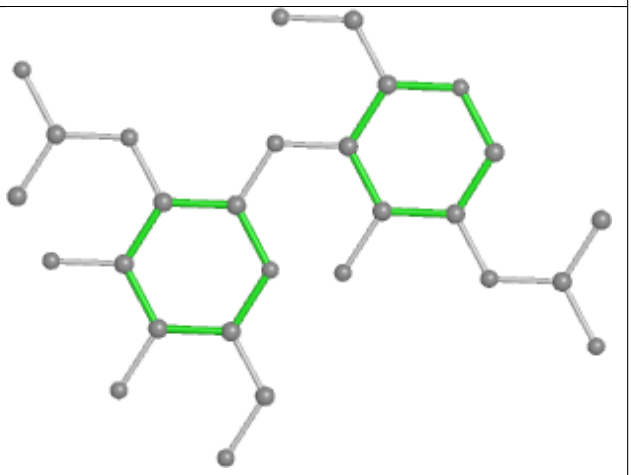
Bond lengths



Bond angles

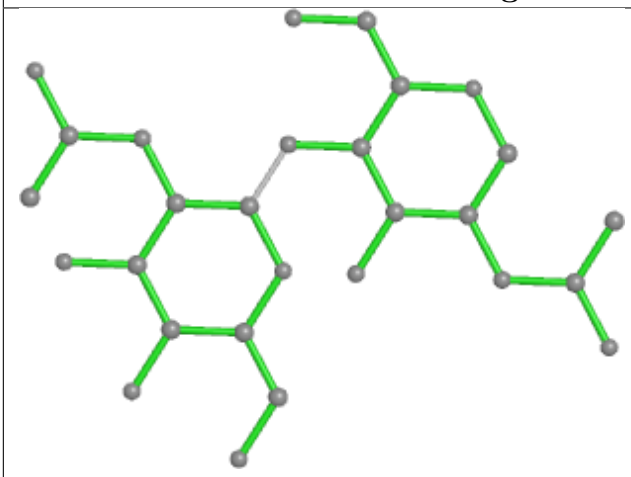


Torsions

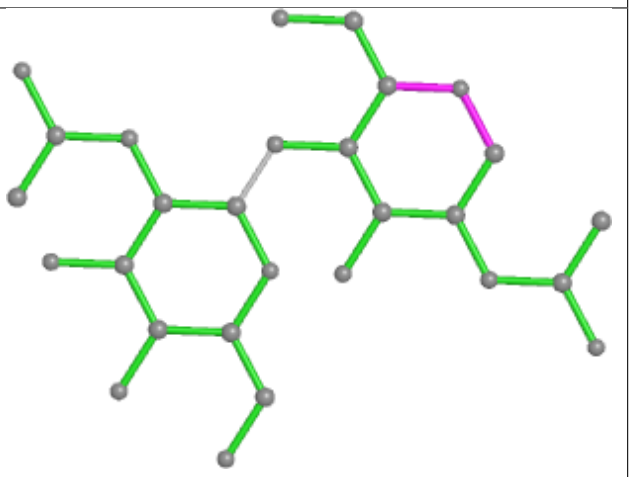


Rings

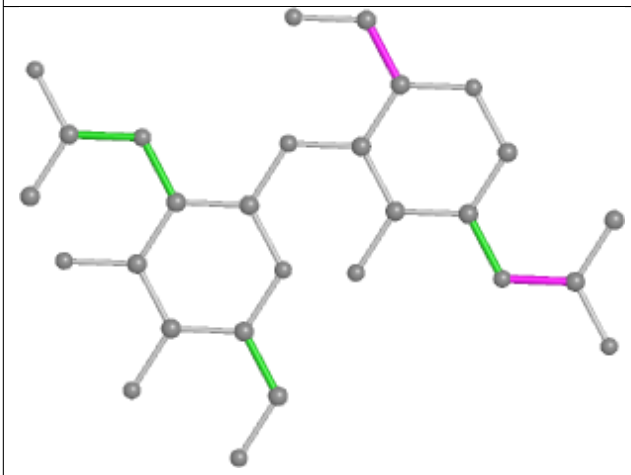
Oligosaccharide Chain I



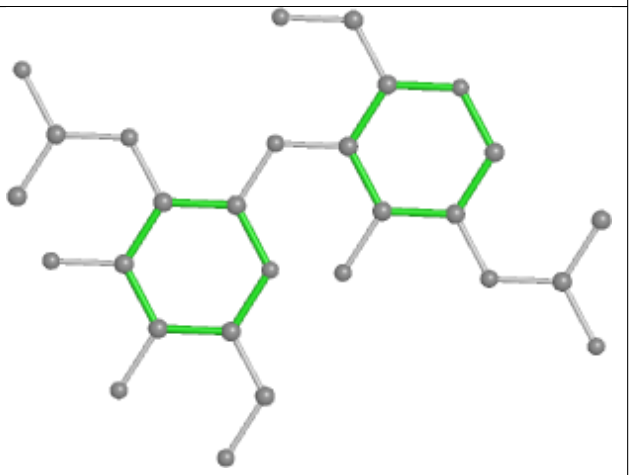
Bond lengths



Bond angles

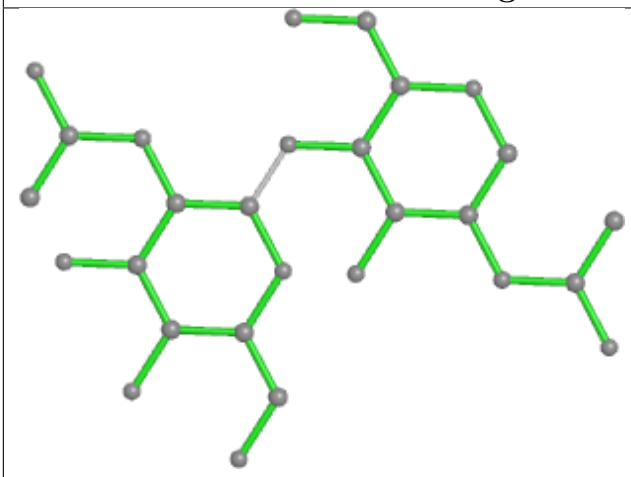


Torsions

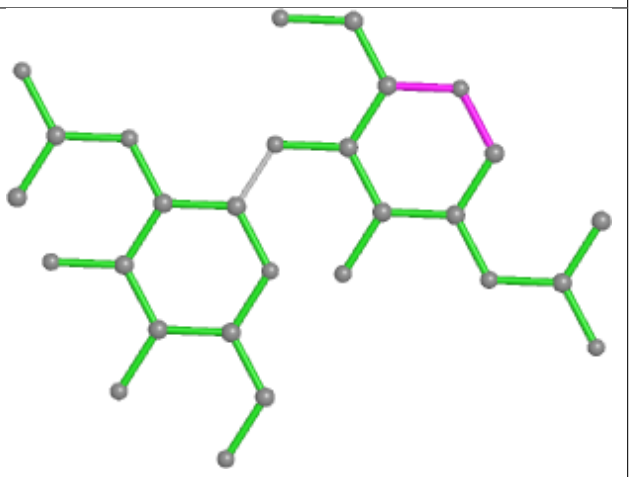


Rings

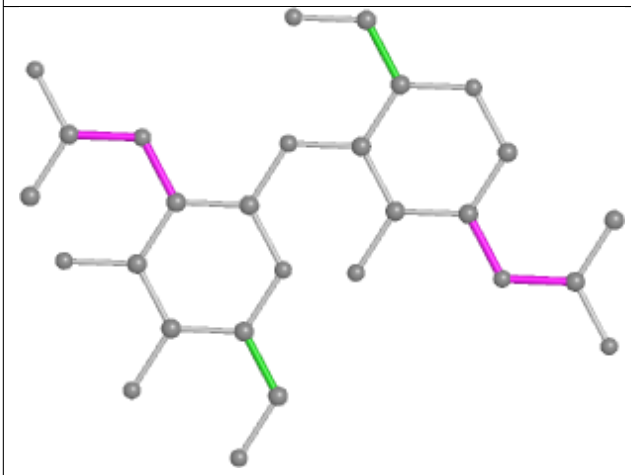
Oligosaccharide Chain J



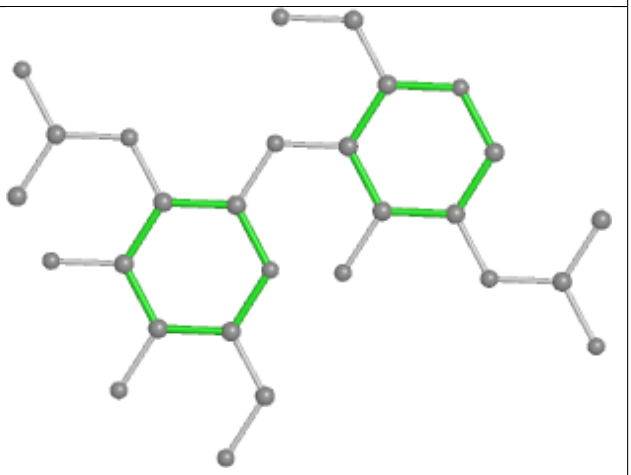
Bond lengths



Bond angles

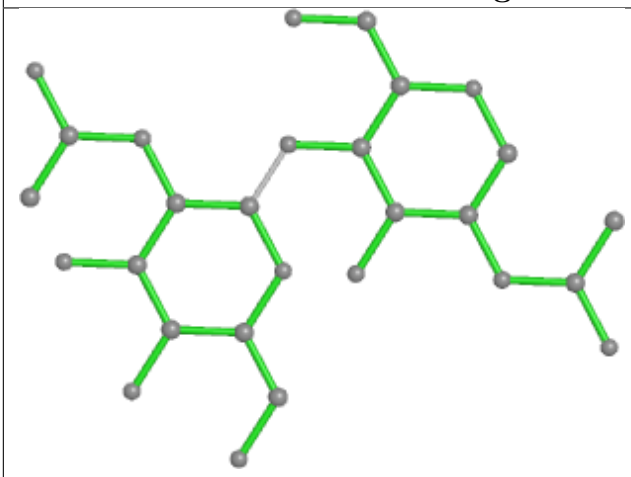


Torsions

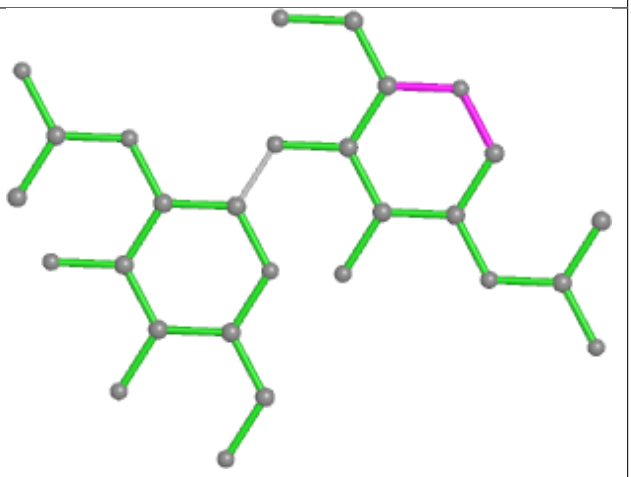


Rings

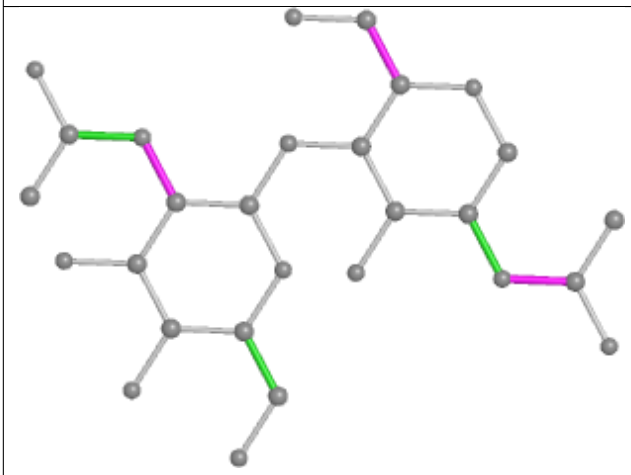
Oligosaccharide Chain K



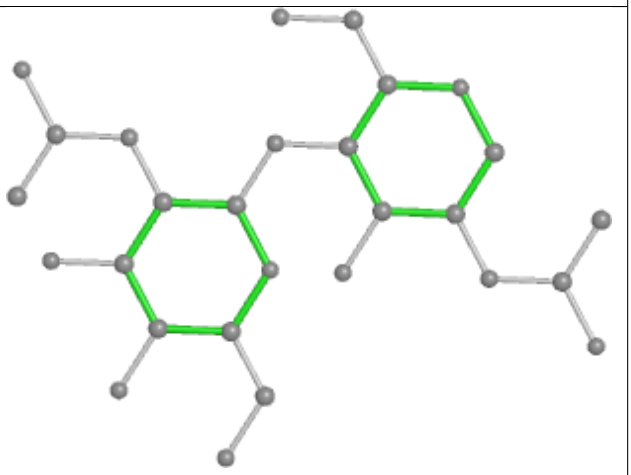
Bond lengths



Bond angles

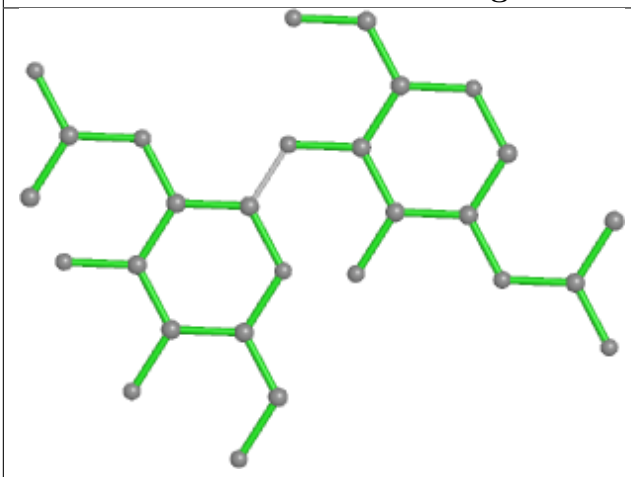


Torsions

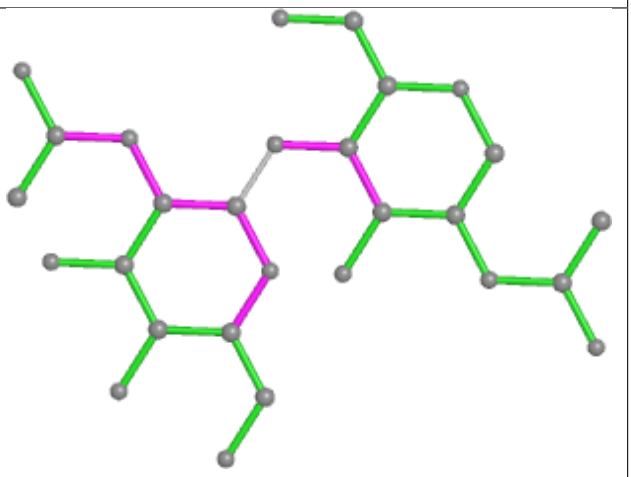


Rings

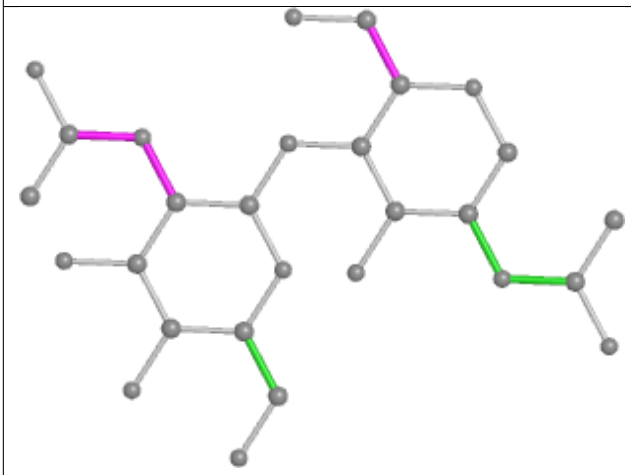
Oligosaccharide Chain M



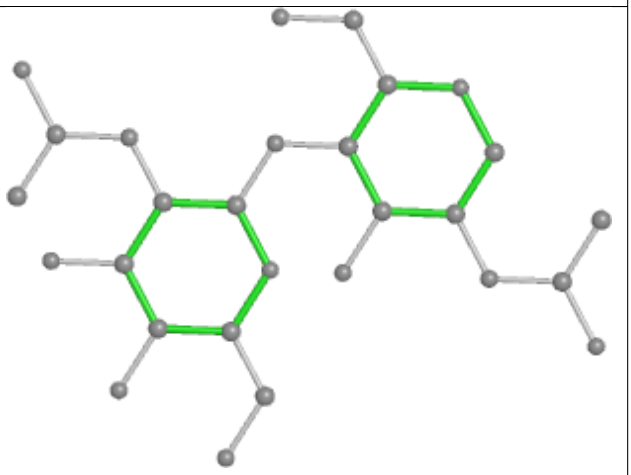
Bond lengths



Bond angles

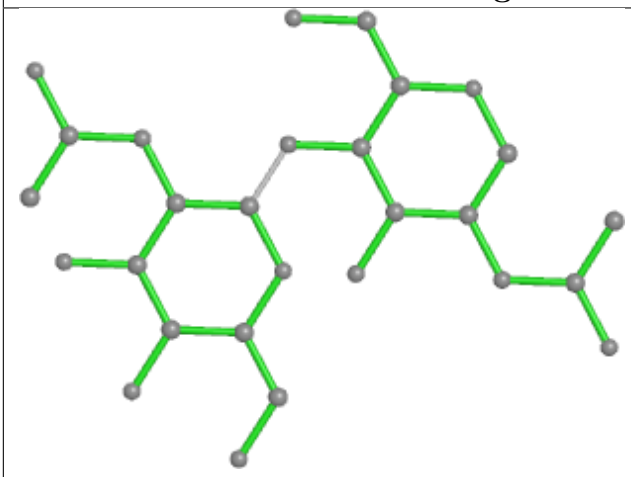


Torsions

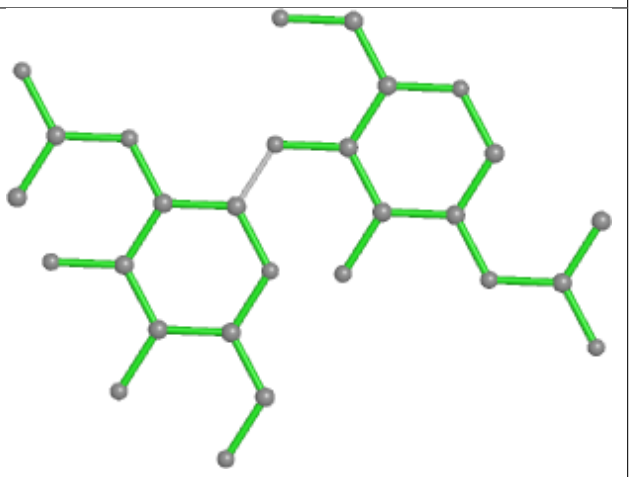


Rings

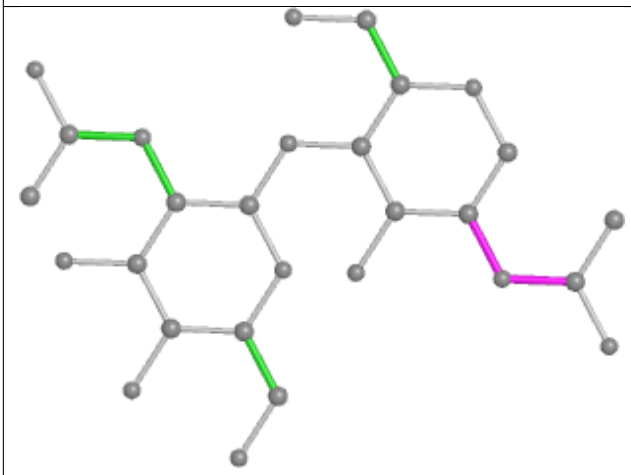
Oligosaccharide Chain N



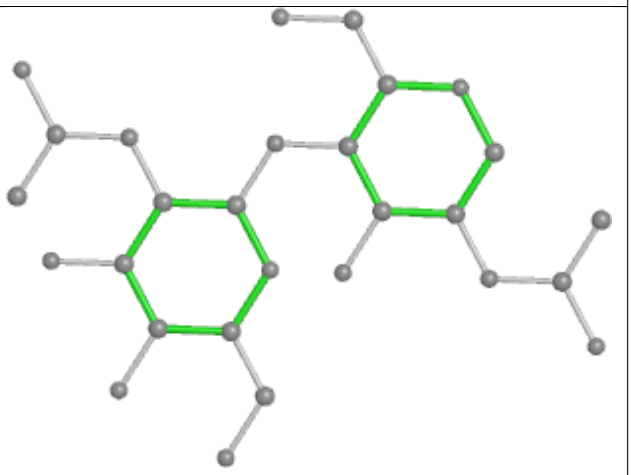
Bond lengths



Bond angles

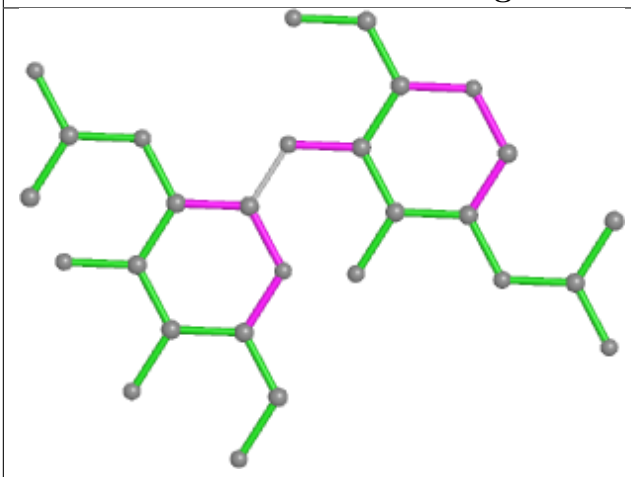


Torsions

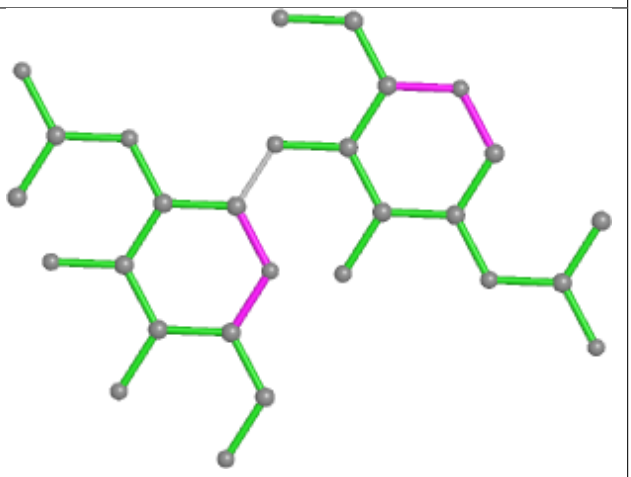


Rings

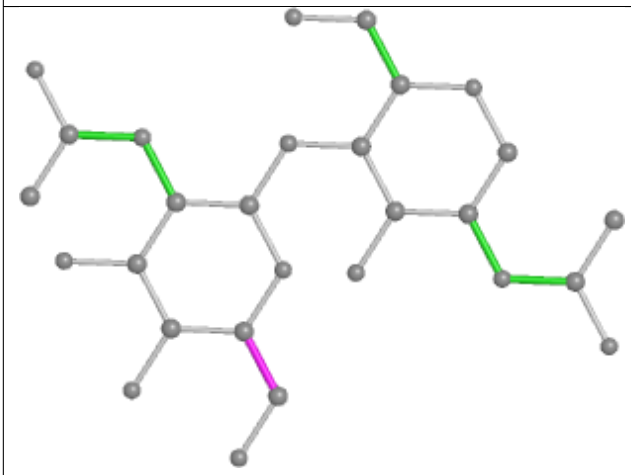
Oligosaccharide Chain O



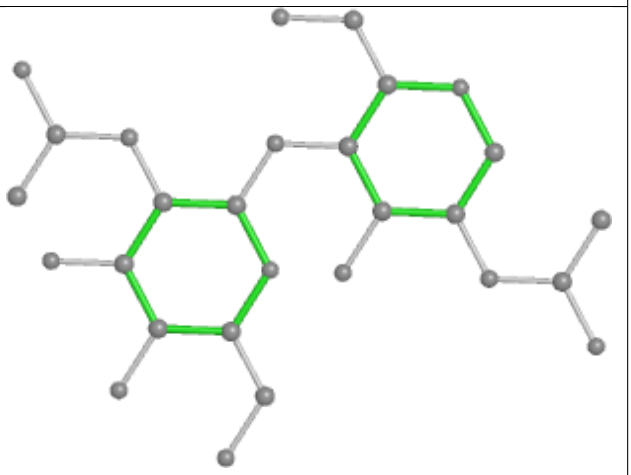
Bond lengths



Bond angles

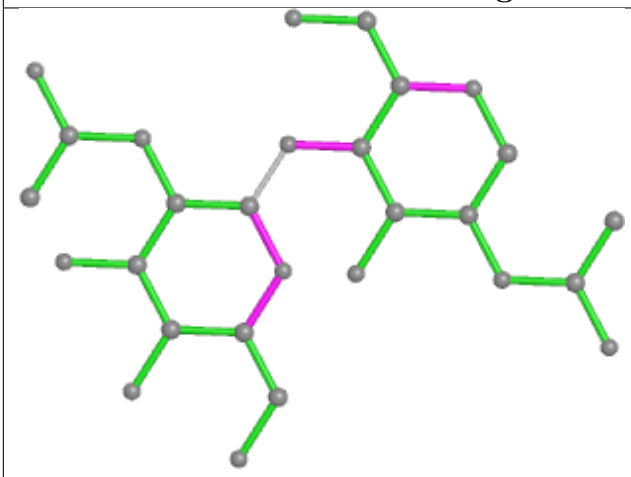


Torsions

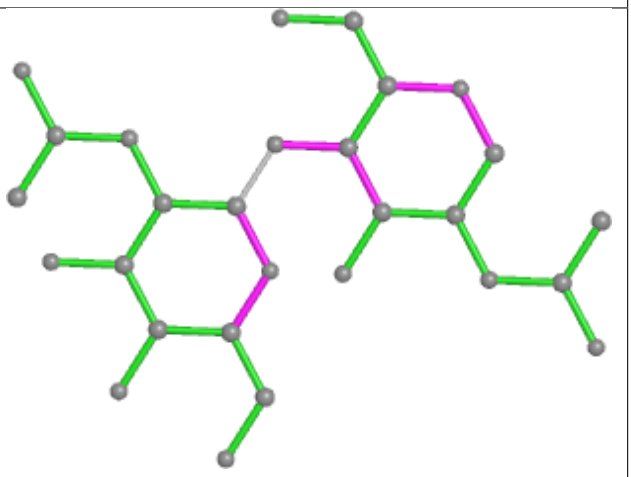


Rings

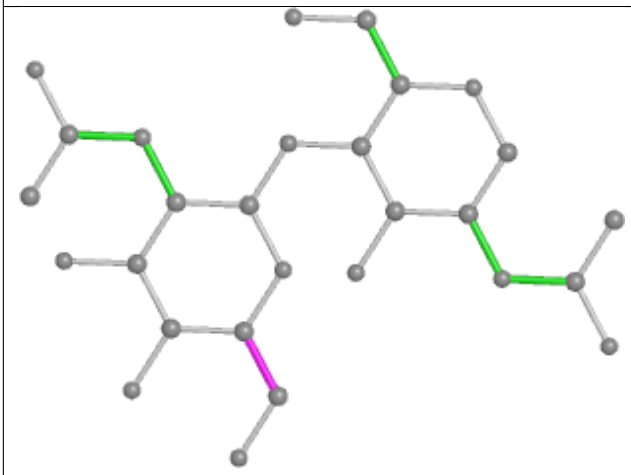
Oligosaccharide Chain P



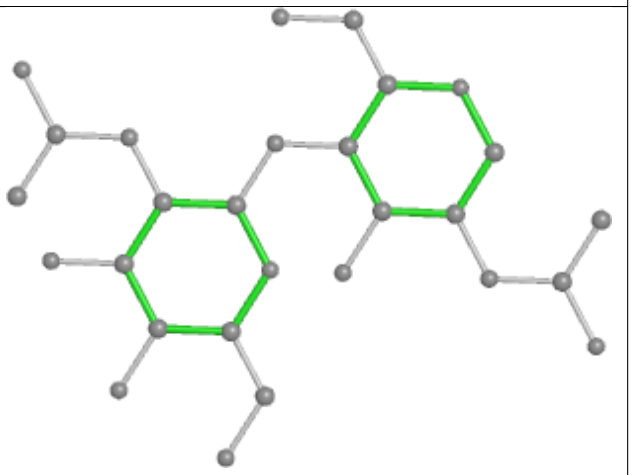
Bond lengths



Bond angles

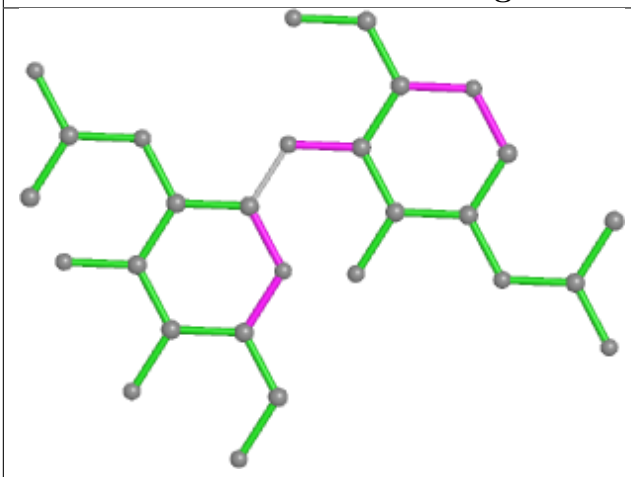


Torsions

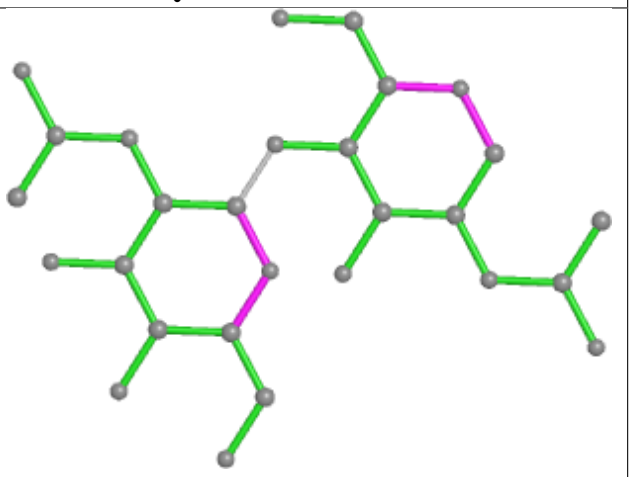


