Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 12:10 PM JST

PDB ID	:	7XTZ
EMDB ID	:	EMD-33453
Title	:	Structure of SARS-CoV-2 Spike Protein with Engineered x3 Disulfide (x3(D427C, V987C) and single Arg S1/S2 cleavage site), Locked-1 Conformation
Authors	:	Qu, K.; Chen, Q.; Ciazynska, K.A.; Liu, B.; Zhang, X.; Wang, J.; He, Y.; Guan, J.; He, J.; Liu, T.; Zhang, X.; Carter, A.P.; Xiong, X.; Briggs, J.A.G.
Deposited on	:	2022-05-18
Resolution	:	2.80 Å(reported)
Based on initial model	:	6ZP2

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:

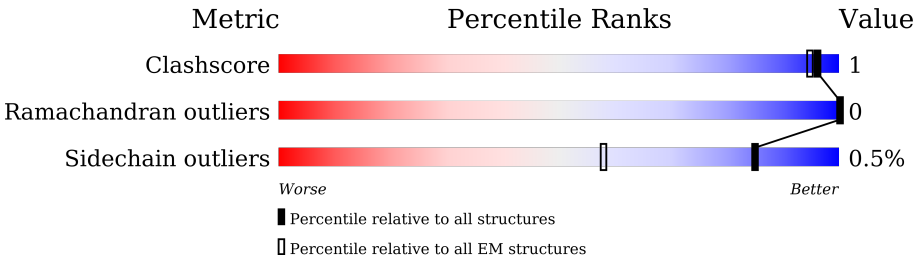
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1128	95%
1	B	1128	95%
1	C	1128	95%
2	D	2	100%
2	E	2	50% 100%
2	F	2	50% 100%
2	G	2	100%

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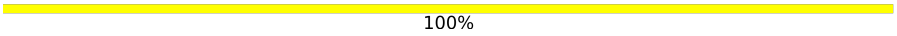
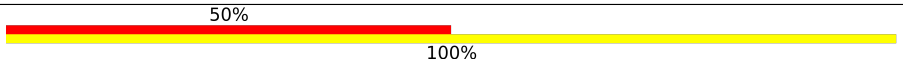
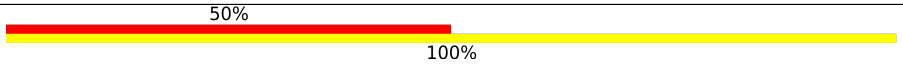
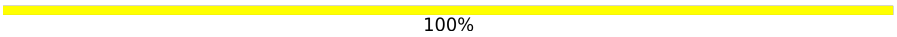
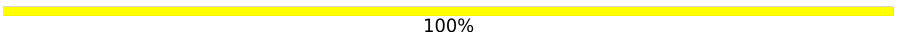
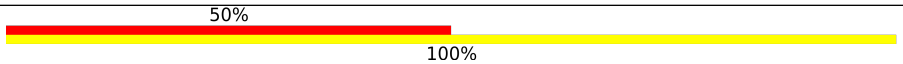
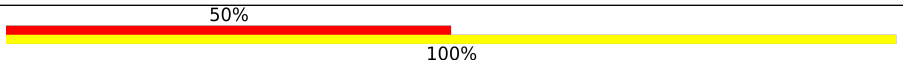
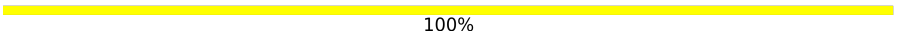
Mol	Chain	Length	Quality of chain
2	H	2	
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
2	R	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 52971 atoms, of which 26103 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.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1097	Total	C	H	N	O	S	0	0
			16915	5465	8344	1434	1630	42		
1	B	1097	Total	C	H	N	O	S	0	0
			16915	5465	8344	1434	1630	42		
1	C	1097	Total	C	H	N	O	S	0	0
			16915	5465	8344	1434	1630	42		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	427	CYS	ASP	engineered mutation	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	987	CYS	VAL	engineered mutation	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	427	CYS	ASP	engineered mutation	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	987	CYS	VAL	engineered mutation	UNP P0DTC2
C	10	GLU	-	expression tag	UNP P0DTC2
C	11	THR	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	427	CYS	ASP	engineered mutation	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	987	CYS	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	E	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	G	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	J	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	K	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	L	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	M	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	N	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	O	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	P	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	Q	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

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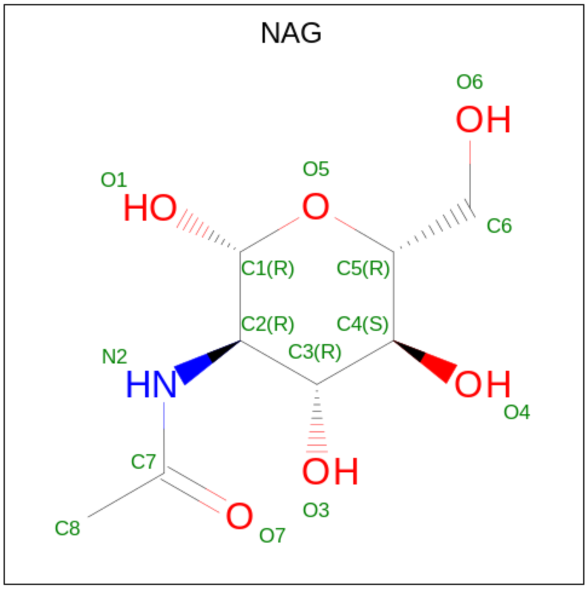
Mol	Chain	Residues	Atoms	AltConf	Trace
2	R	2	Total C H N O 53 16 25 2 10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0

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Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	A	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	B	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0

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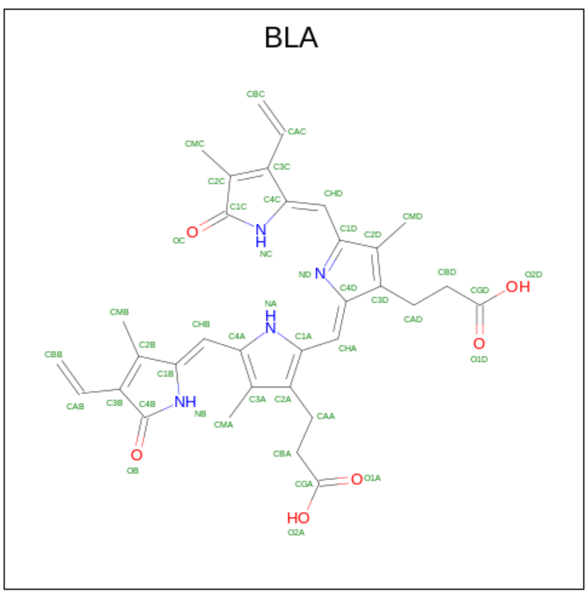
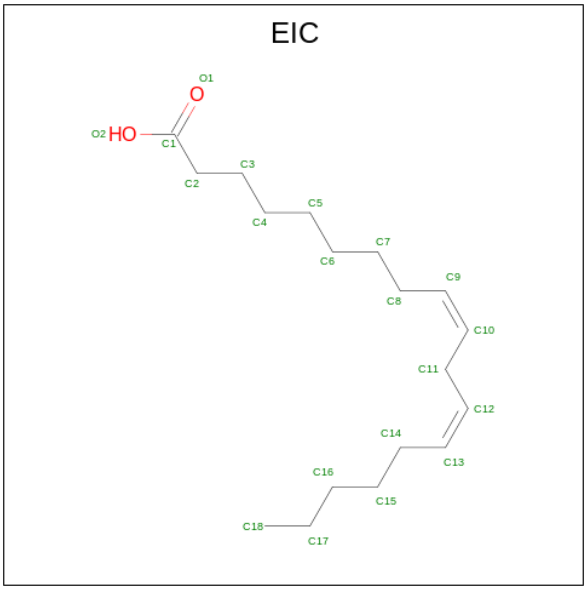
Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0
3	C	1	Total C H N O 27 8 13 1 5	0

- Molecule 4 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C H N O 75 33 32 4 6	0
4	B	1	Total C H N O 75 33 32 4 6	0
4	C	1	Total C H N O 75 33 32 4 6	0

- Molecule 5 is LINOLEIC ACID (three-letter code: EIC) (formula: $C_{18}H_{32}O_2$).



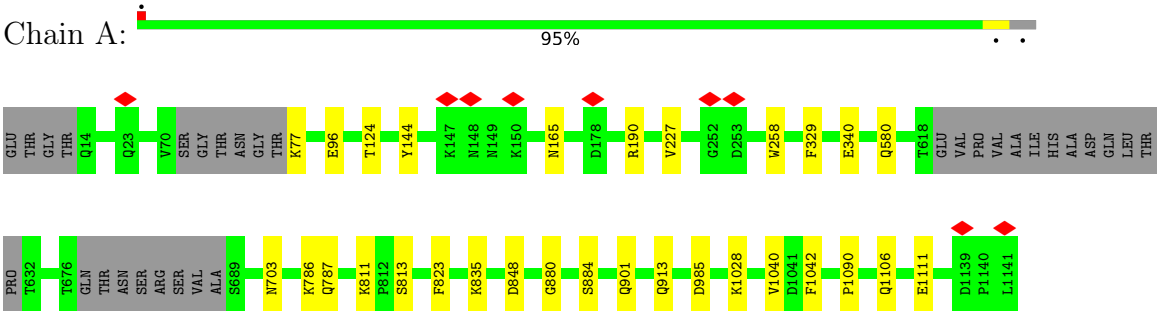
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	O	0
			51	18	31	2	
5	B	1	Total	C	H	O	0
			51	18	31	2	
5	C	1	Total	C	H	O	0
			51	18	31	2	

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.

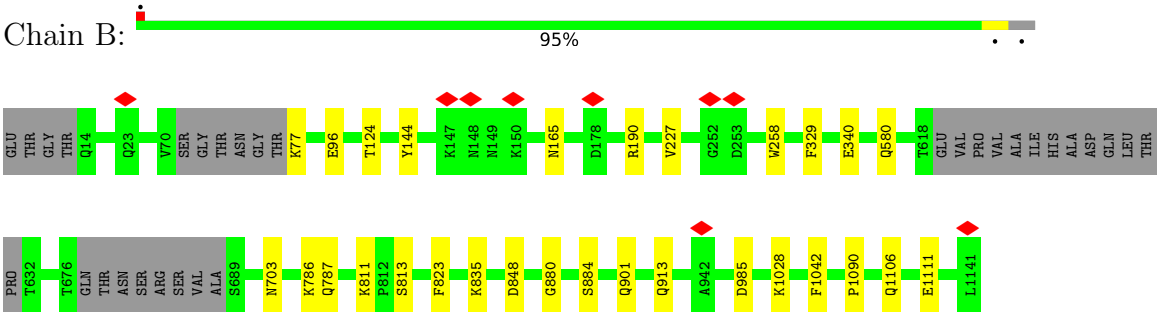
• Molecule 1: Spike glycoprotein

Chain A:



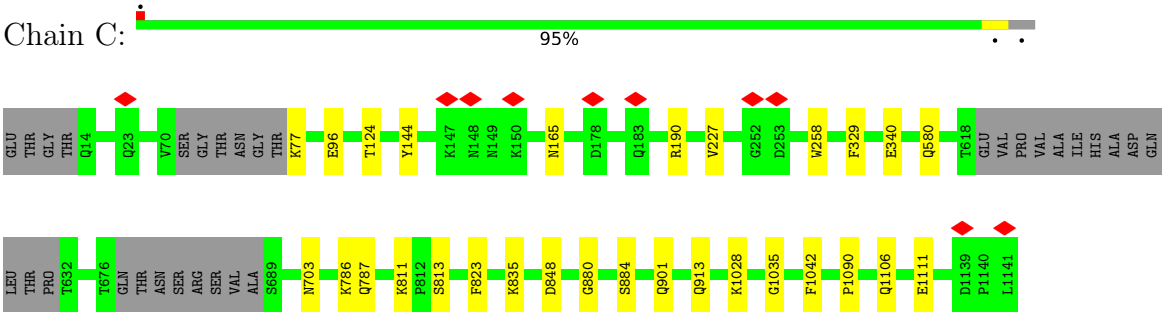
• Molecule 1: Spike glycoprotein

Chain B:



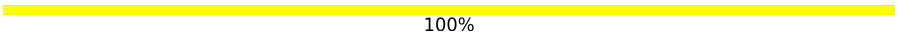
• Molecule 1: Spike glycoprotein

Chain C:



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

Chain D:

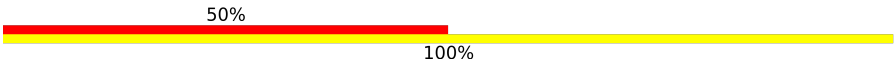


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

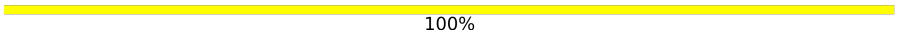
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain G:

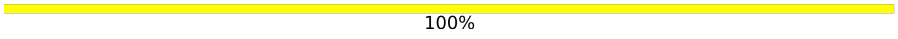


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

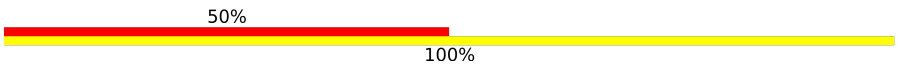
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



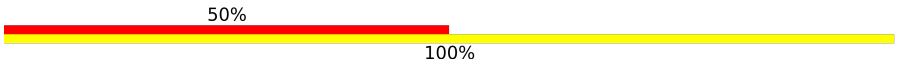
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



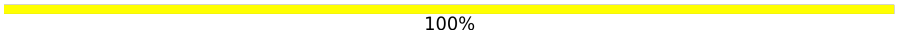
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain L:

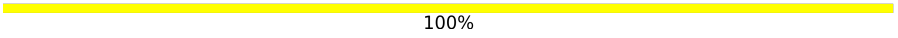


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

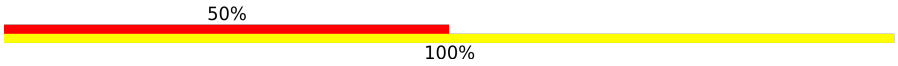
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



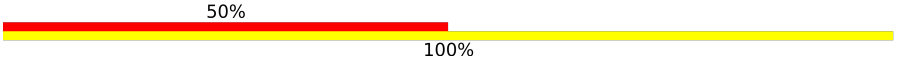
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



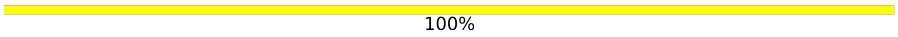
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



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

Chain Q:



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

Chain R:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	80277	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.276	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/8769	0.56	0/11929
1	B	0.29	0/8769	0.56	0/11929
1	C	0.29	0/8769	0.56	0/11929
All	All	0.29	0/26307	0.56	0/35787

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	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ASN	Peptide
1	B	165	ASN	Peptide
1	C	165	ASN	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	8571	8344	8345	16	0
1	B	8571	8344	8345	15	0
1	C	8571	8344	8345	15	0
2	D	28	25	25	0	0
2	E	28	25	25	0	0
2	F	28	25	25	0	0
2	G	28	25	25	0	0
2	H	28	25	25	1	0
2	I	28	25	25	0	0
2	J	28	25	25	0	0
2	K	28	25	25	0	0
2	L	28	25	25	0	0
2	M	28	25	25	1	0
2	N	28	25	25	0	0
2	O	28	25	25	0	0
2	P	28	25	25	0	0
2	Q	28	25	25	0	0
2	R	28	25	25	1	0
3	A	182	169	169	0	0
3	B	182	169	169	1	0
3	C	182	169	169	0	0
4	A	43	32	32	0	0
4	B	43	32	32	0	0
4	C	43	32	32	0	0
5	A	20	31	31	0	0
5	B	20	31	31	0	0
5	C	20	31	31	0	0
All	All	26868	26103	26106	40	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 (40) 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:787:GLN:OE1	1:C:703:ASN:ND2	2.20	0.74
1:A:703:ASN:ND2	1:C:787:GLN:OE1	2.21	0.74
1:A:787:GLN:OE1	1:B:703:ASN:ND2	2.21	0.74
1:A:96:GLU:OE1	1:A:190:ARG:NH1	2.25	0.69
1:B:96:GLU:OE1	1:B:190:ARG:NH1	2.25	0.69
1:A:811:LYS:NZ	1:A:813:SER:OG	2.26	0.68
1:C:96:GLU:OE1	1:C:190:ARG:NH1	2.25	0.68
1:A:1090:PRO:O	1:C:913:GLN:NE2	2.29	0.66
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.29	0.66
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.30	0.65
1:A:77:LYS:NZ	1:A:258:TRP:O	2.30	0.64
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.31	0.63
1:B:77:LYS:NZ	1:B:258:TRP:O	2.30	0.63
1:C:77:LYS:NZ	1:C:258:TRP:O	2.30	0.62
1:C:811:LYS:NZ	1:C:813:SER:OG	2.33	0.62
1:B:811:LYS:NZ	1:B:813:SER:OG	2.33	0.61
1:A:913:GLN:NE2	1:B:1090:PRO:O	2.33	0.61
1:B:913:GLN:NE2	1:C:1090:PRO:O	2.37	0.58
1:B:329:PHE:O	1:B:580:GLN:NE2	2.39	0.56
1:A:880:GLY:O	1:A:884:SER:OG	2.22	0.54
1:A:124:THR:OG1	2:H:1:NAG:N2	2.42	0.53
1:C:835:LYS:NZ	1:C:848:ASP:OD2	2.42	0.53
1:C:329:PHE:O	1:C:580:GLN:NE2	2.42	0.52
1:C:124:THR:OG1	2:R:1:NAG:N2	2.42	0.52
1:B:1106:GLN:NE2	1:B:1111:GLU:OE1	2.43	0.52
1:A:1106:GLN:NE2	1:A:1111:GLU:OE1	2.43	0.51
1:B:124:THR:OG1	2:M:1:NAG:N2	2.42	0.51
1:A:835:LYS:NZ	1:A:848:ASP:OD2	2.44	0.51
1:A:329:PHE:O	1:A:580:GLN:NE2	2.43	0.50
1:B:835:LYS:NZ	1:B:848:ASP:OD2	2.45	0.49
1:C:1106:GLN:NE2	1:C:1111:GLU:OE1	2.45	0.49
1:C:880:GLY:O	1:C:884:SER:OG	2.24	0.49
1:A:340:GLU:N	1:A:340:GLU:OE1	2.47	0.47
1:B:880:GLY:O	1:B:884:SER:OG	2.24	0.47
3:B:1613:NAG:O7	3:B:1613:NAG:O3	2.30	0.46
1:B:340:GLU:OE1	1:B:340:GLU:N	2.47	0.44
1:A:1040:VAL:HG21	1:C:1035:GLY:HA3	2.00	0.44
1:C:340:GLU:OE1	1:C:340:GLU:N	2.48	0.43
1:A:985:ASP:OD1	1:A:985:ASP:N	2.55	0.40
1:B:985:ASP:OD1	1:B:985:ASP:N	2.54	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	1089/1128 (96%)	1054 (97%)	35 (3%)	0	100	100
1	B	1089/1128 (96%)	1055 (97%)	34 (3%)	0	100	100
1	C	1089/1128 (96%)	1055 (97%)	34 (3%)	0	100	100
All	All	3267/3384 (96%)	3164 (97%)	103 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	954/979 (97%)	949 (100%)	5 (0%)	86	95
1	B	954/979 (97%)	949 (100%)	5 (0%)	86	95
1	C	954/979 (97%)	949 (100%)	5 (0%)	86	95
All	All	2862/2937 (97%)	2847 (100%)	15 (0%)	85	95

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	TYR
1	A	227	VAL
1	A	786	LYS
1	A	823	PHE
1	A	901	GLN

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Mol	Chain	Res	Type
1	B	144	TYR
1	B	227	VAL
1	B	786	LYS
1	B	823	PHE
1	B	901	GLN
1	C	144	TYR
1	C	227	VAL
1	C	786	LYS
1	C	823	PHE
1	C	901	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	703	ASN
1	B	703	ASN
1	C	703	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

