Full wwPDB EM Validation Report ⓘ

Dec 26, 2022 – 04:16 PM JST

PDB ID	:	7WGV
EMDB ID	:	EMD-32490
Title	:	SARS-CoV-2 spike glycoprotein trimer in closed state
Authors	:	Zhu, Y.; Tai, L.; Yin, G.; Sun, F.
Deposited on	:	2021-12-29
Resolution	:	3.20 Å(reported)

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

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

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

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

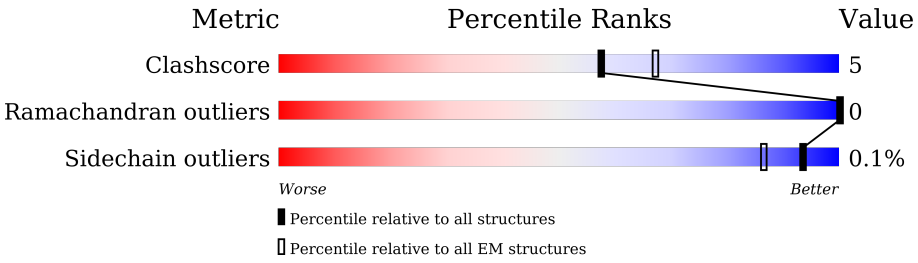
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.20 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	A	1204	81% 10% 8%
1	B	1204	81% 10% 8%
1	C	1204	82% 10% 8%
2	D	2	100%
2	E	2	50% 100%
2	F	2	50% 50% 50%
2	G	2	100%
2	H	2	100%

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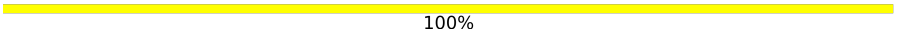
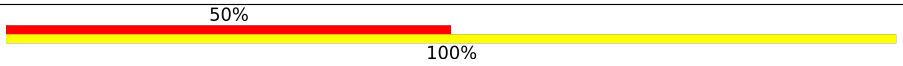
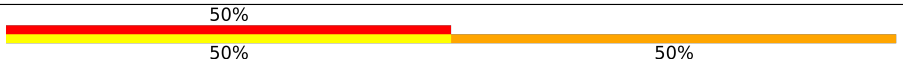
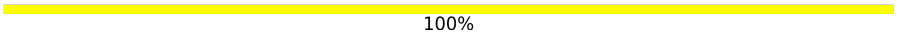
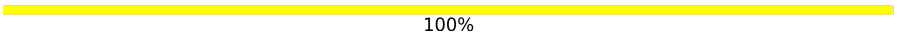
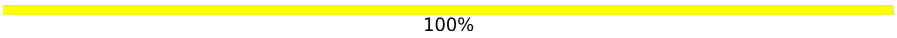
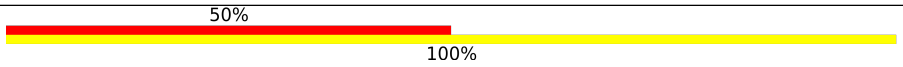
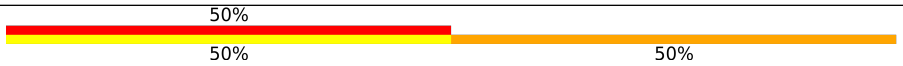
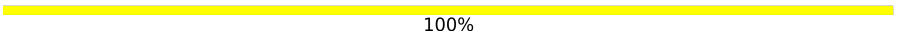
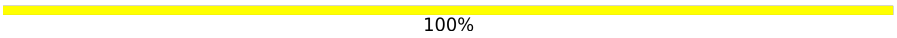
Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
2	R	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26931 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1103	Total	C	N	O	S	0	0
			8620	5496	1441	1643	40		
1	B	1103	Total	C	N	O	S	0	0
			8620	5496	1441	1643	40		
1	C	1103	Total	C	N	O	S	0	0
			8620	5496	1441	1643	40		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	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	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		

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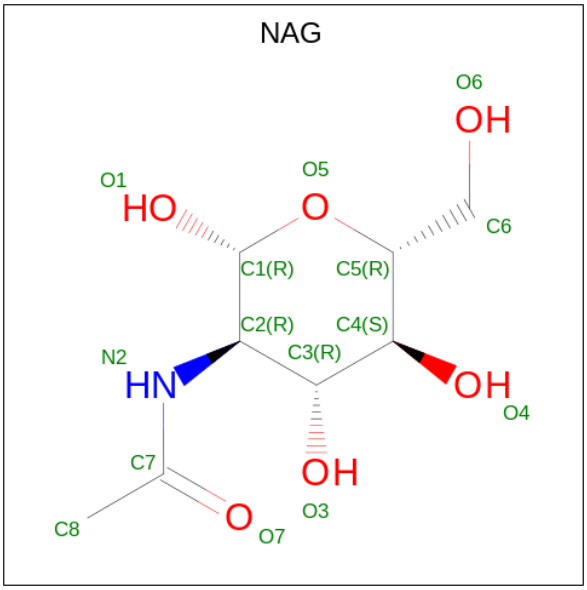
Mol	Chain	Residues	Atoms				AltConf	Trace
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	N	O	0
			154	88	11	55	
3	A	1	Total	C	N	O	0
			154	88	11	55	
3	A	1	Total	C	N	O	0
			154	88	11	55	

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Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 154 88 11 55	0
3	A	1	Total C N O 154 88 11 55	0
3	A	1	Total C N O 154 88 11 55	0
3	A	1	Total C N O 154 88 11 55	0
3	A	1	Total C N O 154 88 11 55	0
3	A	1	Total C N O 154 88 11 55	0
3	A	1	Total C N O 154 88 11 55	0
3	A	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	B	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0

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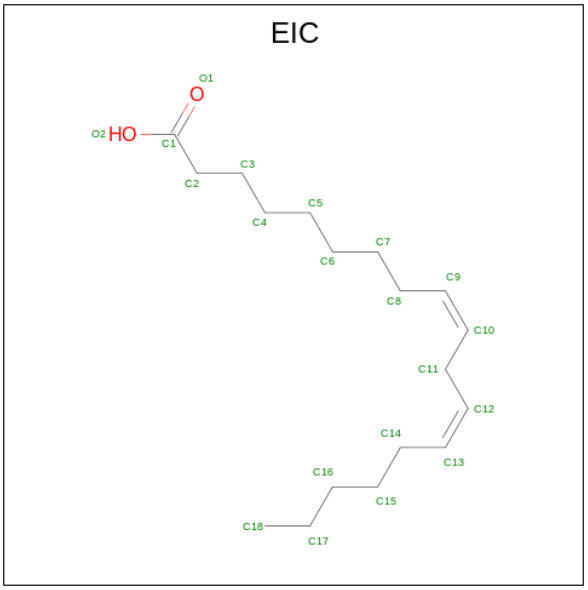
Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0

- Molecule 4 is LINOLEIC ACID (three-letter code: EIC) (formula: $C_{18}H_{32}O_2$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 20 18 2	0
4	B	1	Total C O 20 18 2	0

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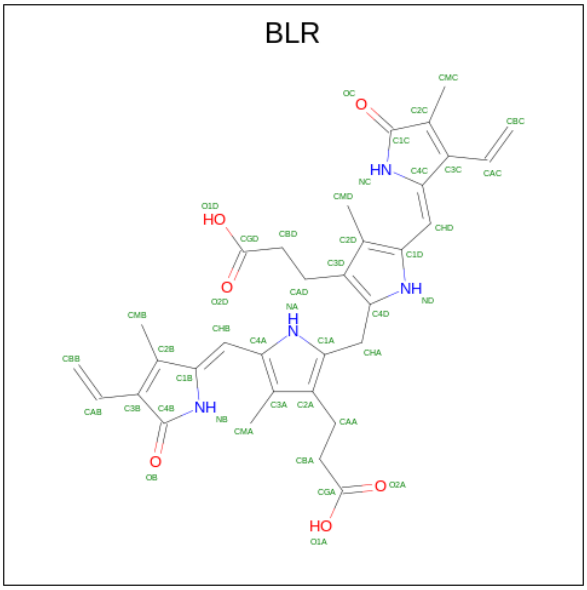
Mol	Chain	Residues	Atoms			AltConf
4	C	1	Total 20	C 18	O 2	0

- Molecule 5 is 3-[5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-2-[[5-[(Z)-(3-ethenyl-4-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1H-pyrrol-2-yl]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (three-letter code: BLR) (formula: $C_{33}H_{36}N_4O_6$).



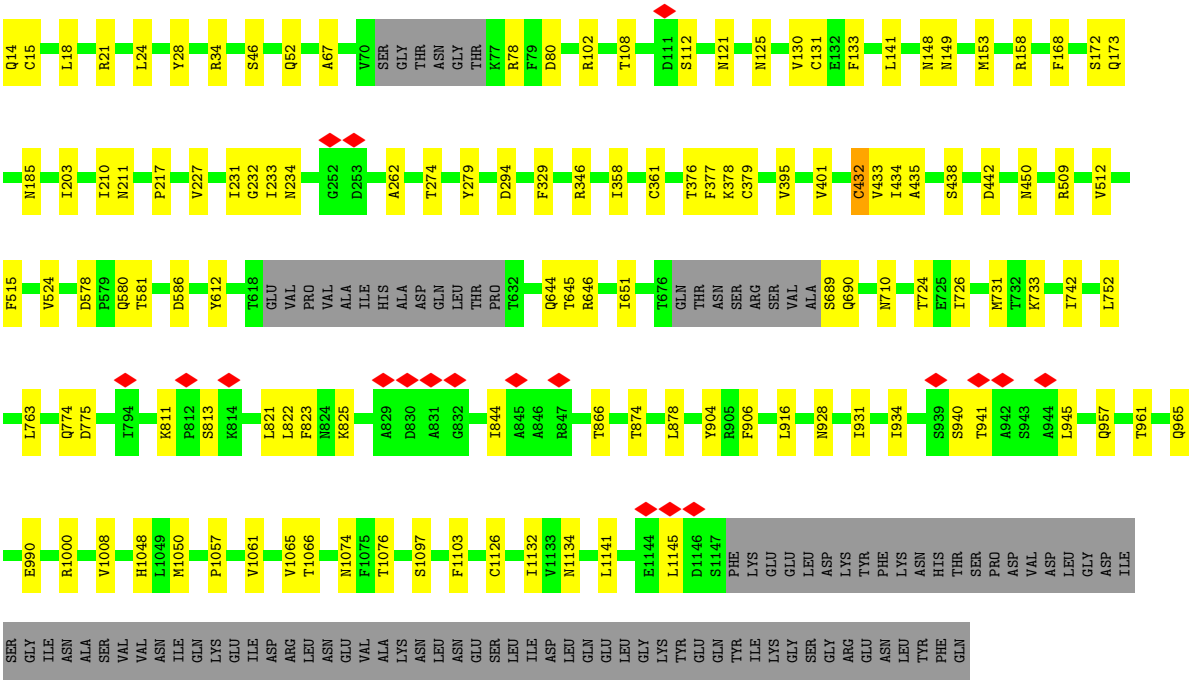
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 43	C 33	N 4	O 6	0
5	B	1	Total 43	C 33	N 4	O 6	0
5	C	1	Total 43	C 33	N 4	O 6	0

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.

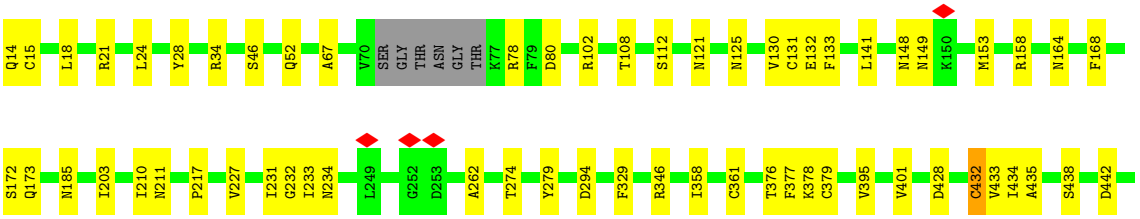
• Molecule 1: Spike glycoprotein

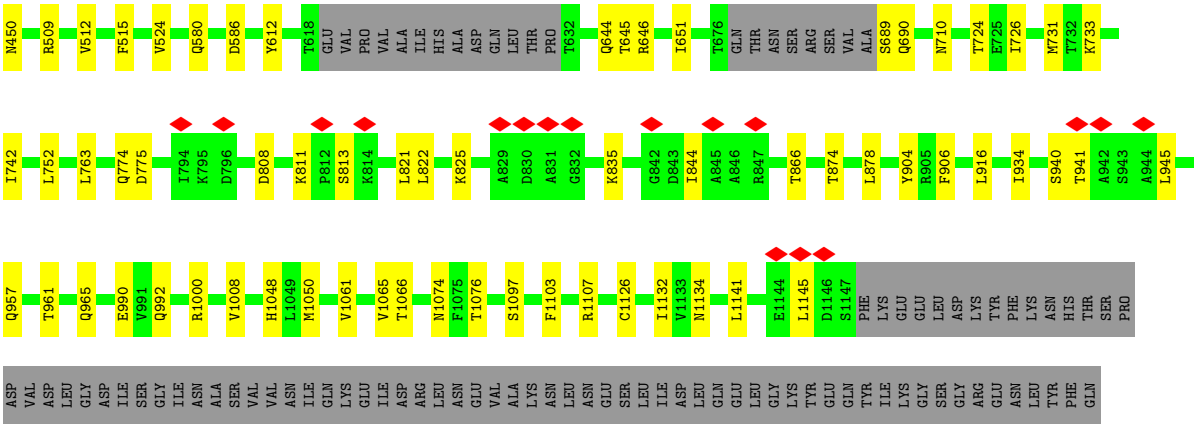
Chain A:



• Molecule 1: Spike glycoprotein

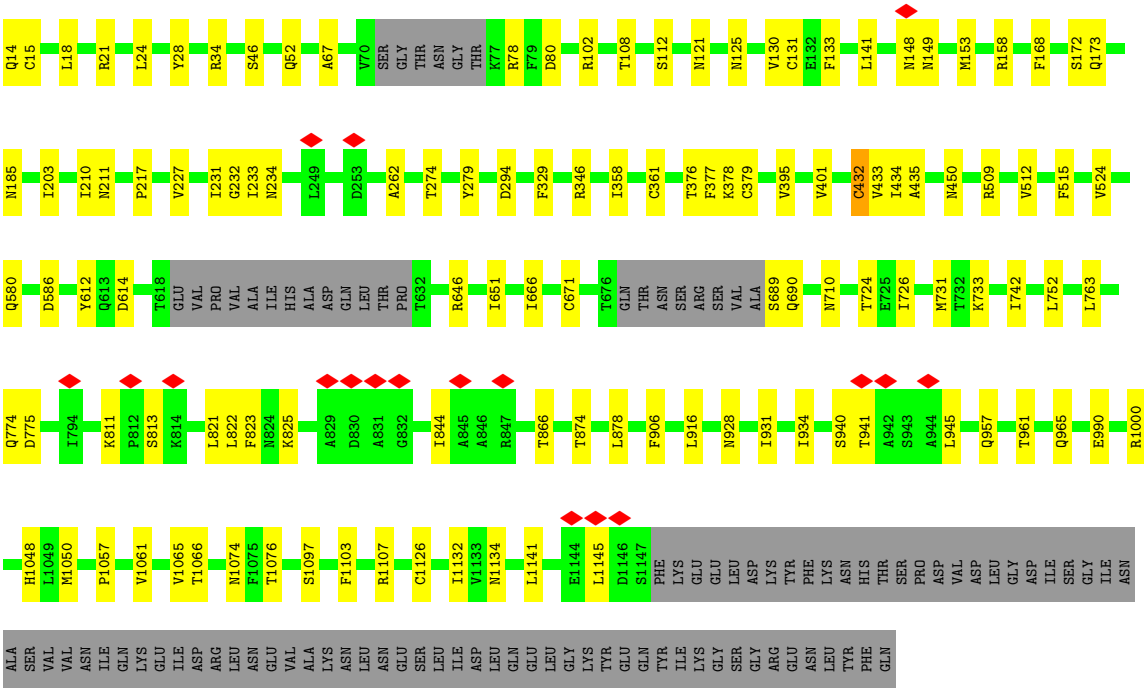
Chain B:





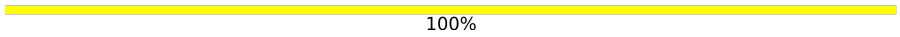
• Molecule 1: Spike glycoprotein

Chain C:



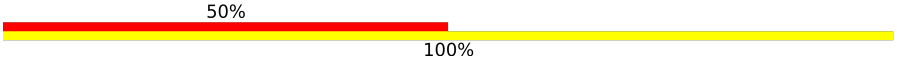
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain E:

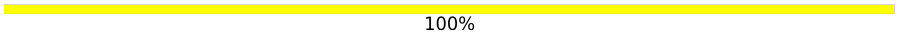


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

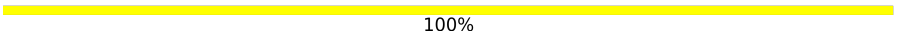
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



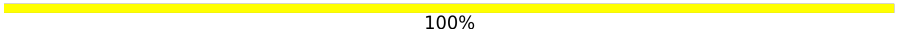
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



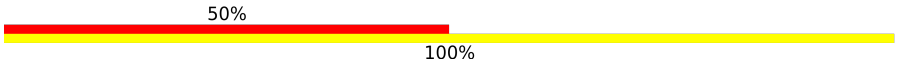
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain J:

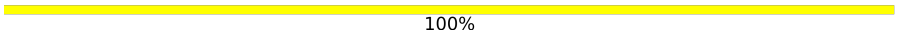


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

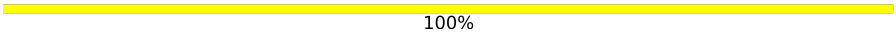
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



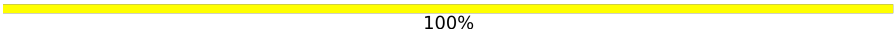
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



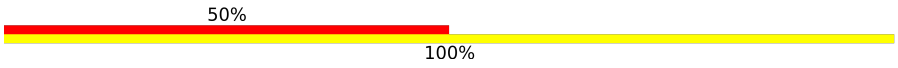
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain O:

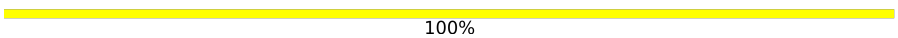


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

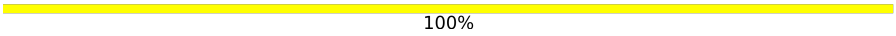
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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, Not provided	
Number of particles used	42115	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	5.278	Depositor
Minimum map value	-2.955	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.140	Depositor
Recommended contour level	0.633	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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, BLR, EIC

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	0.26	0/8819	0.48	1/12000 (0.0%)
1	B	0.26	0/8819	0.48	1/12000 (0.0%)
1	C	0.26	0/8819	0.48	1/12000 (0.0%)
All	All	0.26	0/26457	0.48	3/36000 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	432	CYS	CA-CB-SG	7.44	127.39	114.00
1	A	432	CYS	CA-CB-SG	7.44	127.39	114.00
1	C	432	CYS	CA-CB-SG	7.43	127.37	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8620	0	8392	75	0
1	B	8620	0	8392	78	0
1	C	8620	0	8392	76	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	1	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
3	A	154	0	143	4	0
3	B	154	0	143	4	0
3	C	154	0	143	4	0
4	A	20	0	31	0	0
4	B	20	0	31	0	0
4	C	20	0	31	0	0
5	A	43	0	34	17	0
5	B	43	0	34	16	0
5	C	43	0	34	16	0
All	All	26931	0	26175	266	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 5.