Rings

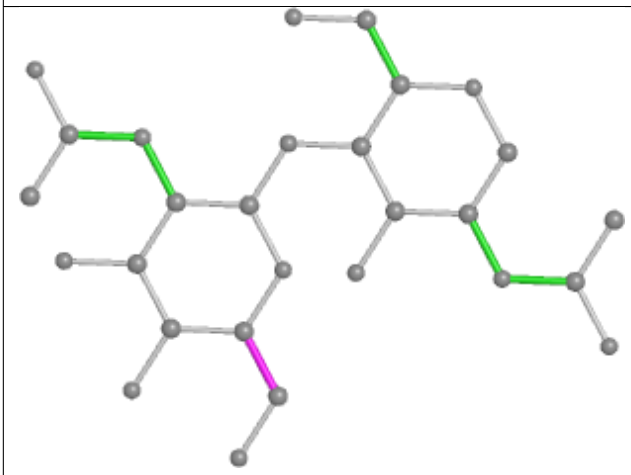
Oligosaccharide Chain Q



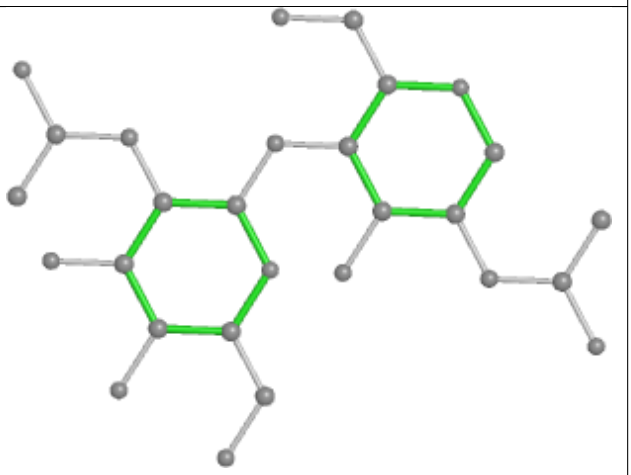
Bond lengths



Bond angles

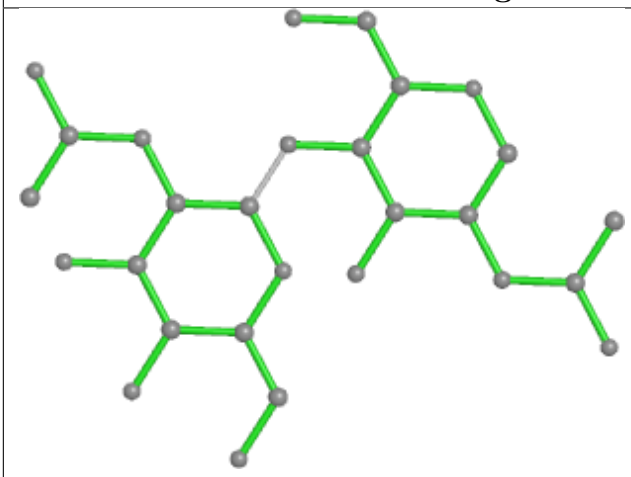


Torsions

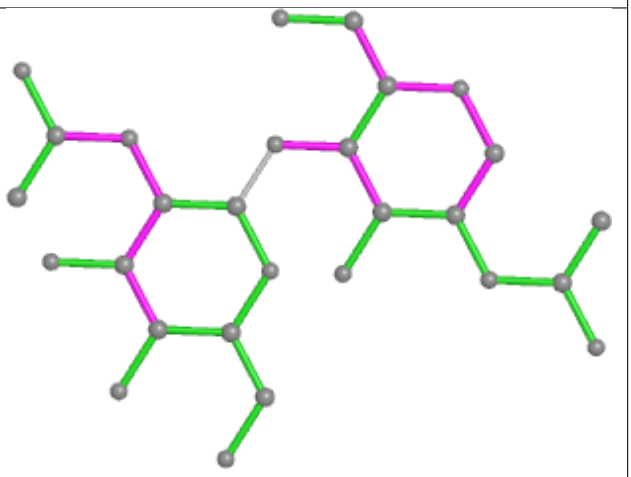


Rings

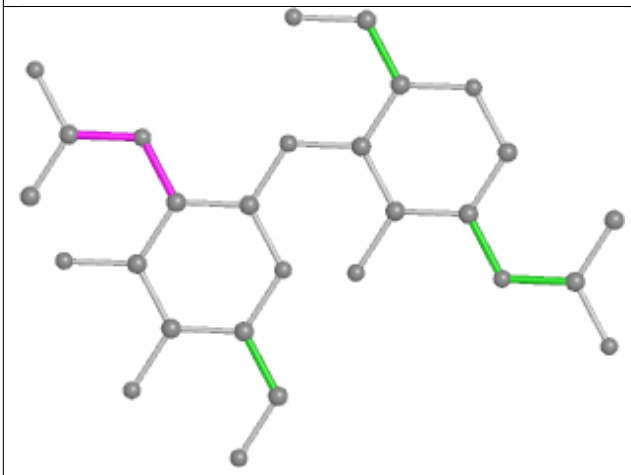
Oligosaccharide Chain R



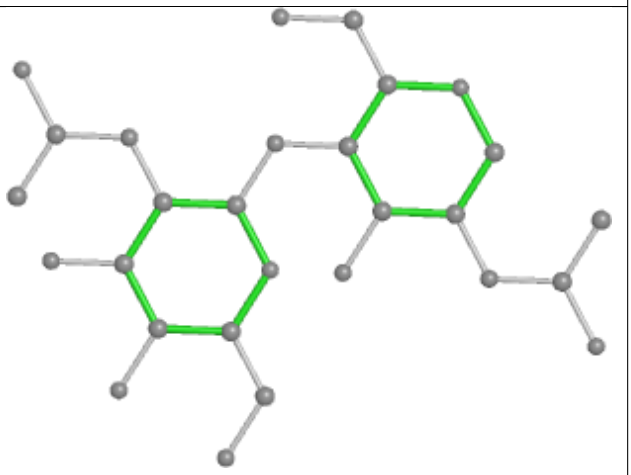
Bond lengths



Bond angles

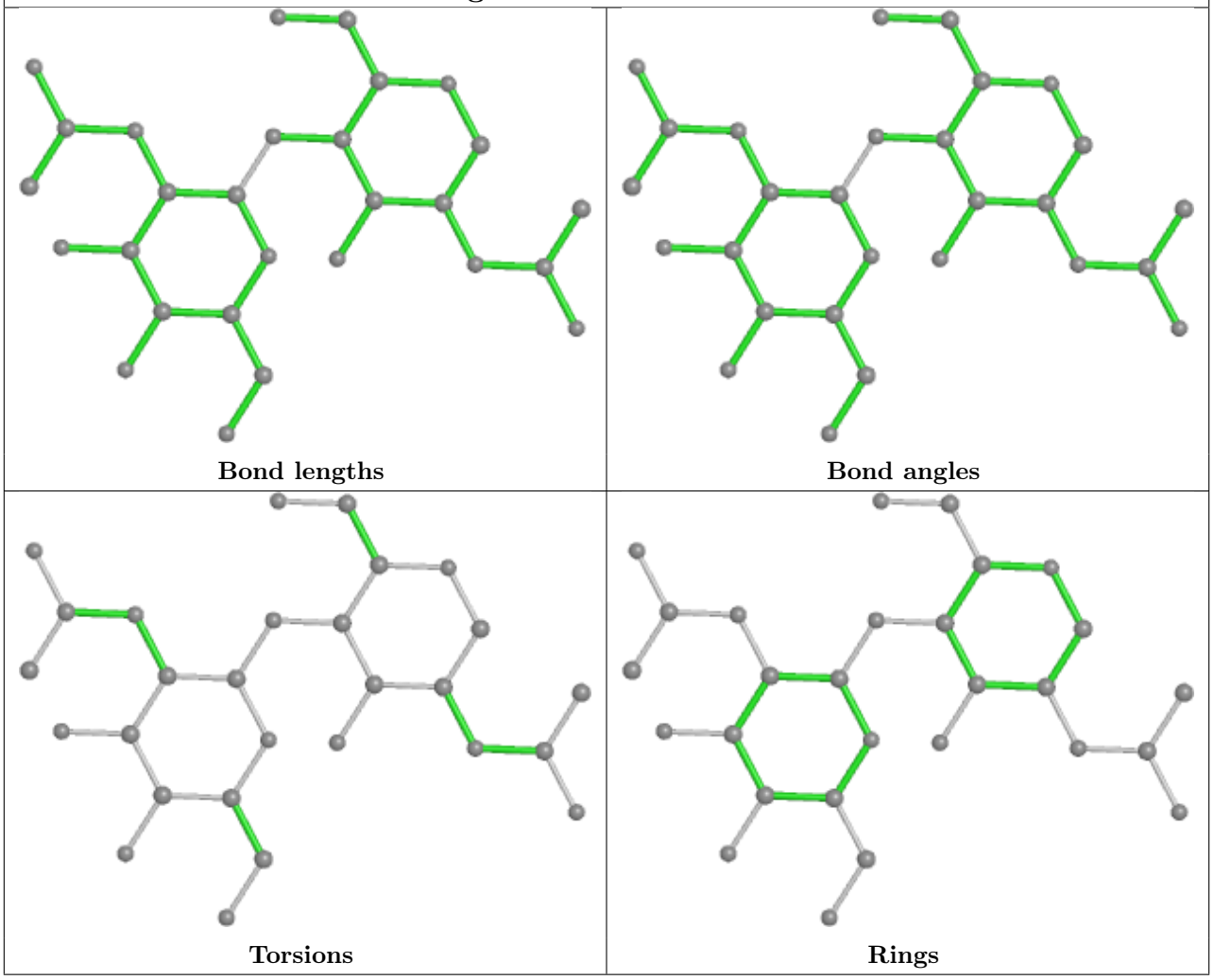


Torsions



Rings

Oligosaccharide Chain U



5.6 Ligand geometry (i)

31 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	$\#\|Z\| > 2$
5	NAG	C	1305	3	14,14,15	1.25	2 (14%)	17,19,21	0.95	1 (5%)
5	NAG	B	1207	3	14,14,15	1.28	3 (21%)	17,19,21	0.64	0
5	NAG	A	1311	3	14,14,15	1.26	2 (14%)	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	C	1311	3	14,14,15	1.16	1 (7%)	17,19,21	0.69	0
5	NAG	B	1204	3	14,14,15	1.15	1 (7%)	17,19,21	0.93	0
5	NAG	A	1304	3	14,14,15	1.26	2 (14%)	17,19,21	1.02	1 (5%)
5	NAG	C	1306	3	14,14,15	1.25	2 (14%)	17,19,21	0.66	0
5	NAG	A	1301	3	14,14,15	1.18	2 (14%)	17,19,21	1.03	1 (5%)
5	NAG	B	1205	3	14,14,15	1.31	3 (21%)	17,19,21	1.06	1 (5%)
5	NAG	A	1303	3	14,14,15	1.35	3 (21%)	17,19,21	1.15	1 (5%)
5	NAG	A	1309	3	14,14,15	1.13	1 (7%)	17,19,21	0.62	0
5	NAG	B	1201	3	14,14,15	1.15	1 (7%)	17,19,21	0.75	0
5	NAG	A	1305	3	14,14,15	1.27	1 (7%)	17,19,21	0.82	1 (5%)
5	NAG	C	1309	3	14,14,15	1.23	2 (14%)	17,19,21	0.75	1 (5%)
5	NAG	C	1308	3	14,14,15	1.23	2 (14%)	17,19,21	0.85	1 (5%)
5	NAG	A	1310	3	14,14,15	0.99	0	17,19,21	0.84	1 (5%)
5	NAG	B	1203	3	14,14,15	1.27	2 (14%)	17,19,21	0.96	0
5	NAG	B	1202	3	14,14,15	1.33	4 (28%)	17,19,21	1.15	1 (5%)
5	NAG	C	1302	3	14,14,15	1.24	3 (21%)	17,19,21	0.88	0
5	NAG	C	1310	3	14,14,15	1.10	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	B	1208	3	14,14,15	1.30	3 (21%)	17,19,21	1.26	1 (5%)