30 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	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	2.13	4 (28%)	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	2	2	14,14,15	2.16	4 (28%)	17,19,21	0.99	1 (5%)
2	NAG	E	1	1,2	14,14,15	2.20	4 (28%)	17,19,21	1.03	1 (5%)
2	NAG	E	2	2	14,14,15	2.16	4 (28%)	17,19,21	0.99	1 (5%)
2	NAG	F	1	1,2	14,14,15	2.17	4 (28%)	17,19,21	0.99	1 (5%)
2	NAG	F	2	2	14,14,15	2.17	4 (28%)	17,19,21	0.98	1 (5%)
2	NAG	G	1	1,2	14,14,15	2.12	4 (28%)	17,19,21	1.10	0
2	NAG	G	2	2	14,14,15	2.16	4 (28%)	17,19,21	1.05	2 (11%)
2	NAG	H	1	1,2	14,14,15	2.17	4 (28%)	17,19,21	1.10	1 (5%)
2	NAG	H	2	2	14,14,15	2.21	4 (28%)	17,19,21	1.34	1 (5%)
2	NAG	I	1	1,2	14,14,15	2.12	4 (28%)	17,19,21	0.96	1 (5%)
2	NAG	I	2	2	14,14,15	2.17	4 (28%)	17,19,21	0.99	1 (5%)
2	NAG	J	1	1,2	14,14,15	2.21	4 (28%)	17,19,21	1.04	1 (5%)
2	NAG	J	2	2	14,14,15	2.16	4 (28%)	17,19,21	0.97	1 (5%)
2	NAG	K	1	1,2	14,14,15	2.17	4 (28%)	17,19,21	0.99	1 (5%)
2	NAG	K	2	2	14,14,15	2.17	4 (28%)	17,19,21	0.98	1 (5%)
2	NAG	L	1	1,2	14,14,15	2.12	4 (28%)	17,19,21	1.13	0
2	NAG	L	2	2	14,14,15	2.15	4 (28%)	17,19,21	1.06	2 (11%)
2	NAG	M	1	1,2	14,14,15	2.17	4 (28%)	17,19,21	1.11	1 (5%)
2	NAG	M	2	2	14,14,15	2.20	4 (28%)	17,19,21	1.35	1 (5%)
2	NAG	N	1	1,2	14,14,15	2.14	4 (28%)	17,19,21	0.97	1 (5%)
2	NAG	N	2	2	14,14,15	2.15	4 (28%)	17,19,21	0.99	1 (5%)
2	NAG	O	1	1,2	14,14,15	2.19	4 (28%)	17,19,21	1.04	1 (5%)
2	NAG	O	2	2	14,14,15	2.17	4 (28%)	17,19,21	0.99	1 (5%)
2	NAG	P	1	1,2	14,14,15	2.16	4 (28%)	17,19,21	0.99	1 (5%)
2	NAG	P	2	2	14,14,15	2.17	4 (28%)	17,19,21	0.98	1 (5%)
2	NAG	Q	1	1,2	14,14,15	2.12	4 (28%)	17,19,21	1.13	0
2	NAG	Q	2	2	14,14,15	2.17	4 (28%)	17,19,21	1.06	1 (5%)
2	NAG	R	1	1,2	14,14,15	2.17	4 (28%)	17,19,21	1.09	1 (5%)
2	NAG	R	2	2	14,14,15	2.20	4 (28%)	17,19,21	1.34	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
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	1/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	NAG	O5-C1	5.51	1.52	1.43
2	E	1	NAG	O5-C1	5.47	1.52	1.43
2	O	1	NAG	O5-C1	5.45	1.52	1.43
2	P	1	NAG	O5-C1	5.33	1.52	1.43
2	F	1	NAG	O5-C1	5.33	1.52	1.43
2	K	1	NAG	O5-C1	5.31	1.52	1.43
2	F	2	NAG	O5-C1	5.30	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	2	NAG	O5-C1	5.30	1.52	1.43
2	H	1	NAG	O5-C1	5.30	1.52	1.43
2	I	2	NAG	O5-C1	5.29	1.52	1.43
2	Q	2	NAG	O5-C1	5.28	1.52	1.43
2	M	1	NAG	O5-C1	5.28	1.52	1.43
2	G	2	NAG	O5-C1	5.28	1.52	1.43
2	R	1	NAG	O5-C1	5.27	1.52	1.43
2	K	2	NAG	O5-C1	5.25	1.52	1.43
2	D	2	NAG	O5-C1	5.24	1.52	1.43
2	R	2	NAG	O5-C1	5.24	1.52	1.43
2	M	2	NAG	O5-C1	5.23	1.52	1.43
2	N	1	NAG	O5-C1	5.22	1.52	1.43
2	H	2	NAG	O5-C1	5.21	1.52	1.43
2	O	2	NAG	O5-C1	5.20	1.52	1.43
2	E	2	NAG	O5-C1	5.20	1.52	1.43
2	J	2	NAG	O5-C1	5.20	1.52	1.43
2	N	2	NAG	O5-C1	5.19	1.52	1.43
2	D	1	NAG	O5-C1	5.17	1.52	1.43
2	L	2	NAG	O5-C1	5.17	1.52	1.43
2	I	1	NAG	O5-C1	5.15	1.51	1.43
2	Q	1	NAG	O5-C1	5.07	1.51	1.43
2	G	1	NAG	O5-C1	5.07	1.51	1.43
2	L	1	NAG	O5-C1	5.05	1.51	1.43
2	H	2	NAG	C7-N2	4.11	1.48	1.34
2	R	2	NAG	C7-N2	4.08	1.48	1.34
2	M	2	NAG	C7-N2	4.08	1.48	1.34
2	E	2	NAG	C7-N2	4.00	1.48	1.34
2	J	2	NAG	C7-N2	3.99	1.48	1.34
2	D	1	NAG	C7-N2	3.97	1.48	1.34
2	K	2	NAG	C7-N2	3.97	1.48	1.34
2	O	2	NAG	C7-N2	3.97	1.48	1.34
2	F	2	NAG	C7-N2	3.96	1.48	1.34
2	P	2	NAG	C7-N2	3.96	1.48	1.34
2	N	2	NAG	C7-N2	3.95	1.47	1.34
2	L	2	NAG	C7-N2	3.95	1.47	1.34
2	E	1	NAG	C7-N2	3.95	1.47	1.34
2	I	1	NAG	C7-N2	3.95	1.47	1.34
2	D	2	NAG	C7-N2	3.94	1.47	1.34
2	N	1	NAG	C7-N2	3.94	1.47	1.34
2	J	1	NAG	C7-N2	3.93	1.47	1.34
2	Q	2	NAG	C7-N2	3.93	1.47	1.34
2	K	1	NAG	C7-N2	3.93	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	C7-N2	3.93	1.47	1.34
2	F	1	NAG	C7-N2	3.92	1.47	1.34
2	O	1	NAG	C7-N2	3.92	1.47	1.34
2	R	1	NAG	C7-N2	3.92	1.47	1.34
2	M	1	NAG	C7-N2	3.92	1.47	1.34
2	G	2	NAG	C7-N2	3.92	1.47	1.34
2	H	1	NAG	C7-N2	3.91	1.47	1.34
2	P	1	NAG	C7-N2	3.90	1.47	1.34
2	Q	1	NAG	C7-N2	3.90	1.47	1.34
2	G	1	NAG	C7-N2	3.89	1.47	1.34
2	L	1	NAG	C7-N2	3.89	1.47	1.34
2	H	2	NAG	C2-N2	3.29	1.51	1.46
2	M	2	NAG	C2-N2	3.26	1.51	1.46
2	R	2	NAG	C2-N2	3.25	1.51	1.46
2	O	2	NAG	C2-N2	3.18	1.51	1.46
2	N	1	NAG	C2-N2	3.15	1.51	1.46
2	E	2	NAG	C2-N2	3.15	1.51	1.46
2	D	2	NAG	C2-N2	3.14	1.51	1.46
2	I	2	NAG	C2-N2	3.13	1.51	1.46
2	J	2	NAG	C2-N2	3.13	1.51	1.46
2	Q	2	NAG	C2-N2	3.12	1.51	1.46
2	L	2	NAG	C2-N2	3.11	1.51	1.46
2	K	2	NAG	C2-N2	3.11	1.51	1.46
2	K	1	NAG	C2-N2	3.11	1.51	1.46
2	N	2	NAG	C2-N2	3.10	1.51	1.46
2	F	1	NAG	C2-N2	3.10	1.51	1.46
2	F	2	NAG	C2-N2	3.09	1.51	1.46
2	P	2	NAG	C2-N2	3.09	1.51	1.46
2	D	1	NAG	C2-N2	3.07	1.51	1.46
2	M	1	NAG	C2-N2	3.07	1.51	1.46
2	P	1	NAG	C2-N2	3.05	1.51	1.46
2	I	1	NAG	C2-N2	3.05	1.51	1.46
2	G	2	NAG	C2-N2	3.04	1.51	1.46
2	R	1	NAG	C2-N2	3.04	1.51	1.46
2	J	1	NAG	C2-N2	3.04	1.51	1.46
2	E	1	NAG	C2-N2	3.03	1.51	1.46
2	H	1	NAG	C2-N2	3.03	1.51	1.46
2	L	1	NAG	C2-N2	3.02	1.51	1.46
2	O	1	NAG	C2-N2	3.01	1.51	1.46
2	G	1	NAG	C2-N2	3.00	1.51	1.46
2	Q	1	NAG	C2-N2	2.98	1.51	1.46
2	L	1	NAG	O7-C7	-2.20	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O7-C7	-2.19	1.18	1.23
2	Q	1	NAG	O7-C7	-2.19	1.18	1.23
2	I	2	NAG	O7-C7	-2.16	1.18	1.23
2	I	1	NAG	O7-C7	-2.16	1.18	1.23
2	O	1	NAG	O7-C7	-2.16	1.18	1.23
2	H	1	NAG	O7-C7	-2.16	1.18	1.23
2	L	2	NAG	O7-C7	-2.15	1.18	1.23
2	D	1	NAG	O7-C7	-2.14	1.18	1.23
2	E	1	NAG	O7-C7	-2.14	1.18	1.23
2	H	2	NAG	O7-C7	-2.14	1.18	1.23
2	N	2	NAG	O7-C7	-2.14	1.18	1.23
2	P	2	NAG	O7-C7	-2.13	1.18	1.23
2	Q	2	NAG	O7-C7	-2.13	1.18	1.23
2	D	2	NAG	O7-C7	-2.13	1.18	1.23
2	G	2	NAG	O7-C7	-2.12	1.18	1.23
2	K	2	NAG	O7-C7	-2.12	1.18	1.23
2	M	1	NAG	O7-C7	-2.12	1.18	1.23
2	R	2	NAG	O7-C7	-2.12	1.18	1.23
2	J	2	NAG	O7-C7	-2.12	1.18	1.23
2	R	1	NAG	O7-C7	-2.12	1.18	1.23
2	P	1	NAG	O7-C7	-2.11	1.18	1.23
2	J	1	NAG	O7-C7	-2.11	1.18	1.23
2	K	1	NAG	O7-C7	-2.11	1.18	1.23
2	F	2	NAG	O7-C7	-2.11	1.18	1.23
2	M	2	NAG	O7-C7	-2.10	1.18	1.23
2	O	2	NAG	O7-C7	-2.10	1.18	1.23
2	N	1	NAG	O7-C7	-2.10	1.18	1.23
2	F	1	NAG	O7-C7	-2.10	1.18	1.23
2	E	2	NAG	O7-C7	-2.08	1.18	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	2	NAG	C8-C7-N2	3.92	122.74	116.10
2	R	2	NAG	C8-C7-N2	3.89	122.68	116.10
2	H	2	NAG	C8-C7-N2	3.87	122.65	116.10
2	Q	2	NAG	C8-C7-N2	2.32	120.02	116.10
2	L	2	NAG	C8-C7-N2	2.30	120.00	116.10
2	G	2	NAG	C8-C7-N2	2.30	119.99	116.10
2	F	1	NAG	C8-C7-N2	2.17	119.78	116.10
2	P	1	NAG	C8-C7-N2	2.17	119.77	116.10
2	K	1	NAG	C8-C7-N2	2.16	119.75	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1	NAG	C8-C7-N2	2.16	119.75	116.10
2	M	1	NAG	C8-C7-N2	2.15	119.74	116.10
2	D	1	NAG	C8-C7-N2	2.15	119.74	116.10
2	N	1	NAG	C8-C7-N2	2.14	119.72	116.10
2	H	1	NAG	C8-C7-N2	2.13	119.70	116.10
2	R	1	NAG	C8-C7-N2	2.11	119.67	116.10
2	P	2	NAG	C8-C7-N2	2.11	119.66	116.10
2	K	2	NAG	C8-C7-N2	2.10	119.65	116.10
2	F	2	NAG	C8-C7-N2	2.09	119.64	116.10
2	N	2	NAG	C8-C7-N2	2.09	119.64	116.10
2	I	2	NAG	C8-C7-N2	2.09	119.63	116.10
2	D	2	NAG	C8-C7-N2	2.08	119.63	116.10
2	O	1	NAG	C8-C7-N2	2.07	119.61	116.10
2	E	1	NAG	C8-C7-N2	2.07	119.60	116.10
2	J	1	NAG	C8-C7-N2	2.07	119.60	116.10
2	L	2	NAG	C2-N2-C7	-2.07	119.96	122.90
2	E	2	NAG	C8-C7-N2	2.01	119.51	116.10
2	O	2	NAG	C8-C7-N2	2.01	119.50	116.10
2	G	2	NAG	C2-N2-C7	-2.01	120.05	122.90
2	J	2	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	R	2	NAG	C8-C7-N2-C2
2	R	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6

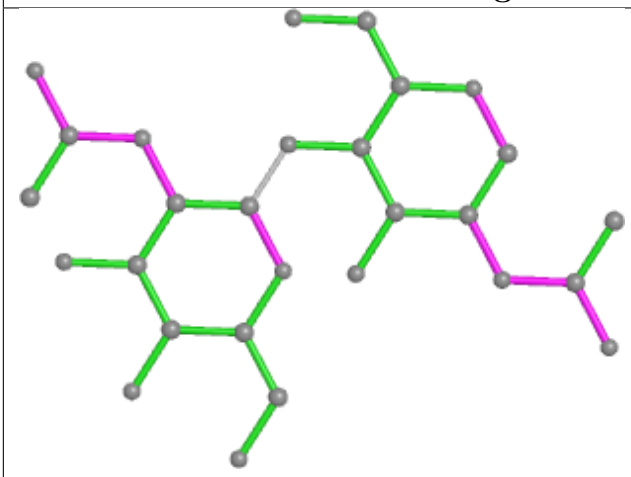
There are no ring outliers.

3 monomers are involved in 3 short contacts:

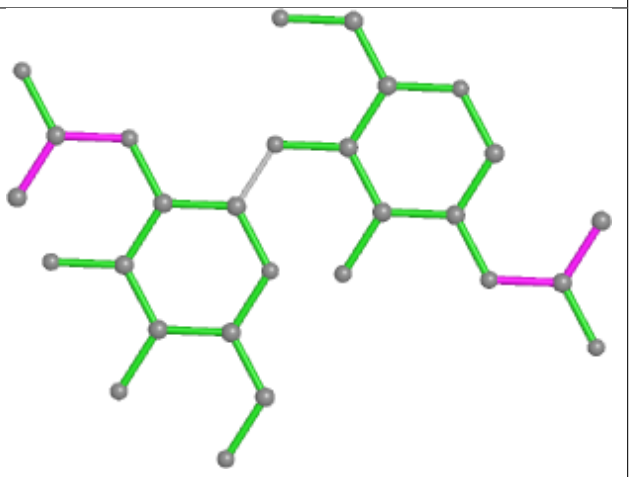
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	1	NAG	1	0
2	M	1	NAG	1	0
2	H	1	NAG	1	0