All (266) 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)
5:A:1313:BLR:CMA	5:A:1313:BLR:C3A	1.75	1.64
5:B:1313:BLR:C4D	5:B:1313:BLR:CHA	1.78	1.62
5:B:1313:BLR:CMA	5:B:1313:BLR:C3A	1.75	1.62
5:A:1313:BLR:C4D	5:A:1313:BLR:CHA	1.78	1.59
5:C:1313:BLR:CMA	5:C:1313:BLR:C3A	1.75	1.58
5:B:1313:BLR:CAA	5:B:1313:BLR:C2A	1.80	1.57
5:C:1313:BLR:CAA	5:C:1313:BLR:CBA	1.82	1.57
5:A:1313:BLR:CAA	5:A:1313:BLR:C2A	1.79	1.56
5:C:1313:BLR:C4D	5:C:1313:BLR:CHA	1.78	1.55
5:A:1313:BLR:CAA	5:A:1313:BLR:CBA	1.82	1.55
5:C:1313:BLR:CAA	5:C:1313:BLR:C2A	1.80	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1313:BLR:CAA	5:B:1313:BLR:CBA	1.82	1.52
5:A:1313:BLR:CMB	5:A:1313:BLR:C2B	1.95	1.44
5:B:1313:BLR:CMB	5:B:1313:BLR:C2B	1.95	1.42
5:C:1313:BLR:CMB	5:C:1313:BLR:C2B	1.95	1.42
5:B:1313:BLR:CBD	5:B:1313:BLR:CAD	1.97	1.41
5:C:1313:BLR:CBD	5:C:1313:BLR:CAD	1.97	1.41
5:A:1313:BLR:CAD	5:A:1313:BLR:CBD	1.97	1.40
5:C:1313:BLR:C4D	5:C:1313:BLR:C3D	1.77	1.37
5:B:1313:BLR:C4D	5:B:1313:BLR:C3D	1.77	1.36
5:A:1313:BLR:CHA	5:A:1313:BLR:C1A	2.06	1.34
5:C:1313:BLR:CHA	5:C:1313:BLR:C1A	2.06	1.33
5:B:1313:BLR:CHA	5:B:1313:BLR:C1A	2.06	1.32
5:A:1313:BLR:C4D	5:A:1313:BLR:C3D	1.77	1.27
5:C:1313:BLR:CHA	5:C:1313:BLR:ND	2.10	1.14
5:A:1313:BLR:CHA	5:A:1313:BLR:ND	2.10	1.14
5:B:1313:BLR:CHA	5:B:1313:BLR:ND	2.10	1.13
1:C:379:CYS:HA	1:C:432:CYS:CB	2.12	0.80
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.64	0.80
1:A:379:CYS:HA	1:A:432:CYS:CB	2.12	0.80
1:B:379:CYS:HA	1:B:432:CYS:CB	2.12	0.80
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.64	0.80
1:A:379:CYS:HA	1:A:432:CYS:HB3	1.64	0.78
5:C:1313:BLR:CHA	5:C:1313:BLR:H28	1.97	0.77
1:A:646:ARG:HH22	1:C:866:THR:HG21	1.49	0.77
1:A:866:THR:HG21	1:B:646:ARG:HH22	1.53	0.74
1:B:866:THR:HG21	1:C:646:ARG:HH22	1.53	0.74
5:A:1313:BLR:CHA	5:A:1313:BLR:H28	1.97	0.74
5:B:1313:BLR:CHA	5:B:1313:BLR:H28	1.97	0.73
1:A:18:LEU:HD12	1:A:21:ARG:HH21	1.57	0.70
1:A:731:MET:HG2	1:A:774:GLN:HE21	1.58	0.68
1:C:18:LEU:HD12	1:C:21:ARG:HH21	1.57	0.68
1:B:18:LEU:HD12	1:B:21:ARG:HH21	1.57	0.68
1:B:731:MET:HG2	1:B:774:GLN:HE21	1.58	0.67
1:C:125:ASN:ND2	1:C:172:SER:O	2.29	0.66
1:C:731:MET:HG2	1:C:774:GLN:HE21	1.58	0.66
1:A:34:ARG:NH2	1:A:217:PRO:O	2.29	0.66
1:B:34:ARG:NH2	1:B:217:PRO:O	2.29	0.66
1:A:125:ASN:ND2	1:A:172:SER:O	2.29	0.66
1:C:34:ARG:NH2	1:C:217:PRO:O	2.29	0.65
1:B:125:ASN:ND2	1:B:172:SER:O	2.29	0.65
1:C:78:ARG:NH2	1:C:80:ASP:OD2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:ASN:HB2	3:B:1304:NAG:N2	2.13	0.64
1:A:185:ASN:ND2	1:A:211:ASN:O	2.30	0.63
1:C:1074:ASN:HB2	3:C:1304:NAG:N2	2.13	0.63
1:A:78:ARG:NH2	1:A:80:ASP:OD2	2.31	0.63
1:B:78:ARG:NH2	1:B:80:ASP:OD2	2.31	0.63
1:C:185:ASN:ND2	1:C:211:ASN:O	2.30	0.63
1:B:185:ASN:ND2	1:B:211:ASN:O	2.30	0.62
1:A:1074:ASN:HB2	3:A:1304:NAG:N2	2.13	0.62
1:A:379:CYS:HA	1:A:432:CYS:HB2	1.82	0.61
1:B:28:TYR:HB2	3:B:1311:NAG:H61	1.82	0.61
1:C:378:LYS:O	1:C:432:CYS:HB2	2.01	0.61
1:A:378:LYS:O	1:A:432:CYS:HB2	2.01	0.61
1:C:28:TYR:HB2	3:C:1311:NAG:H61	1.82	0.61
1:C:379:CYS:HA	1:C:432:CYS:HB2	1.82	0.61
1:B:379:CYS:HA	1:B:432:CYS:HB2	1.82	0.60
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.83	0.60
1:A:28:TYR:HB2	3:A:1311:NAG:H61	1.82	0.60
5:A:1313:BLR:C1A	5:A:1313:BLR:H28	2.15	0.60
1:B:378:LYS:O	1:B:432:CYS:HB2	2.01	0.60
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.83	0.60
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.84	0.60
5:B:1313:BLR:C1A	5:B:1313:BLR:H28	2.15	0.59
5:C:1313:BLR:C1A	5:C:1313:BLR:H28	2.15	0.59
1:A:329:PHE:O	1:A:580:GLN:NE2	2.37	0.58
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.85	0.58
1:C:329:PHE:O	1:C:580:GLN:NE2	2.37	0.58
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.85	0.58
1:B:329:PHE:O	1:B:580:GLN:NE2	2.37	0.57
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.85	0.56
5:C:1313:BLR:CAA	5:C:1313:BLR:CGA	2.83	0.56
1:A:1141:LEU:HD23	1:A:1145:LEU:HD23	1.88	0.55
1:B:24:LEU:HD12	1:B:78:ARG:HH11	1.72	0.55
5:A:1313:BLR:CAA	5:A:1313:BLR:CGA	2.83	0.55
1:C:24:LEU:HD12	1:C:78:ARG:HH11	1.72	0.55
1:C:52:GLN:OE1	1:C:274:THR:OG1	2.15	0.55
1:B:1141:LEU:HD23	1:B:1145:LEU:HD23	1.88	0.55
1:A:24:LEU:HD12	1:A:78:ARG:HH11	1.72	0.55
1:C:358:ILE:HB	1:C:395:VAL:HG23	1.88	0.54
1:C:1141:LEU:HD23	1:C:1145:LEU:HD23	1.88	0.54
1:B:358:ILE:HB	1:B:395:VAL:HG23	1.89	0.54
1:A:153:MET:HE1	3:A:1312:NAG:H4	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HB	1:A:395:VAL:HG23	1.89	0.54
5:A:1313:BLR:CBD	5:A:1313:BLR:C3D	2.84	0.53
1:B:52:GLN:OE1	1:B:274:THR:OG1	2.15	0.53
1:B:1076:THR:HG23	1:B:1097:SER:HB3	1.91	0.52
1:A:46:SER:HA	1:A:279:TYR:O	2.10	0.52
1:C:153:MET:HE1	3:C:1312:NAG:H4	1.90	0.52
1:A:1076:THR:HG23	1:A:1097:SER:HB3	1.91	0.52
1:C:46:SER:HA	1:C:279:TYR:O	2.10	0.52
1:C:1076:THR:HG23	1:C:1097:SER:HB3	1.91	0.52
1:A:689:SER:OG	1:A:690:GLN:N	2.43	0.52
1:B:46:SER:HA	1:B:279:TYR:O	2.10	0.52
1:B:153:MET:HE1	3:B:1312:NAG:H4	1.90	0.52
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.45	0.52
1:B:121:ASN:ND2	5:B:1313:BLR:H24	2.25	0.51
1:A:121:ASN:ND2	5:A:1313:BLR:H24	2.25	0.51
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.45	0.51
1:B:689:SER:OG	1:B:690:GLN:N	2.43	0.51
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.45	0.51
1:B:203:ILE:HB	1:B:227:VAL:HG12	1.93	0.51
5:B:1313:BLR:CAA	5:B:1313:BLR:CGA	2.83	0.51
1:C:121:ASN:ND2	5:C:1313:BLR:H24	2.25	0.51
1:C:130:VAL:HB	1:C:168:PHE:HB2	1.93	0.51
1:B:130:VAL:HB	1:B:168:PHE:HB2	1.93	0.51
1:A:203:ILE:HB	1:A:227:VAL:HG12	1.92	0.50
1:A:14:GLN:O	1:A:158:ARG:NH1	2.45	0.50
1:A:130:VAL:HB	1:A:168:PHE:HB2	1.93	0.50
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.93	0.50
5:C:1313:BLR:CBD	5:C:1313:BLR:C3D	2.84	0.50
1:B:14:GLN:O	1:B:158:ARG:NH1	2.45	0.50
1:B:361:CYS:HB2	1:B:524:VAL:HG13	1.94	0.50
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.94	0.50
1:B:108:THR:OG1	1:B:234:ASN:O	2.30	0.50
1:C:203:ILE:HB	1:C:227:VAL:HG12	1.93	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.50
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.93	0.50
1:C:689:SER:OG	1:C:690:GLN:N	2.43	0.50
1:C:731:MET:HG2	1:C:774:GLN:NE2	2.25	0.50
1:C:14:GLN:O	1:C:158:ARG:NH1	2.45	0.50
1:C:1103:PHE:HZ	3:C:1305:NAG:H62	1.77	0.49
1:C:395:VAL:HG12	1:C:515:PHE:HB3	1.93	0.49
1:A:395:VAL:HG12	1:A:515:PHE:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:VAL:HG12	1:B:515:PHE:HB3	1.93	0.49
1:B:1103:PHE:HZ	3:B:1305:NAG:H62	1.77	0.49
5:B:1313:BLR:H22	5:B:1313:BLR:H18	1.94	0.49
1:C:67:ALA:O	1:C:262:ALA:HA	2.13	0.49
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.93	0.49
1:A:724:THR:OG1	1:A:934:ILE:HD11	2.13	0.49
5:A:1313:BLR:H22	5:A:1313:BLR:H18	1.95	0.49
5:B:1313:BLR:CBD	5:B:1313:BLR:C3D	2.84	0.49
1:C:210:ILE:HG21	1:C:217:PRO:HG3	1.94	0.49
1:A:52:GLN:OE1	1:A:274:THR:OG1	2.15	0.49
1:B:210:ILE:HG21	1:B:217:PRO:HG3	1.95	0.49
1:A:108:THR:OG1	1:A:234:ASN:O	2.30	0.49
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.46	0.49
5:C:1313:BLR:H22	5:C:1313:BLR:H18	1.95	0.49
1:A:361:CYS:HB2	1:A:524:VAL:HG13	1.94	0.49
1:C:108:THR:OG1	1:C:234:ASN:O	2.30	0.49
1:C:131:CYS:HB3	1:C:133:PHE:CE2	2.49	0.48
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.46	0.48
1:A:131:CYS:HB3	1:A:133:PHE:CE2	2.48	0.48
1:B:67:ALA:O	1:B:262:ALA:HA	2.13	0.48
1:B:131:CYS:HB3	1:B:133:PHE:CE2	2.48	0.48
1:C:361:CYS:HB2	1:C:524:VAL:HG13	1.94	0.48
1:A:67:ALA:O	1:A:262:ALA:HA	2.13	0.48
1:A:1103:PHE:HZ	3:A:1305:NAG:H62	1.77	0.48
1:C:724:THR:OG1	1:C:934:ILE:HD11	2.13	0.48
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.46	0.48
1:B:724:THR:OG1	1:B:934:ILE:HD11	2.13	0.48
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.94	0.48
1:A:586:ASP:HB2	1:C:844:ILE:HD12	1.94	0.48
1:B:346:ARG:HH22	1:B:450:ASN:HB3	1.78	0.48
1:A:346:ARG:HH22	1:A:450:ASN:HB3	1.78	0.48
1:C:346:ARG:HH22	1:C:450:ASN:HB3	1.78	0.48
1:A:210:ILE:HG21	1:A:217:PRO:HG3	1.95	0.48
1:A:733:LYS:NZ	1:A:775:ASP:OD2	2.40	0.48
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.96	0.47
1:A:731:MET:HG2	1:A:774:GLN:NE2	2.25	0.47
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.96	0.47
1:C:821:LEU:O	1:C:825:LYS:HG2	2.15	0.47
1:A:821:LEU:O	1:A:825:LYS:HG2	2.15	0.47
1:B:844:ILE:HD12	1:C:586:ASP:HB2	1.96	0.47
1:B:731:MET:HG2	1:B:774:GLN:NE2	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.40	0.47
1:A:844:ILE:HD12	1:B:586:ASP:HB2	1.96	0.46
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.96	0.46
5:B:1313:BLR:CMA	5:B:1313:BLR:C2A	2.67	0.46
1:C:376:THR:HB	1:C:435:ALA:HB3	1.97	0.46
1:A:376:THR:HB	1:A:435:ALA:HB3	1.97	0.46
1:B:376:THR:HB	1:B:435:ALA:HB3	1.98	0.46
1:B:710:ASN:O	1:B:1076:THR:HA	2.16	0.46
1:A:710:ASN:O	1:A:1076:THR:HA	2.16	0.46
1:B:102:ARG:HD2	1:B:141:LEU:HD13	1.98	0.46
1:B:821:LEU:O	1:B:825:LYS:HG2	2.15	0.46
1:C:15:CYS:HA	1:C:158:ARG:HD3	1.98	0.46
1:B:112:SER:O	1:B:112:SER:OG	2.33	0.45
1:C:231:ILE:HG13	1:C:232:GLY:N	2.31	0.45
1:C:710:ASN:O	1:C:1076:THR:HA	2.16	0.45
1:A:15:CYS:HA	1:A:158:ARG:HD3	1.98	0.45
1:A:102:ARG:HD2	1:A:141:LEU:HD13	1.98	0.45
1:A:231:ILE:HD12	1:A:233:ILE:HD12	1.99	0.45
1:A:231:ILE:HG13	1:A:232:GLY:N	2.31	0.45
1:B:231:ILE:HD12	1:B:233:ILE:HD12	1.99	0.45
1:B:294:ASP:N	1:B:294:ASP:OD1	2.50	0.45
1:A:294:ASP:OD1	1:A:294:ASP:N	2.50	0.44
1:B:231:ILE:HG13	1:B:232:GLY:N	2.31	0.44
1:C:102:ARG:HD2	1:C:141:LEU:HD13	1.98	0.44
1:A:433:VAL:HG22	1:A:512:VAL:HG22	2.00	0.44
1:A:1134:ASN:OD1	2:F:1:NAG:N2	2.51	0.44
1:B:15:CYS:HA	1:B:158:ARG:HD3	1.98	0.44
1:C:231:ILE:HD12	1:C:233:ILE:HD12	1.99	0.44
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.40	0.44
1:C:294:ASP:OD1	1:C:294:ASP:N	2.50	0.44
1:C:1134:ASN:OD1	2:P:1:NAG:N2	2.51	0.44
5:A:1313:BLR:C3A	5:A:1313:BLR:CAA	2.69	0.44
1:C:433:VAL:HG22	1:C:512:VAL:HG22	2.00	0.44
1:A:172:SER:OG	1:A:173:GLN:N	2.51	0.43
1:C:172:SER:OG	1:C:173:GLN:N	2.51	0.43
1:A:752:LEU:HD11	1:A:990:GLU:HG2	2.00	0.43
1:B:961:THR:O	1:B:965:GLN:HG3	2.18	0.43
1:A:961:THR:O	1:A:965:GLN:HG3	2.18	0.43
1:B:1134:ASN:OD1	2:K:1:NAG:N2	2.51	0.43
1:C:752:LEU:HD11	1:C:990:GLU:HG2	2.00	0.43
1:B:433:VAL:HG22	1:B:512:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1313:BLR:CMA	5:A:1313:BLR:C2A	2.67	0.43
1:B:752:LEU:HD11	1:B:990:GLU:HG2	2.00	0.43
1:B:835:LYS:H	1:C:614:ASP:HB2	1.83	0.43
1:C:961:THR:O	1:C:965:GLN:HG3	2.18	0.43
1:B:172:SER:OG	1:B:173:GLN:N	2.51	0.43
1:B:438:SER:OG	1:B:442:ASP:OD2	2.35	0.43
1:B:148:ASN:OD1	1:B:149:ASN:N	2.52	0.43
1:B:428:ASP:OD1	1:B:428:ASP:N	2.46	0.43
1:C:112:SER:O	1:C:112:SER:OG	2.33	0.43
1:C:148:ASN:OD1	1:C:149:ASN:N	2.52	0.43
1:A:112:SER:O	1:A:112:SER:OG	2.33	0.43
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	2.02	0.42
1:B:811:LYS:HE2	1:B:813:SER:HB2	2.02	0.42
1:A:904:TYR:CE2	1:B:1107:ARG:HD3	2.55	0.42
1:A:811:LYS:HE2	1:A:813:SER:HB2	2.02	0.42
1:B:644:GLN:NE2	1:B:645:THR:O	2.48	0.42
1:C:811:LYS:HE2	1:C:813:SER:HB2	2.02	0.42
1:B:808:ASP:OD1	1:B:808:ASP:N	2.51	0.42
1:B:1050:MET:HG2	1:B:1065:VAL:HB	2.02	0.42
1:C:874:THR:O	1:C:878:LEU:HD23	2.21	0.41
1:C:612:TYR:HE2	1:C:651:ILE:HD12	1.86	0.41
1:A:612:TYR:HE2	1:A:651:ILE:HD12	1.86	0.41
1:A:940:SER:OG	1:A:941:THR:N	2.54	0.41
1:A:1050:MET:HG2	1:A:1065:VAL:HB	2.02	0.41
1:C:666:ILE:HG12	1:C:671:CYS:HA	2.03	0.41
1:A:148:ASN:OD1	1:A:149:ASN:N	2.52	0.41
5:C:1313:BLR:CMA	5:C:1313:BLR:C2A	2.67	0.41
1:A:928:ASN:O	1:A:931:ILE:HG22	2.21	0.41
1:B:874:THR:O	1:B:878:LEU:HD23	2.21	0.41
1:B:940:SER:OG	1:B:941:THR:N	2.54	0.41
1:C:940:SER:OG	1:C:941:THR:N	2.54	0.41
1:A:644:GLN:NE2	1:A:645:THR:O	2.48	0.41
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	2.01	0.41
1:B:377:PHE:HD1	1:B:434:ILE:HG12	1.86	0.41
1:C:377:PHE:HD1	1:C:434:ILE:HG12	1.86	0.41
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	2.02	0.41
1:A:578:ASP:HB3	1:A:581:THR:O	2.21	0.40
1:B:992:GLN:H	1:B:992:GLN:HG2	1.65	0.40
1:C:823:PHE:CD1	1:C:1057:PRO:HD3	2.56	0.40
1:C:906:PHE:HD2	1:C:916:LEU:HB2	1.86	0.40
1:C:928:ASN:O	1:C:931:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1050:MET:HG2	1:C:1065:VAL:HB	2.02	0.40
1:A:874:THR:O	1:A:878:LEU:HD23	2.21	0.40
1:B:612:TYR:HE2	1:B:651:ILE:HD12	1.86	0.40
1:B:904:TYR:CE2	1:C:1107:ARG:HD3	2.56	0.40
1:A:377:PHE:HD1	1:A:434:ILE:HG12	1.86	0.40
1:A:438:SER:OG	1:A:442:ASP:OD2	2.35	0.40
1:A:823:PHE:CD1	1:A:1057:PRO:HD3	2.56	0.40
1:B:132:GLU:HB2	1:B:164:ASN:O	2.22	0.40
1:C:130:VAL:HG13	1:C:233:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1095/1204 (91%)	1060 (97%)	35 (3%)	0	100	100
1	B	1095/1204 (91%)	1060 (97%)	35 (3%)	0	100	100
1	C	1095/1204 (91%)	1060 (97%)	35 (3%)	0	100	100
All	All	3285/3612 (91%)	3180 (97%)	105 (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	960/1049 (92%)	959 (100%)	1 (0%)	93	98
1	B	960/1049 (92%)	959 (100%)	1 (0%)	93	98
1	C	960/1049 (92%)	959 (100%)	1 (0%)	93	98
All	All	2880/3147 (92%)	2877 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	957	GLN
1	B	957	GLN
1	C	957	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	774	GLN
1	A	1002	GLN
1	B	774	GLN
1	B	1002	GLN
1	C	774	GLN
1	C	1002	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	1.97	3 (21%)	17,19,21	1.17	1 (5%)
2	NAG	D	2	2	14,14,15	2.02	3 (21%)	17,19,21	1.11	2 (11%)
2	NAG	E	1	2	14,14,15	2.01	3 (21%)	17,19,21	1.25	2 (11%)
2	NAG	E	2	2	14,14,15	2.01	3 (21%)	17,19,21	1.14	2 (11%)
2	NAG	F	1	1,2	14,14,15	2.03	3 (21%)	17,19,21	1.20	1 (5%)
2	NAG	F	2	2	14,14,15	2.04	3 (21%)	17,19,21	1.12	2 (11%)
2	NAG	G	1	1,2	14,14,15	2.00	3 (21%)	17,19,21	1.10	1 (5%)
2	NAG	G	2	2	14,14,15	2.01	3 (21%)	17,19,21	1.18	2 (11%)
2	NAG	H	1	2	14,14,15	2.00	3 (21%)	17,19,21	1.08	2 (11%)
2	NAG	H	2	2	14,14,15	2.03	3 (21%)	17,19,21	1.15	1 (5%)
2	NAG	I	1	1,2	14,14,15	1.96	3 (21%)	17,19,21	1.17	1 (5%)
2	NAG	I	2	2	14,14,15	2.02	3 (21%)	17,19,21	1.11	2 (11%)
2	NAG	J	1	2	14,14,15	2.01	3 (21%)	17,19,21	1.25	2 (11%)
2	NAG	J	2	2	14,14,15	2.01	3 (21%)	17,19,21	1.13	2 (11%)
2	NAG	K	1	1,2	14,14,15	2.03	3 (21%)	17,19,21	1.19	1 (5%)
2	NAG	K	2	2	14,14,15	2.03	3 (21%)	17,19,21	1.12	2 (11%)
2	NAG	L	1	1,2	14,14,15	1.99	3 (21%)	17,19,21	1.10	1 (5%)
2	NAG	L	2	2	14,14,15	2.03	3 (21%)	17,19,21	1.18	2 (11%)
2	NAG	M	1	2	14,14,15	1.99	3 (21%)	17,19,21	1.08	2 (11%)
2	NAG	M	2	2	14,14,15	2.01	3 (21%)	17,19,21	1.15	1 (5%)
2	NAG	N	1	1,2	14,14,15	1.96	3 (21%)	17,19,21	1.17	1 (5%)
2	NAG	N	2	2	14,14,15	2.01	3 (21%)	17,19,21	1.11	2 (11%)
2	NAG	O	1	2	14,14,15	2.01	3 (21%)	17,19,21	1.25	2 (11%)
2	NAG	O	2	2	14,14,15	2.02	3 (21%)	17,19,21	1.13	2 (11%)
2	NAG	P	1	1,2	14,14,15	2.01	3 (21%)	17,19,21	1.20	1 (5%)
2	NAG	P	2	2	14,14,15	2.03	3 (21%)	17,19,21	1.12	2 (11%)
2	NAG	Q	1	1,2	14,14,15	2.00	3 (21%)	17,19,21	1.09	1 (5%)
2	NAG	Q	2	2	14,14,15	2.03	3 (21%)	17,19,21	1.18	2 (11%)
2	NAG	R	1	2	14,14,15	1.99	3 (21%)	17,19,21	1.08	2 (11%)
2	NAG	R	2	2	14,14,15	2.02	3 (21%)	17,19,21	1.16	2 (11%)