5	NAG	B	1209	3	14,14,15	1.16	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	C	1301	3	14,14,15	1.04	1 (7%)	17,19,21	0.85	1 (5%)
5	NAG	B	1206	3	14,14,15	1.20	2 (14%)	17,19,21	0.92	1 (5%)
5	NAG	A	1307	3	14,14,15	1.22	1 (7%)	17,19,21	0.70	0
5	NAG	C	1304	3	14,14,15	1.26	2 (14%)	17,19,21	1.11	1 (5%)
5	NAG	C	1303	3	14,14,15	1.23	1 (7%)	17,19,21	0.89	1 (5%)
5	NAG	C	1307	3	14,14,15	1.14	1 (7%)	17,19,21	0.73	0
5	NAG	A	1308	3	14,14,15	1.28	2 (14%)	17,19,21	1.17	2 (11%)
5	NAG	A	1306	3	14,14,15	1.27	3 (21%)	17,19,21	0.75	0
5	NAG	A	1302	3	14,14,15	1.33	3 (21%)	17,19,21	1.07	1 (5%)

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
5	NAG	C	1305	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1207	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1311	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1311	3	-	1/6/23/26	0/1/1/1
5	NAG	B	1204	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	3	-	1/6/23/26	0/1/1/1
5	NAG	B	1205	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	3	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1201	3	-	1/6/23/26	0/1/1/1
5	NAG	A	1305	3	-	1/6/23/26	0/1/1/1
5	NAG	C	1309	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1308	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1310	3	-	1/6/23/26	0/1/1/1
5	NAG	B	1203	3	-	1/6/23/26	0/1/1/1
5	NAG	B	1202	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	3	-	4/6/23/26	0/1/1/1
5	NAG	C	1310	3	-	1/6/23/26	0/1/1/1
5	NAG	B	1208	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1209	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1206	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1303	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1307	3	-	1/6/23/26	0/1/1/1
5	NAG	A	1308	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	3	-	1/6/23/26	0/1/1/1
5	NAG	A	1302	3	-	2/6/23/26	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1308	NAG	O5-C5	3.05	1.49	1.43