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

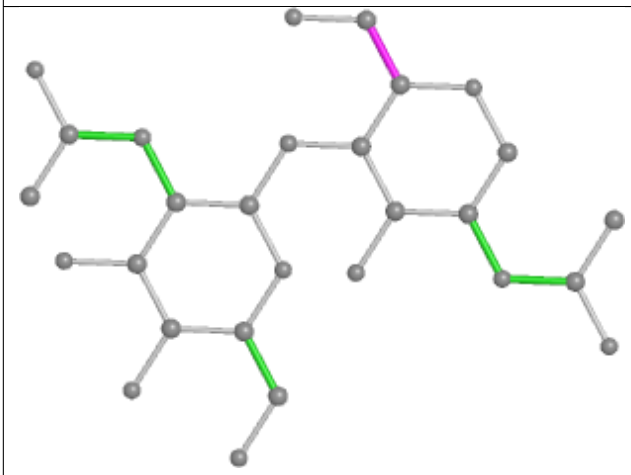
Oligosaccharide Chain D



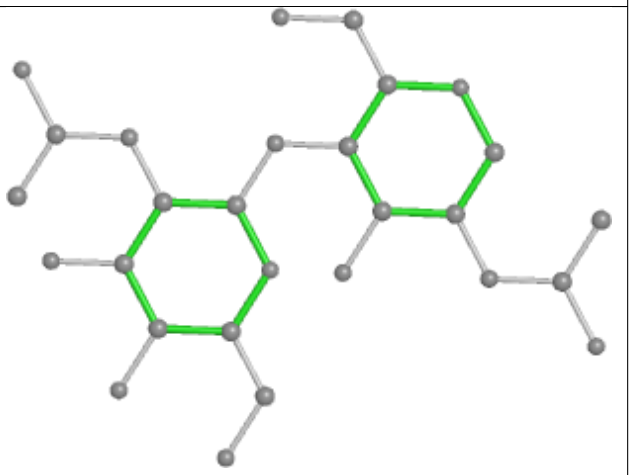
Bond lengths



Bond angles

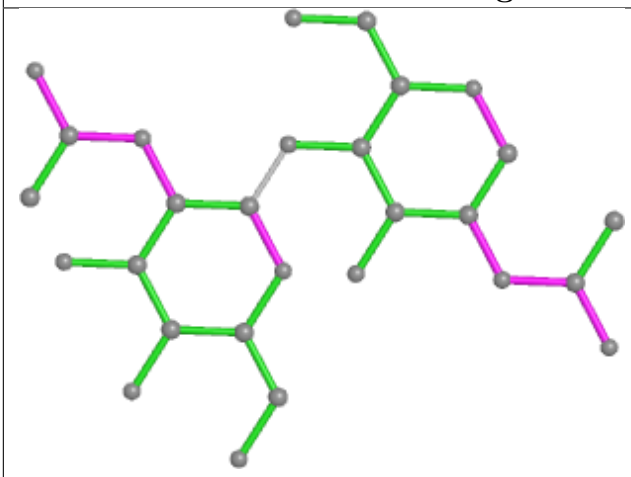


Torsions

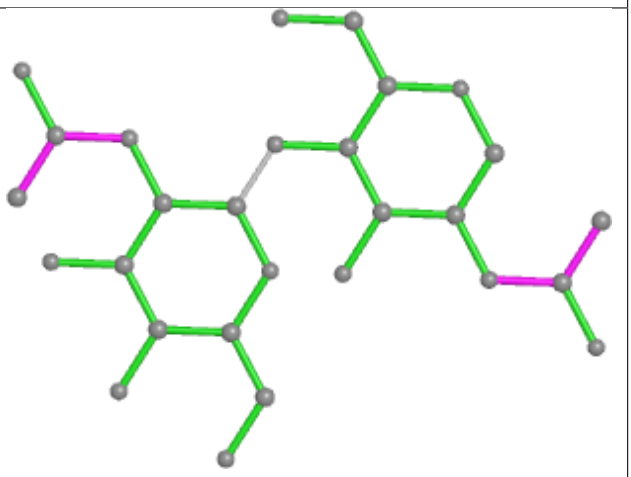


Rings

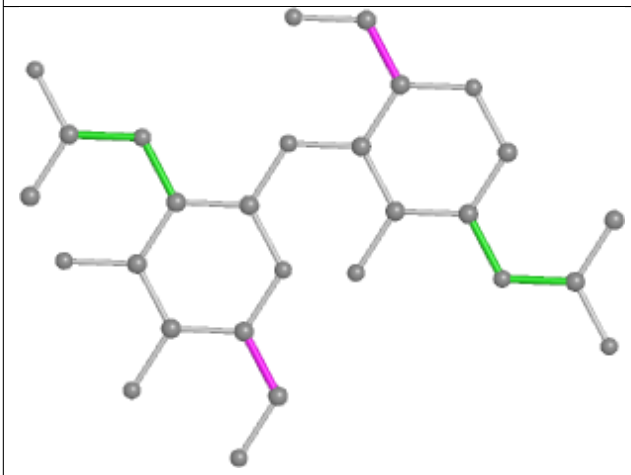
Oligosaccharide Chain E



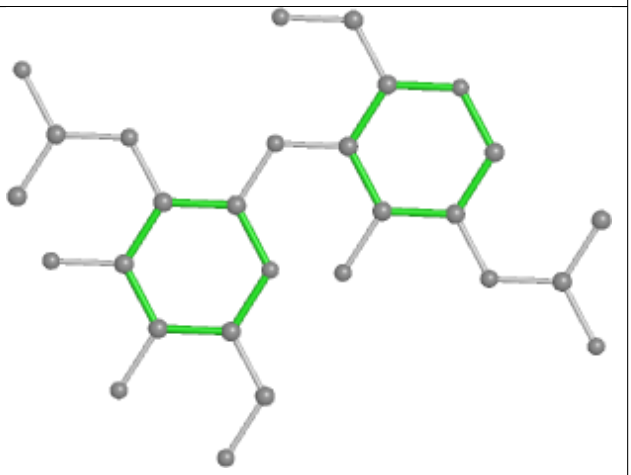
Bond lengths



Bond angles

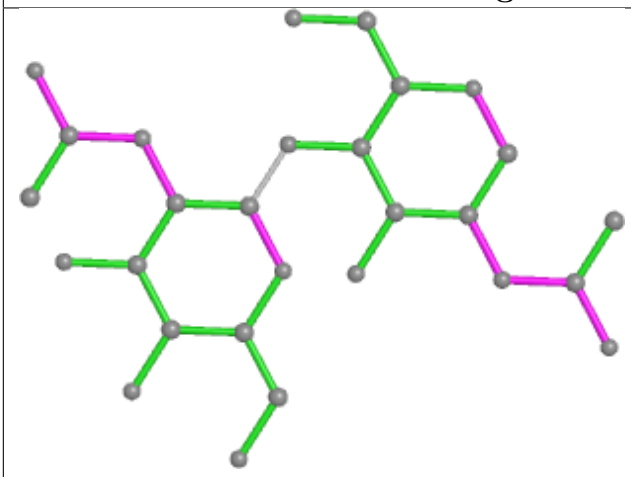


Torsions

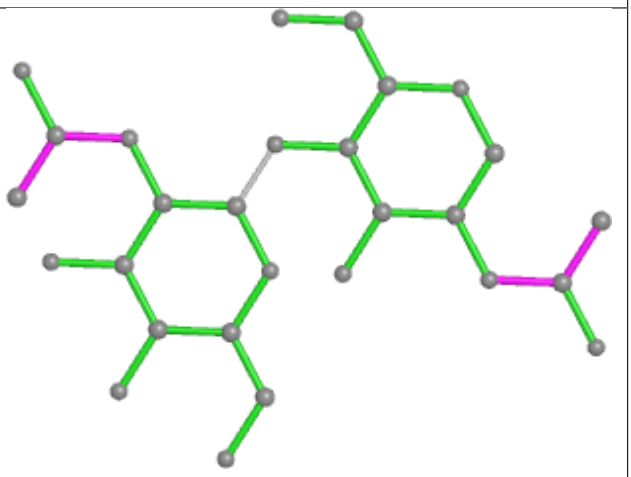


Rings

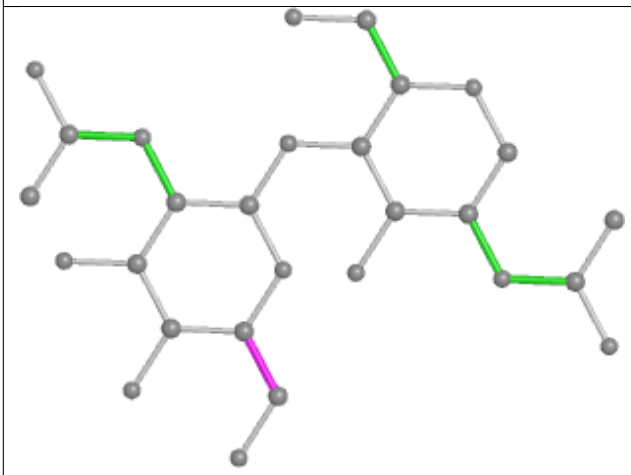
Oligosaccharide Chain F



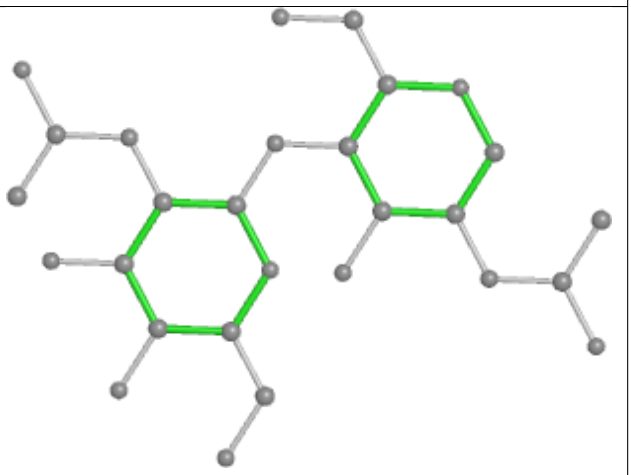
Bond lengths



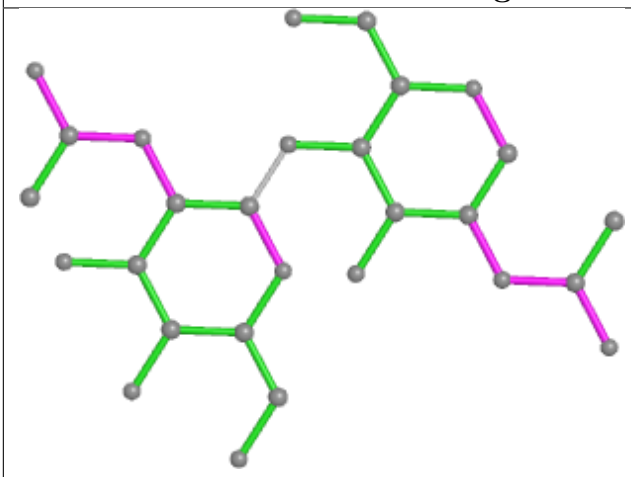
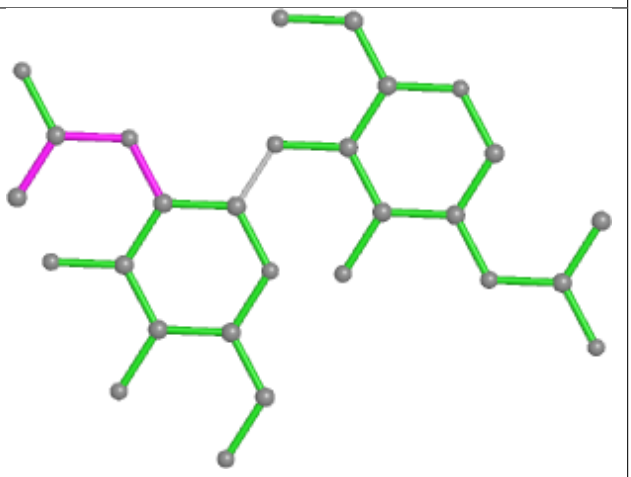
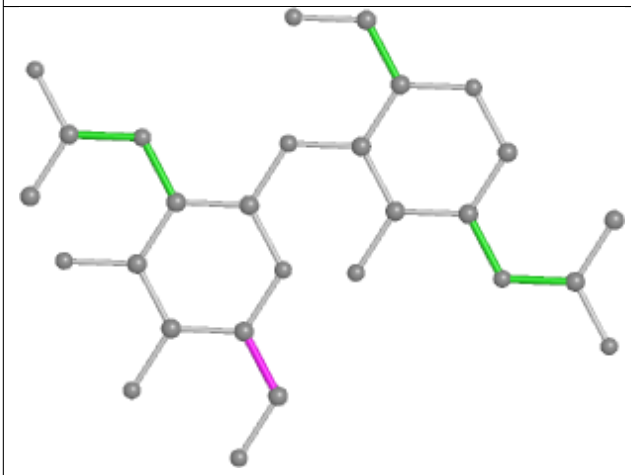
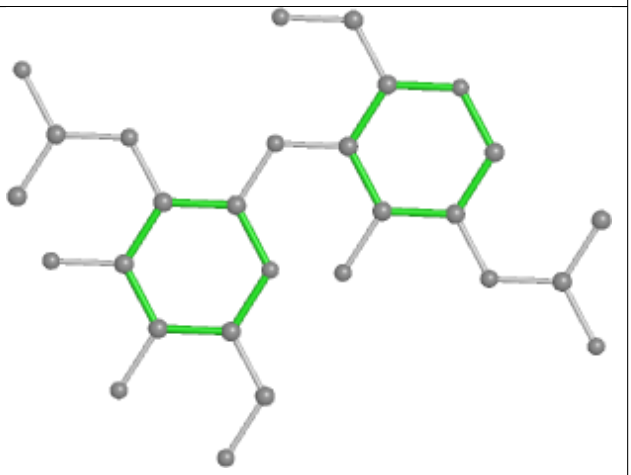
Bond angles



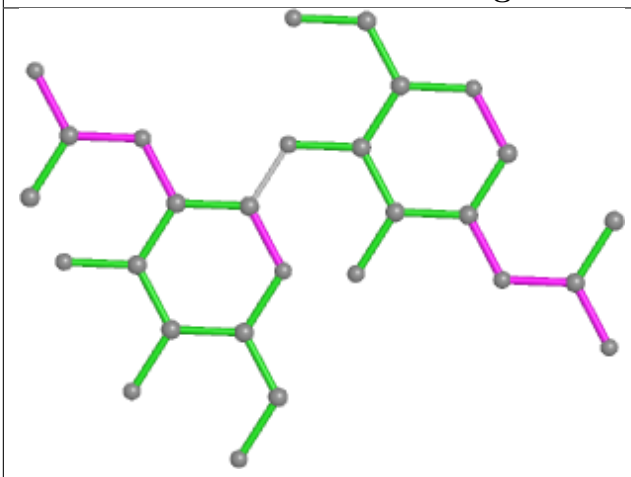
Torsions



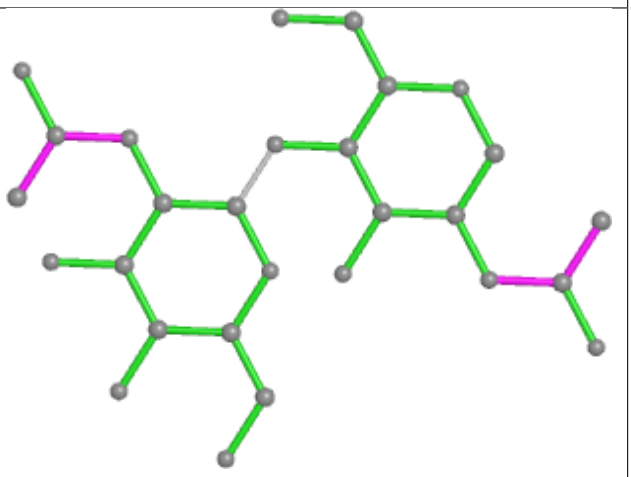
Rings

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

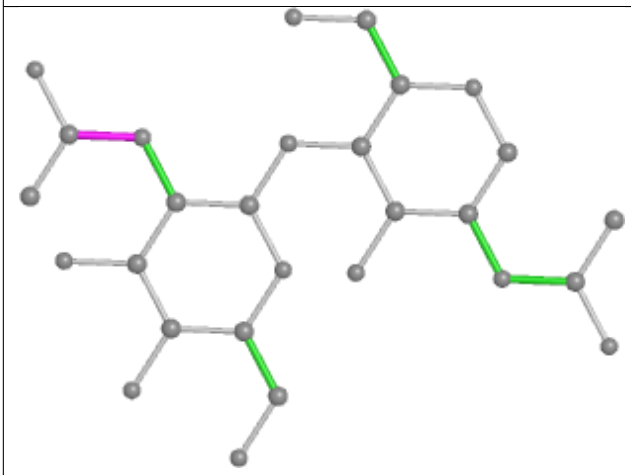
Oligosaccharide Chain H



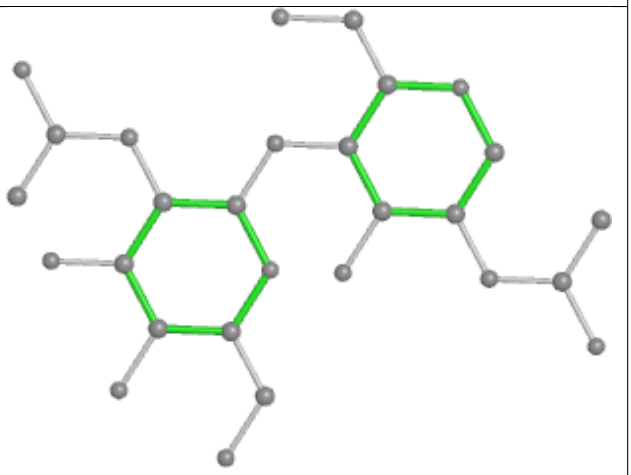
Bond lengths



Bond angles

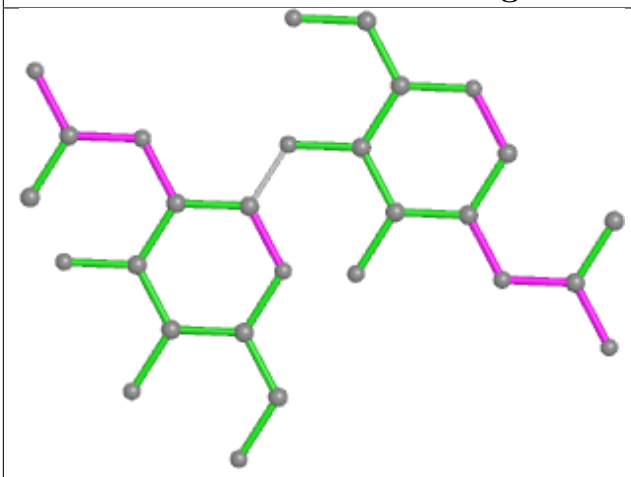


Torsions

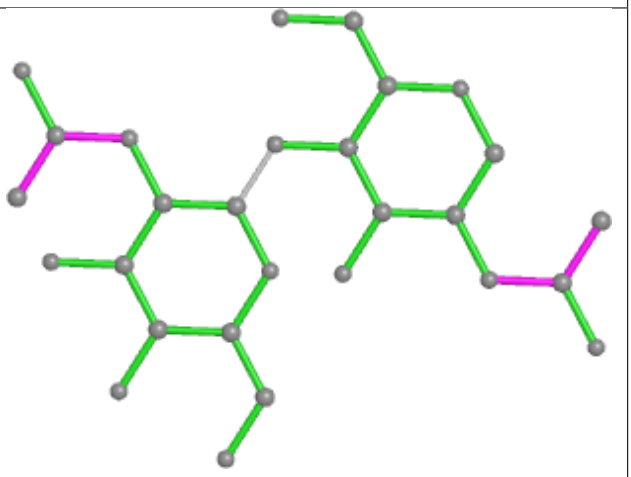


Rings

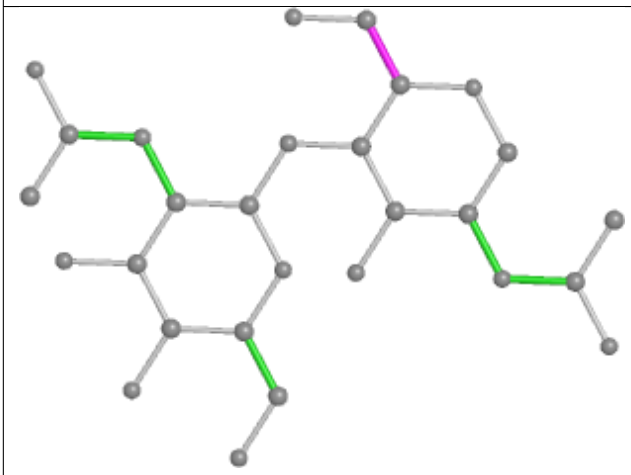
Oligosaccharide Chain I



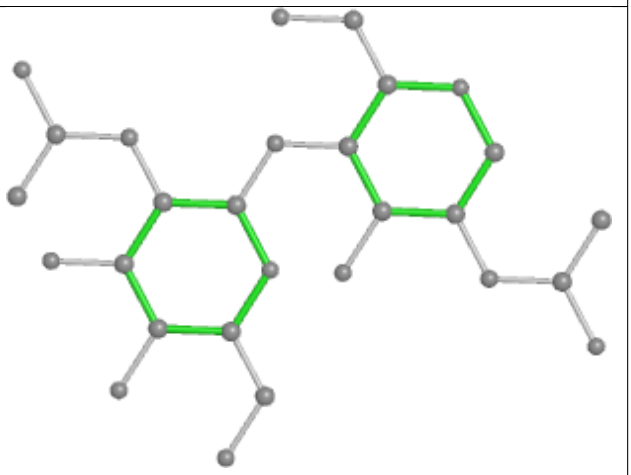
Bond lengths



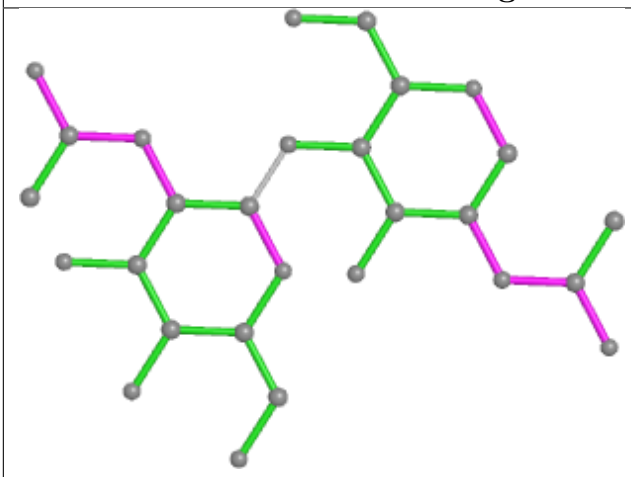
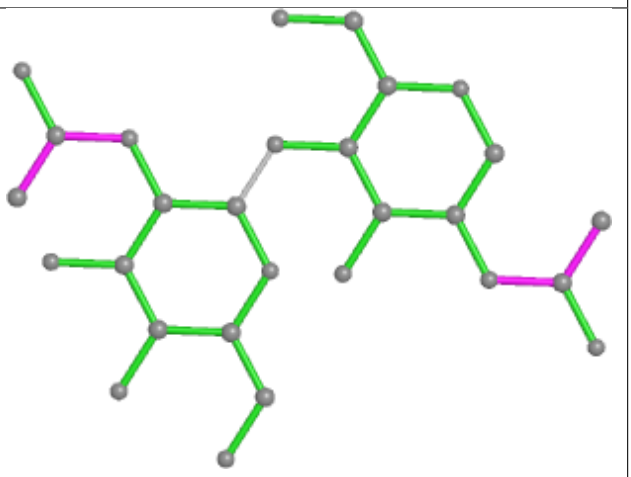
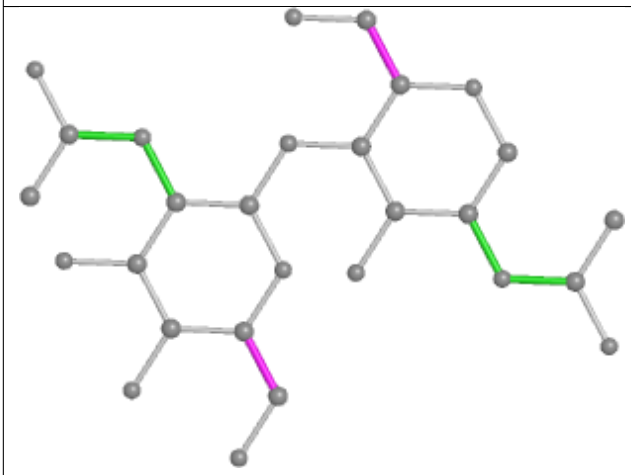
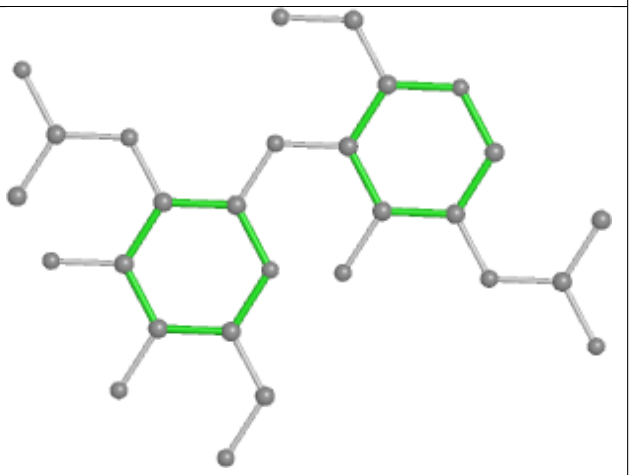
Bond angles

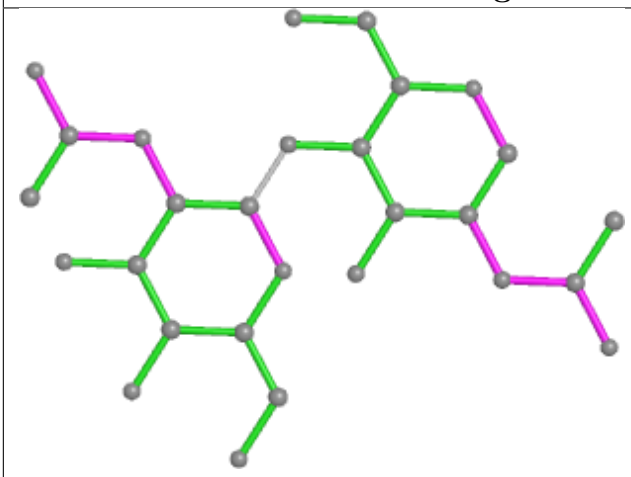
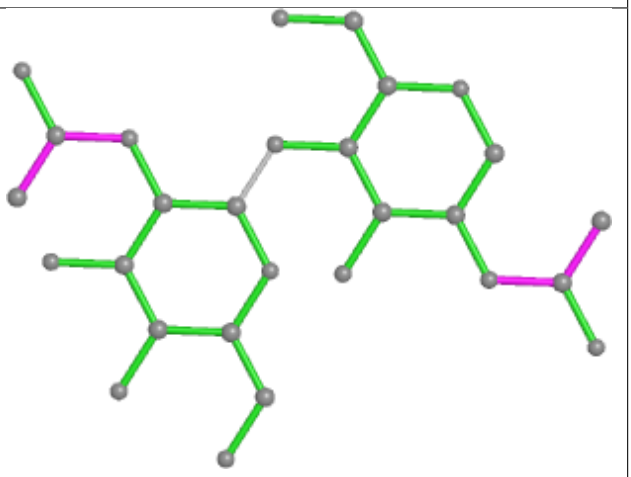
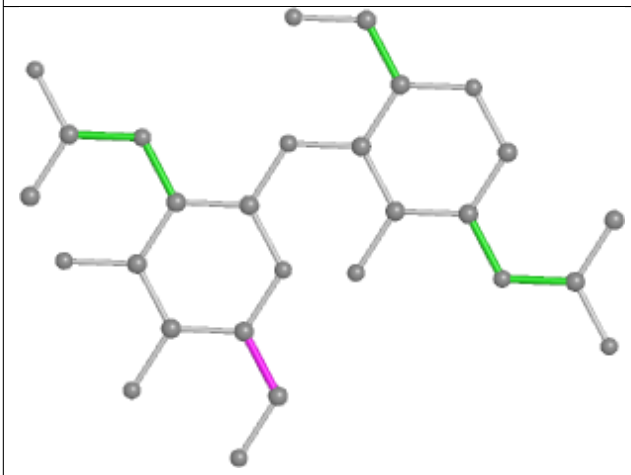
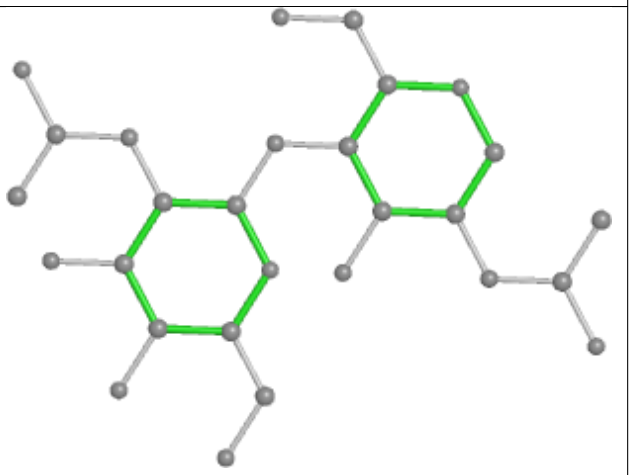


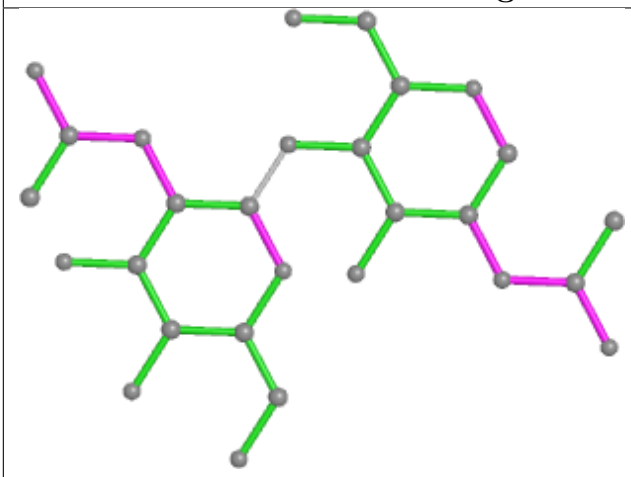
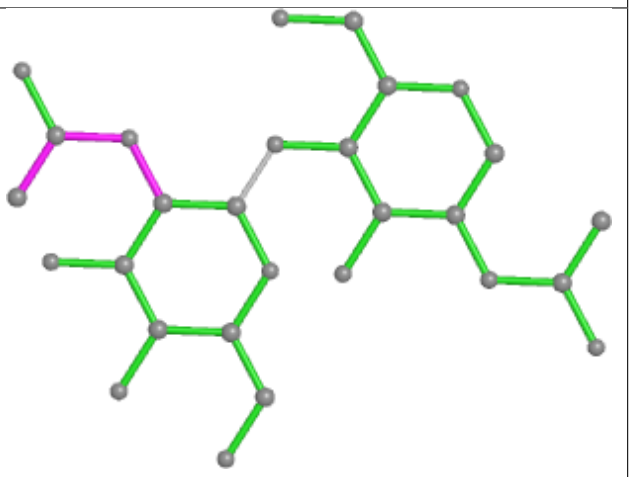
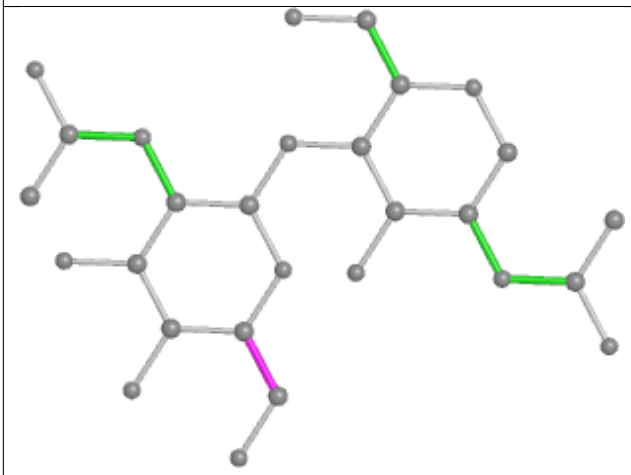
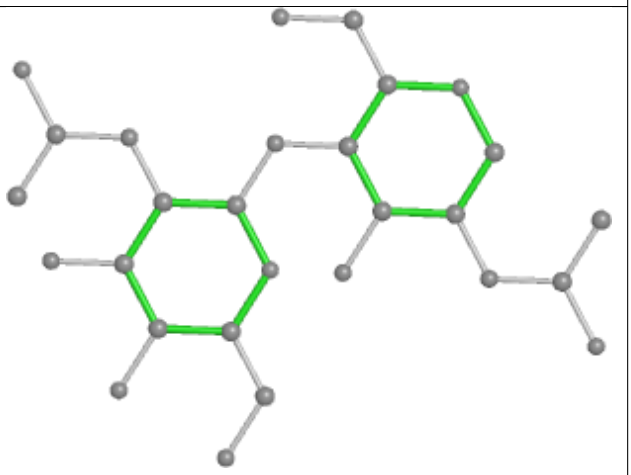
Torsions