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	-	2/6/23/26	0/1/1/1
2	NAG	E	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	2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	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	2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	4/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	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	2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	4/6/23/26	0/1/1/1

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	O5-C1	5.37	1.52	1.43
2	K	2	NAG	O5-C1	5.31	1.52	1.43
2	K	1	NAG	O5-C1	5.29	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	2	NAG	O5-C1	5.29	1.52	1.43
2	F	1	NAG	O5-C1	5.29	1.52	1.43
2	D	2	NAG	O5-C1	5.27	1.52	1.43
2	H	2	NAG	O5-C1	5.27	1.52	1.43
2	I	2	NAG	O5-C1	5.26	1.52	1.43
2	Q	2	NAG	O5-C1	5.25	1.52	1.43
2	E	2	NAG	O5-C1	5.25	1.52	1.43
2	O	2	NAG	O5-C1	5.25	1.52	1.43
2	M	2	NAG	O5-C1	5.25	1.52	1.43
2	J	2	NAG	O5-C1	5.24	1.52	1.43
2	R	2	NAG	O5-C1	5.24	1.52	1.43
2	G	1	NAG	O5-C1	5.24	1.52	1.43
2	L	2	NAG	O5-C1	5.24	1.52	1.43
2	P	1	NAG	O5-C1	5.23	1.52	1.43
2	N	2	NAG	O5-C1	5.23	1.52	1.43
2	Q	1	NAG	O5-C1	5.22	1.52	1.43
2	L	1	NAG	O5-C1	5.21	1.52	1.43
2	G	2	NAG	O5-C1	5.20	1.52	1.43
2	E	1	NAG	O5-C1	5.15	1.51	1.43
2	H	1	NAG	O5-C1	5.15	1.51	1.43
2	R	1	NAG	O5-C1	5.15	1.51	1.43
2	O	1	NAG	O5-C1	5.14	1.51	1.43
2	J	1	NAG	O5-C1	5.14	1.51	1.43
2	M	1	NAG	O5-C1	5.10	1.51	1.43
2	D	1	NAG	O5-C1	5.06	1.51	1.43
2	I	1	NAG	O5-C1	5.05	1.51	1.43
2	N	1	NAG	O5-C1	5.03	1.51	1.43
2	L	2	NAG	C7-N2	3.19	1.45	1.34
2	D	2	NAG	C7-N2	3.18	1.45	1.34
2	O	1	NAG	C7-N2	3.18	1.45	1.34
2	J	1	NAG	C7-N2	3.18	1.45	1.34
2	Q	1	NAG	C7-N2	3.18	1.45	1.34
2	Q	2	NAG	C7-N2	3.18	1.45	1.34
2	K	2	NAG	C7-N2	3.18	1.45	1.34
2	R	1	NAG	C7-N2	3.18	1.45	1.34
2	P	2	NAG	C7-N2	3.18	1.45	1.34
2	R	2	NAG	C7-N2	3.18	1.45	1.34
2	H	2	NAG	C7-N2	3.17	1.45	1.34
2	I	1	NAG	C7-N2	3.17	1.45	1.34
2	M	2	NAG	C7-N2	3.17	1.45	1.34
2	G	2	NAG	C7-N2	3.17	1.45	1.34
2	H	1	NAG	C7-N2	3.17	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1	NAG	C7-N2	3.17	1.45	1.34
2	E	2	NAG	C7-N2	3.16	1.45	1.34
2	G	1	NAG	C7-N2	3.16	1.45	1.34
2	D	1	NAG	C7-N2	3.16	1.45	1.34
2	N	1	NAG	C7-N2	3.16	1.45	1.34
2	J	2	NAG	C7-N2	3.16	1.45	1.34
2	I	2	NAG	C7-N2	3.16	1.45	1.34
2	P	1	NAG	C7-N2	3.16	1.45	1.34
2	E	1	NAG	C7-N2	3.15	1.45	1.34
2	N	2	NAG	C7-N2	3.15	1.45	1.34
2	O	2	NAG	C7-N2	3.15	1.45	1.34
2	K	1	NAG	C7-N2	3.15	1.45	1.34
2	L	1	NAG	C7-N2	3.15	1.45	1.34
2	F	1	NAG	C7-N2	3.15	1.45	1.34
2	F	2	NAG	C7-N2	3.14	1.45	1.34
2	F	1	NAG	C2-N2	2.90	1.51	1.46
2	K	1	NAG	C2-N2	2.89	1.51	1.46
2	F	2	NAG	C2-N2	2.87	1.51	1.46
2	D	1	NAG	C2-N2	2.87	1.51	1.46
2	O	2	NAG	C2-N2	2.87	1.51	1.46
2	H	2	NAG	C2-N2	2.86	1.51	1.46
2	L	2	NAG	C2-N2	2.86	1.51	1.46
2	Q	2	NAG	C2-N2	2.86	1.51	1.46
2	P	2	NAG	C2-N2	2.85	1.51	1.46
2	N	2	NAG	C2-N2	2.84	1.51	1.46
2	M	1	NAG	C2-N2	2.84	1.51	1.46
2	H	1	NAG	C2-N2	2.83	1.51	1.46
2	P	1	NAG	C2-N2	2.83	1.51	1.46
2	K	2	NAG	C2-N2	2.83	1.51	1.46
2	R	2	NAG	C2-N2	2.83	1.51	1.46
2	N	1	NAG	C2-N2	2.82	1.51	1.46
2	O	1	NAG	C2-N2	2.82	1.51	1.46
2	E	2	NAG	C2-N2	2.82	1.51	1.46
2	G	2	NAG	C2-N2	2.81	1.51	1.46
2	I	2	NAG	C2-N2	2.81	1.51	1.46
2	Q	1	NAG	C2-N2	2.81	1.51	1.46
2	G	1	NAG	C2-N2	2.81	1.51	1.46
2	J	2	NAG	C2-N2	2.81	1.51	1.46
2	E	1	NAG	C2-N2	2.81	1.51	1.46
2	M	2	NAG	C2-N2	2.81	1.51	1.46
2	D	2	NAG	C2-N2	2.80	1.51	1.46
2	R	1	NAG	C2-N2	2.79	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	NAG	C2-N2	2.78	1.51	1.46
2	I	1	NAG	C2-N2	2.78	1.51	1.46
2	L	1	NAG	C2-N2	2.77	1.51	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	2	NAG	C8-C7-N2	2.45	120.24	116.10
2	R	2	NAG	C8-C7-N2	2.45	120.24	116.10
2	M	2	NAG	C8-C7-N2	2.43	120.21	116.10
2	H	1	NAG	C8-C7-N2	2.40	120.16	116.10
2	Q	2	NAG	C8-C7-N2	2.39	120.15	116.10
2	R	1	NAG	C8-C7-N2	2.39	120.15	116.10
2	L	2	NAG	C8-C7-N2	2.39	120.14	116.10
2	F	1	NAG	C8-C7-N2	2.38	120.13	116.10
2	F	2	NAG	C8-C7-N2	2.38	120.12	116.10
2	J	1	NAG	C8-C7-N2	2.37	120.12	116.10
2	E	1	NAG	C8-C7-N2	2.37	120.12	116.10
2	G	2	NAG	C2-N2-C7	-2.37	119.52	122.90
2	M	1	NAG	C8-C7-N2	2.37	120.11	116.10
2	O	1	NAG	C8-C7-N2	2.37	120.11	116.10
2	O	1	NAG	C2-N2-C7	-2.37	119.53	122.90
2	E	2	NAG	C8-C7-N2	2.37	120.10	116.10
2	J	2	NAG	C8-C7-N2	2.36	120.10	116.10
2	G	2	NAG	C8-C7-N2	2.36	120.10	116.10
2	P	2	NAG	C8-C7-N2	2.36	120.10	116.10
2	J	1	NAG	C2-N2-C7	-2.36	119.54	122.90
2	K	2	NAG	C8-C7-N2	2.36	120.09	116.10
2	P	1	NAG	C8-C7-N2	2.35	120.09	116.10
2	I	2	NAG	C8-C7-N2	2.35	120.08	116.10
2	K	1	NAG	C8-C7-N2	2.35	120.08	116.10
2	E	1	NAG	C2-N2-C7	-2.35	119.56	122.90
2	Q	2	NAG	C2-N2-C7	-2.35	119.56	122.90
2	O	2	NAG	C8-C7-N2	2.34	120.07	116.10
2	D	2	NAG	C8-C7-N2	2.34	120.07	116.10
2	N	2	NAG	C8-C7-N2	2.34	120.06	116.10
2	L	2	NAG	C2-N2-C7	-2.34	119.57	122.90
2	D	1	NAG	C8-C7-N2	2.30	119.99	116.10
2	I	1	NAG	C8-C7-N2	2.30	119.99	116.10
2	N	1	NAG	C8-C7-N2	2.30	119.99	116.10
2	L	1	NAG	C8-C7-N2	2.25	119.91	116.10
2	G	1	NAG	C8-C7-N2	2.25	119.91	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	1	NAG	C8-C7-N2	2.24	119.89	116.10
2	M	1	NAG	C2-N2-C7	-2.20	119.77	122.90
2	R	1	NAG	C2-N2-C7	-2.20	119.77	122.90
2	K	2	NAG	C2-N2-C7	-2.20	119.78	122.90
2	J	2	NAG	C2-N2-C7	-2.19	119.79	122.90
2	P	2	NAG	C2-N2-C7	-2.18	119.80	122.90
2	O	2	NAG	C2-N2-C7	-2.18	119.80	122.90
2	E	2	NAG	C2-N2-C7	-2.18	119.80	122.90
2	H	1	NAG	C2-N2-C7	-2.17	119.81	122.90
2	F	2	NAG	C2-N2-C7	-2.16	119.83	122.90
2	N	2	NAG	C2-N2-C7	-2.04	120.00	122.90
2	D	2	NAG	C2-N2-C7	-2.02	120.03	122.90
2	I	2	NAG	C2-N2-C7	-2.00	120.05	122.90
2	R	2	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (48) 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	D	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
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	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-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	F	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	P	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-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	H	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6

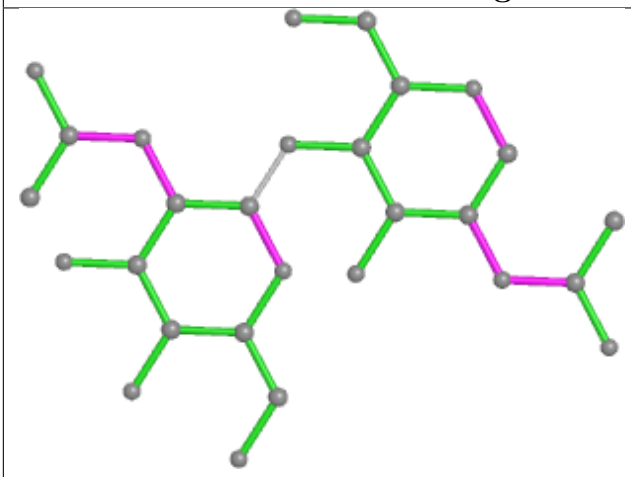
There are no ring outliers.