5	A	1303	NAG	O5-C5	2.85	1.49	1.43
5	B	1205	NAG	O5-C5	2.81	1.49	1.43
5	C	1303	NAG	O5-C5	2.79	1.49	1.43
5	B	1208	NAG	O5-C5	2.79	1.49	1.43
5	C	1308	NAG	O5-C5	2.78	1.49	1.43
5	C	1305	NAG	O5-C5	2.76	1.49	1.43
5	A	1311	NAG	O5-C5	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1304	NAG	O5-C5	2.70	1.48	1.43
5	B	1201	NAG	O5-C5	2.70	1.48	1.43
5	B	1202	NAG	O5-C5	2.70	1.48	1.43
5	A	1302	NAG	O5-C5	2.65	1.48	1.43
5	B	1207	NAG	O5-C5	2.62	1.48	1.43
5	C	1307	NAG	O5-C5	2.62	1.48	1.43
5	A	1304	NAG	O5-C5	2.60	1.48	1.43
5	A	1306	NAG	O5-C5	2.60	1.48	1.43
5	C	1302	NAG	O5-C5	2.57	1.48	1.43
5	B	1208	NAG	O5-C1	2.53	1.47	1.43
5	A	1307	NAG	O5-C5	2.52	1.48	1.43
5	B	1203	NAG	O5-C5	2.51	1.48	1.43
5	A	1305	NAG	O5-C5	2.49	1.48	1.43
5	A	1302	NAG	C1-C2	2.46	1.56	1.52
5	B	1206	NAG	O5-C5	2.46	1.48	1.43
5	A	1303	NAG	C1-C2	2.41	1.55	1.52
5	C	1306	NAG	O5-C5	2.41	1.48	1.43
5	B	1209	NAG	O5-C5	2.38	1.48	1.43
5	A	1301	NAG	O5-C5	2.37	1.48	1.43
5	B	1203	NAG	C1-C2	2.36	1.55	1.52
5	C	1309	NAG	C1-C2	2.34	1.55	1.52
5	C	1304	NAG	C1-C2	2.32	1.55	1.52
5	B	1207	NAG	C1-C2	2.31	1.55	1.52
5	A	1309	NAG	O5-C5	2.28	1.48	1.43
5	A	1304	NAG	C1-C2	2.26	1.55	1.52
5	C	1309	NAG	O5-C5	2.25	1.48	1.43
5	C	1311	NAG	O5-C5	2.25	1.48	1.43
5	C	1302	NAG	C1-C2	2.22	1.55	1.52
5	B	1202	NAG	O5-C1	2.21	1.47	1.43
5	B	1206	NAG	C1-C2	2.18	1.55	1.52
5	A	1302	NAG	O5-C1	2.18	1.47	1.43
5	B	1205	NAG	C1-C2	2.16	1.55	1.52
5	B	1205	NAG	O5-C1	2.15	1.47	1.43
5	B	1204	NAG	O5-C5	2.11	1.47	1.43
5	C	1302	NAG	O5-C1	2.10	1.47	1.43
5	A	1306	NAG	O5-C1	2.10	1.47	1.43
5	A	1303	NAG	O5-C1	2.08	1.47	1.43
5	C	1301	NAG	O5-C5	2.07	1.47	1.43
5	C	1305	NAG	O5-C1	2.07	1.47	1.43
5	C	1308	NAG	C1-C2	2.07	1.55	1.52
5	A	1311	NAG	O5-C1	2.06	1.47	1.43
5	A	1301	NAG	C1-C2	2.05	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1306	NAG	O5-C1	2.05	1.47	1.43
5	C	1310	NAG	O5-C5	2.04	1.47	1.43