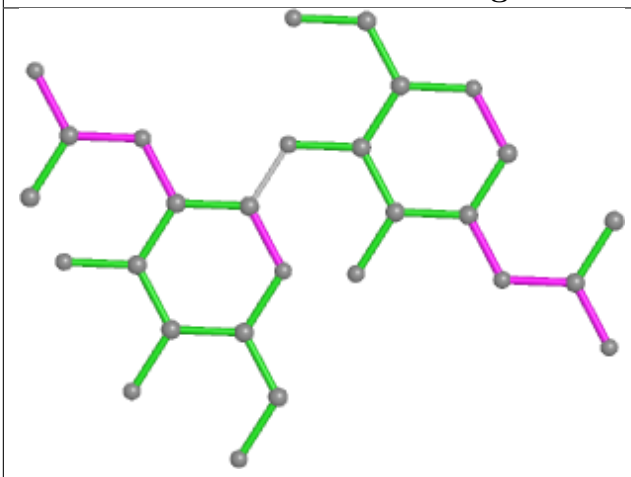
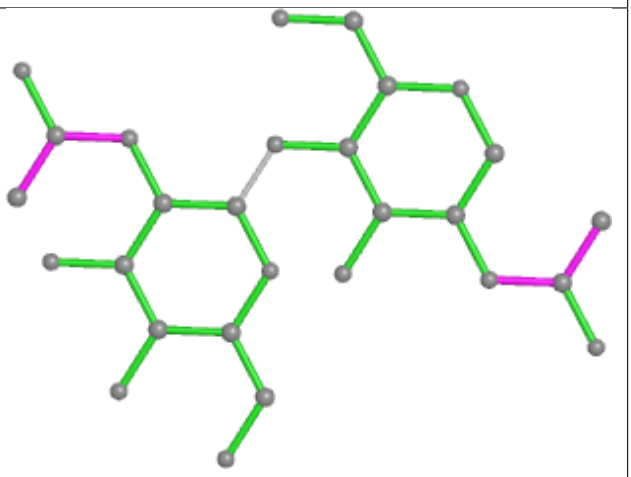
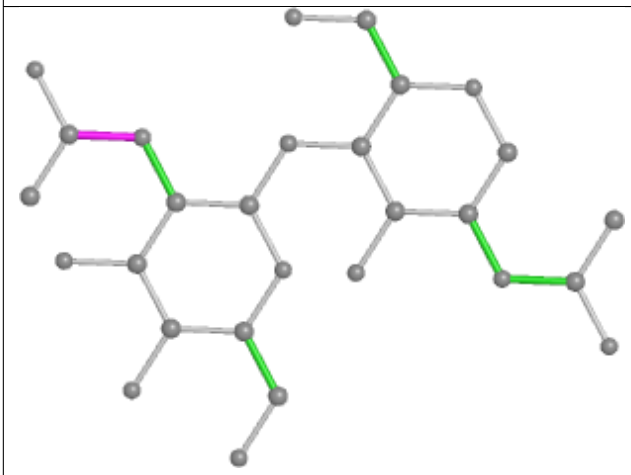
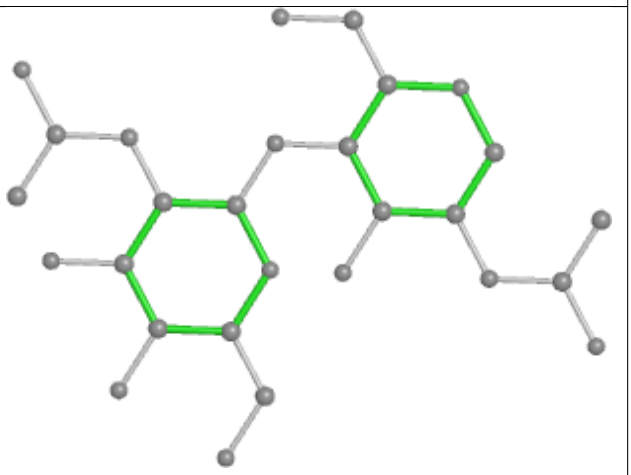


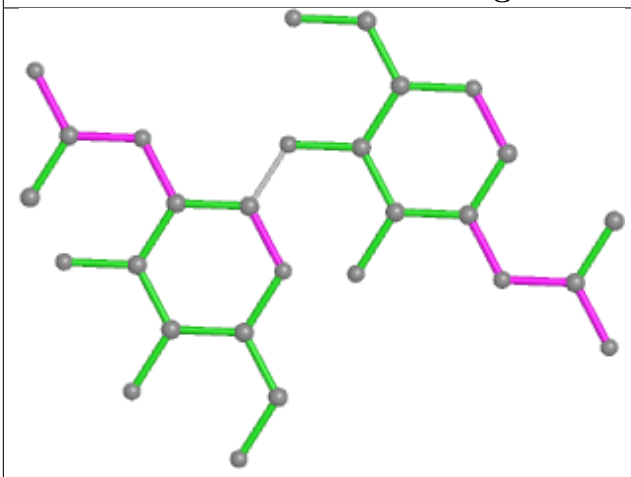
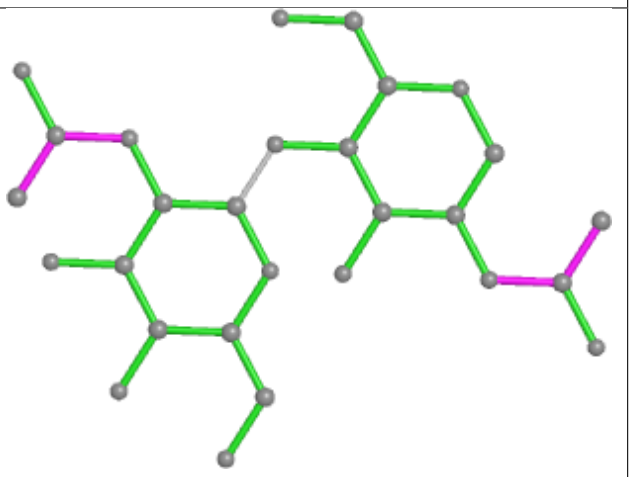
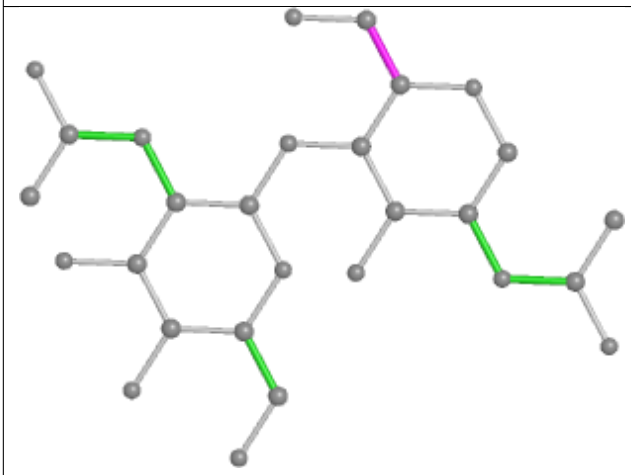
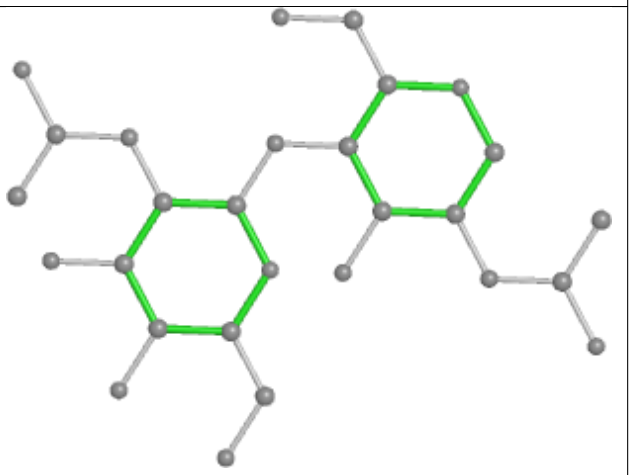
Rings

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

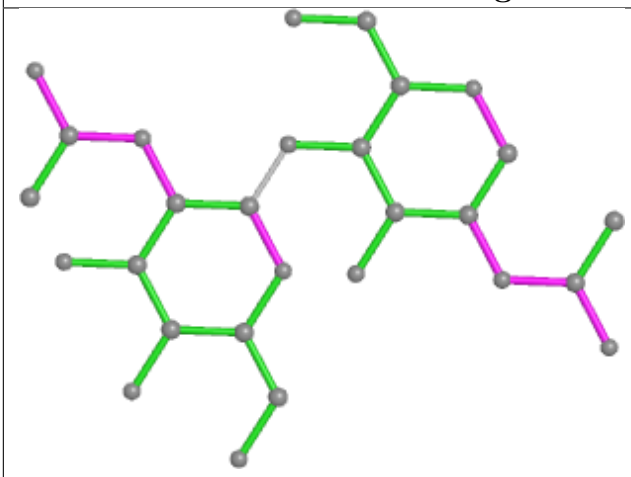
Oligosaccharide Chain K	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

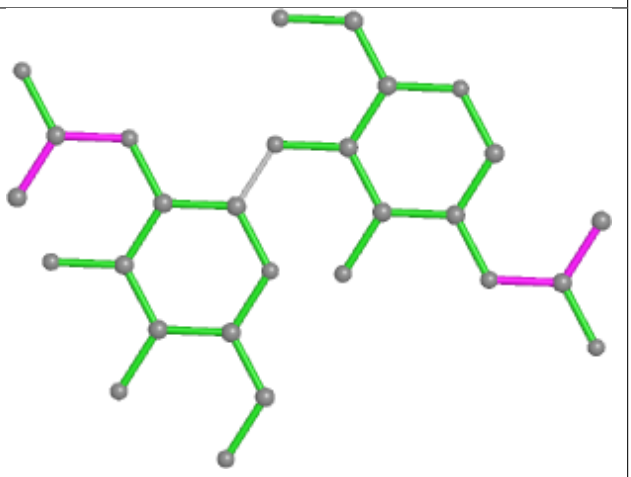
Oligosaccharide Chain M	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

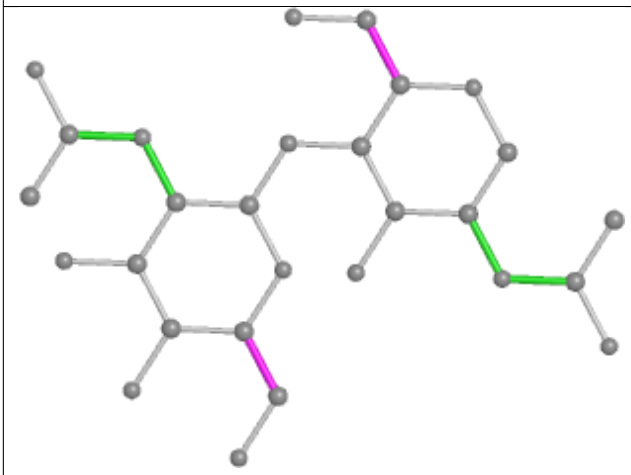
Oligosaccharide Chain O



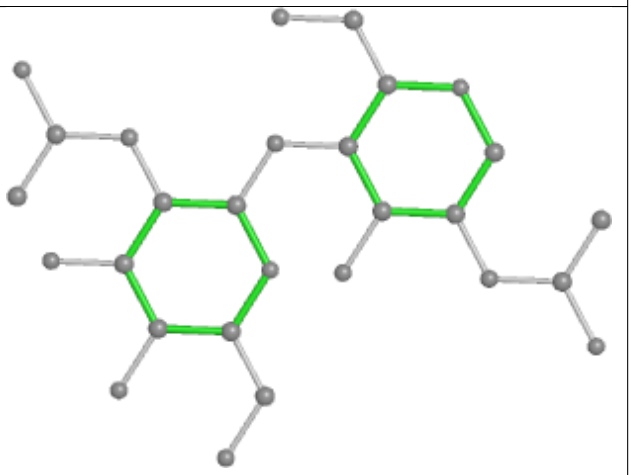
Bond lengths



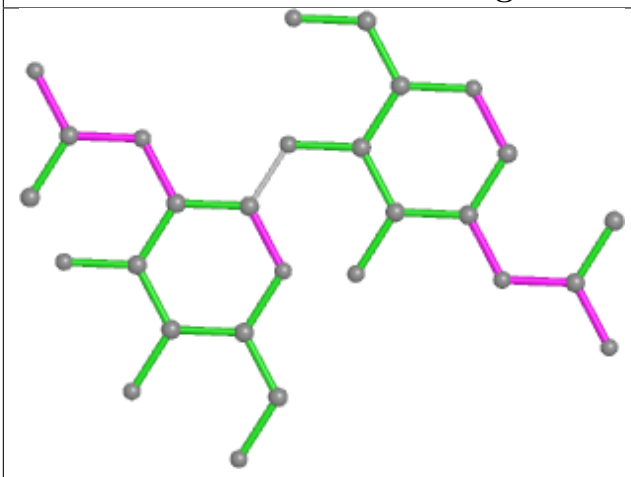
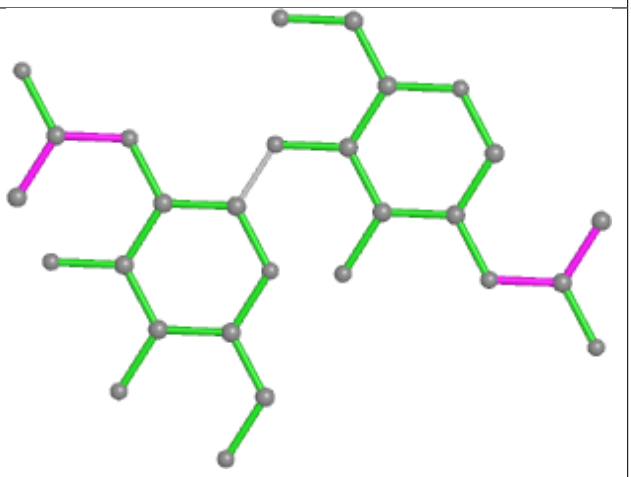
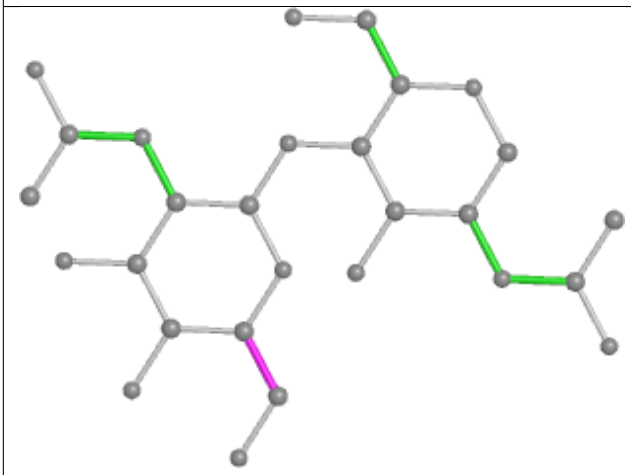
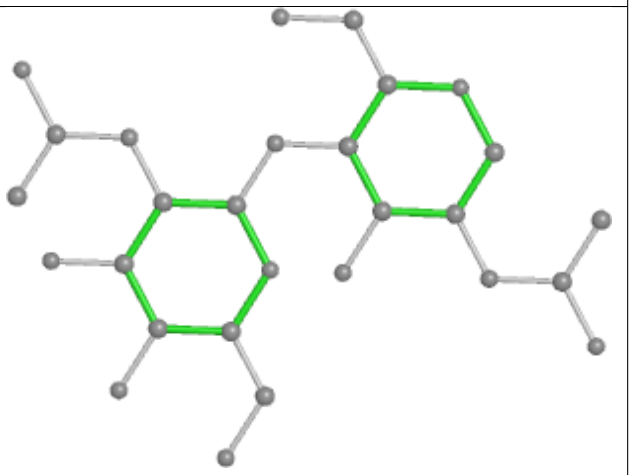
Bond angles



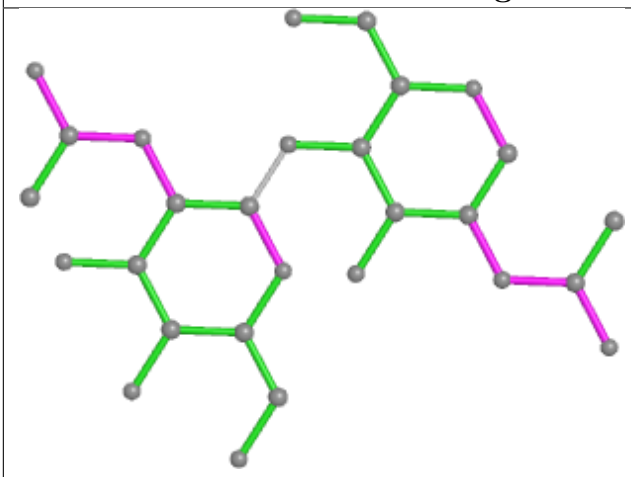
Torsions



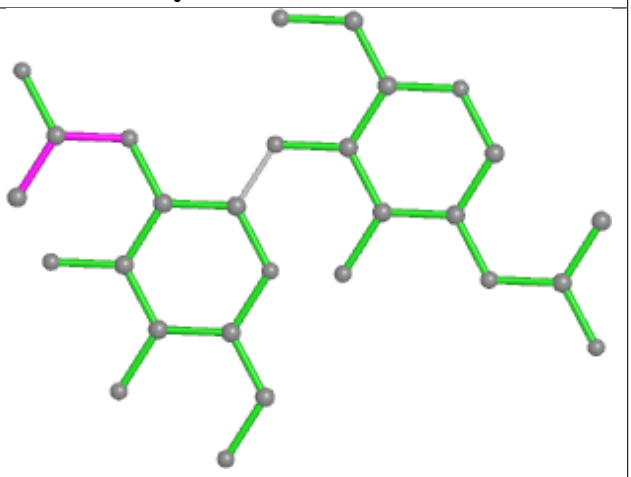
Rings

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

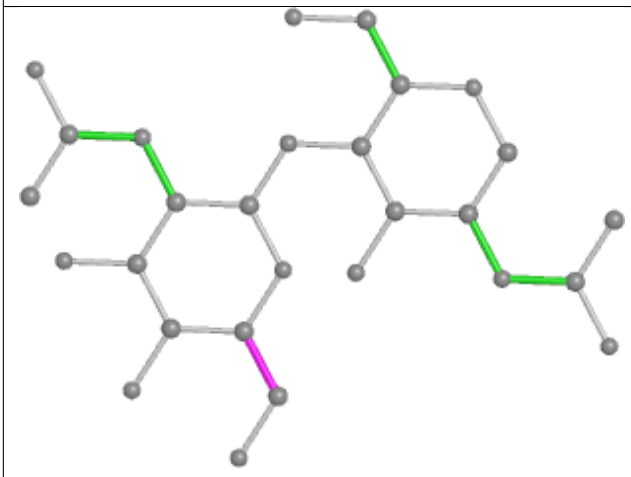
Oligosaccharide Chain Q



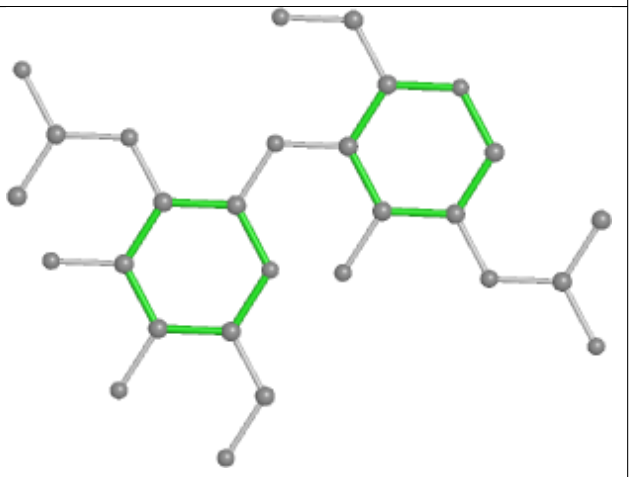
Bond lengths



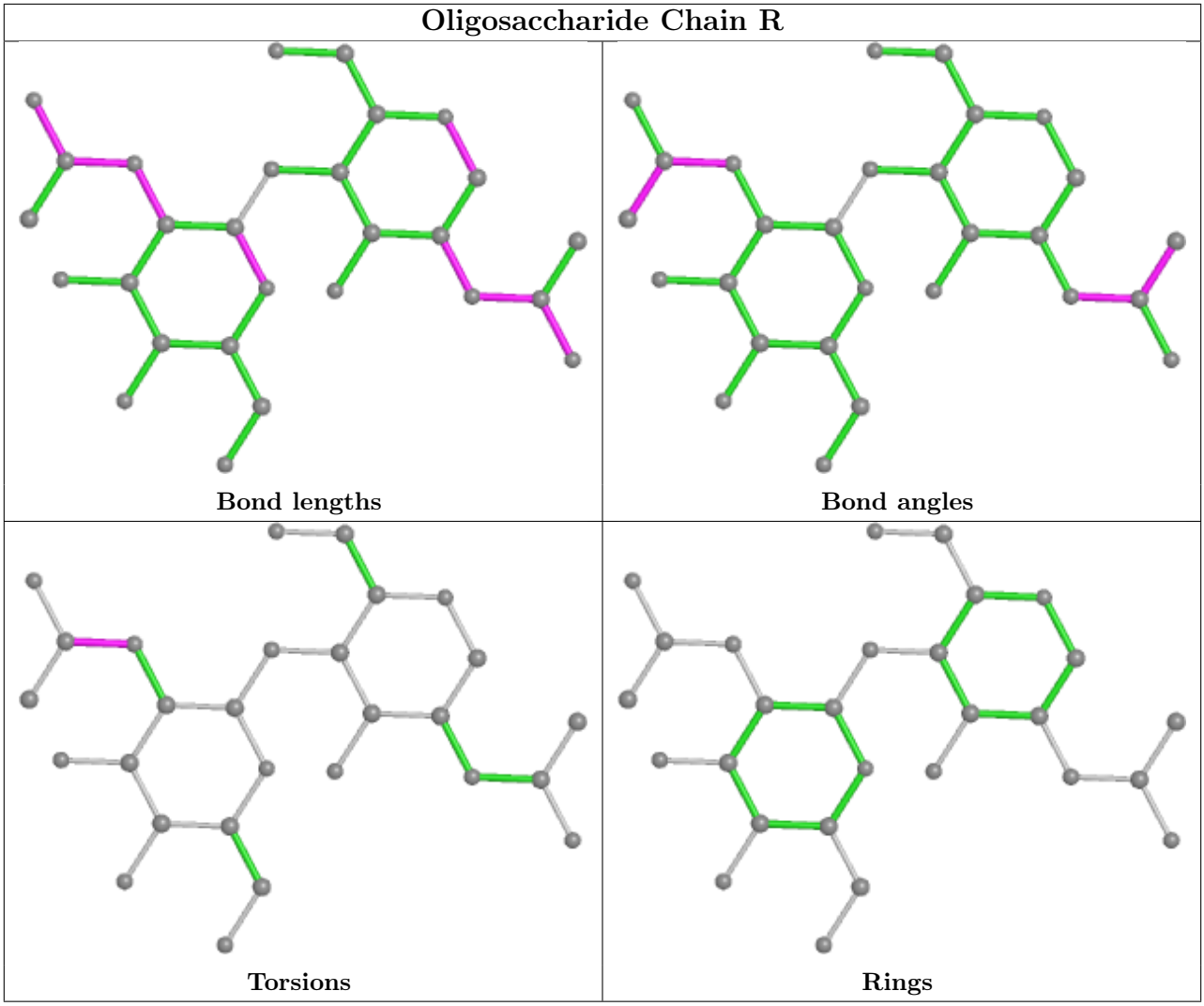
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