3 monomers are involved in 3 short contacts:

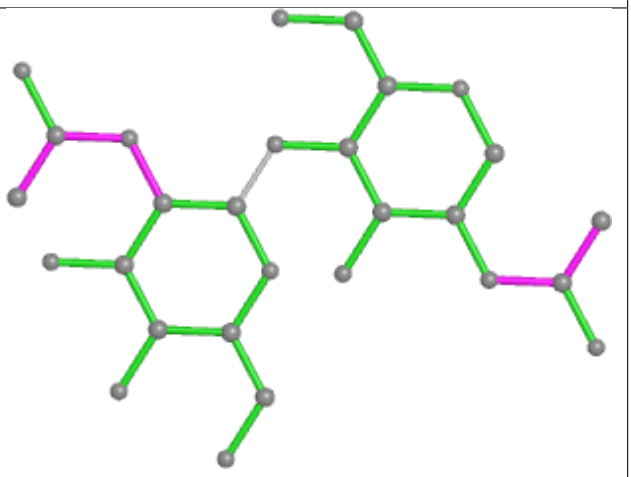
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	1	0
2	F	1	NAG	1	0
2	P	1	NAG	1	0

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

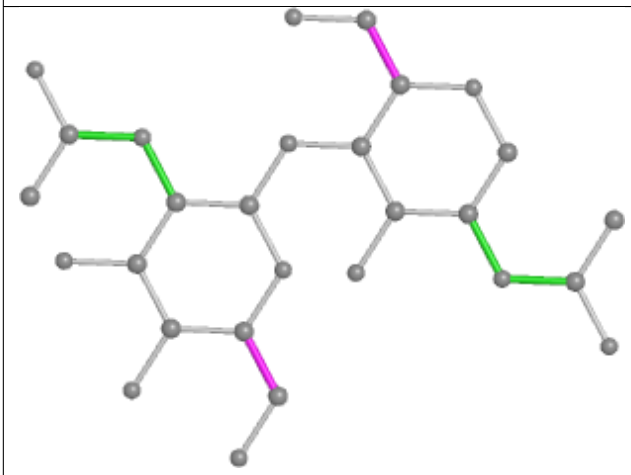
Oligosaccharide Chain D



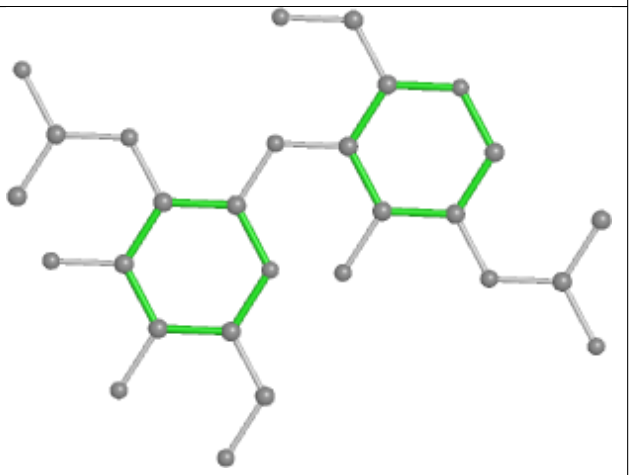
Bond lengths



Bond angles

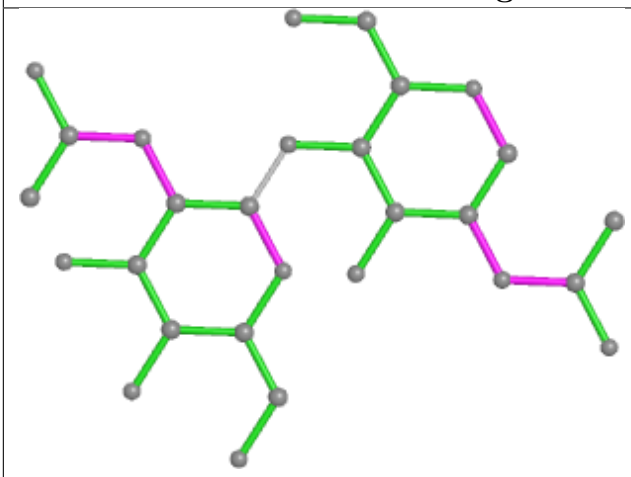


Torsions

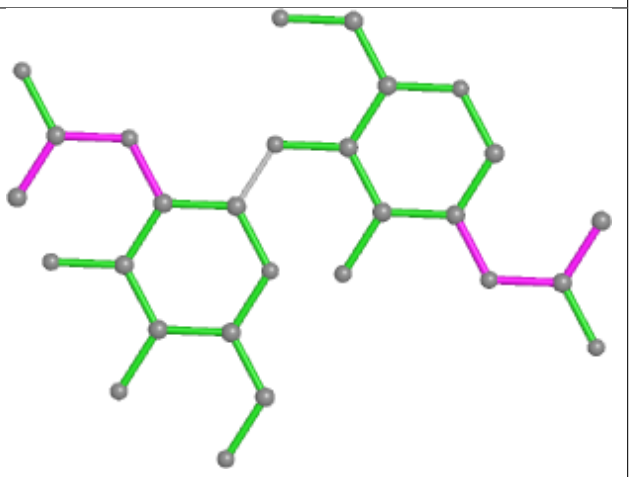


Rings

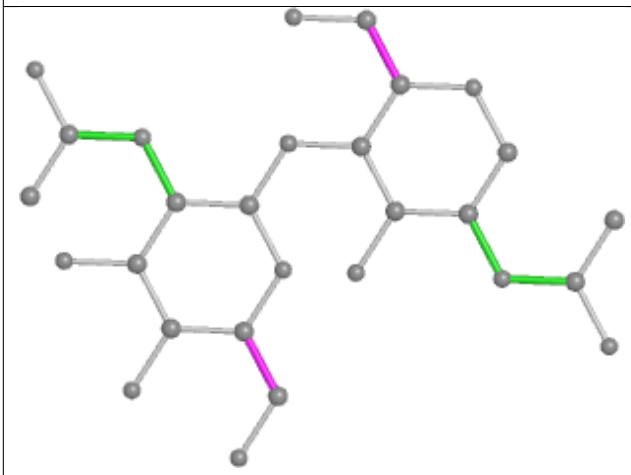
Oligosaccharide Chain E



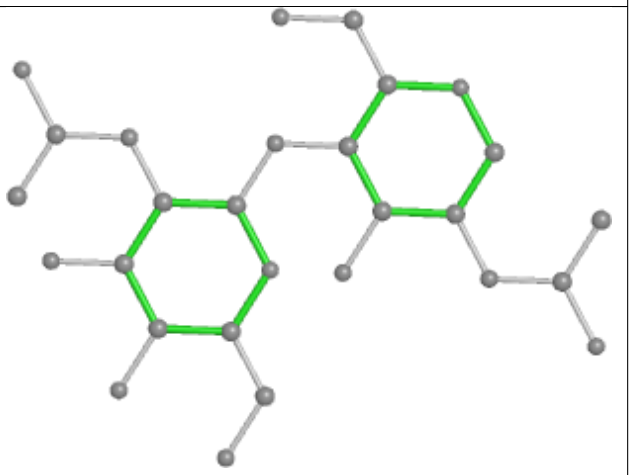
Bond lengths



Bond angles

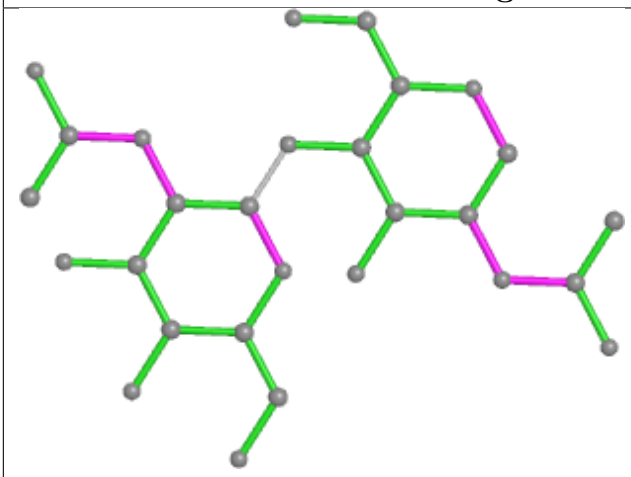


Torsions

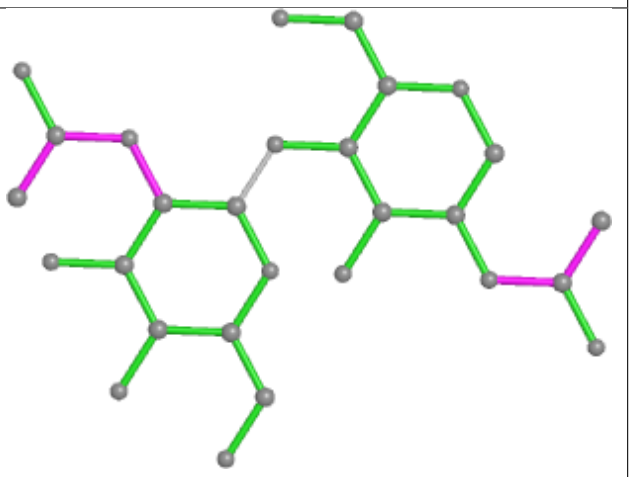


Rings

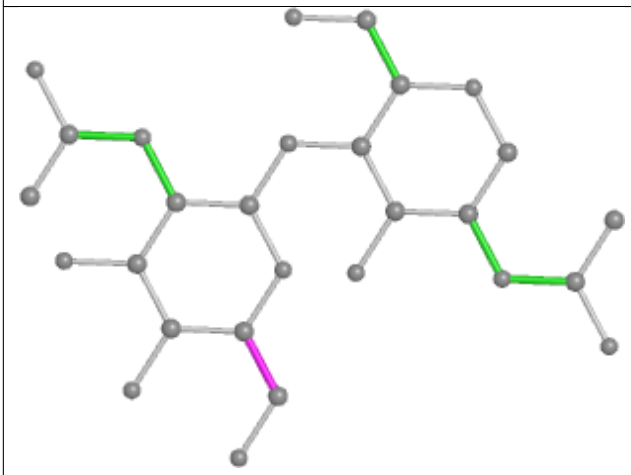
Oligosaccharide Chain F



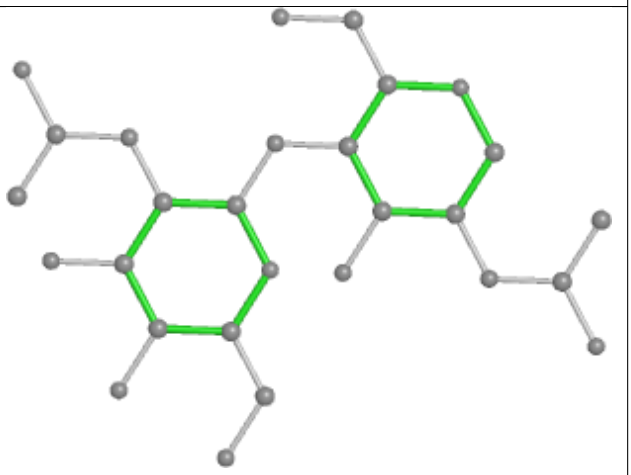
Bond lengths



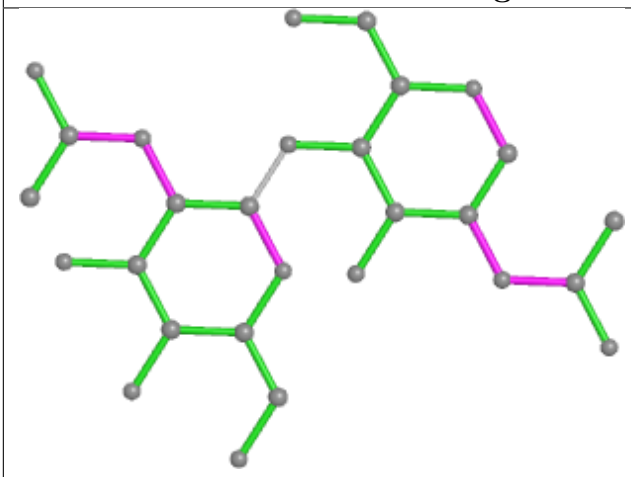
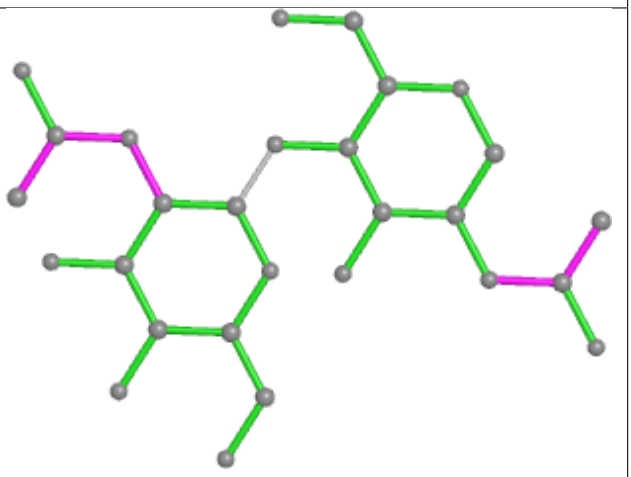
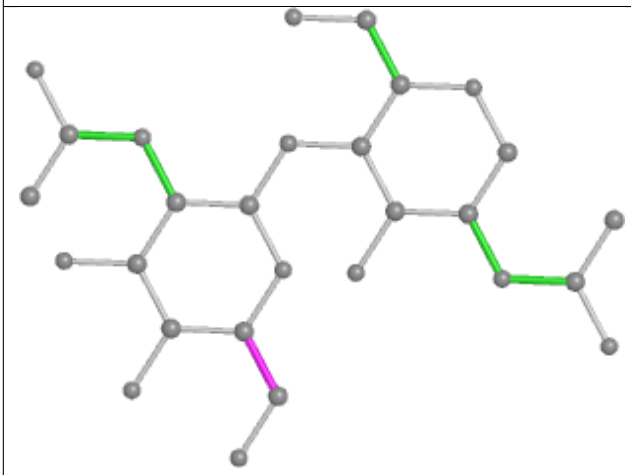
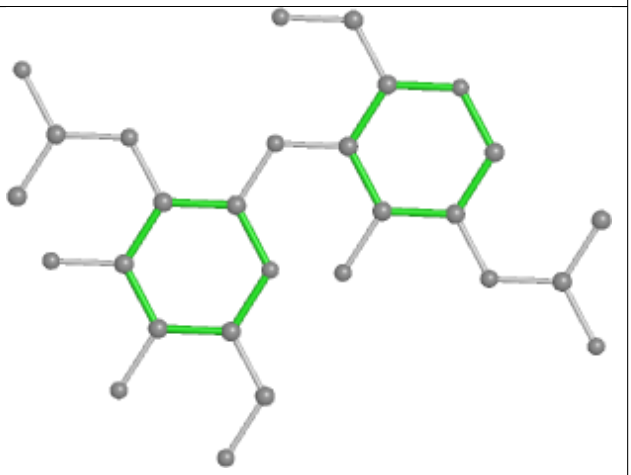
Bond angles