5	B	1208	NAG	C1-C2	2.03	1.55	1.52
5	B	1202	NAG	C1-C2	2.02	1.55	1.52
5	A	1306	NAG	C1-C2	2.02	1.55	1.52
5	B	1202	NAG	C8-C7	2.01	1.54	1.50
5	B	1207	NAG	C8-C7	2.01	1.54	1.50
5	A	1308	NAG	C1-C2	2.00	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1208	NAG	C1-O5-C5	4.63	118.47	112.19
5	B	1202	NAG	C1-O5-C5	4.10	117.75	112.19
5	C	1304	NAG	C1-O5-C5	4.02	117.64	112.19
5	A	1303	NAG	C1-O5-C5	3.72	117.24	112.19
5	B	1209	NAG	C1-O5-C5	3.63	117.12	112.19
5	A	1301	NAG	C1-O5-C5	3.45	116.86	112.19
5	A	1302	NAG	C1-O5-C5	3.25	116.59	112.19
5	C	1305	NAG	C1-O5-C5	3.04	116.31	112.19
5	C	1310	NAG	C1-O5-C5	2.97	116.21	112.19
5	B	1205	NAG	C1-O5-C5	2.79	115.97	112.19
5	A	1310	NAG	C1-O5-C5	2.70	115.85	112.19
5	C	1303	NAG	C1-O5-C5	2.64	115.77	112.19
5	C	1308	NAG	C1-O5-C5	2.53	115.63	112.19
5	A	1308	NAG	O5-C1-C2	-2.50	107.34	111.29
5	A	1308	NAG	C1-O5-C5	2.44	115.49	112.19
5	B	1206	NAG	C1-O5-C5	2.40	115.45	112.19
5	C	1309	NAG	C1-O5-C5	2.30	115.30	112.19
5	C	1301	NAG	C1-O5-C5	2.29	115.29	112.19
5	A	1311	NAG	C1-O5-C5	2.09	115.03	112.19
5	A	1305	NAG	C1-O5-C5	2.04	114.95	112.19
5	A	1304	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1302	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	B	1201	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1305	NAG	O5-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	C	1311	NAG	O5-C5-C6-O6
5	A	1310	NAG	O5-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	C	1310	NAG	O5-C5-C6-O6
5	C	1302	NAG	C1-C2-N2-C7
5	A	1302	NAG	C1-C2-N2-C7
5	C	1302	NAG	C4-C5-C6-O6
5	B	1203	NAG	C1-C2-N2-C7
5	A	1302	NAG	C3-C2-N2-C7
5	C	1302	NAG	C3-C2-N2-C7
5	A	1301	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1309	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	796:ASP	C	797:PHE	N	2.12
1	C	806:LEU	C	807:PRO	N	1.71
1	C	800:PHE	C	801:ASN	N	1.14
1	C	1129:VAL	C	1130:ILE	N	0.97
1	C	801:ASN	C	802:PHE	N	0.87