45 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	$\#\|Z\| > 2$
3	NAG	B	1614	1	14,14,15	2.14	4 (28%)	17,19,21	1.04	1 (5%)
3	NAG	B	1602	1	14,14,15	2.18	4 (28%)	17,19,21	1.13	1 (5%)
3	NAG	C	1610	1	14,14,15	2.17	4 (28%)	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1207	1	14,14,15	2.18	4 (28%)	17,19,21	1.01	1 (5%)
3	NAG	C	1609	1	14,14,15	2.17	4 (28%)	17,19,21	1.07	1 (5%)
4	BLA	A	1214	-	42,46,46	3.53	19 (45%)	53,67,67	1.83	10 (18%)
3	NAG	B	1611	1	14,14,15	2.19	4 (28%)	17,19,21	1.11	2 (11%)
3	NAG	A	1209	1	14,14,15	2.16	4 (28%)	17,19,21	0.97	1 (5%)
3	NAG	A	1204	1	14,14,15	2.17	4 (28%)	17,19,21	0.97	1 (5%)
5	EIC	C	1601	-	19,19,19	0.90	0	19,19,19	1.00	1 (5%)
3	NAG	C	1608	1	14,14,15	2.16	4 (28%)	17,19,21	1.01	1 (5%)
3	NAG	A	1202	1	14,14,15	2.18	4 (28%)	17,19,21	0.97	1 (5%)
3	NAG	C	1604	1	14,14,15	2.12	4 (28%)	17,19,21	1.09	2 (11%)
3	NAG	A	1208	1	14,14,15	2.16	4 (28%)	17,19,21	1.06	1 (5%)
3	NAG	A	1211	1	14,14,15	2.17	4 (28%)	17,19,21	0.94	1 (5%)
3	NAG	B	1610	1	14,14,15	2.16	4 (28%)	17,19,21	0.97	1 (5%)
4	BLA	B	1615	-	42,46,46	3.53	19 (45%)	53,67,67	1.83	10 (18%)
3	NAG	B	1612	1	14,14,15	2.16	4 (28%)	17,19,21	0.96	1 (5%)
3	NAG	B	1606	1	14,14,15	2.17	4 (28%)	17,19,21	1.03	1 (5%)
3	NAG	B	1604	1	14,14,15	2.13	4 (28%)	17,19,21	1.09	2 (11%)
3	NAG	A	1205	1	14,14,15	2.16	4 (28%)	17,19,21	1.02	1 (5%)
3	NAG	B	1605	1	14,14,15	2.16	4 (28%)	17,19,21	0.96	1 (5%)
3	NAG	A	1201	1	14,14,15	2.20	4 (28%)	17,19,21	1.11	1 (5%)
3	NAG	B	1607	1	14,14,15	2.17	4 (28%)	17,19,21	1.00	1 (5%)
3	NAG	A	1212	1	14,14,15	2.21	4 (28%)	17,19,21	1.21	2 (11%)
3	NAG	C	1614	1	14,14,15	2.14	4 (28%)	17,19,21	1.04	1 (5%)
3	NAG	B	1613	1	14,14,15	2.19	4 (28%)	17,19,21	1.23	2 (11%)
3	NAG	C	1602	1	14,14,15	2.19	4 (28%)	17,19,21	1.14	1 (5%)
3	NAG	C	1606	1	14,14,15	2.16	4 (28%)	17,19,21	1.02	1 (5%)
5	EIC	A	1215	-	19,19,19	0.87	0	19,19,19	0.93	1 (5%)
3	NAG	A	1210	1	14,14,15	2.20	4 (28%)	17,19,21	1.11	1 (5%)
3	NAG	B	1603	1	14,14,15	2.18	4 (28%)	17,19,21	0.97	1 (5%)
4	BLA	C	1615	-	42,46,46	3.53	19 (45%)	53,67,67	1.84	11 (20%)
3	NAG	C	1607	1	14,14,15	2.16	4 (28%)	17,19,21	0.96	1 (5%)
3	NAG	C	1612	1	14,14,15	2.16	4 (28%)	17,19,21	0.94	1 (5%)
3	NAG	B	1608	1	14,14,15	2.17	4 (28%)	17,19,21	1.01	1 (5%)
5	EIC	B	1601	-	19,19,19	0.88	0	19,19,19	0.96	1 (5%)
3	NAG	C	1605	1	14,14,15	2.16	4 (28%)	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1213	1	14,14,15	2.14	4 (28%)	17,19,21	1.04	1 (5%)
3	NAG	C	1611	1	14,14,15	2.19	4 (28%)	17,19,21	1.12	1 (5%)
3	NAG	B	1609	1	14,14,15	2.18	4 (28%)	17,19,21	1.06	1 (5%)
3	NAG	C	1613	1	14,14,15	2.20	4 (28%)	17,19,21	1.23	2 (11%)
3	NAG	A	1203	1	14,14,15	2.12	4 (28%)	17,19,21	1.09	2 (11%)
3	NAG	A	1206	1	14,14,15	2.17	4 (28%)	17,19,21	0.98	1 (5%)
3	NAG	C	1603	1	14,14,15	2.17	4 (28%)	17,19,21	0.97	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
3	NAG	B	1614	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1602	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1610	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1207	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1609	1	-	0/6/23/26	0/1/1/1
4	BLA	A	1214	-	-	14/26/74/74	0/4/4/4
3	NAG	B	1611	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1209	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
5	EIC	C	1601	-	-	8/17/17/17	-
3	NAG	C	1608	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1208	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1211	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1610	1	-	2/6/23/26	0/1/1/1
4	BLA	B	1615	-	-	14/26/74/74	0/4/4/4
3	NAG	B	1612	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1606	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1605	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1201	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1607	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1212	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1614	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1613	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1602	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1606	1	-	2/6/23/26	0/1/1/1
5	EIC	A	1215	-	-	8/17/17/17	-
3	NAG	A	1210	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1603	1	-	2/6/23/26	0/1/1/1
4	BLA	C	1615	-	-	14/26/74/74	0/4/4/4
3	NAG	C	1607	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1612	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1608	1	-	0/6/23/26	0/1/1/1
5	EIC	B	1601	-	-	8/17/17/17	-
3	NAG	C	1605	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1213	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1611	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1609	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1613	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1206	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1603	1	-	2/6/23/26	0/1/1/1

All (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1615	BLA	C4C-NC	9.73	1.54	1.37
4	A	1214	BLA	C4C-NC	9.72	1.54	1.37
4	B	1615	BLA	C4C-NC	9.71	1.54	1.37
4	A	1214	BLA	C1B-NB	9.66	1.54	1.37
4	C	1615	BLA	C1B-NB	9.63	1.53	1.37
4	B	1615	BLA	C1B-NB	9.62	1.53	1.37
4	C	1615	BLA	C4B-NB	7.30	1.53	1.38
4	A	1214	BLA	C4B-NB	7.28	1.53	1.38
4	B	1615	BLA	C4B-NB	7.26	1.53	1.38
4	A	1214	BLA	C1C-NC	7.26	1.53	1.38
4	B	1615	BLA	C1C-NC	7.23	1.53	1.38
4	C	1615	BLA	C1C-NC	7.19	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	NAG	O5-C1	5.55	1.52	1.43
4	A	1214	BLA	C4D-ND	5.54	1.50	1.38
4	B	1615	BLA	C4D-ND	5.53	1.50	1.38
3	C	1613	NAG	O5-C1	5.51	1.52	1.43
3	C	1602	NAG	O5-C1	5.50	1.52	1.43
3	A	1212	NAG	O5-C1	5.50	1.52	1.43
4	C	1615	BLA	C4D-ND	5.49	1.50	1.38
3	B	1602	NAG	O5-C1	5.47	1.52	1.43
3	B	1613	NAG	O5-C1	5.46	1.52	1.43
3	A	1210	NAG	O5-C1	5.35	1.52	1.43
3	B	1603	NAG	O5-C1	5.35	1.52	1.43
3	A	1202	NAG	O5-C1	5.35	1.52	1.43
3	A	1207	NAG	O5-C1	5.35	1.52	1.43
3	C	1603	NAG	O5-C1	5.34	1.52	1.43
3	B	1611	NAG	O5-C1	5.33	1.52	1.43
3	B	1607	NAG	O5-C1	5.33	1.52	1.43
3	C	1611	NAG	O5-C1	5.33	1.52	1.43
3	C	1605	NAG	O5-C1	5.32	1.52	1.43
3	B	1606	NAG	O5-C1	5.32	1.52	1.43
4	A	1214	BLA	CHD-C1D	5.31	1.52	1.40
3	B	1608	NAG	O5-C1	5.30	1.52	1.43
3	A	1204	NAG	O5-C1	5.30	1.52	1.43
3	A	1206	NAG	O5-C1	5.30	1.52	1.43
3	C	1612	NAG	O5-C1	5.30	1.52	1.43
3	B	1605	NAG	O5-C1	5.29	1.52	1.43
4	B	1615	BLA	CHD-C1D	5.29	1.52	1.40
3	C	1608	NAG	O5-C1	5.29	1.52	1.43
3	A	1211	NAG	O5-C1	5.28	1.52	1.43
3	C	1610	NAG	O5-C1	5.28	1.52	1.43
3	C	1606	NAG	O5-C1	5.28	1.52	1.43
4	C	1615	BLA	CHD-C1D	5.28	1.52	1.40
3	B	1612	NAG	O5-C1	5.27	1.52	1.43
4	B	1615	BLA	C3D-C2D	5.27	1.47	1.36
3	C	1607	NAG	O5-C1	5.27	1.52	1.43
3	A	1205	NAG	O5-C1	5.27	1.52	1.43
3	B	1614	NAG	O5-C1	5.26	1.52	1.43
4	C	1615	BLA	C3D-C2D	5.26	1.47	1.36
3	A	1213	NAG	O5-C1	5.25	1.52	1.43
3	B	1610	NAG	O5-C1	5.25	1.52	1.43
4	A	1214	BLA	C3D-C2D	5.25	1.47	1.36
3	A	1209	NAG	O5-C1	5.24	1.52	1.43
3	B	1609	NAG	O5-C1	5.22	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1614	NAG	O5-C1	5.20	1.52	1.43
3	C	1609	NAG	O5-C1	5.17	1.52	1.43
3	B	1604	NAG	O5-C1	5.17	1.52	1.43
3	A	1208	NAG	O5-C1	5.16	1.52	1.43
3	A	1203	NAG	O5-C1	5.13	1.51	1.43
3	C	1604	NAG	O5-C1	5.12	1.51	1.43
4	C	1615	BLA	C4D-C3D	5.08	1.53	1.45
4	A	1214	BLA	C4D-C3D	5.03	1.53	1.45
4	B	1615	BLA	C4D-C3D	5.00	1.53	1.45
4	C	1615	BLA	C1D-ND	4.61	1.47	1.36
4	B	1615	BLA	C1D-ND	4.59	1.47	1.36
4	A	1214	BLA	C1D-ND	4.56	1.47	1.36
3	A	1208	NAG	C7-N2	4.00	1.48	1.34
3	B	1609	NAG	C7-N2	3.99	1.48	1.34
3	C	1611	NAG	C7-N2	3.99	1.48	1.34
3	A	1210	NAG	C7-N2	3.99	1.48	1.34
3	C	1609	NAG	C7-N2	3.99	1.48	1.34
3	B	1611	NAG	C7-N2	3.97	1.48	1.34
3	C	1614	NAG	C7-N2	3.96	1.48	1.34
3	A	1209	NAG	C7-N2	3.96	1.48	1.34
3	B	1613	NAG	C7-N2	3.96	1.48	1.34
3	A	1204	NAG	C7-N2	3.96	1.48	1.34
3	C	1610	NAG	C7-N2	3.96	1.47	1.34
3	A	1211	NAG	C7-N2	3.96	1.47	1.34
3	B	1605	NAG	C7-N2	3.95	1.47	1.34
3	B	1610	NAG	C7-N2	3.95	1.47	1.34
3	A	1202	NAG	C7-N2	3.95	1.47	1.34
3	B	1607	NAG	C7-N2	3.95	1.47	1.34
3	B	1612	NAG	C7-N2	3.95	1.47	1.34
3	A	1213	NAG	C7-N2	3.95	1.47	1.34
3	A	1212	NAG	C7-N2	3.94	1.47	1.34
3	C	1605	NAG	C7-N2	3.94	1.47	1.34
3	B	1608	NAG	C7-N2	3.94	1.47	1.34
3	C	1603	NAG	C7-N2	3.94	1.47	1.34
3	A	1206	NAG	C7-N2	3.94	1.47	1.34
3	C	1612	NAG	C7-N2	3.94	1.47	1.34
3	C	1607	NAG	C7-N2	3.93	1.47	1.34
3	B	1603	NAG	C7-N2	3.93	1.47	1.34
3	C	1613	NAG	C7-N2	3.93	1.47	1.34
3	B	1604	NAG	C7-N2	3.92	1.47	1.34
3	B	1606	NAG	C7-N2	3.92	1.47	1.34
3	B	1614	NAG	C7-N2	3.92	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1608	NAG	C7-N2	3.92	1.47	1.34
3	C	1606	NAG	C7-N2	3.92	1.47	1.34
3	C	1604	NAG	C7-N2	3.91	1.47	1.34
3	A	1207	NAG	C7-N2	3.91	1.47	1.34
3	A	1205	NAG	C7-N2	3.91	1.47	1.34
3	A	1203	NAG	C7-N2	3.90	1.47	1.34
3	A	1201	NAG	C7-N2	3.90	1.47	1.34
3	C	1602	NAG	C7-N2	3.88	1.47	1.34
3	B	1602	NAG	C7-N2	3.88	1.47	1.34
4	B	1615	BLA	C1A-CHA	3.38	1.54	1.41
4	C	1615	BLA	C1A-CHA	3.38	1.54	1.41
4	A	1214	BLA	C1A-CHA	3.36	1.54	1.41
3	A	1212	NAG	C2-N2	3.27	1.51	1.46
3	B	1613	NAG	C2-N2	3.21	1.51	1.46
3	C	1613	NAG	C2-N2	3.20	1.51	1.46
3	B	1611	NAG	C2-N2	3.18	1.51	1.46
3	C	1609	NAG	C2-N2	3.17	1.51	1.46
3	B	1610	NAG	C2-N2	3.16	1.51	1.46
3	A	1210	NAG	C2-N2	3.16	1.51	1.46
4	A	1214	BLA	C4A-CHB	3.16	1.53	1.41
3	B	1609	NAG	C2-N2	3.16	1.51	1.46
3	C	1611	NAG	C2-N2	3.15	1.51	1.46
4	C	1615	BLA	C4A-CHB	3.14	1.53	1.41
3	B	1603	NAG	C2-N2	3.13	1.51	1.46
3	A	1209	NAG	C2-N2	3.13	1.51	1.46
4	B	1615	BLA	C4A-CHB	3.13	1.53	1.41
3	C	1612	NAG	C2-N2	3.12	1.51	1.46
3	C	1610	NAG	C2-N2	3.12	1.51	1.46
3	A	1208	NAG	C2-N2	3.11	1.51	1.46
4	A	1214	BLA	CHA-C4D	-3.11	1.32	1.35
3	A	1207	NAG	C2-N2	3.10	1.51	1.46
3	B	1605	NAG	C2-N2	3.10	1.51	1.46
3	A	1202	NAG	C2-N2	3.09	1.51	1.46
3	A	1205	NAG	C2-N2	3.08	1.51	1.46
3	A	1211	NAG	C2-N2	3.08	1.51	1.46
3	C	1607	NAG	C2-N2	3.08	1.51	1.46
3	A	1206	NAG	C2-N2	3.08	1.51	1.46
3	B	1612	NAG	C2-N2	3.08	1.51	1.46
3	C	1614	NAG	C2-N2	3.07	1.51	1.46
4	C	1615	BLA	CHA-C4D	-3.07	1.32	1.35
3	B	1614	NAG	C2-N2	3.07	1.51	1.46
3	C	1605	NAG	C2-N2	3.07	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1606	NAG	C2-N2	3.07	1.51	1.46
3	A	1204	NAG	C2-N2	3.06	1.51	1.46
3	C	1603	NAG	C2-N2	3.06	1.51	1.46
3	A	1213	NAG	C2-N2	3.06	1.51	1.46
4	B	1615	BLA	CHA-C4D	-3.06	1.32	1.35
3	C	1608	NAG	C2-N2	3.06	1.51	1.46
3	B	1608	NAG	C2-N2	3.05	1.51	1.46
3	B	1607	NAG	C2-N2	3.04	1.51	1.46
3	C	1606	NAG	C2-N2	3.04	1.51	1.46
3	C	1602	NAG	C2-N2	3.03	1.51	1.46
3	B	1602	NAG	C2-N2	3.01	1.51	1.46
3	A	1203	NAG	C2-N2	2.99	1.51	1.46
3	C	1604	NAG	C2-N2	2.98	1.51	1.46
3	A	1201	NAG	C2-N2	2.97	1.51	1.46
3	B	1604	NAG	C2-N2	2.96	1.51	1.46
4	C	1615	BLA	OC-C1C	-2.85	1.18	1.23
4	A	1214	BLA	OC-C1C	-2.85	1.18	1.23
4	B	1615	BLA	OC-C1C	-2.80	1.18	1.23
4	C	1615	BLA	OB-C4B	-2.66	1.18	1.23
4	A	1214	BLA	OB-C4B	-2.62	1.18	1.23
4	B	1615	BLA	OB-C4B	-2.57	1.18	1.23
4	A	1214	BLA	C1B-C2B	2.53	1.49	1.45
4	B	1615	BLA	C1B-C2B	2.51	1.49	1.45
4	C	1615	BLA	C1B-C2B	2.51	1.49	1.45
4	C	1615	BLA	C3B-C2B	2.49	1.42	1.37
4	B	1615	BLA	C3B-C2B	2.49	1.42	1.37
4	A	1214	BLA	C3B-C2B	2.48	1.42	1.37
4	B	1615	BLA	C3C-C2C	2.47	1.42	1.37
4	A	1214	BLA	C3C-C2C	2.43	1.42	1.37
4	C	1615	BLA	C3C-C2C	2.41	1.42	1.37
4	C	1615	BLA	CHD-C4C	-2.40	1.32	1.38
4	A	1214	BLA	CHD-C4C	-2.38	1.32	1.38
4	B	1615	BLA	CHD-C4C	-2.38	1.32	1.38
4	C	1615	BLA	C3C-C4C	2.30	1.49	1.45
4	B	1615	BLA	C3C-C4C	2.24	1.49	1.45
4	A	1214	BLA	C3C-C4C	2.20	1.49	1.45
3	B	1609	NAG	O7-C7	-2.19	1.18	1.23
3	C	1609	NAG	O7-C7	-2.18	1.18	1.23
3	A	1210	NAG	O7-C7	-2.18	1.18	1.23
3	A	1208	NAG	O7-C7	-2.17	1.18	1.23
3	B	1607	NAG	O7-C7	-2.17	1.18	1.23
3	C	1608	NAG	O7-C7	-2.16	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1203	NAG	O7-C7	-2.16	1.18	1.23
3	C	1610	NAG	O7-C7	-2.16	1.18	1.23
3	B	1604	NAG	O7-C7	-2.16	1.18	1.23
3	C	1607	NAG	O7-C7	-2.16	1.18	1.23
3	A	1207	NAG	O7-C7	-2.16	1.18	1.23
3	A	1204	NAG	O7-C7	-2.15	1.18	1.23
3	C	1613	NAG	O7-C7	-2.15	1.18	1.23
3	A	1212	NAG	O7-C7	-2.15	1.18	1.23
3	B	1608	NAG	O7-C7	-2.14	1.18	1.23
3	B	1610	NAG	O7-C7	-2.14	1.18	1.23
3	B	1613	NAG	O7-C7	-2.14	1.18	1.23
3	A	1206	NAG	O7-C7	-2.14	1.18	1.23
3	B	1606	NAG	O7-C7	-2.14	1.18	1.23
3	C	1606	NAG	O7-C7	-2.13	1.18	1.23
3	B	1605	NAG	O7-C7	-2.13	1.18	1.23
3	C	1612	NAG	O7-C7	-2.13	1.18	1.23
3	C	1611	NAG	O7-C7	-2.13	1.18	1.23
3	B	1612	NAG	O7-C7	-2.13	1.18	1.23
3	A	1211	NAG	O7-C7	-2.13	1.18	1.23
3	A	1209	NAG	O7-C7	-2.13	1.18	1.23
3	A	1205	NAG	O7-C7	-2.13	1.18	1.23
3	C	1604	NAG	O7-C7	-2.12	1.18	1.23
3	B	1603	NAG	O7-C7	-2.12	1.18	1.23
3	A	1213	NAG	O7-C7	-2.12	1.18	1.23
3	C	1603	NAG	O7-C7	-2.12	1.18	1.23
3	A	1202	NAG	O7-C7	-2.11	1.18	1.23
3	C	1605	NAG	O7-C7	-2.11	1.18	1.23
3	C	1602	NAG	O7-C7	-2.11	1.18	1.23
3	B	1611	NAG	O7-C7	-2.11	1.18	1.23
3	C	1614	NAG	O7-C7	-2.11	1.18	1.23
3	A	1201	NAG	O7-C7	-2.10	1.18	1.23
3	B	1614	NAG	O7-C7	-2.09	1.18	1.23
3	B	1602	NAG	O7-C7	-2.08	1.18	1.23