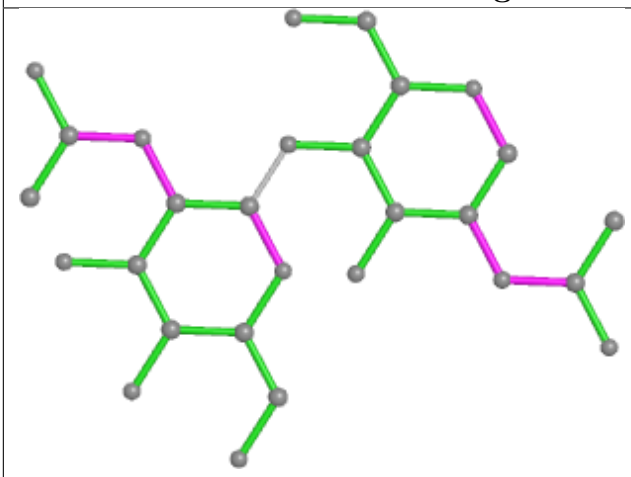
Torsions



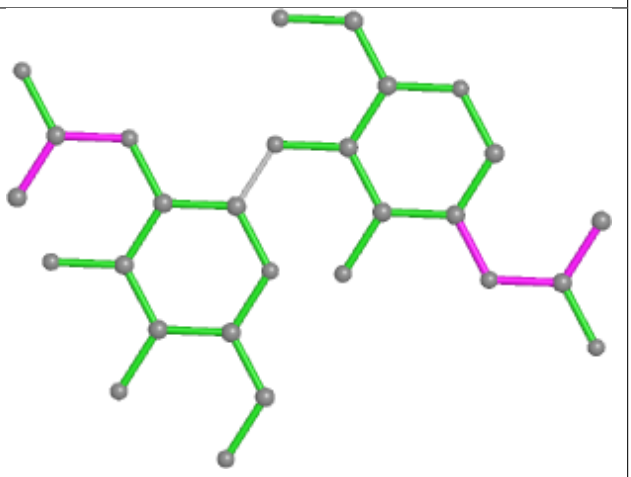
Rings

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

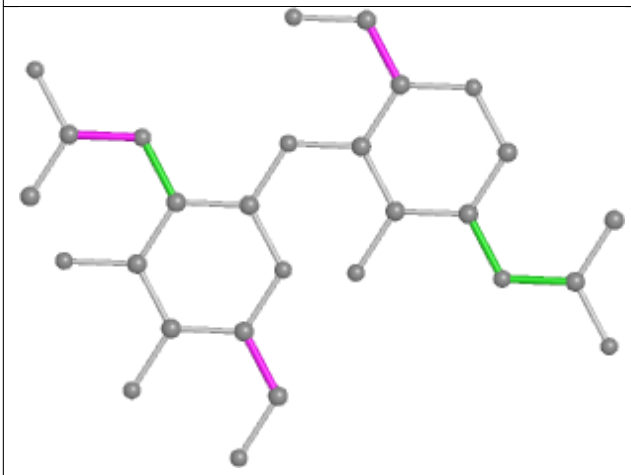
Oligosaccharide Chain H



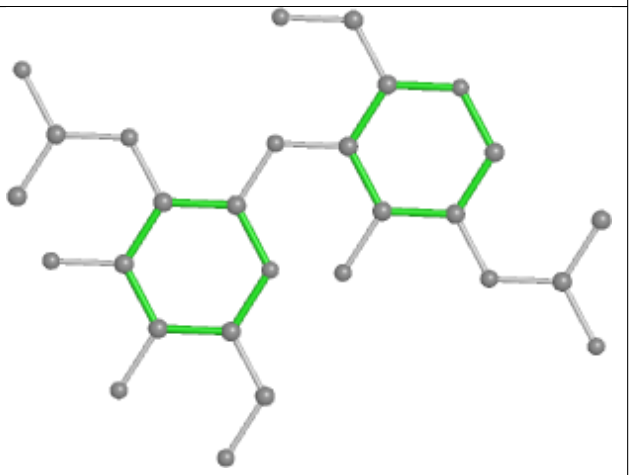
Bond lengths



Bond angles

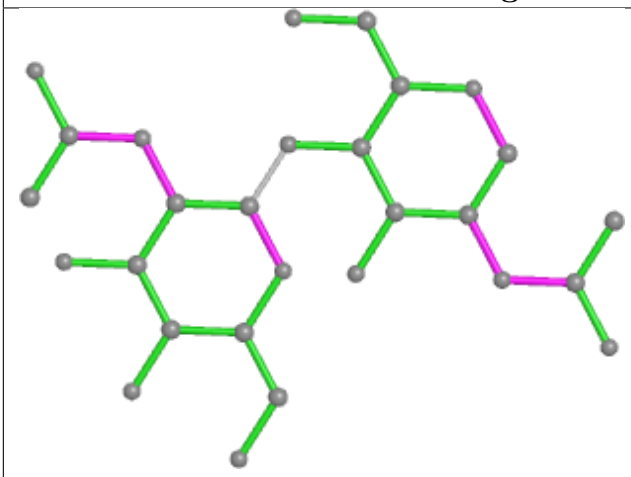


Torsions

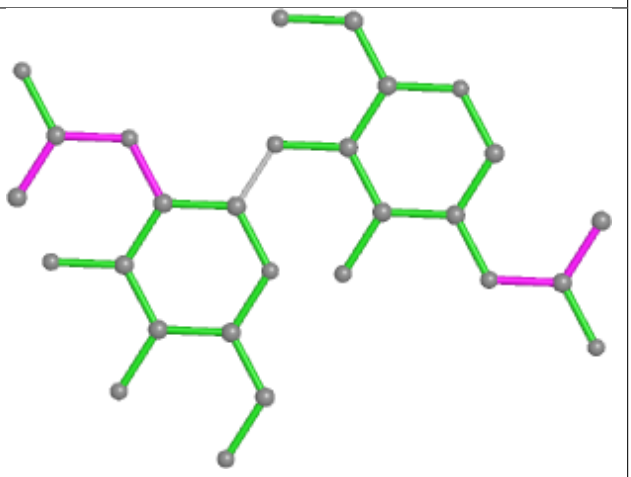


Rings

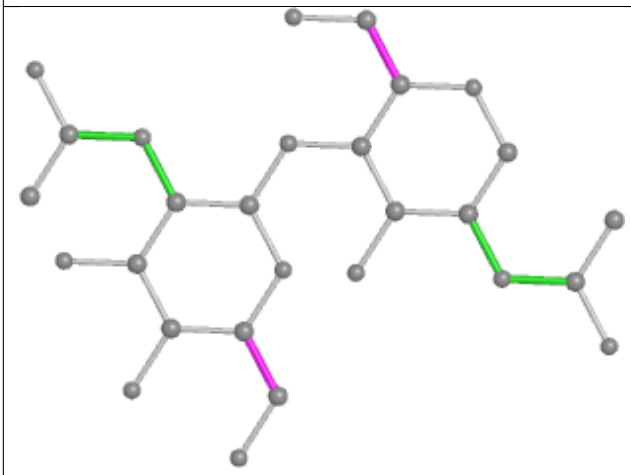
Oligosaccharide Chain I



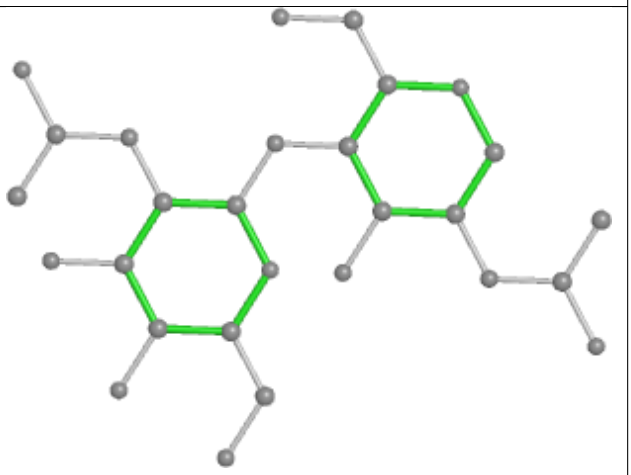
Bond lengths



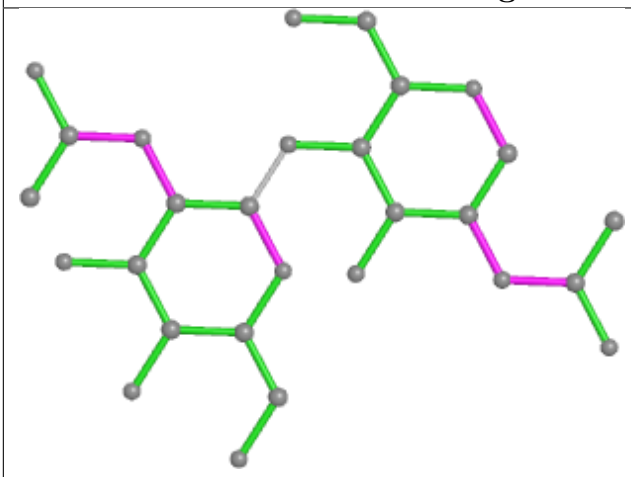
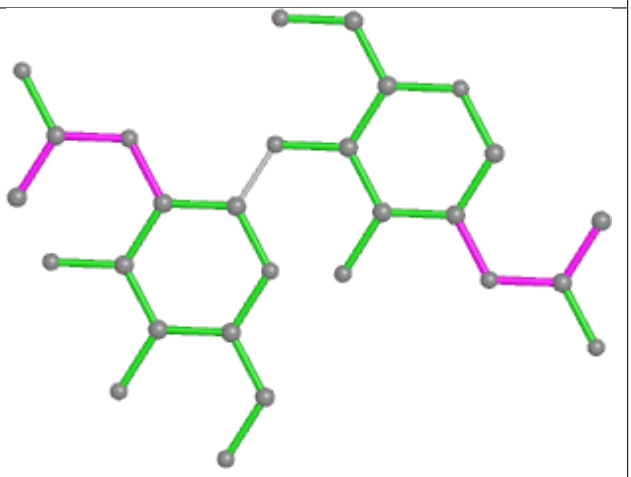
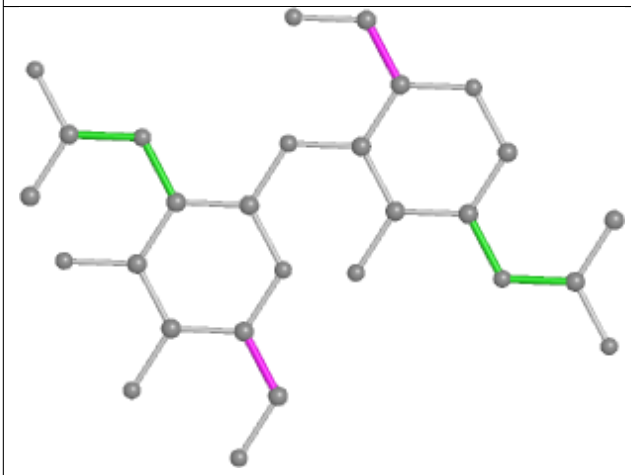
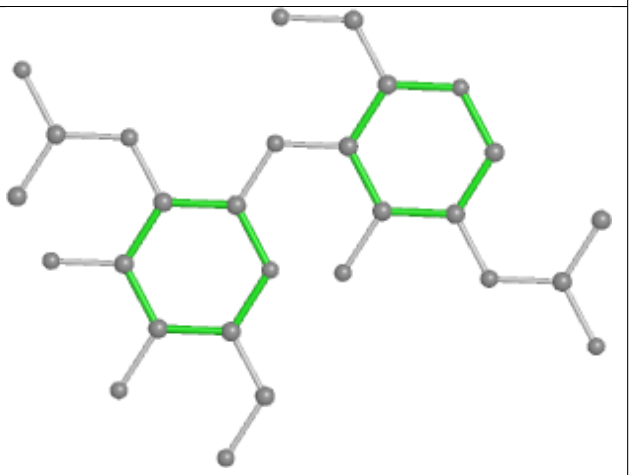
Bond angles