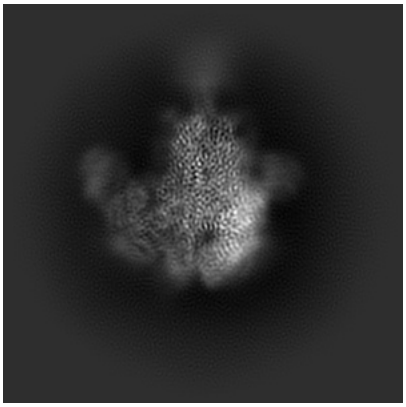
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23248. These allow visual inspection of the internal detail of the map and identification of artifacts.

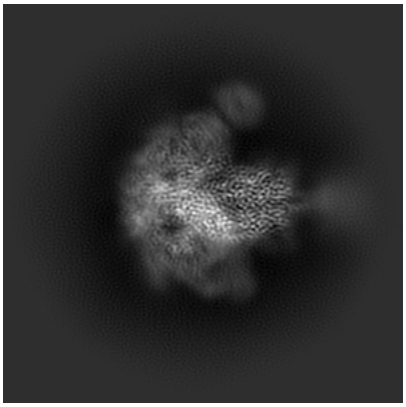
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

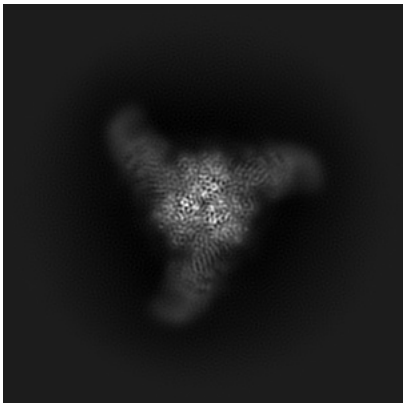
6.1.1 Primary map



X



Y

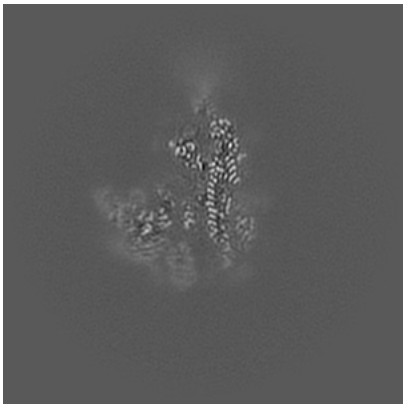


Z

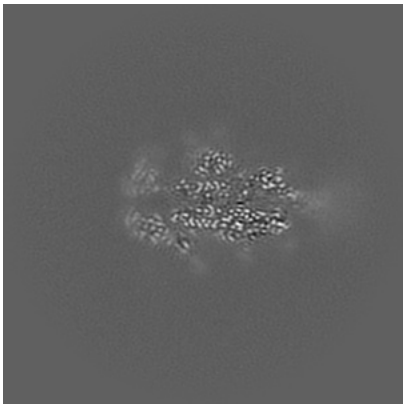
The images above show the map projected in three orthogonal directions.

6.2 Central slices

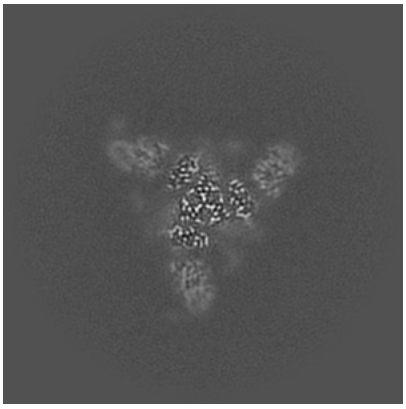
6.2.1 Primary map



X Index: 160



Y Index: 160

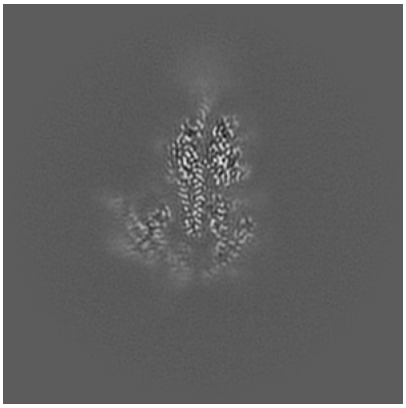


Z Index: 160

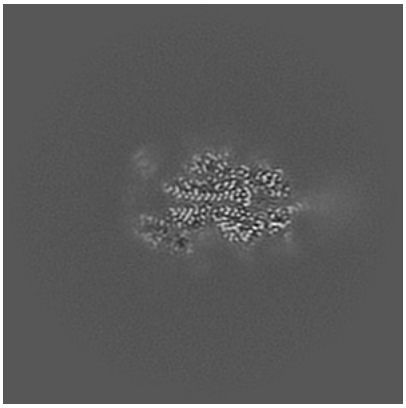
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

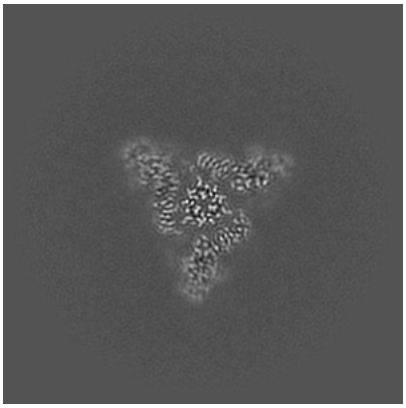
6.3.1 Primary map



X Index: 166



Y Index: 155

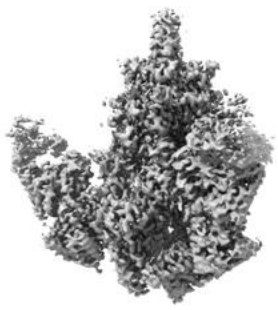


Z Index: 145

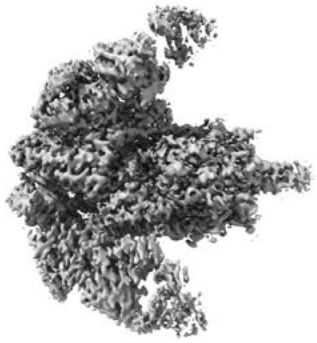
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.274. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