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1615	BLA	C1A-CHA-C4D	-7.33	120.06	128.81
4	B	1615	BLA	C1A-CHA-C4D	-7.30	120.09	128.81
4	A	1214	BLA	C1A-CHA-C4D	-7.29	120.10	128.81
4	C	1615	BLA	C3D-C4D-ND	-3.94	104.32	110.05
4	A	1214	BLA	C3D-C4D-ND	-3.93	104.33	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1615	BLA	C3D-C4D-ND	-3.93	104.34	110.05
4	B	1615	BLA	C4C-CHD-C1D	-3.70	119.04	128.08
4	C	1615	BLA	C4C-CHD-C1D	-3.70	119.05	128.08
4	A	1214	BLA	C4C-CHD-C1D	-3.69	119.05	128.08
4	A	1214	BLA	C4C-NC-C1C	-2.56	107.41	110.67
5	C	1601	EIC	C11-C10-C9	-2.54	102.09	123.57
4	B	1615	BLA	C4C-NC-C1C	-2.53	107.44	110.67
4	C	1615	BLA	C4C-NC-C1C	-2.51	107.48	110.67
3	C	1609	NAG	C8-C7-N2	2.49	120.31	116.10
3	A	1208	NAG	C8-C7-N2	2.42	120.20	116.10
3	B	1609	NAG	C8-C7-N2	2.41	120.17	116.10
3	A	1212	NAG	C1-C2-N2	-2.38	106.42	110.49
4	A	1214	BLA	CHA-C4D-ND	-2.38	125.53	128.83
4	B	1615	BLA	CHA-C4D-ND	-2.37	125.54	128.83
4	A	1214	BLA	C1B-NB-C4B	-2.37	107.65	110.67
3	B	1613	NAG	C1-C2-N2	-2.36	106.45	110.49
4	B	1615	BLA	C1B-NB-C4B	-2.36	107.66	110.67
3	C	1604	NAG	C8-C7-N2	2.34	120.06	116.10
4	C	1615	BLA	C1B-NB-C4B	-2.34	107.69	110.67
4	C	1615	BLA	CHA-C4D-ND	-2.33	125.59	128.83
3	C	1613	NAG	C1-C2-N2	-2.33	106.50	110.49
3	B	1604	NAG	C8-C7-N2	2.33	120.04	116.10
4	A	1214	BLA	C4D-C3D-C2D	2.29	109.32	106.78
4	A	1214	BLA	C3B-C2B-C1B	2.28	110.78	108.03
4	B	1615	BLA	C4D-C3D-C2D	2.28	109.31	106.78
3	A	1203	NAG	C8-C7-N2	2.27	119.94	116.10
4	C	1615	BLA	C4D-C3D-C2D	2.27	109.30	106.78
4	C	1615	BLA	C3B-C2B-C1B	2.26	110.76	108.03
4	B	1615	BLA	C3B-C2B-C1B	2.25	110.74	108.03
4	C	1615	BLA	C4B-C3B-C2B	2.21	110.77	107.92
3	C	1605	NAG	C8-C7-N2	2.20	119.82	116.10
3	B	1608	NAG	C8-C7-N2	2.19	119.81	116.10
5	B	1601	EIC	C11-C10-C9	-2.19	105.09	123.57
3	C	1608	NAG	C8-C7-N2	2.19	119.80	116.10
4	B	1615	BLA	C4B-C3B-C2B	2.18	110.73	107.92
4	A	1214	BLA	C4B-C3B-C2B	2.17	110.72	107.92
3	B	1614	NAG	C8-C7-N2	2.17	119.78	116.10
3	B	1607	NAG	C8-C7-N2	2.17	119.77	116.10
3	A	1205	NAG	C8-C7-N2	2.16	119.76	116.10
3	A	1212	NAG	C8-C7-N2	2.16	119.75	116.10
3	A	1204	NAG	C8-C7-N2	2.16	119.75	116.10
3	A	1207	NAG	C8-C7-N2	2.15	119.75	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1605	NAG	C8-C7-N2	2.15	119.75	116.10
3	B	1606	NAG	C8-C7-N2	2.15	119.74	116.10
3	A	1206	NAG	C8-C7-N2	2.14	119.73	116.10
3	C	1606	NAG	C8-C7-N2	2.14	119.73	116.10
3	B	1613	NAG	C8-C7-N2	2.14	119.72	116.10
3	B	1612	NAG	C8-C7-N2	2.14	119.72	116.10
3	C	1613	NAG	C8-C7-N2	2.14	119.72	116.10
3	C	1614	NAG	C8-C7-N2	2.14	119.72	116.10
3	C	1607	NAG	C8-C7-N2	2.13	119.71	116.10
3	A	1213	NAG	C8-C7-N2	2.13	119.71	116.10
3	B	1602	NAG	C8-C7-N2	2.13	119.70	116.10
3	A	1211	NAG	C8-C7-N2	2.12	119.68	116.10
3	C	1602	NAG	C8-C7-N2	2.11	119.67	116.10
3	A	1201	NAG	C8-C7-N2	2.10	119.66	116.10
3	C	1612	NAG	C8-C7-N2	2.10	119.65	116.10
3	C	1603	NAG	C8-C7-N2	2.08	119.63	116.10
4	A	1214	BLA	CHA-C4D-C3D	2.08	130.13	125.32
4	B	1615	BLA	CHA-C4D-C3D	2.08	130.12	125.32
3	B	1604	NAG	C2-N2-C7	-2.07	119.95	122.90
4	C	1615	BLA	CHA-C4D-C3D	2.06	130.09	125.32
3	A	1203	NAG	C2-N2-C7	-2.06	119.97	122.90
3	B	1611	NAG	C8-C7-N2	2.06	119.59	116.10
3	C	1604	NAG	C2-N2-C7	-2.06	119.97	122.90
3	C	1611	NAG	C8-C7-N2	2.06	119.58	116.10
3	B	1603	NAG	C8-C7-N2	2.05	119.57	116.10
3	A	1202	NAG	C8-C7-N2	2.04	119.55	116.10
5	A	1215	EIC	C11-C10-C9	-2.03	106.40	123.57
3	A	1209	NAG	C8-C7-N2	2.03	119.53	116.10
3	A	1210	NAG	C8-C7-N2	2.02	119.53	116.10
3	B	1611	NAG	C1-O5-C5	2.02	114.93	112.19
3	B	1610	NAG	C8-C7-N2	2.02	119.52	116.10
4	C	1615	BLA	C4D-ND-C1D	2.01	110.30	106.51
3	C	1610	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1212	NAG	C1-C2-N2-C7
3	B	1613	NAG	C1-C2-N2-C7
3	C	1613	NAG	C1-C2-N2-C7
4	A	1214	BLA	NA-C1A-CHA-C4D

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Mol	Chain	Res	Type	Atoms
4	A	1214	BLA	C2A-C1A-CHA-C4D
4	A	1214	BLA	NA-C4A-CHB-C1B
4	A	1214	BLA	C3A-C4A-CHB-C1B
4	A	1214	BLA	C2C-C3C-CAC-CBC
4	A	1214	BLA	C4C-C3C-CAC-CBC
4	B	1615	BLA	NA-C1A-CHA-C4D
4	B	1615	BLA	C2A-C1A-CHA-C4D
4	B	1615	BLA	NA-C4A-CHB-C1B
4	B	1615	BLA	C3A-C4A-CHB-C1B
4	B	1615	BLA	C2C-C3C-CAC-CBC
4	B	1615	BLA	C4C-C3C-CAC-CBC
4	C	1615	BLA	NA-C1A-CHA-C4D
4	C	1615	BLA	C2A-C1A-CHA-C4D
4	C	1615	BLA	NA-C4A-CHB-C1B
4	C	1615	BLA	C3A-C4A-CHB-C1B
4	C	1615	BLA	C2C-C3C-CAC-CBC
4	C	1615	BLA	C4C-C3C-CAC-CBC
3	C	1612	NAG	O5-C5-C6-O6
3	A	1211	NAG	O5-C5-C6-O6
3	B	1612	NAG	O5-C5-C6-O6
3	A	1213	NAG	O5-C5-C6-O6
3	C	1607	NAG	O5-C5-C6-O6
3	C	1614	NAG	O5-C5-C6-O6
3	B	1614	NAG	O5-C5-C6-O6
3	A	1206	NAG	O5-C5-C6-O6
3	B	1607	NAG	O5-C5-C6-O6
3	B	1610	NAG	O5-C5-C6-O6
3	A	1209	NAG	O5-C5-C6-O6
3	A	1210	NAG	O5-C5-C6-O6
3	B	1611	NAG	O5-C5-C6-O6
3	C	1606	NAG	O5-C5-C6-O6
3	C	1611	NAG	O5-C5-C6-O6
3	A	1205	NAG	O5-C5-C6-O6
3	B	1606	NAG	O5-C5-C6-O6
3	C	1610	NAG	O5-C5-C6-O6
3	A	1209	NAG	C4-C5-C6-O6
3	B	1610	NAG	C4-C5-C6-O6
3	A	1213	NAG	C4-C5-C6-O6
3	C	1610	NAG	C4-C5-C6-O6
3	A	1211	NAG	C4-C5-C6-O6
3	B	1614	NAG	C4-C5-C6-O6
3	C	1612	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1614	NAG	C4-C5-C6-O6
3	A	1204	NAG	O5-C5-C6-O6
3	B	1605	NAG	O5-C5-C6-O6
3	C	1605	NAG	O5-C5-C6-O6
3	C	1607	NAG	C4-C5-C6-O6
3	A	1206	NAG	C4-C5-C6-O6
3	B	1607	NAG	C4-C5-C6-O6
3	B	1612	NAG	C4-C5-C6-O6
3	B	1603	NAG	C4-C5-C6-O6
3	B	1605	NAG	C4-C5-C6-O6
3	C	1603	NAG	C4-C5-C6-O6
3	B	1611	NAG	C4-C5-C6-O6
3	C	1611	NAG	C4-C5-C6-O6
3	A	1202	NAG	C4-C5-C6-O6
3	A	1204	NAG	C4-C5-C6-O6
3	A	1205	NAG	C4-C5-C6-O6
3	A	1210	NAG	C4-C5-C6-O6
3	B	1606	NAG	C4-C5-C6-O6
3	C	1605	NAG	C4-C5-C6-O6
3	C	1606	NAG	C4-C5-C6-O6
3	B	1603	NAG	O5-C5-C6-O6
3	C	1603	NAG	O5-C5-C6-O6
5	A	1215	EIC	C6-C7-C8-C9
5	B	1601	EIC	C6-C7-C8-C9
5	C	1601	EIC	C6-C7-C8-C9
3	A	1202	NAG	O5-C5-C6-O6
5	A	1215	EIC	C13-C14-C15-C16
5	B	1601	EIC	C13-C14-C15-C16
5	C	1601	EIC	C13-C14-C15-C16
4	A	1214	BLA	C4B-C3B-CAB-CBB
4	B	1615	BLA	C4B-C3B-CAB-CBB
4	C	1615	BLA	C4B-C3B-CAB-CBB
4	A	1214	BLA	C2B-C3B-CAB-CBB
4	B	1615	BLA	C2B-C3B-CAB-CBB
4	C	1615	BLA	C2B-C3B-CAB-CBB
3	B	1613	NAG	C4-C5-C6-O6
5	A	1215	EIC	C9-C10-C11-C12
5	B	1601	EIC	C9-C10-C11-C12
5	C	1601	EIC	C9-C10-C11-C12
3	A	1212	NAG	C4-C5-C6-O6
3	C	1613	NAG	C4-C5-C6-O6
5	A	1215	EIC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	B	1601	EIC	C2-C3-C4-C5
5	C	1601	EIC	C2-C3-C4-C5
4	A	1214	BLA	ND-C4D-CHA-C1A
4	B	1615	BLA	ND-C4D-CHA-C1A
4	C	1615	BLA	ND-C4D-CHA-C1A
5	B	1601	EIC	C14-C15-C16-C17
5	C	1601	EIC	C14-C15-C16-C17
5	A	1215	EIC	C14-C15-C16-C17
3	A	1212	NAG	C3-C2-N2-C7
3	B	1613	NAG	C3-C2-N2-C7
3	C	1613	NAG	C3-C2-N2-C7
4	B	1615	BLA	CAD-CBD-CGD-O1D
4	C	1615	BLA	CAD-CBD-CGD-O1D
4	A	1214	BLA	CAD-CBD-CGD-O1D
4	C	1615	BLA	CAD-CBD-CGD-O2D
4	A	1214	BLA	CAD-CBD-CGD-O2D
4	B	1615	BLA	CAD-CBD-CGD-O2D
5	B	1601	EIC	O2-C1-C2-C3
4	A	1214	BLA	ND-C1D-CHD-C4C
4	B	1615	BLA	ND-C1D-CHD-C4C
4	C	1615	BLA	ND-C1D-CHD-C4C
5	A	1215	EIC	O2-C1-C2-C3
5	C	1601	EIC	O2-C1-C2-C3
5	B	1601	EIC	O1-C1-C2-C3
5	C	1601	EIC	O1-C1-C2-C3
3	B	1613	NAG	O5-C5-C6-O6
5	A	1215	EIC	O1-C1-C2-C3
4	C	1615	BLA	CAA-CBA-CGA-O2A
4	A	1214	BLA	CAA-CBA-CGA-O2A
4	B	1615	BLA	CAA-CBA-CGA-O2A
5	A	1215	EIC	C12-C13-C14-C15
5	B	1601	EIC	C12-C13-C14-C15
5	C	1601	EIC	C12-C13-C14-C15
4	A	1214	BLA	CAA-CBA-CGA-O1A
4	B	1615	BLA	CAA-CBA-CGA-O1A
4	C	1615	BLA	CAA-CBA-CGA-O1A

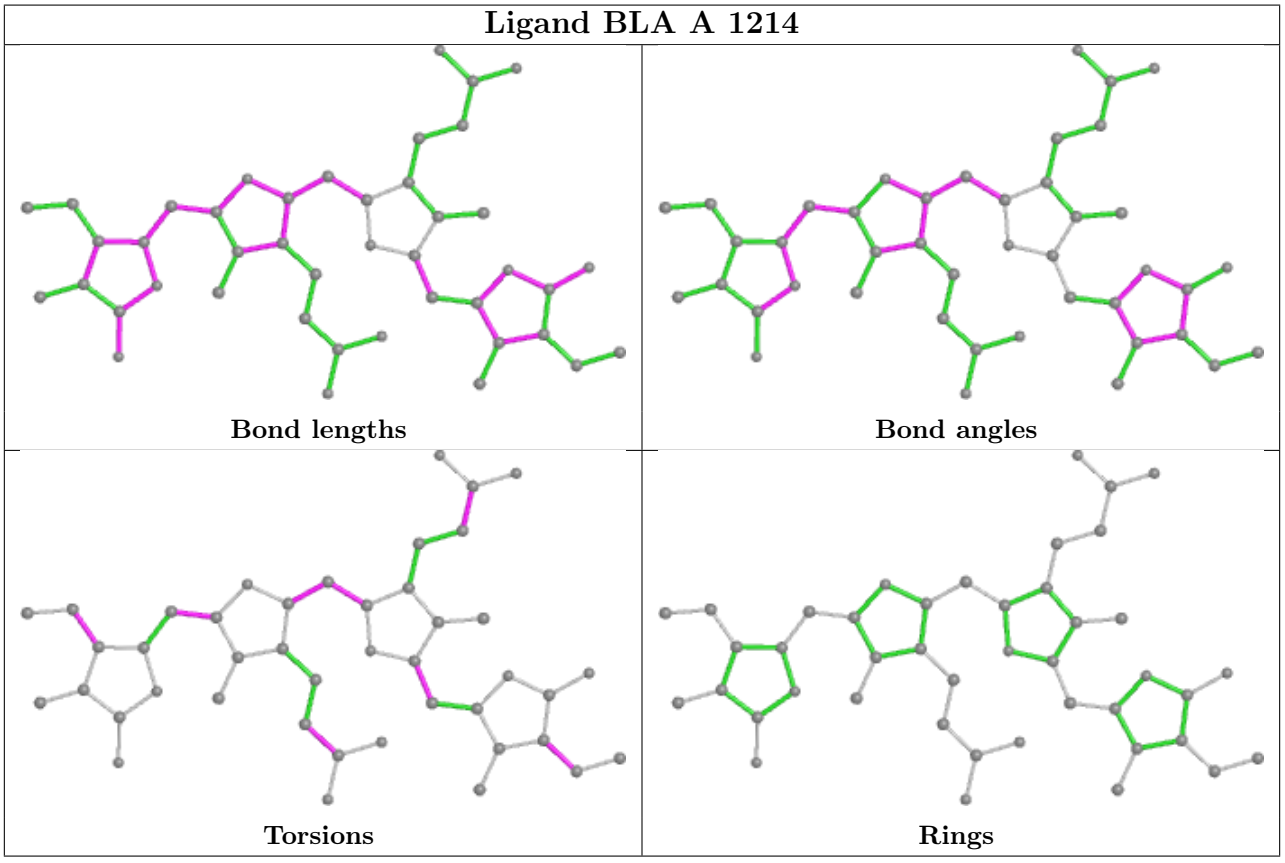
There are no ring outliers.

1 monomer is involved in 1 short contact:

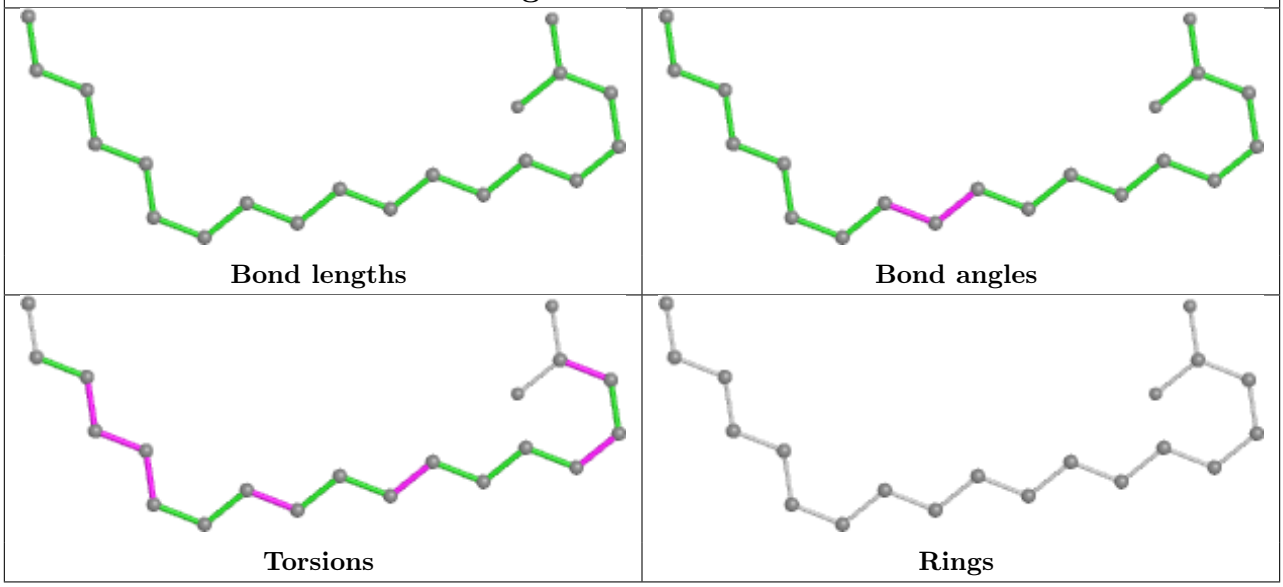
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1613	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