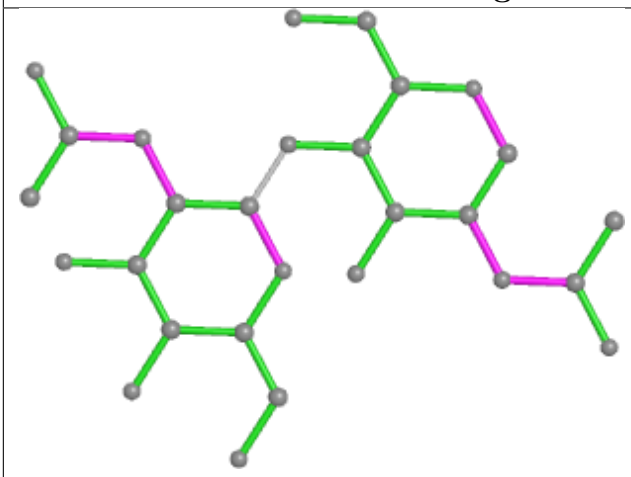
Torsions



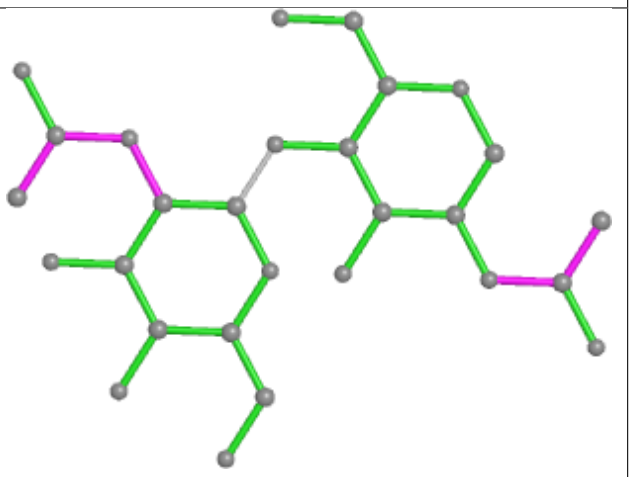
Rings

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

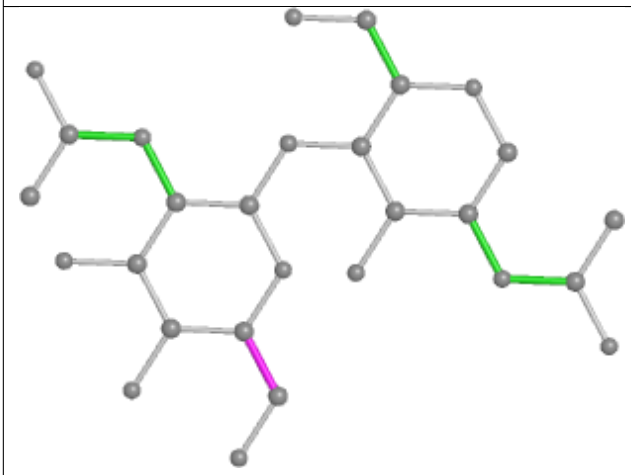
Oligosaccharide Chain K



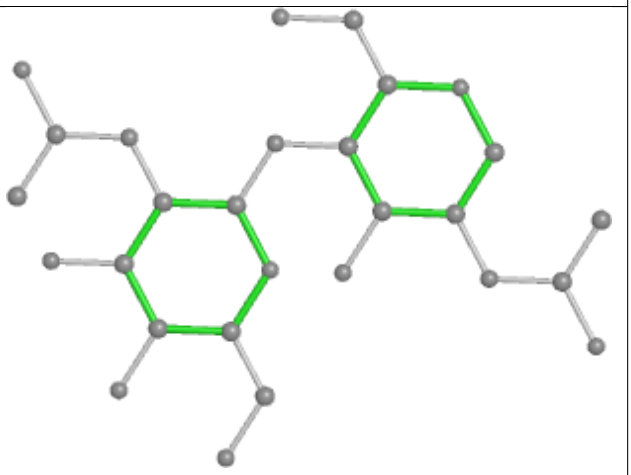
Bond lengths



Bond angles

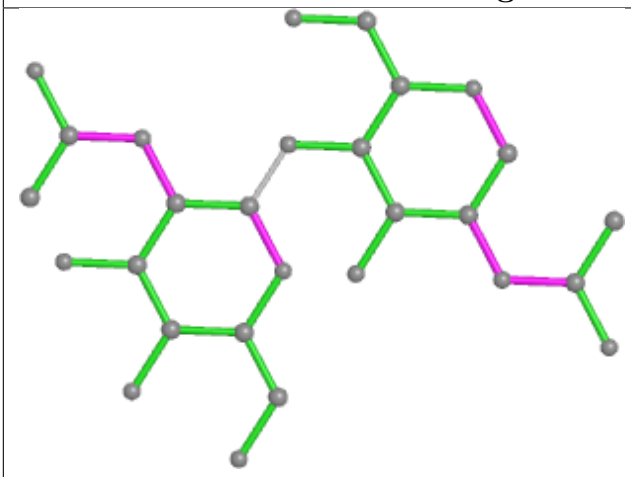


Torsions

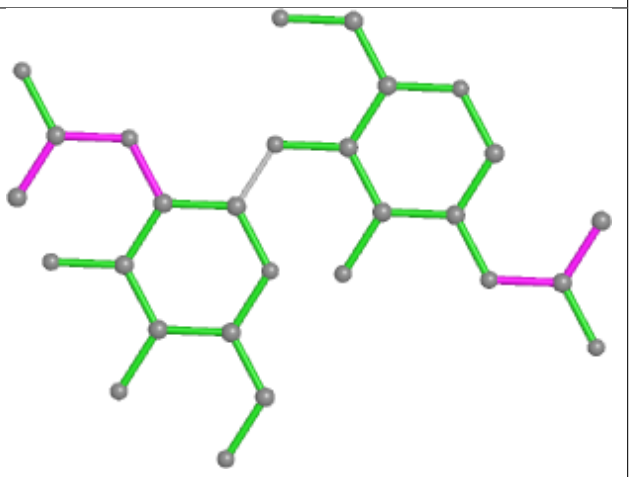


Rings

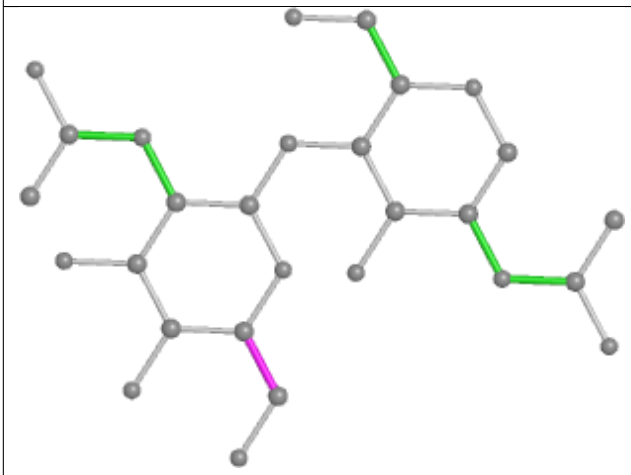
Oligosaccharide Chain L



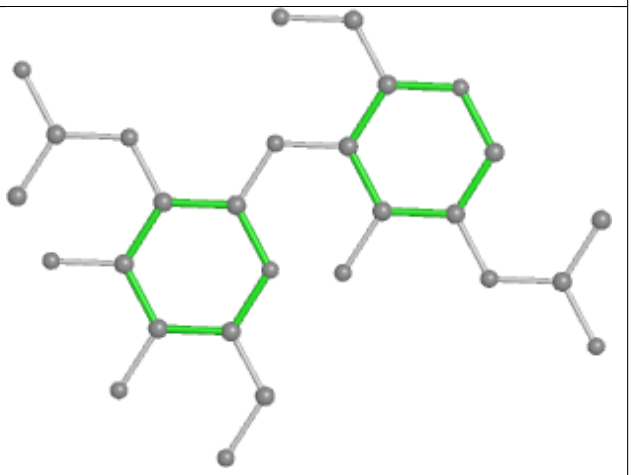
Bond lengths



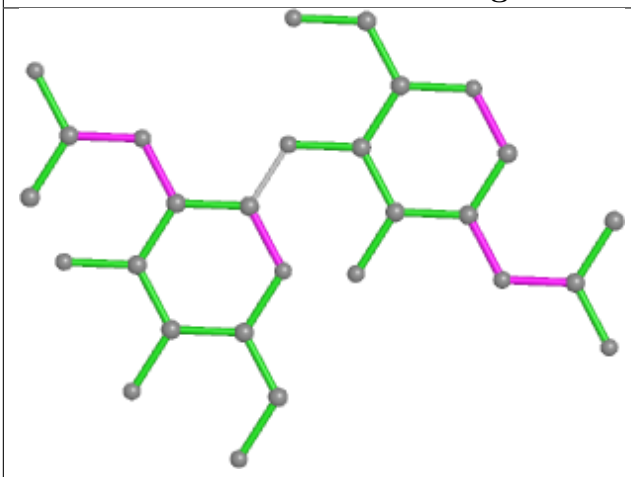
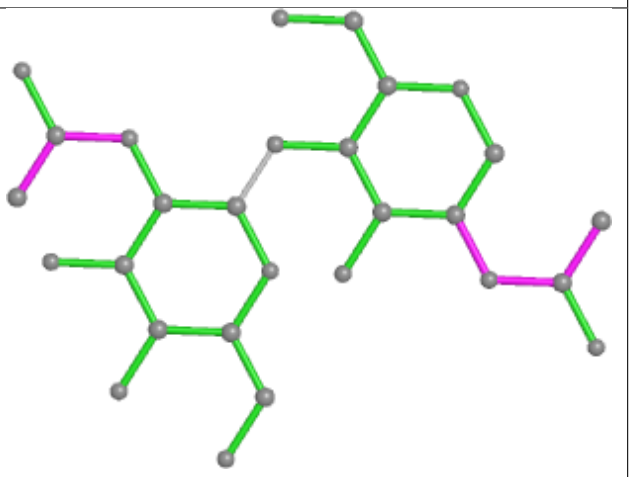
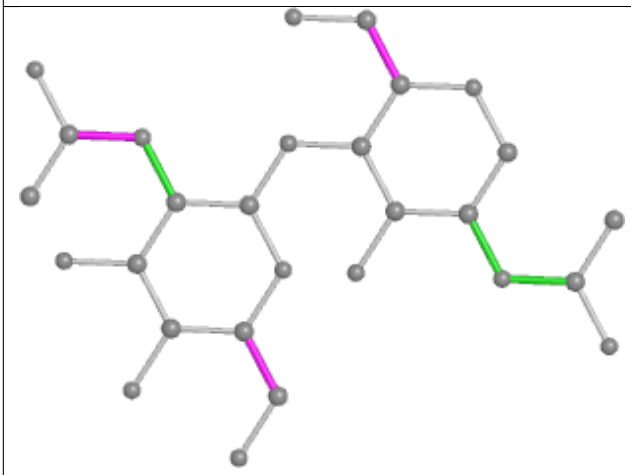
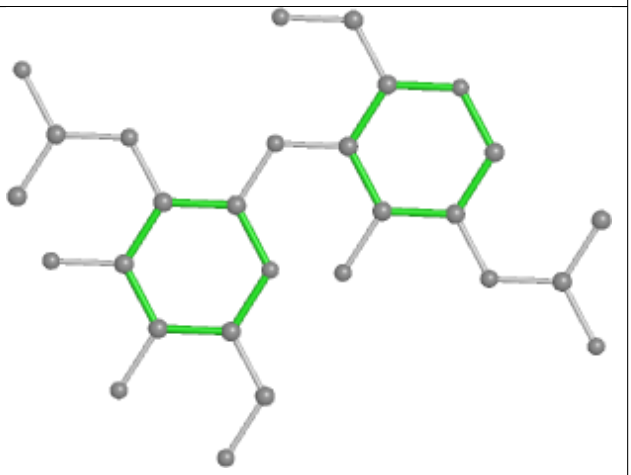
Bond angles



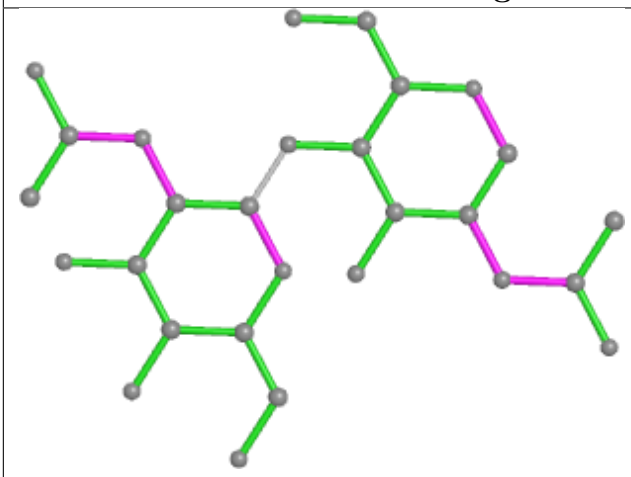
Torsions



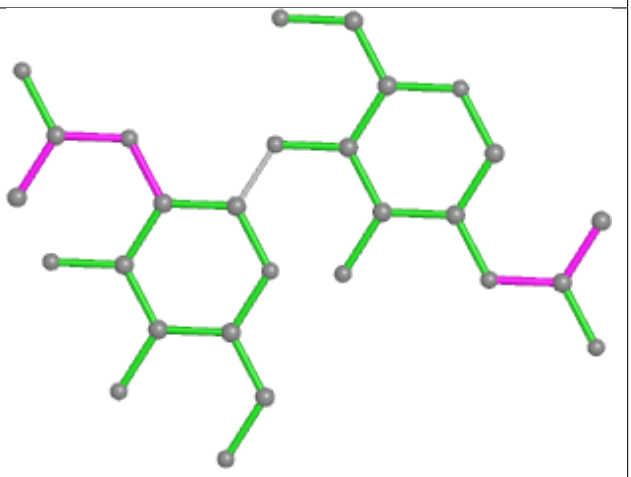
Rings

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

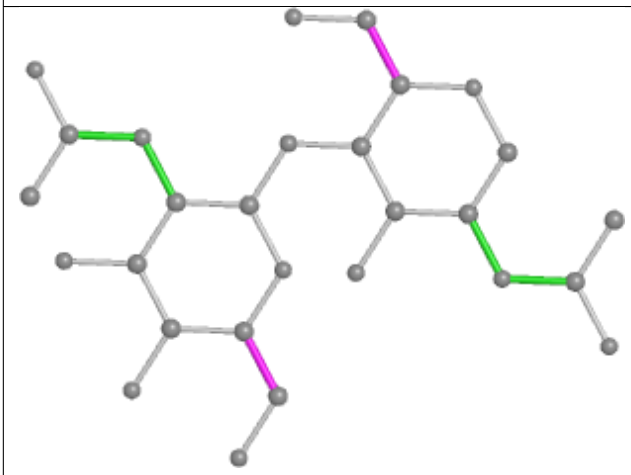
Oligosaccharide Chain N



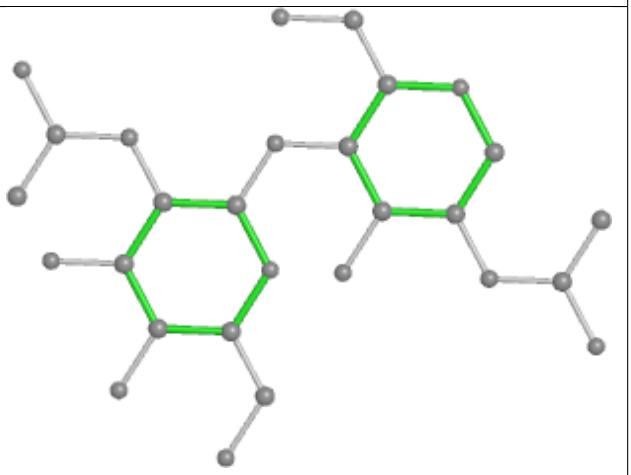
Bond lengths



Bond angles

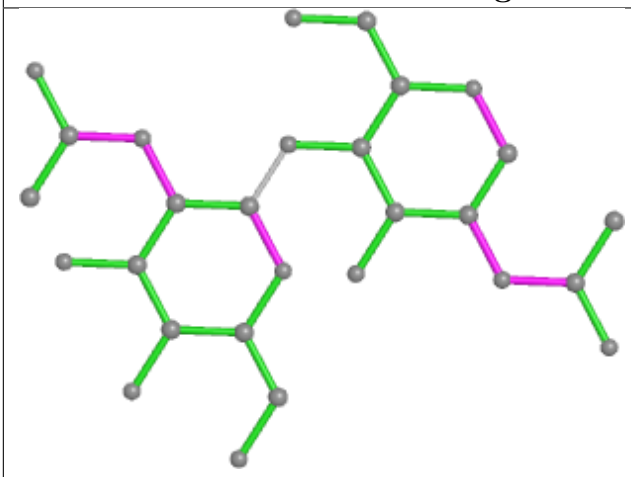


Torsions

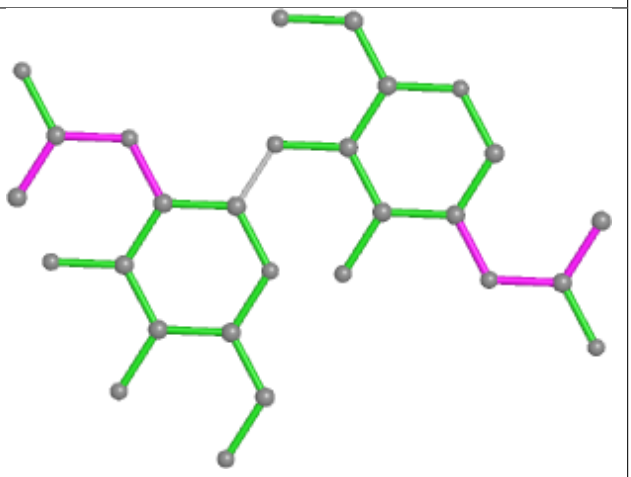


Rings

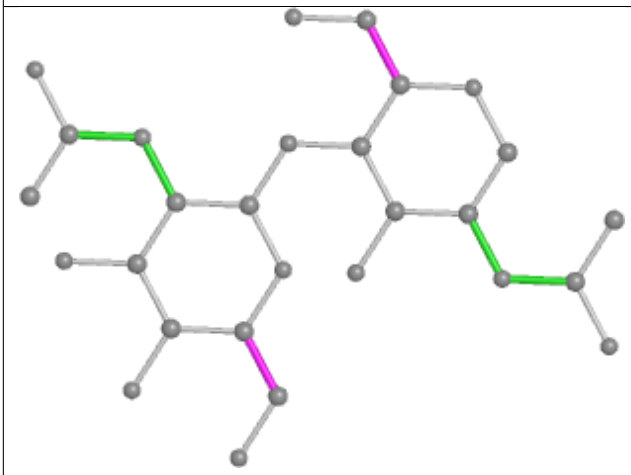
Oligosaccharide Chain O



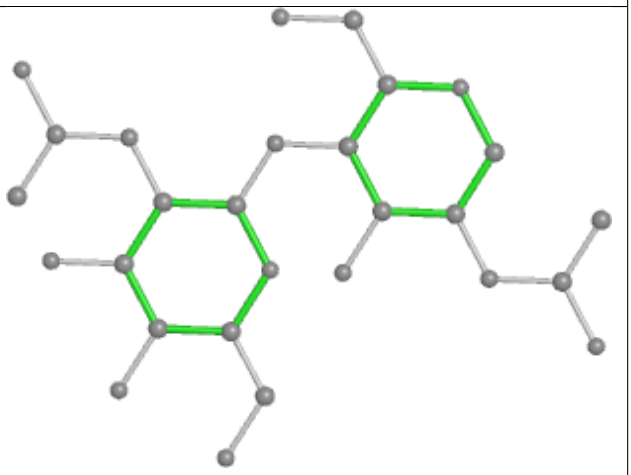
Bond lengths



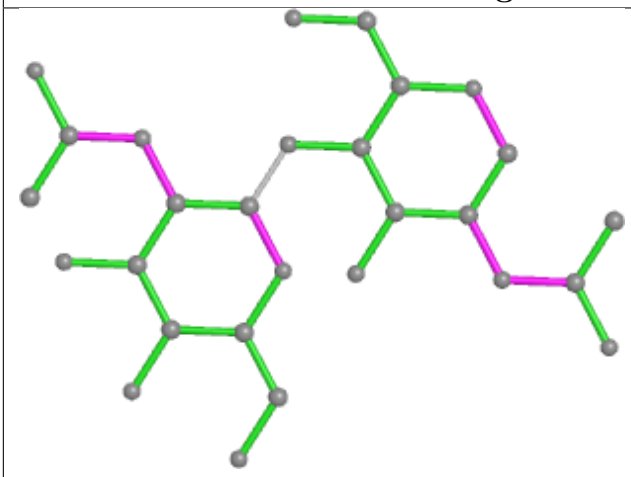
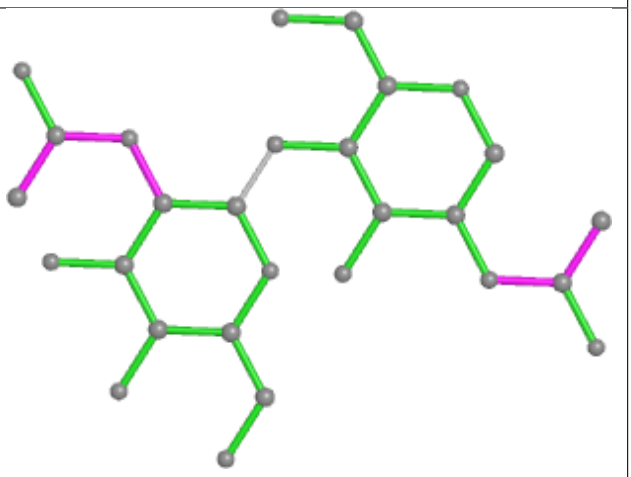
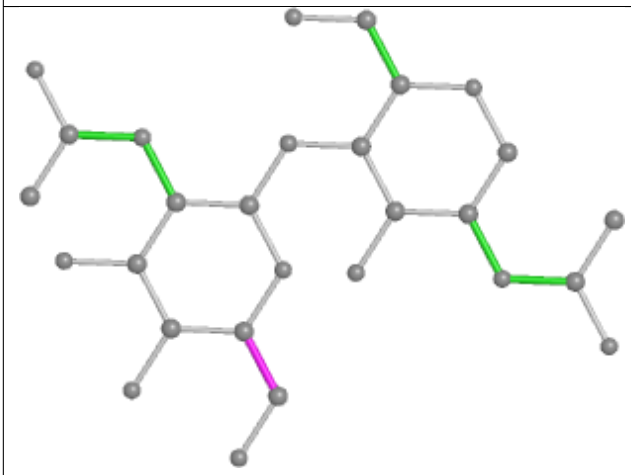
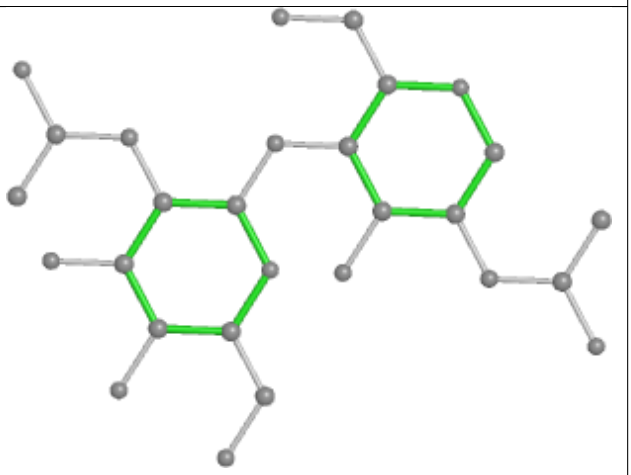
Bond angles