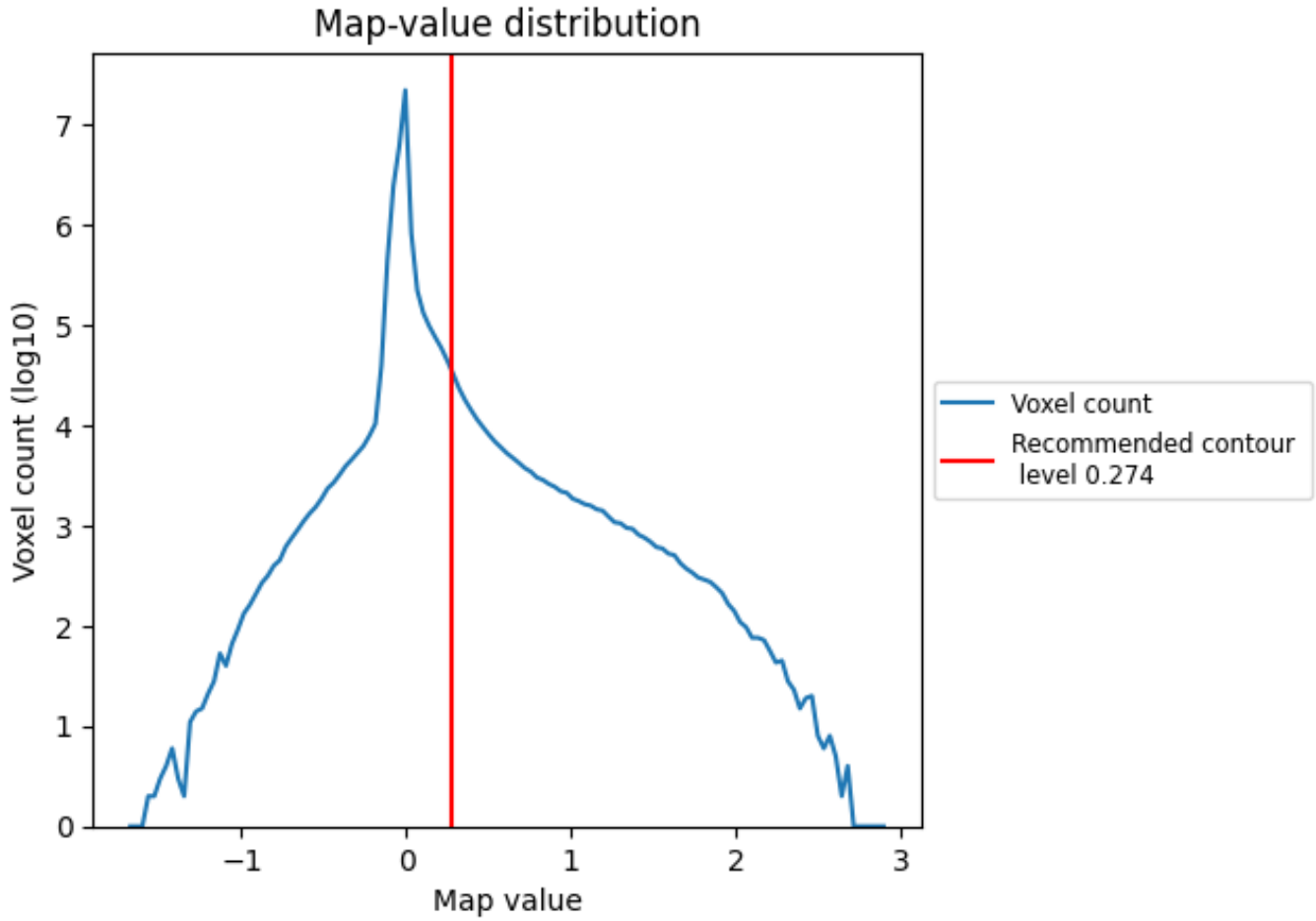
6.5 Mask visualisation (i)

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

7 Map analysis

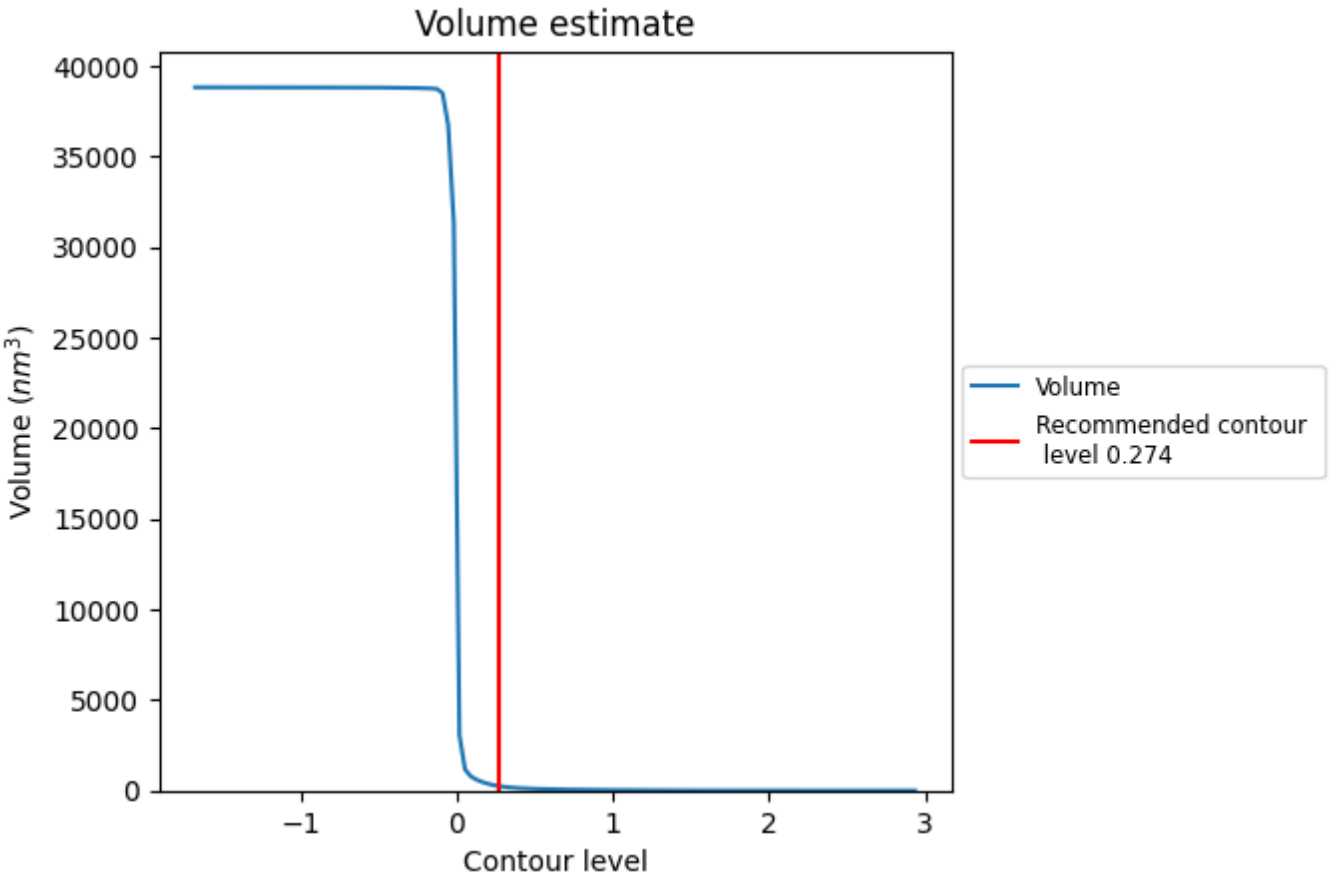
This section contains the results of statistical analysis of the map.

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.

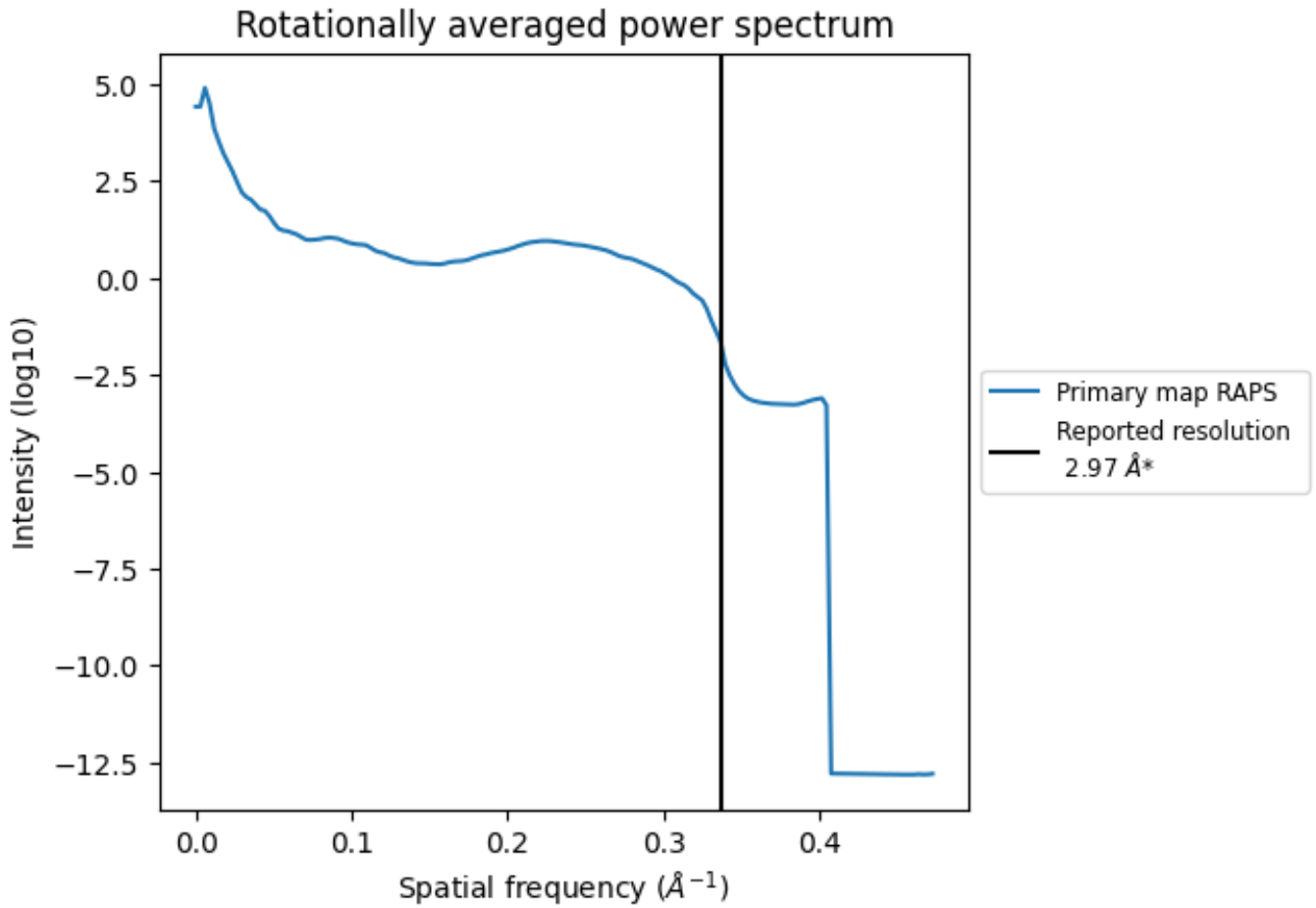
7.2 Volume estimate



The volume at the recommended contour level is 240 nm^3; this corresponds to an approximate mass of 217 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 0.337 Å^{-1}