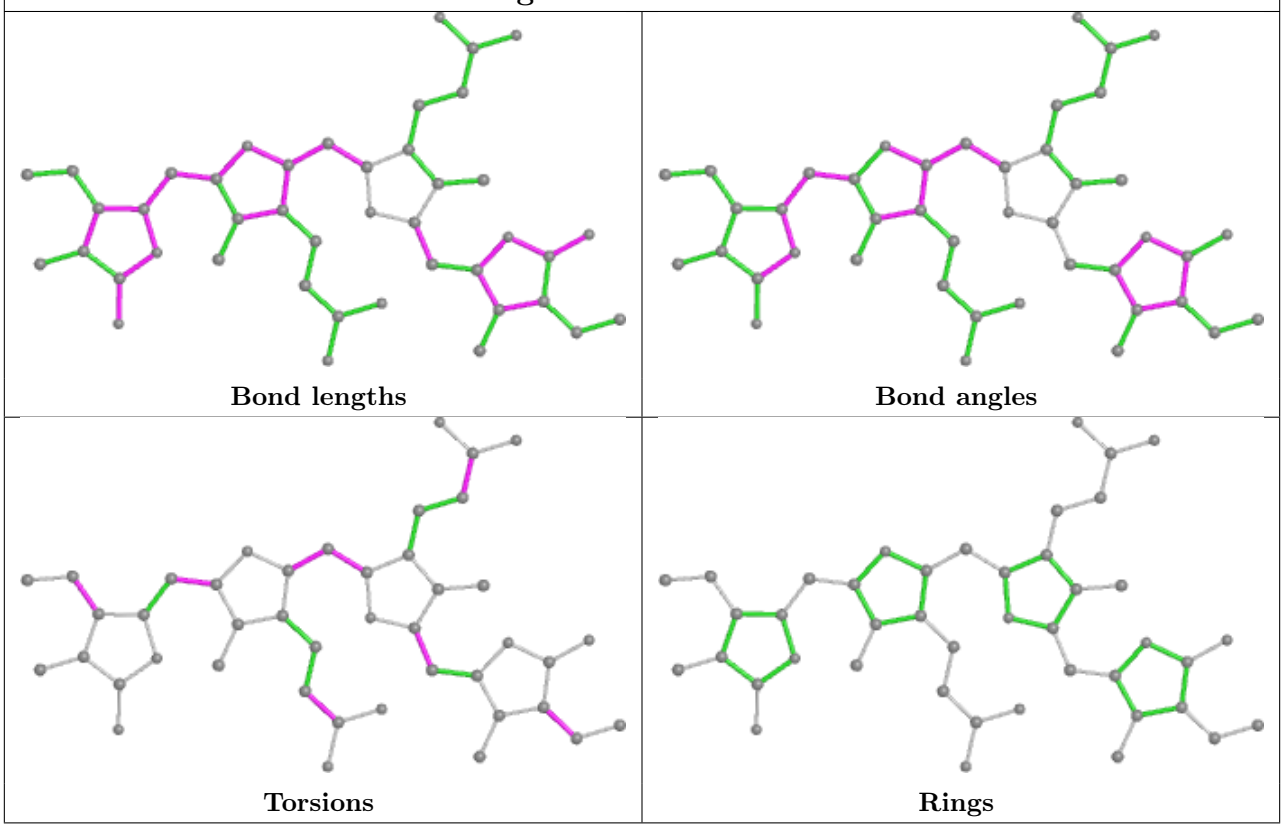
Ligand BLA A 1214



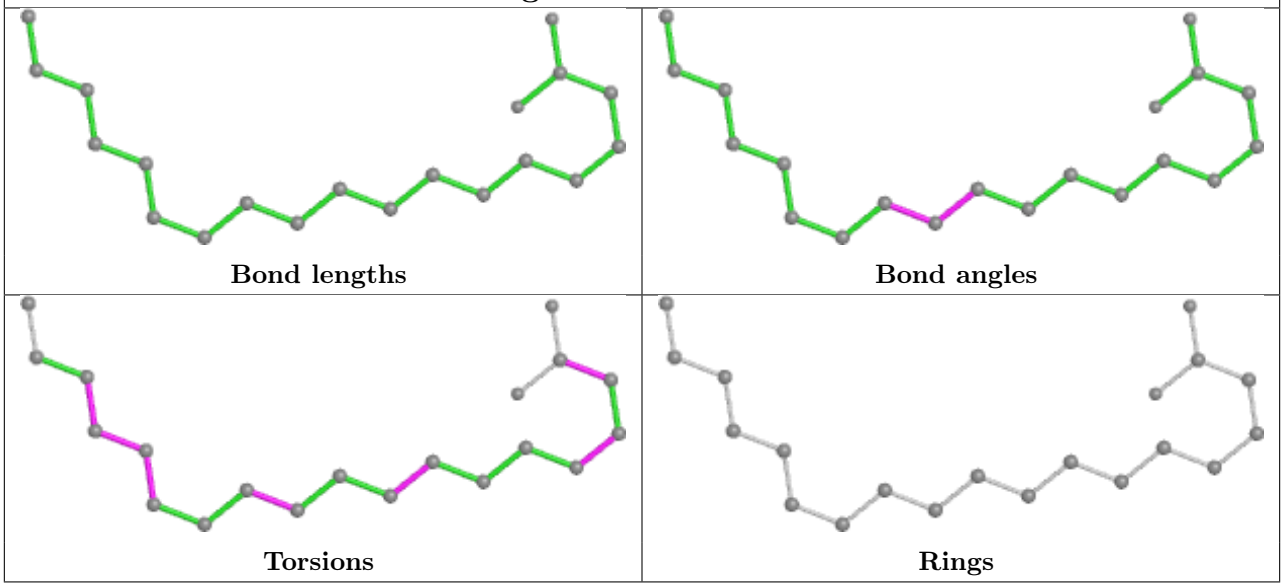
Ligand EIC C 1601



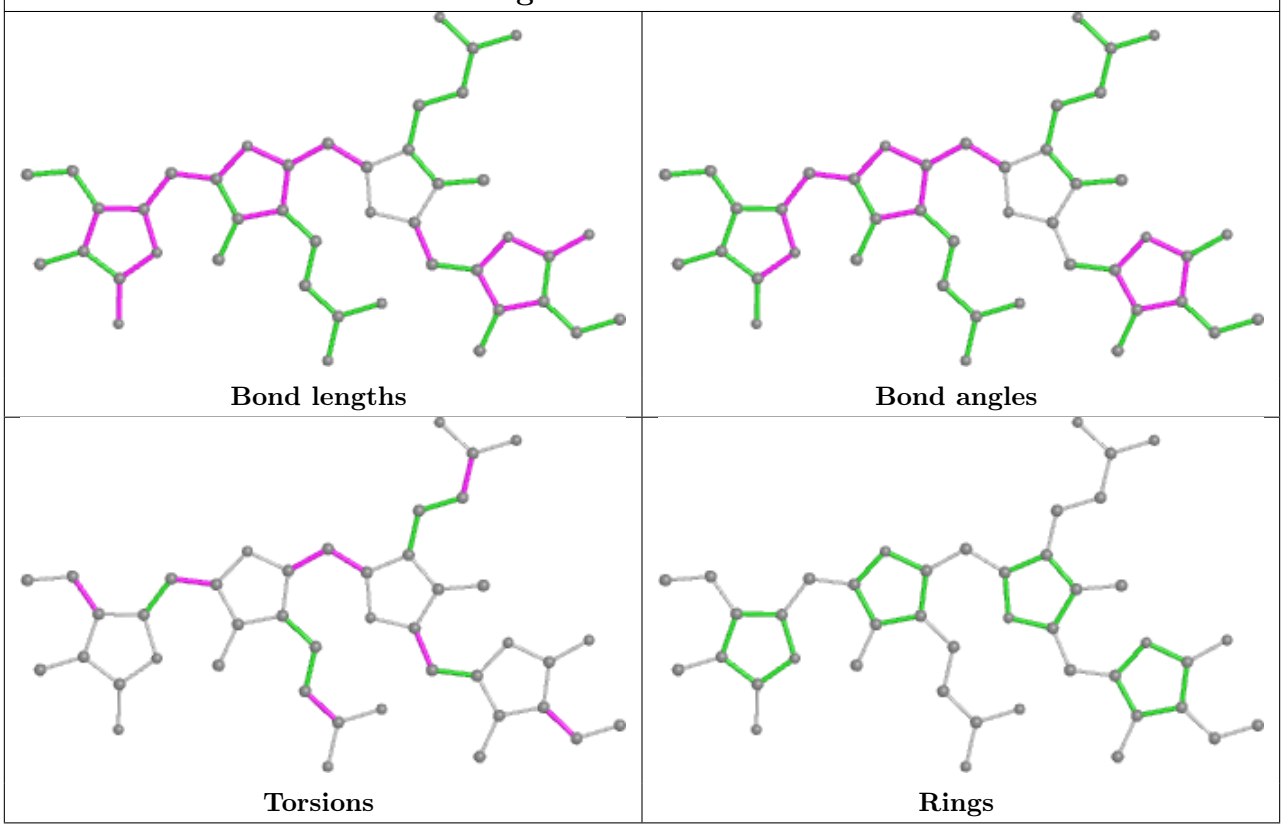
Ligand BLA B 1615



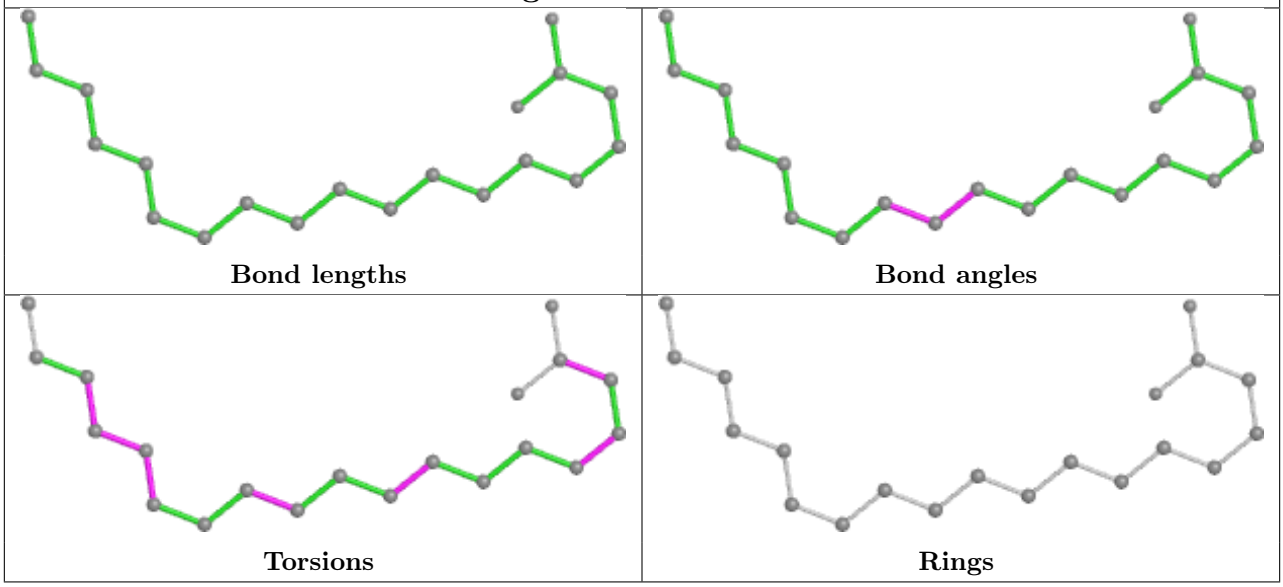
Ligand EIC A 1215



Ligand BLA C 1615



Ligand EIC B 1601



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.

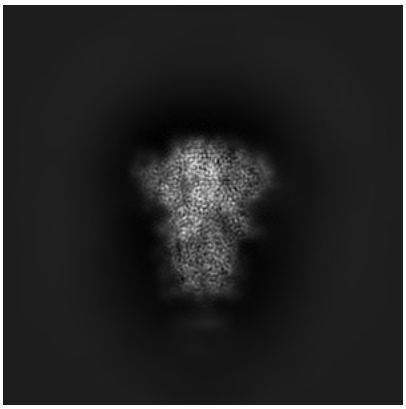
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33453. These allow visual inspection of the internal detail of the map and identification of artifacts.

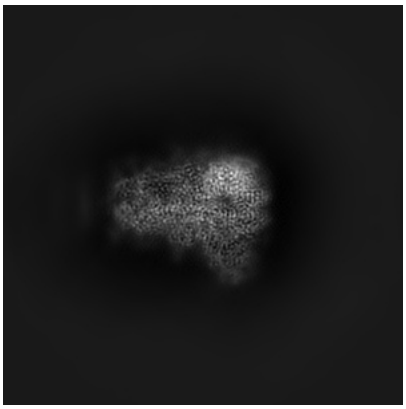
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

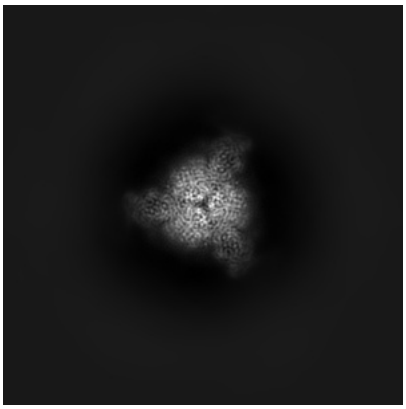
6.1.1 Primary map



X

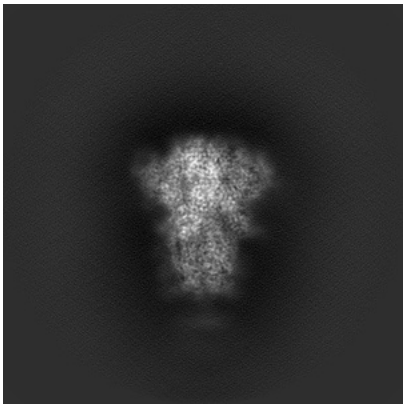


Y

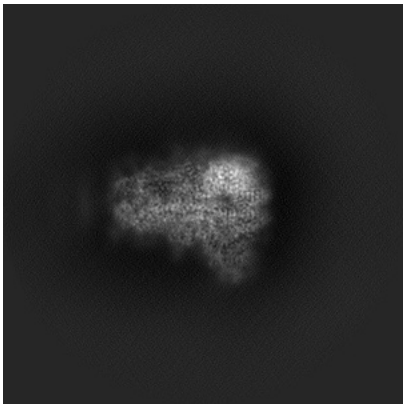


Z

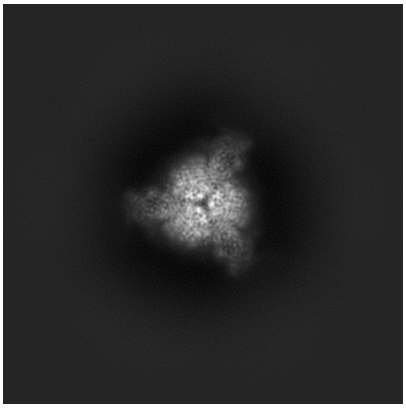
6.1.2 Raw map



X



Y



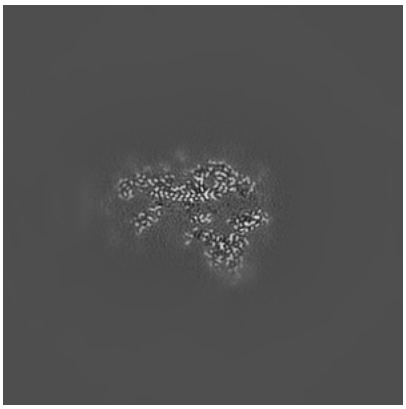
Z

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

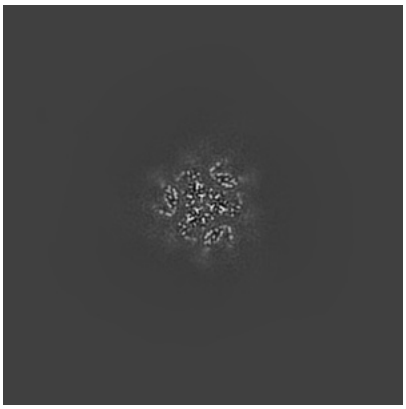
6.2 Central slices (i)

6.2.1 Primary map

X Index: 180

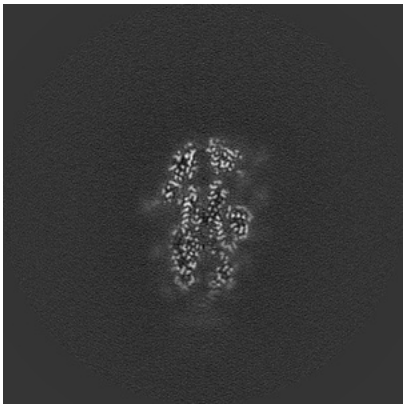


Y Index: 180

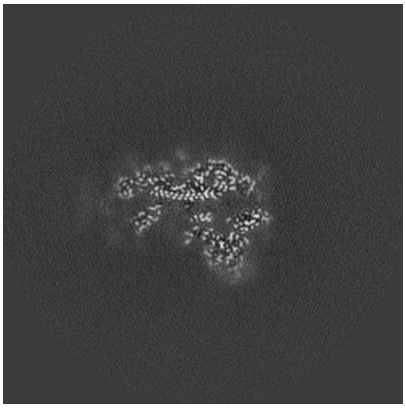


Z Index: 180

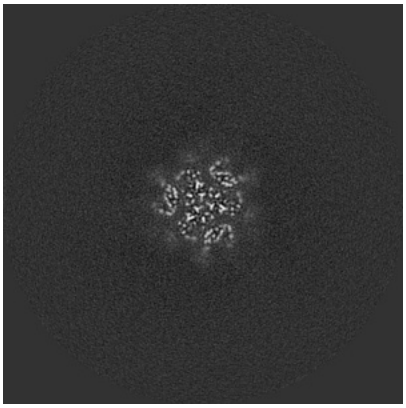
6.2.2 Raw map



X Index: 180



Y Index: 180

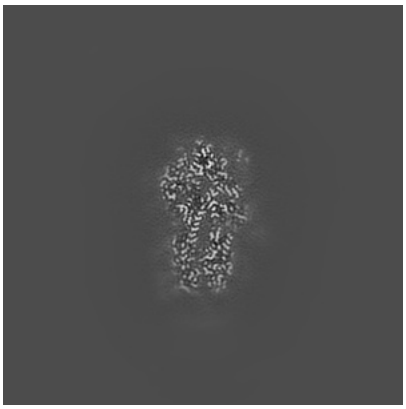


Z Index: 180

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

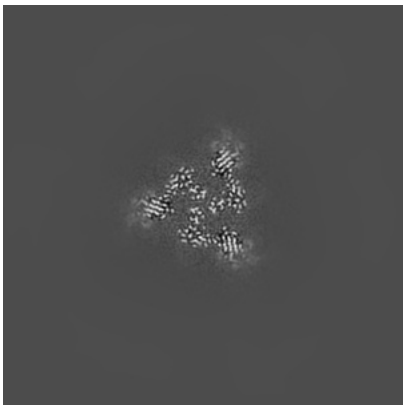
6.3 Largest variance slices (i)

6.3.1 Primary map



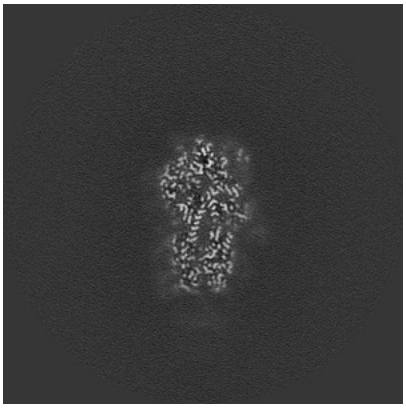
X Index: 169

Y Index: 186

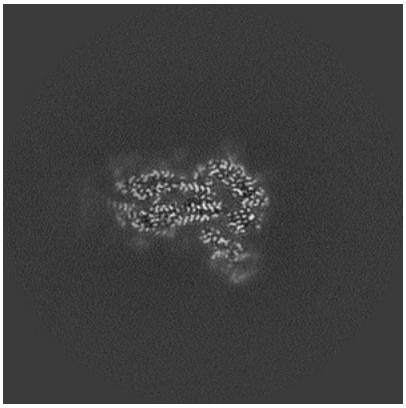


Z Index: 195

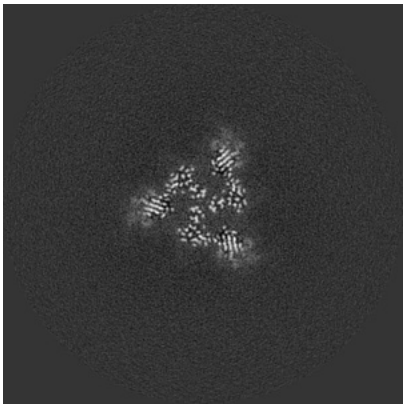
6.3.2 Raw map



X Index: 169



Y Index: 188

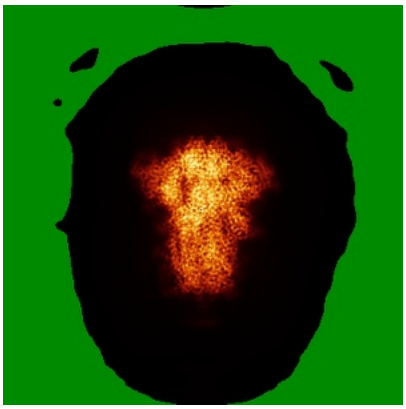


Z Index: 195

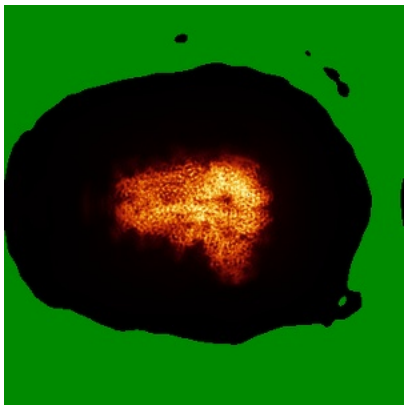
The images above show the largest variance slices of the map in three orthogonal directions.

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

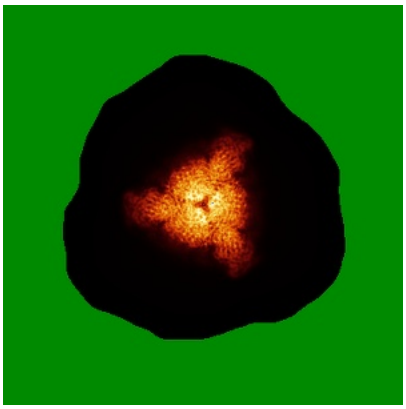
6.4.1 Primary map



X

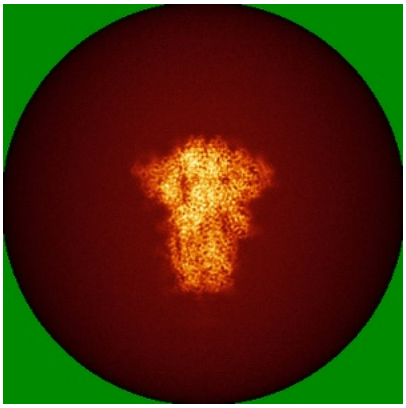


Y

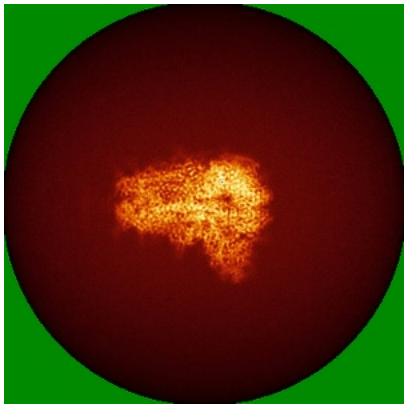


Z

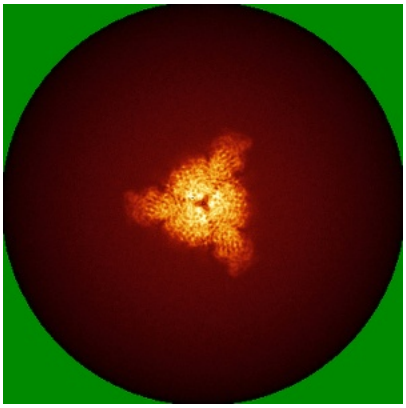
6.4.2 Raw map



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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