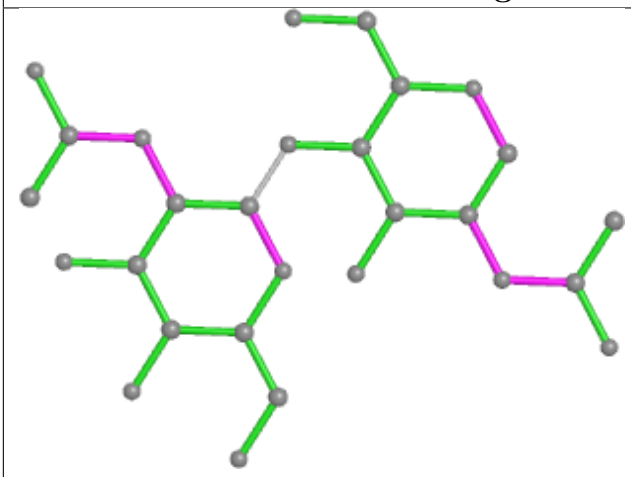
Torsions



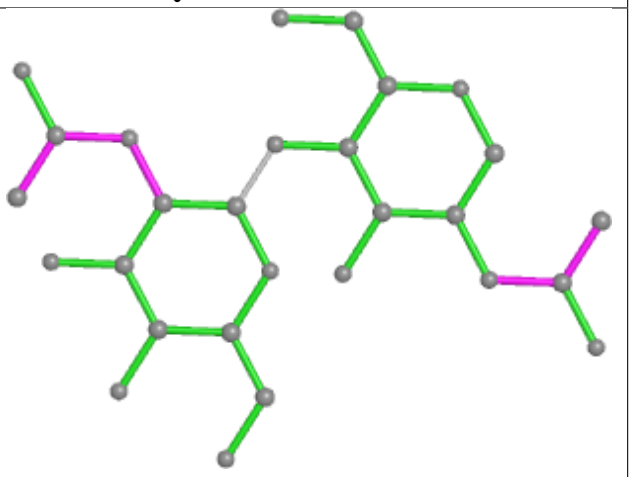
Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

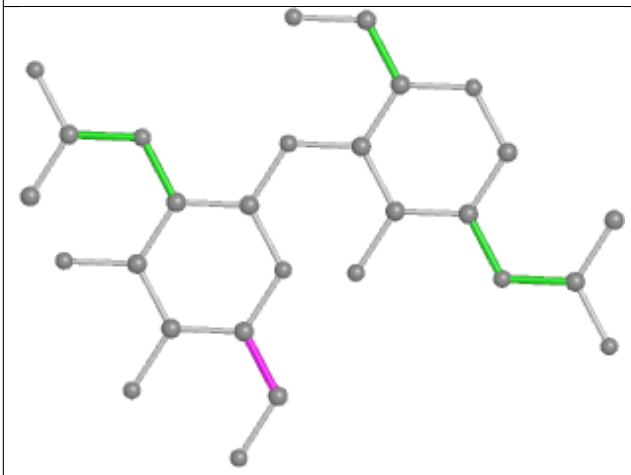
Oligosaccharide Chain Q



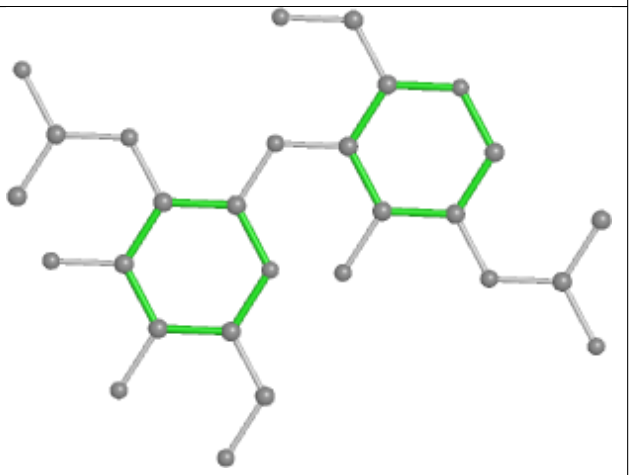
Bond lengths



Bond angles

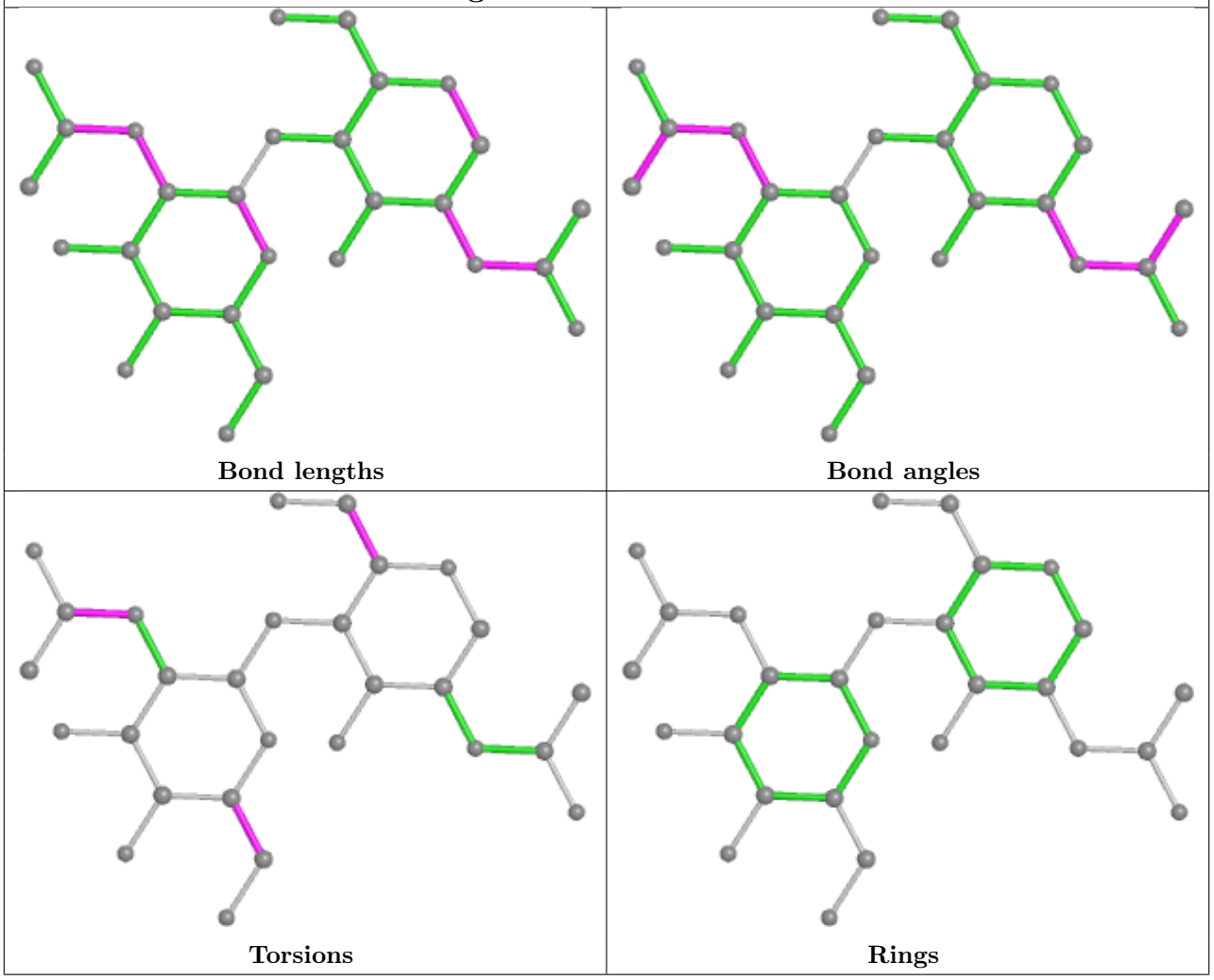


Torsions



Rings

Oligosaccharide Chain R



5.6 Ligand geometry (i)

39 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	C	1303	1	14,14,15	2.01	4 (28%)	17,19,21	1.81	3 (17%)
3	NAG	C	1310	1	14,14,15	2.05	3 (21%)	17,19,21	1.12	2 (11%)
3	NAG	A	1308	1	14,14,15	2.04	3 (21%)	17,19,21	1.11	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	1302	1	14,14,15	1.96	3 (21%)	17,19,21	1.89	4 (23%)
3	NAG	C	1312	1	14,14,15	1.99	3 (21%)	17,19,21	1.45	2 (11%)
3	NAG	A	1305	1	14,14,15	2.07	3 (21%)	17,19,21	1.19	3 (17%)
3	NAG	B	1306	1	14,14,15	1.98	3 (21%)	17,19,21	1.33	2 (11%)
3	NAG	B	1310	1	14,14,15	2.05	4 (28%)	17,19,21	1.12	2 (11%)
3	NAG	A	1307	1	14,14,15	2.02	3 (21%)	17,19,21	1.12	1 (5%)
3	NAG	C	1305	1	14,14,15	2.07	3 (21%)	17,19,21	1.19	3 (17%)
3	NAG	B	1303	1	14,14,15	2.02	4 (28%)	17,19,21	1.81	3 (17%)
3	NAG	C	1311	1	14,14,15	2.04	3 (21%)	17,19,21	1.28	1 (5%)
3	NAG	A	1303	1	14,14,15	2.02	4 (28%)	17,19,21	1.81	3 (17%)
3	NAG	B	1308	1	14,14,15	2.05	3 (21%)	17,19,21	1.12	2 (11%)
3	NAG	C	1301	1	14,14,15	2.09	3 (21%)	17,19,21	1.23	2 (11%)
3	NAG	B	1307	1	14,14,15	2.03	3 (21%)	17,19,21	1.12	2 (11%)
3	NAG	B	1304	1	14,14,15	2.17	3 (21%)	17,19,21	1.73	3 (17%)
3	NAG	A	1301	1	14,14,15	2.08	3 (21%)	17,19,21	1.22	2 (11%)
4	EIC	A	1309	-	19,19,19	0.85	0	19,19,19	1.31	1 (5%)
3	NAG	A	1304	1	14,14,15	2.18	3 (21%)	17,19,21	1.73	3 (17%)
3	NAG	C	1304	1	14,14,15	2.17	3 (21%)	17,19,21	1.74	3 (17%)
5	BLR	B	1313	-	40,46,46	15.52	32 (80%)	44,67,67	5.41	14 (31%)
4	EIC	C	1309	-	19,19,19	0.85	0	19,19,19	1.31	1 (5%)
3	NAG	B	1312	1	14,14,15	1.99	3 (21%)	17,19,21	1.44	2 (11%)
3	NAG	A	1306	1	14,14,15	1.99	3 (21%)	17,19,21	1.33	2 (11%)
3	NAG	A	1312	1	14,14,15	1.99	3 (21%)	17,19,21	1.44	2 (11%)
5	BLR	C	1313	-	40,46,46	15.52	32 (80%)	44,67,67	5.41	15 (34%)
4	EIC	B	1309	-	19,19,19	0.85	0	19,19,19	1.31	1 (5%)
3	NAG	B	1302	1	14,14,15	1.97	3 (21%)	17,19,21	1.89	4 (23%)
3	NAG	C	1302	1	14,14,15	1.95	3 (21%)	17,19,21	1.89	4 (23%)
3	NAG	A	1311	1	14,14,15	2.04	4 (28%)	17,19,21	1.28	1 (5%)
3	NAG	C	1308	1	14,14,15	2.04	3 (21%)	17,19,21	1.12	2 (11%)
3	NAG	B	1301	1	14,14,15	2.08	3 (21%)	17,19,21	1.22	2 (11%)
3	NAG	B	1311	1	14,14,15	2.04	4 (28%)	17,19,21	1.28	1 (5%)
3	NAG	C	1306	1	14,14,15	1.99	3 (21%)	17,19,21	1.32	2 (11%)
3	NAG	C	1307	1	14,14,15	2.02	3 (21%)	17,19,21	1.12	1 (5%)
5	BLR	A	1313	-	40,46,46	15.53	32 (80%)	44,67,67	5.41	14 (31%)
3	NAG	A	1310	1	14,14,15	2.04	3 (21%)	17,19,21	1.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1305	1	14,14,15	2.06	3 (21%)	17,19,21	1.20	3 (17%)

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	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	EIC	A	1309	-	-	8/17/17/17	-
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
5	BLR	B	1313	-	-	15/24/58/58	0/4/4/4
4	EIC	C	1309	-	-	8/17/17/17	-
3	NAG	B	1312	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	4/6/23/26	0/1/1/1
5	BLR	C	1313	-	-	15/24/58/58	0/4/4/4
4	EIC	B	1309	-	-	8/17/17/17	-
3	NAG	B	1302	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
5	BLR	A	1313	-	-	15/24/58/58	0/4/4/4
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1