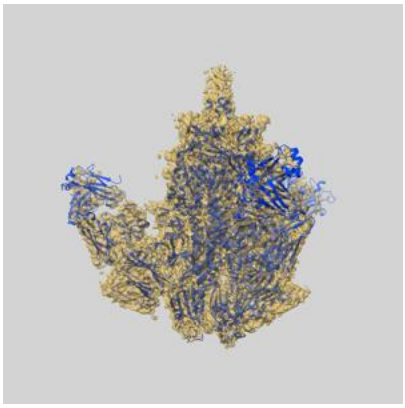
8 Fourier-Shell correlation (i)

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

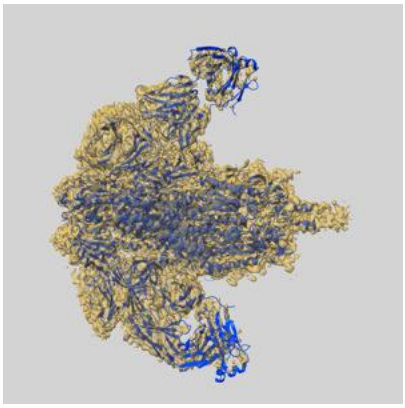
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23248 and PDB model 7LAB. Per-residue inclusion information can be found in section 3 on page 8.

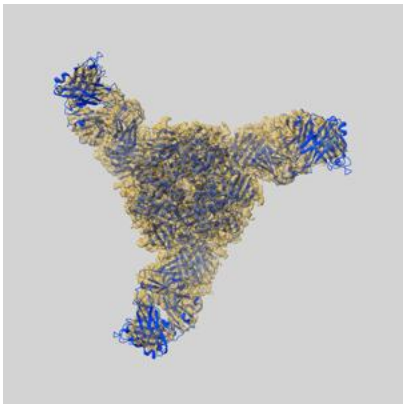
9.1 Map-model overlay



X



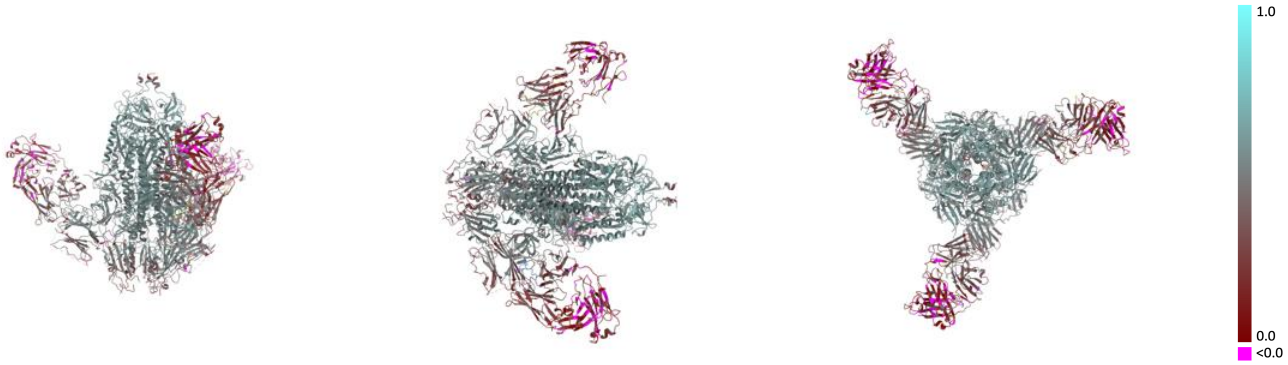
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.274 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.

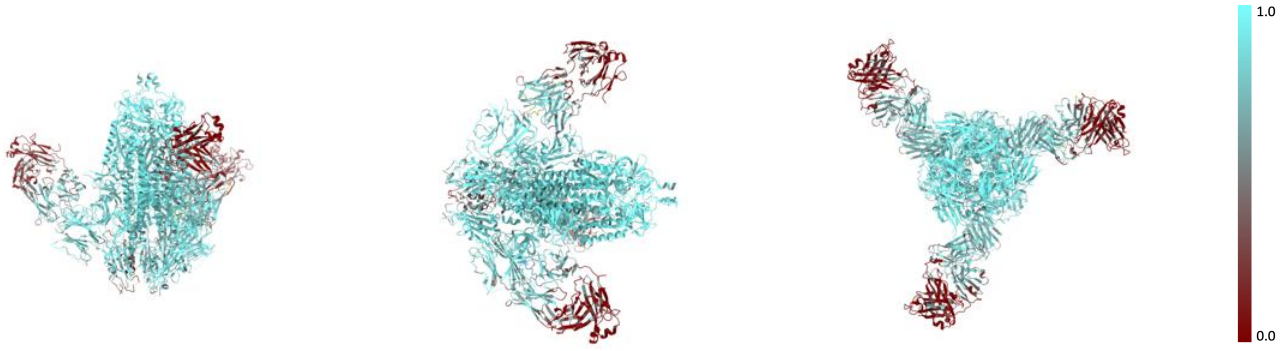
9.2 Q-score mapped to coordinate model (i)



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.

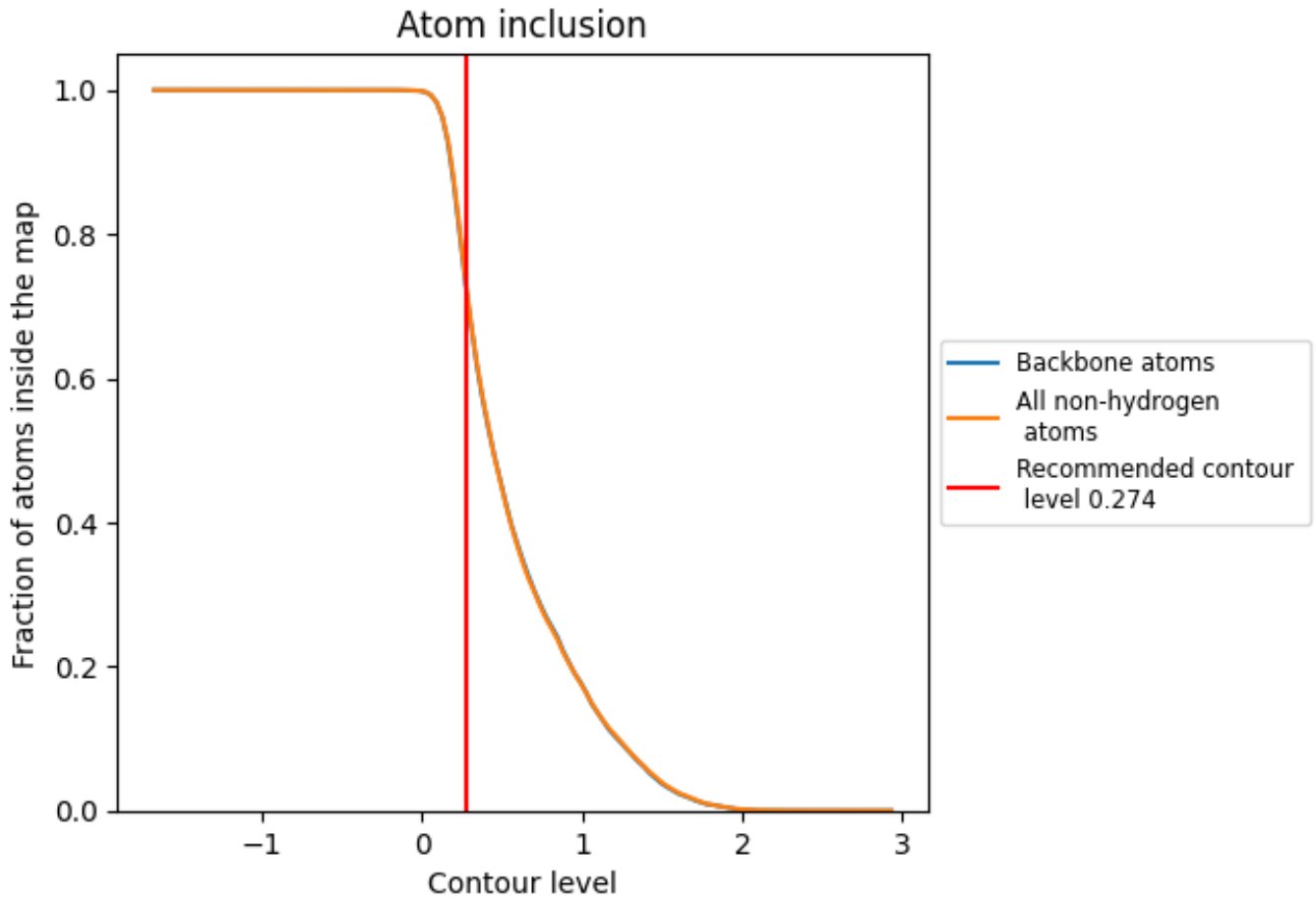
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.274).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.274) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7325	0.4290
A	0.8719	0.5050
B	0.8461	0.5070
C	0.8813	0.5120
D	0.6786	0.4340
E	0.8214	0.4720
F	0.2857	0.4090
G	0.7857	0.4350
H	0.4146	0.2350
I	0.8214	0.4150
J	0.7143	0.3970
K	0.8571	0.3990
L	0.3989	0.2490
M	0.7857	0.4620
N	0.6429	0.4610
O	0.2500	0.3880
P	0.8571	0.5280
Q	0.7500	0.4230
R	0.6429	0.3200
S	0.4163	0.2370
T	0.4068	0.2140
U	0.7857	0.5060
X	0.4123	0.2660
Y	0.4194	0.2370