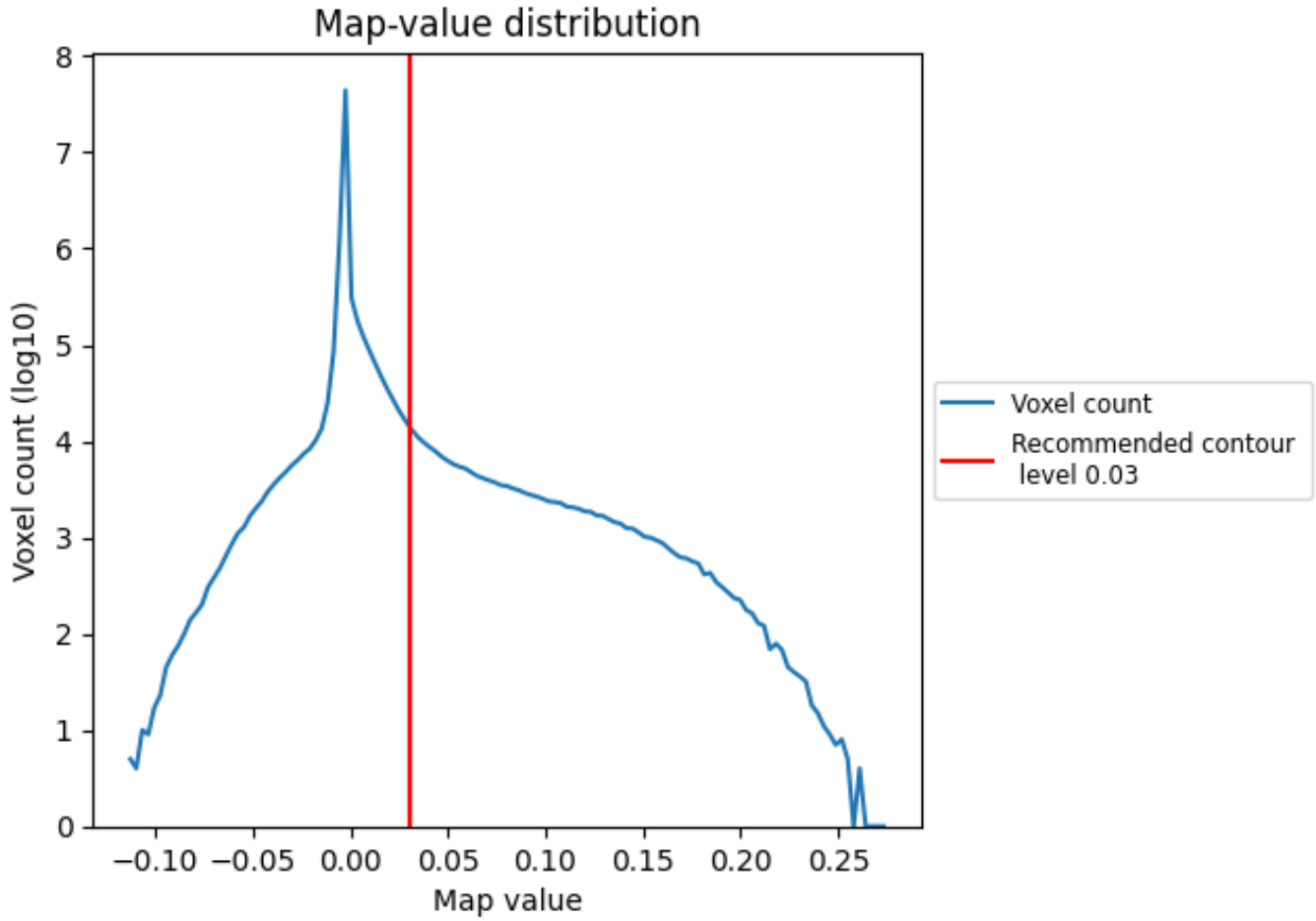
6.6 Mask visualisation (i)

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

7 Map analysis

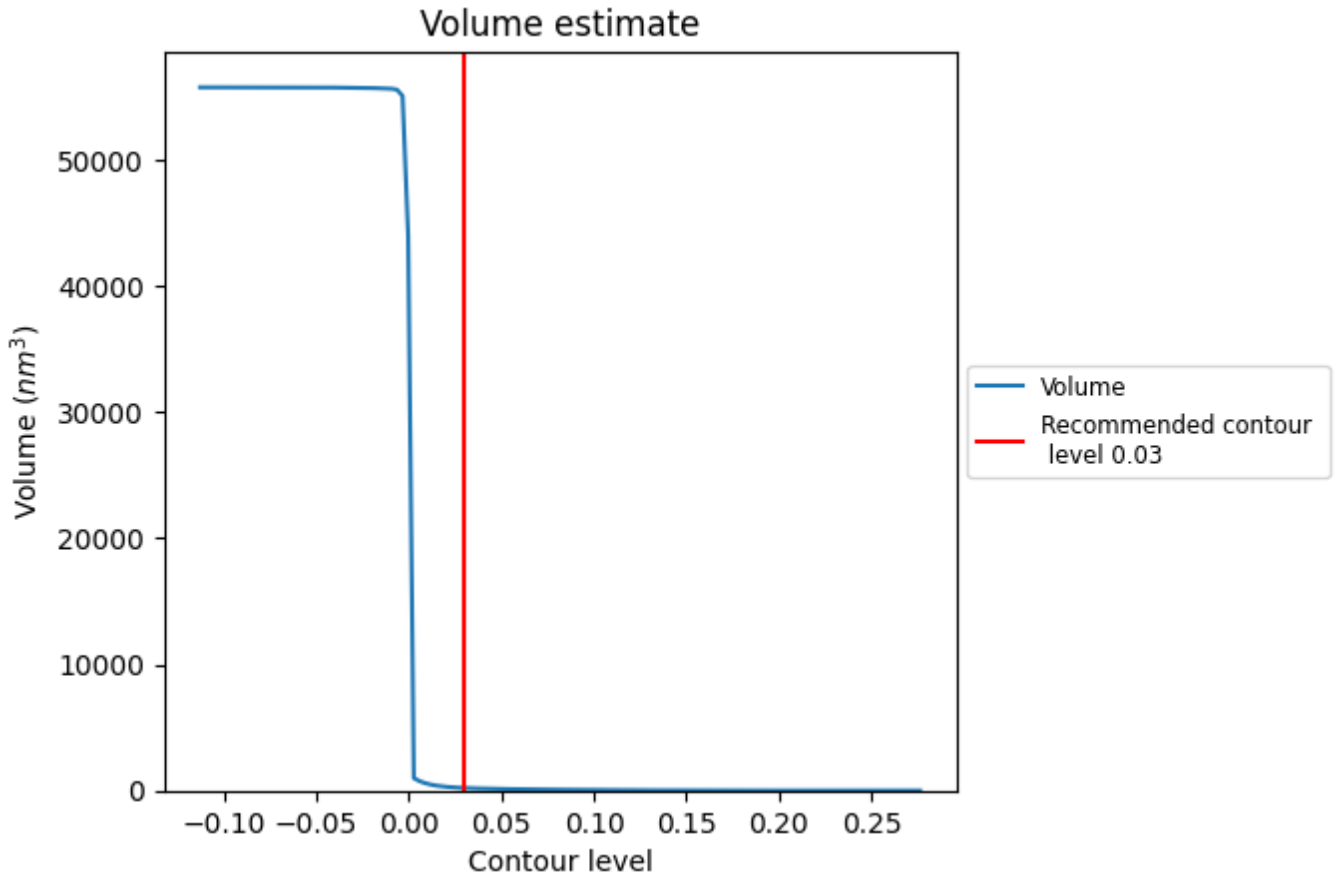
This section contains the results of statistical analysis of the map.

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.

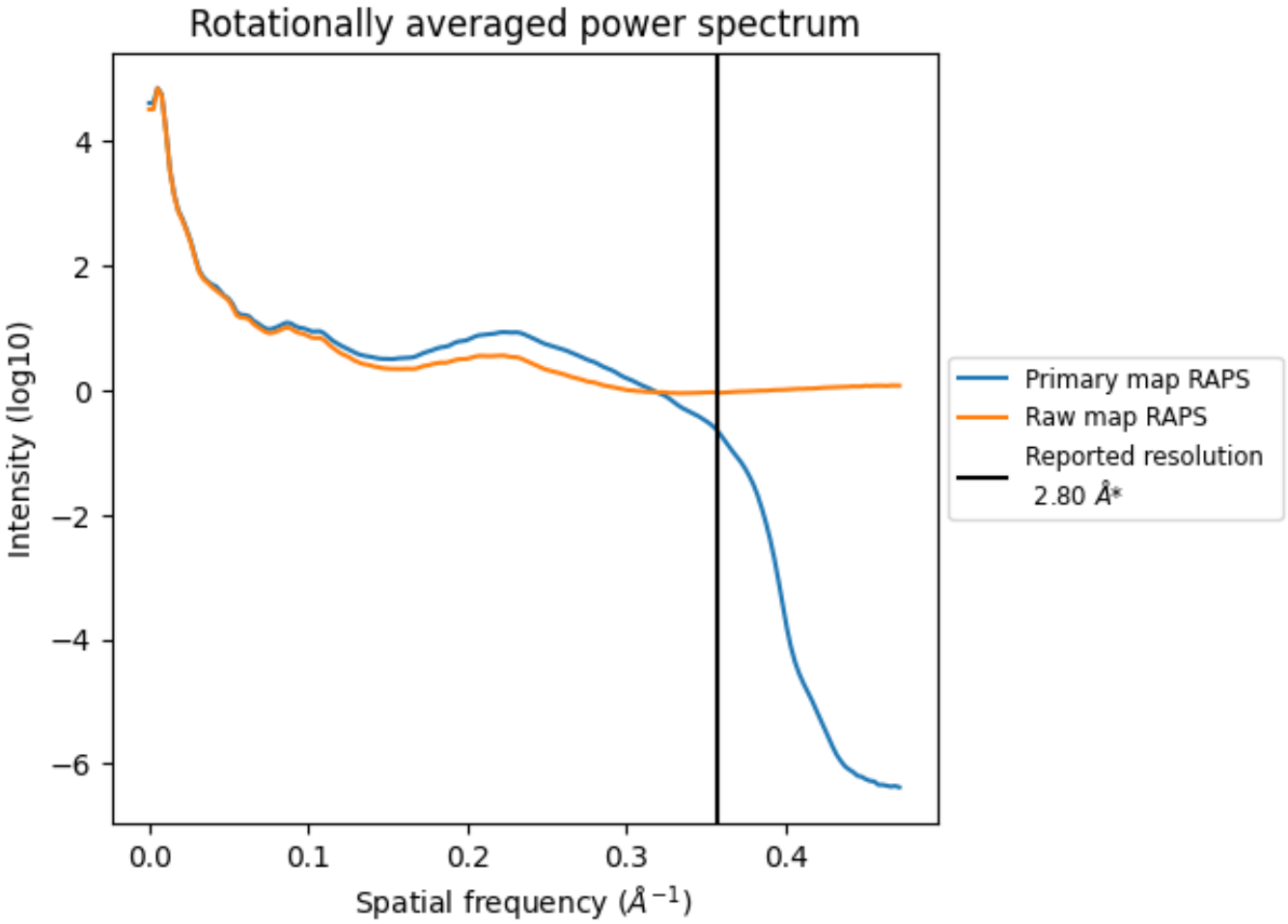
7.2 Volume estimate



The volume at the recommended contour level is 204 nm^3; this corresponds to an approximate mass of 184 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)

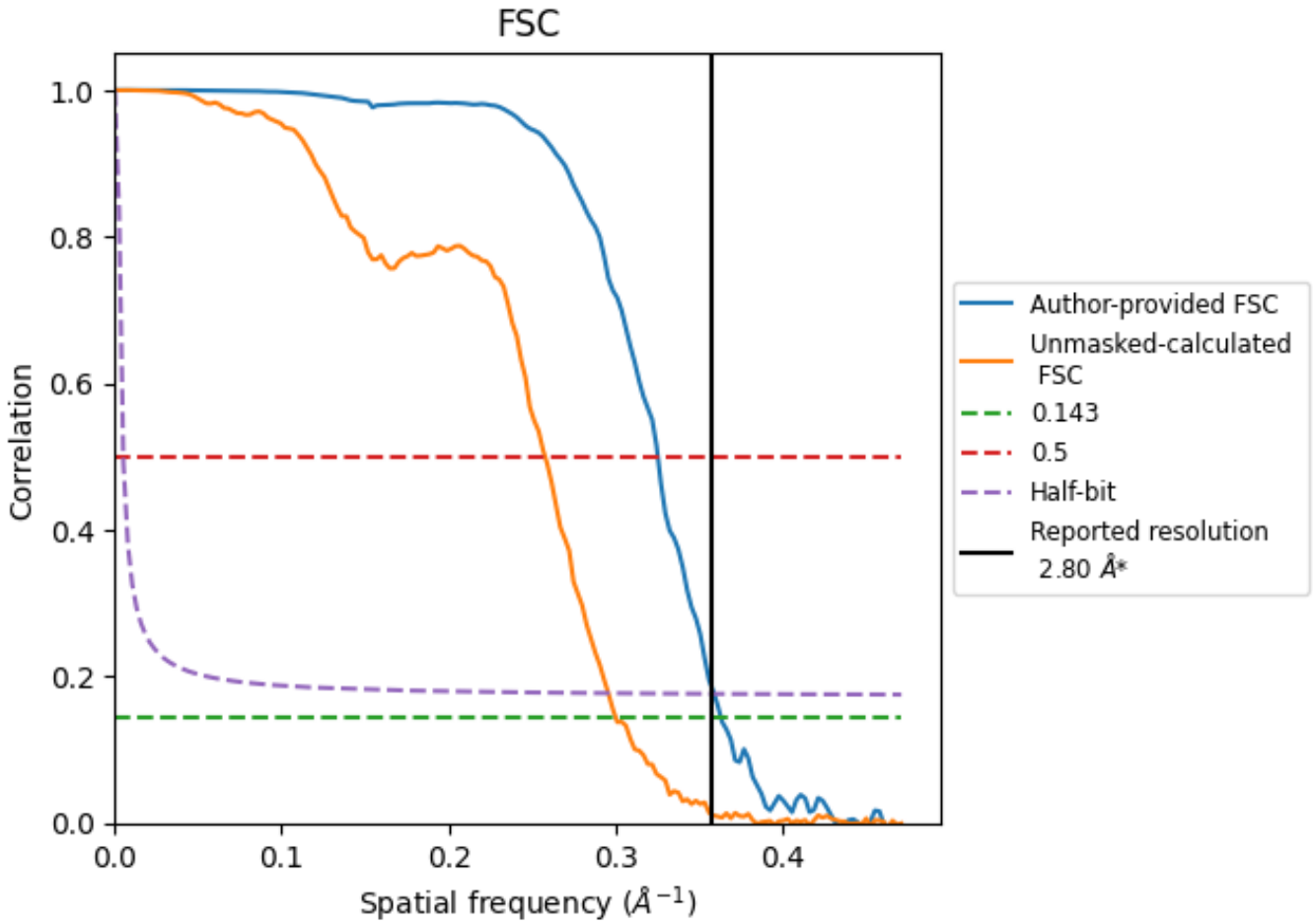


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

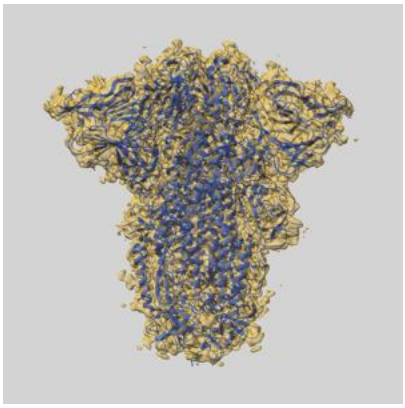
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.75	3.07	2.78
Unmasked-calculated*	3.33	3.88	3.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.33 differs from the reported value 2.8 by more than 10 %

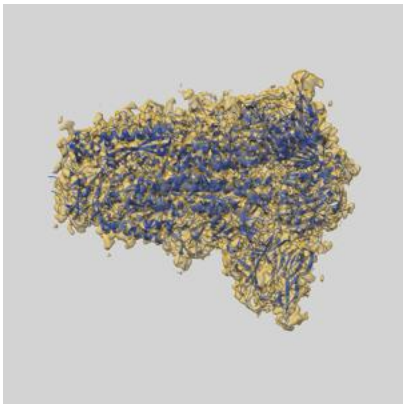
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33453 and PDB model 7XTZ. Per-residue inclusion information can be found in section 3 on page 10.

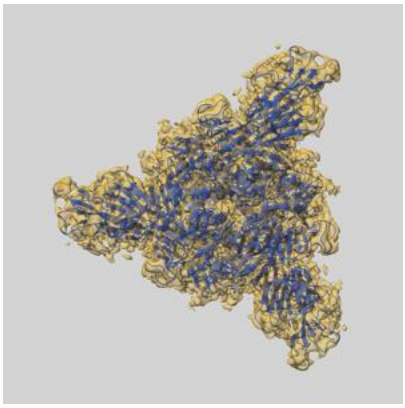
9.1 Map-model overlay



X



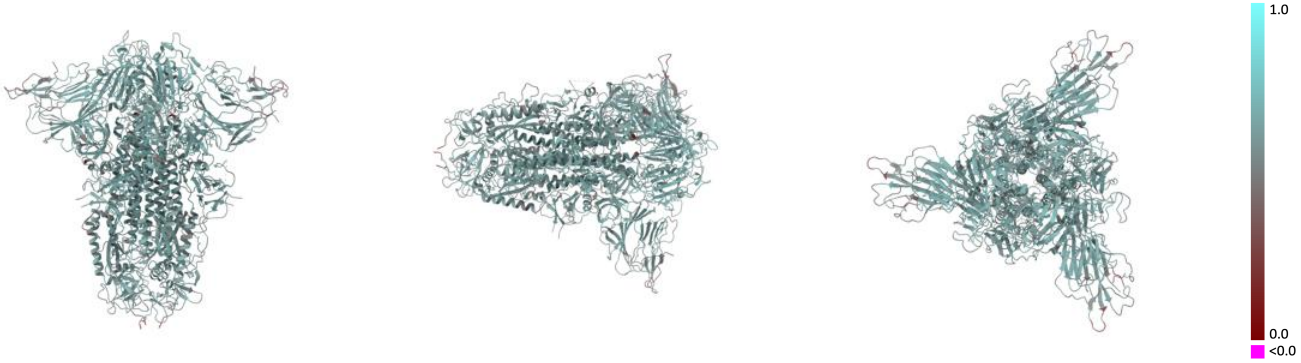
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

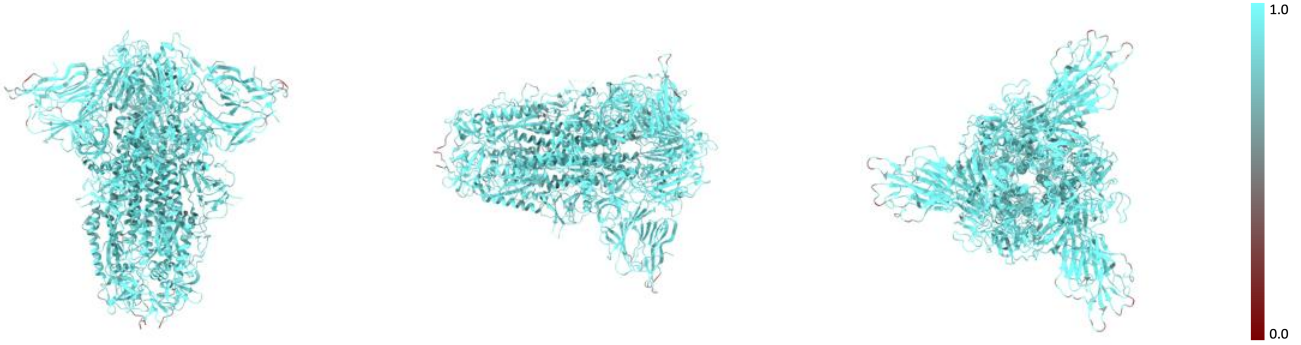
9.2 Q-score mapped to coordinate model (i)



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.

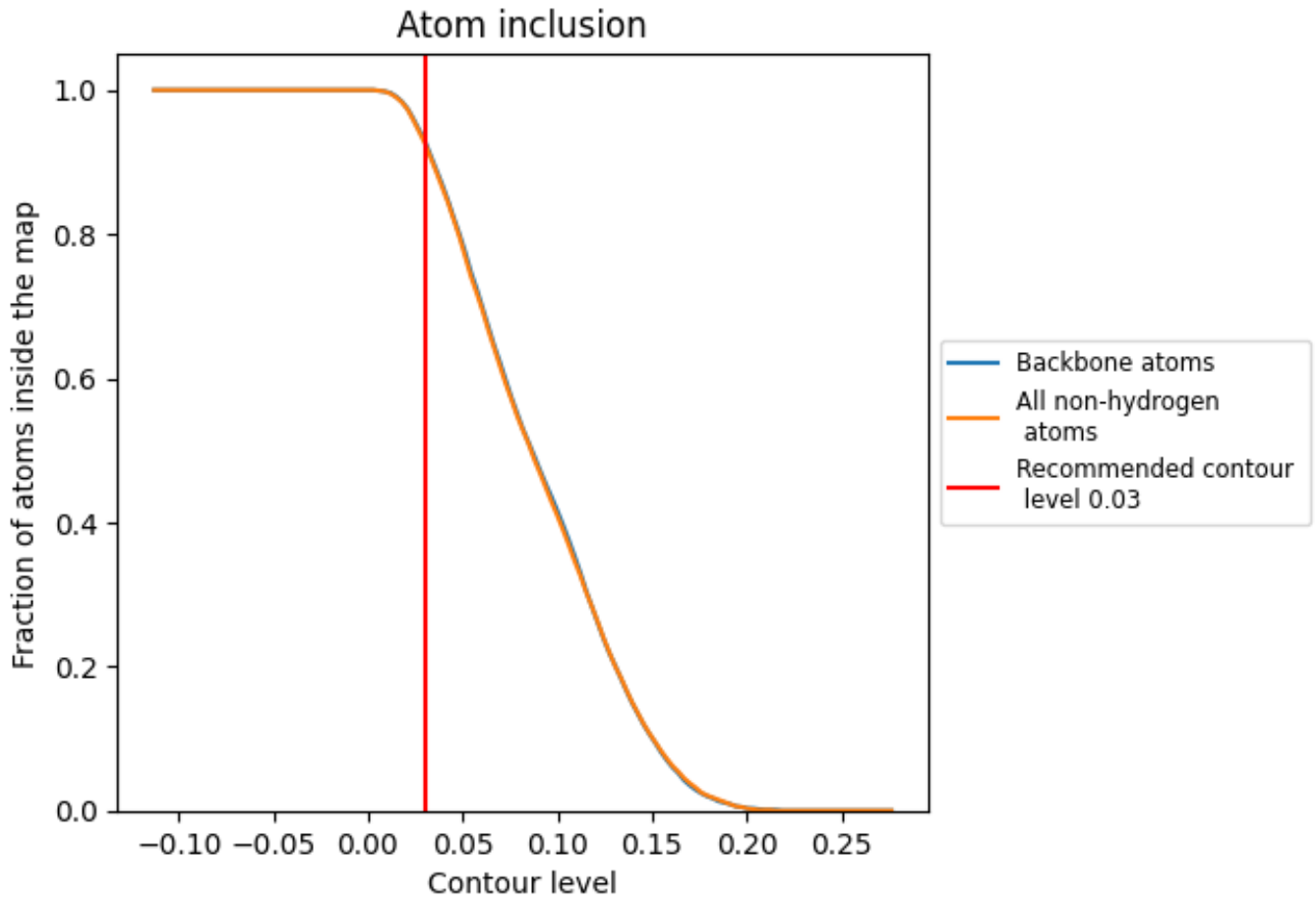
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.5880
A	0.9330	0.5890
B	0.9330	0.5890
C	0.9320	0.5890
D	0.8210	0.5400
E	0.5360	0.4050
F	0.4640	0.4550
G	0.9290	0.5730
H	0.8570	0.5310
I	0.8210	0.5240
J	0.5360	0.3930
K	0.5000	0.4540
L	0.9290	0.5700
M	0.8570	0.5260
N	0.8210	0.5180
O	0.5360	0.4080
P	0.4640	0.4450
Q	0.9290	0.5810
R	0.8210	0.5330