All (201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1313	BLR	CHA-C1A	72.24	2.06	1.51
5	C	1313	BLR	CHA-C1A	72.14	2.06	1.51
5	B	1313	BLR	CHA-C1A	72.13	2.06	1.51
5	C	1313	BLR	CHA-C4D	36.11	1.78	1.51
5	A	1313	BLR	CHA-C4D	36.01	1.78	1.51
5	B	1313	BLR	CHA-C4D	36.01	1.78	1.51
5	B	1313	BLR	C3D-C4D	25.71	1.77	1.39
5	C	1313	BLR	C3D-C4D	25.69	1.77	1.39
5	A	1313	BLR	C3D-C4D	25.69	1.77	1.39
5	C	1313	BLR	CMB-C2B	21.23	1.95	1.50
5	A	1313	BLR	CMB-C2B	21.21	1.95	1.50
5	B	1313	BLR	CMB-C2B	21.17	1.95	1.50
5	B	1313	BLR	CAA-C2A	19.06	1.80	1.52
5	C	1313	BLR	CAA-C2A	19.05	1.80	1.52
5	A	1313	BLR	CAA-C2A	18.98	1.79	1.52
5	A	1313	BLR	CHB-C1B	18.10	1.72	1.34
5	C	1313	BLR	CHB-C1B	18.09	1.72	1.34
5	B	1313	BLR	CHB-C1B	18.07	1.72	1.34
5	B	1313	BLR	C4C-NC	14.39	1.61	1.37
5	A	1313	BLR	C4C-NC	14.39	1.61	1.37
5	C	1313	BLR	C4C-NC	14.35	1.61	1.37
5	A	1313	BLR	C1B-C2B	11.88	1.66	1.45
5	C	1313	BLR	C1B-C2B	11.87	1.66	1.45
5	B	1313	BLR	C1B-C2B	11.87	1.66	1.45
5	C	1313	BLR	CMA-C3A	11.49	1.75	1.51
5	B	1313	BLR	CMA-C3A	11.47	1.75	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1313	BLR	CMA-C3A	11.47	1.75	1.51
5	A	1313	BLR	C4B-NB	11.22	1.61	1.38
5	C	1313	BLR	C4B-NB	11.19	1.61	1.38
5	B	1313	BLR	C4B-NB	11.18	1.61	1.38
5	A	1313	BLR	CMD-C2D	9.66	1.71	1.51
5	B	1313	BLR	CMD-C2D	9.63	1.71	1.51
5	C	1313	BLR	CMD-C2D	9.62	1.71	1.51
5	C	1313	BLR	CAD-CBD	8.91	1.97	1.52
5	B	1313	BLR	CAD-CBD	8.89	1.97	1.52
5	A	1313	BLR	CAD-CBD	8.89	1.97	1.52
5	A	1313	BLR	CHD-C4C	-7.95	1.17	1.34
5	C	1313	BLR	CHD-C4C	-7.94	1.17	1.34
5	B	1313	BLR	CHD-C4C	-7.94	1.17	1.34
5	A	1313	BLR	CAB-C3B	7.41	1.67	1.47
5	A	1313	BLR	C2A-C1A	7.39	1.50	1.39
5	B	1313	BLR	CAB-C3B	7.39	1.67	1.47
5	C	1313	BLR	CAB-C3B	7.38	1.67	1.47
5	C	1313	BLR	C2A-C1A	7.36	1.50	1.39
5	B	1313	BLR	C2A-C1A	7.34	1.50	1.39
5	B	1313	BLR	CBA-CGA	7.04	1.66	1.50
5	A	1313	BLR	CBA-CGA	7.03	1.66	1.50
5	C	1313	BLR	CBA-CGA	7.03	1.66	1.50
5	B	1313	BLR	C1B-NB	6.51	1.48	1.37
5	A	1313	BLR	C1B-NB	6.51	1.48	1.37
5	C	1313	BLR	C1B-NB	6.51	1.48	1.37
5	A	1313	BLR	CAA-CBA	6.04	1.82	1.52
5	B	1313	BLR	CAA-CBA	6.04	1.82	1.52
5	C	1313	BLR	CAA-CBA	6.04	1.82	1.52
5	B	1313	BLR	OB-C4B	-5.99	1.12	1.23
5	C	1313	BLR	OB-C4B	-5.99	1.12	1.23
3	A	1304	NAG	O5-C1	5.96	1.53	1.43
5	A	1313	BLR	OB-C4B	-5.95	1.12	1.23
3	B	1304	NAG	O5-C1	5.94	1.53	1.43
3	C	1304	NAG	O5-C1	5.90	1.53	1.43
3	C	1301	NAG	O5-C1	5.53	1.52	1.43
3	B	1301	NAG	O5-C1	5.53	1.52	1.43
3	A	1301	NAG	O5-C1	5.51	1.52	1.43
3	B	1305	NAG	O5-C1	5.46	1.52	1.43
3	C	1305	NAG	O5-C1	5.46	1.52	1.43
3	A	1305	NAG	O5-C1	5.45	1.52	1.43
5	A	1313	BLR	C1D-CHD	5.41	1.62	1.41
5	C	1313	BLR	C1D-CHD	5.41	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1313	BLR	C1D-CHD	5.40	1.62	1.41
3	C	1311	NAG	O5-C1	5.37	1.52	1.43
3	A	1311	NAG	O5-C1	5.36	1.52	1.43
3	B	1308	NAG	O5-C1	5.36	1.52	1.43
3	B	1311	NAG	O5-C1	5.34	1.52	1.43
3	C	1310	NAG	O5-C1	5.33	1.52	1.43
3	C	1307	NAG	O5-C1	5.32	1.52	1.43
3	C	1308	NAG	O5-C1	5.31	1.52	1.43
3	A	1308	NAG	O5-C1	5.31	1.52	1.43
3	B	1307	NAG	O5-C1	5.31	1.52	1.43
3	B	1310	NAG	O5-C1	5.30	1.52	1.43
3	A	1307	NAG	O5-C1	5.29	1.52	1.43
3	A	1310	NAG	O5-C1	5.28	1.52	1.43
3	C	1312	NAG	O5-C1	5.25	1.52	1.43
3	B	1312	NAG	O5-C1	5.23	1.52	1.43
3	A	1312	NAG	O5-C1	5.19	1.52	1.43
3	A	1306	NAG	O5-C1	5.16	1.52	1.43
3	B	1306	NAG	O5-C1	5.12	1.51	1.43
3	C	1306	NAG	O5-C1	5.11	1.51	1.43
3	B	1302	NAG	O5-C1	5.07	1.51	1.43
3	A	1302	NAG	O5-C1	5.01	1.51	1.43
3	C	1302	NAG	O5-C1	4.99	1.51	1.43
5	C	1313	BLR	C2A-C3A	-4.99	1.22	1.37
5	B	1313	BLR	C2A-C3A	-4.99	1.22	1.37
5	A	1313	BLR	C2A-C3A	-4.95	1.23	1.37
3	B	1303	NAG	O5-C1	4.92	1.51	1.43
3	A	1303	NAG	O5-C1	4.91	1.51	1.43
5	B	1313	BLR	CMC-C2C	-4.91	1.40	1.50
3	C	1303	NAG	O5-C1	4.91	1.51	1.43
5	C	1313	BLR	CMC-C2C	-4.89	1.40	1.50
5	A	1313	BLR	CMC-C2C	-4.86	1.40	1.50
5	A	1313	BLR	CAC-C3C	4.55	1.59	1.47
5	C	1313	BLR	C1C-NC	4.54	1.47	1.38
5	A	1313	BLR	C1C-NC	4.53	1.47	1.38
5	B	1313	BLR	C1C-NC	4.53	1.47	1.38
5	B	1313	BLR	CAC-C3C	4.53	1.59	1.47
5	C	1313	BLR	CAC-C3C	4.51	1.59	1.47
5	A	1313	BLR	CBD-CGD	4.28	1.60	1.50
5	C	1313	BLR	CBD-CGD	4.28	1.60	1.50
5	B	1313	BLR	CBD-CGD	4.28	1.60	1.50
5	C	1313	BLR	OC-C1C	-4.22	1.15	1.23
5	B	1313	BLR	OC-C1C	-4.20	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1313	BLR	OC-C1C	-4.20	1.15	1.23
5	C	1313	BLR	C3B-C2B	-3.88	1.29	1.37
5	A	1313	BLR	C3B-C2B	-3.87	1.29	1.37
5	B	1313	BLR	C3B-C2B	-3.83	1.29	1.37
5	C	1313	BLR	C3D-C2D	-3.77	1.26	1.37
5	A	1313	BLR	C3D-C2D	-3.77	1.26	1.37
5	B	1313	BLR	C3D-C2D	-3.76	1.26	1.37
5	A	1313	BLR	C1C-C2C	-3.44	1.38	1.47
5	B	1313	BLR	C1C-C2C	-3.41	1.38	1.47
5	C	1313	BLR	C1C-C2C	-3.40	1.38	1.47
3	B	1302	NAG	C7-N2	3.34	1.45	1.34
3	C	1302	NAG	C7-N2	3.32	1.45	1.34
3	A	1302	NAG	C7-N2	3.30	1.45	1.34
3	B	1312	NAG	C7-N2	3.28	1.45	1.34
3	A	1312	NAG	C7-N2	3.27	1.45	1.34
3	C	1312	NAG	C7-N2	3.27	1.45	1.34
3	C	1303	NAG	C7-N2	3.23	1.45	1.34
3	A	1303	NAG	C7-N2	3.23	1.45	1.34
3	B	1303	NAG	C7-N2	3.22	1.45	1.34
3	C	1301	NAG	C7-N2	3.21	1.45	1.34
3	B	1304	NAG	C7-N2	3.21	1.45	1.34
3	C	1310	NAG	C7-N2	3.21	1.45	1.34
3	C	1304	NAG	C7-N2	3.20	1.45	1.34
3	B	1306	NAG	C7-N2	3.20	1.45	1.34
3	C	1308	NAG	C7-N2	3.20	1.45	1.34
3	A	1301	NAG	C7-N2	3.20	1.45	1.34
3	A	1304	NAG	C7-N2	3.19	1.45	1.34
3	B	1308	NAG	C7-N2	3.19	1.45	1.34
3	B	1310	NAG	C7-N2	3.18	1.45	1.34
3	C	1306	NAG	C7-N2	3.18	1.45	1.34
3	B	1301	NAG	C7-N2	3.18	1.45	1.34
3	B	1307	NAG	C7-N2	3.17	1.45	1.34
3	C	1307	NAG	C7-N2	3.17	1.45	1.34
3	A	1305	NAG	C7-N2	3.17	1.45	1.34
3	A	1308	NAG	C7-N2	3.17	1.45	1.34
3	A	1306	NAG	C7-N2	3.17	1.45	1.34
3	A	1310	NAG	C7-N2	3.17	1.45	1.34
3	C	1305	NAG	C7-N2	3.16	1.45	1.34
3	B	1311	NAG	C7-N2	3.16	1.45	1.34
3	B	1305	NAG	C7-N2	3.16	1.45	1.34
3	C	1311	NAG	C7-N2	3.16	1.45	1.34
3	A	1307	NAG	C7-N2	3.15	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1311	NAG	C7-N2	3.15	1.45	1.34
3	A	1302	NAG	C2-N2	3.04	1.51	1.46
3	B	1302	NAG	C2-N2	3.02	1.51	1.46
3	A	1312	NAG	C2-N2	3.00	1.51	1.46
3	C	1302	NAG	C2-N2	2.99	1.51	1.46
3	B	1312	NAG	C2-N2	2.98	1.51	1.46
3	C	1312	NAG	C2-N2	2.97	1.51	1.46
3	B	1301	NAG	C2-N2	2.95	1.51	1.46
3	C	1301	NAG	C2-N2	2.92	1.51	1.46
3	A	1301	NAG	C2-N2	2.92	1.51	1.46
3	C	1304	NAG	C2-N2	2.91	1.51	1.46
3	A	1304	NAG	C2-N2	2.90	1.51	1.46
3	A	1303	NAG	C2-N2	2.89	1.51	1.46
3	B	1310	NAG	C2-N2	2.89	1.51	1.46
3	B	1304	NAG	C2-N2	2.88	1.51	1.46
3	A	1305	NAG	C2-N2	2.87	1.51	1.46
3	A	1310	NAG	C2-N2	2.87	1.51	1.46
3	A	1307	NAG	C2-N2	2.87	1.51	1.46
3	C	1305	NAG	C2-N2	2.87	1.51	1.46
3	C	1311	NAG	C2-N2	2.86	1.51	1.46
3	B	1303	NAG	C2-N2	2.86	1.51	1.46
3	C	1306	NAG	C2-N2	2.86	1.51	1.46
3	C	1308	NAG	C2-N2	2.86	1.51	1.46
3	C	1303	NAG	C2-N2	2.85	1.51	1.46
3	C	1310	NAG	C2-N2	2.84	1.51	1.46
3	B	1305	NAG	C2-N2	2.84	1.51	1.46
3	B	1308	NAG	C2-N2	2.83	1.51	1.46
3	A	1311	NAG	C2-N2	2.83	1.51	1.46
3	B	1306	NAG	C2-N2	2.82	1.51	1.46
3	B	1307	NAG	C2-N2	2.82	1.51	1.46
3	A	1306	NAG	C2-N2	2.82	1.51	1.46
3	A	1308	NAG	C2-N2	2.82	1.51	1.46
3	B	1311	NAG	C2-N2	2.78	1.51	1.46
3	C	1307	NAG	C2-N2	2.76	1.51	1.46
5	C	1313	BLR	O2A-CGA	2.69	1.31	1.22
5	B	1313	BLR	O2A-CGA	2.68	1.31	1.22
5	A	1313	BLR	O2A-CGA	2.66	1.31	1.22
5	B	1313	BLR	C4A-CHB	-2.22	1.32	1.41
5	C	1313	BLR	C4A-CHB	-2.21	1.32	1.41
5	A	1313	BLR	C4A-CHB	-2.21	1.32	1.41
3	B	1303	NAG	O5-C5	2.21	1.47	1.43
3	C	1303	NAG	O5-C5	2.19	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1313	BLR	O2D-CGD	2.18	1.29	1.22
3	A	1303	NAG	O5-C5	2.17	1.47	1.43
5	C	1313	BLR	O2D-CGD	2.16	1.29	1.22
5	B	1313	BLR	O2D-CGD	2.14	1.29	1.22
3	A	1311	NAG	O5-C5	2.02	1.47	1.43
3	B	1311	NAG	O5-C5	2.02	1.47	1.43
3	B	1310	NAG	O5-C5	2.01	1.47	1.43

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1313	BLR	CHB-C1B-C2B	24.07	174.51	126.97
5	A	1313	BLR	CHB-C1B-C2B	24.07	174.49	126.97
5	B	1313	BLR	CHB-C1B-C2B	24.05	174.46	126.97
5	B	1313	BLR	CHD-C4C-C3C	-15.62	87.66	127.91
5	C	1313	BLR	CHD-C4C-C3C	-15.61	87.67	127.91
5	A	1313	BLR	CHD-C4C-C3C	-15.60	87.68	127.91
5	A	1313	BLR	CHB-C1B-NB	-13.59	84.75	130.40
5	C	1313	BLR	CHB-C1B-NB	-13.58	84.78	130.40
5	B	1313	BLR	CHB-C1B-NB	-13.58	84.79	130.40
5	B	1313	BLR	CHD-C4C-NC	10.92	167.08	130.40
5	C	1313	BLR	CHD-C4C-NC	10.90	167.03	130.40
5	A	1313	BLR	CHD-C4C-NC	10.90	167.02	130.40
5	A	1313	BLR	C4C-NC-C1C	-5.69	103.42	110.67
5	B	1313	BLR	C4C-NC-C1C	-5.66	103.47	110.67
5	C	1313	BLR	C4C-NC-C1C	-5.66	103.47	110.67
3	C	1304	NAG	C1-O5-C5	5.38	119.49	112.19
3	A	1304	NAG	C1-O5-C5	5.33	119.41	112.19
3	B	1304	NAG	C1-O5-C5	5.33	119.41	112.19
5	C	1313	BLR	C3B-C2B-C1B	4.65	113.65	108.03
3	B	1303	NAG	C1-O5-C5	-4.62	105.94	112.19
5	A	1313	BLR	C3B-C2B-C1B	4.58	113.57	108.03
5	B	1313	BLR	C3B-C2B-C1B	4.57	113.56	108.03
3	C	1303	NAG	C1-O5-C5	-4.57	106.00	112.19
3	A	1303	NAG	C1-O5-C5	-4.57	106.00	112.19
5	C	1313	BLR	C2B-C1B-NB	-4.29	100.70	106.99
5	A	1313	BLR	C2B-C1B-NB	-4.26	100.74	106.99
5	B	1313	BLR	C2B-C1B-NB	-4.26	100.74	106.99
3	B	1302	NAG	C4-C3-C2	3.80	116.58	111.02
3	A	1302	NAG	C4-C3-C2	3.78	116.56	111.02
3	C	1302	NAG	C4-C3-C2	3.77	116.55	111.02
3	B	1302	NAG	C1-O5-C5	-3.76	107.10	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1302	NAG	C1-O5-C5	-3.76	107.10	112.19
3	C	1312	NAG	C4-C3-C2	3.75	116.52	111.02
3	C	1302	NAG	C1-O5-C5	-3.72	107.15	112.19
3	B	1312	NAG	C4-C3-C2	3.72	116.47	111.02
3	A	1312	NAG	C4-C3-C2	3.70	116.45	111.02
3	A	1302	NAG	C3-C4-C5	3.58	116.62	110.24
3	C	1302	NAG	C3-C4-C5	3.57	116.60	110.24
3	B	1302	NAG	C3-C4-C5	3.56	116.59	110.24
4	A	1309	EIC	C11-C10-C9	3.45	152.70	123.57
4	B	1309	EIC	C11-C10-C9	3.45	152.69	123.57
4	C	1309	EIC	C11-C10-C9	3.45	152.69	123.57
3	C	1303	NAG	C3-C4-C5	3.18	115.92	110.24
3	A	1303	NAG	C3-C4-C5	3.17	115.89	110.24
3	B	1303	NAG	C3-C4-C5	3.16	115.87	110.24
5	A	1313	BLR	CBB-CAB-C3B	-3.11	112.15	127.62
5	C	1313	BLR	CBB-CAB-C3B	-3.11	112.16	127.62
5	B	1313	BLR	CBB-CAB-C3B	-3.10	112.17	127.62
5	A	1313	BLR	CBC-CAC-C3C	-2.79	113.76	127.62
5	B	1313	BLR	CBC-CAC-C3C	-2.78	113.76	127.62
5	A	1313	BLR	C4B-C3B-C2B	2.78	111.50	107.92
5	C	1313	BLR	CBC-CAC-C3C	-2.78	113.78	127.62
5	B	1313	BLR	C4B-C3B-C2B	2.77	111.48	107.92
5	C	1313	BLR	C4B-C3B-C2B	2.72	111.41	107.92
5	C	1313	BLR	CBD-CAD-C3D	-2.68	108.04	112.62
5	B	1313	BLR	CBD-CAD-C3D	-2.67	108.07	112.62
3	A	1301	NAG	C2-N2-C7	-2.66	119.11	122.90
5	A	1313	BLR	CBD-CAD-C3D	-2.65	108.09	112.62
3	C	1301	NAG	C2-N2-C7	-2.65	119.13	122.90
5	B	1313	BLR	CAD-C3D-C4D	-2.65	125.44	127.30
5	A	1313	BLR	CAD-C3D-C4D	-2.64	125.44	127.30
3	B	1301	NAG	C2-N2-C7	-2.63	119.15	122.90
3	C	1301	NAG	C8-C7-N2	2.62	120.53	116.10
3	B	1301	NAG	C8-C7-N2	2.60	120.50	116.10
3	A	1301	NAG	C8-C7-N2	2.58	120.47	116.10
5	A	1313	BLR	C1B-NB-C4B	-2.58	107.39	110.67
5	C	1313	BLR	CAD-C3D-C4D	-2.56	125.50	127.30
5	C	1313	BLR	C1B-NB-C4B	-2.54	107.43	110.67
5	B	1313	BLR	C1B-NB-C4B	-2.54	107.44	110.67
3	C	1303	NAG	C8-C7-N2	2.42	120.19	116.10
3	B	1306	NAG	C8-C7-N2	2.41	120.17	116.10
3	B	1310	NAG	C8-C7-N2	2.40	120.17	116.10
3	A	1310	NAG	C8-C7-N2	2.40	120.16	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1306	NAG	C8-C7-N2	2.40	120.16	116.10
3	C	1302	NAG	C8-C7-N2	2.39	120.15	116.10
3	C	1310	NAG	C8-C7-N2	2.39	120.14	116.10
3	A	1302	NAG	C8-C7-N2	2.39	120.14	116.10
3	B	1302	NAG	C8-C7-N2	2.37	120.12	116.10
3	B	1303	NAG	C8-C7-N2	2.37	120.11	116.10
3	C	1308	NAG	C8-C7-N2	2.37	120.11	116.10
3	C	1306	NAG	C8-C7-N2	2.36	120.10	116.10
3	A	1303	NAG	C8-C7-N2	2.36	120.09	116.10
3	A	1308	NAG	C8-C7-N2	2.35	120.08	116.10
3	B	1308	NAG	C8-C7-N2	2.35	120.08	116.10
3	A	1304	NAG	C8-C7-N2	2.35	120.08	116.10
3	B	1305	NAG	C8-C7-N2	2.35	120.08	116.10
3	B	1304	NAG	C8-C7-N2	2.35	120.08	116.10
3	C	1304	NAG	C6-C5-C4	-2.34	107.52	113.00
3	A	1305	NAG	C8-C7-N2	2.34	120.06	116.10
3	C	1305	NAG	C8-C7-N2	2.34	120.06	116.10
3	B	1304	NAG	C6-C5-C4	-2.34	107.53	113.00
3	C	1307	NAG	C8-C7-N2	2.34	120.05	116.10
3	A	1307	NAG	C8-C7-N2	2.33	120.05	116.10
3	C	1304	NAG	C8-C7-N2	2.33	120.05	116.10
3	A	1304	NAG	C6-C5-C4	-2.33	107.55	113.00
3	A	1311	NAG	C8-C7-N2	2.32	120.03	116.10
3	B	1307	NAG	C8-C7-N2	2.32	120.03	116.10
3	C	1311	NAG	C8-C7-N2	2.32	120.02	116.10
3	B	1311	NAG	C8-C7-N2	2.29	119.98	116.10
3	C	1310	NAG	C2-N2-C7	-2.23	119.72	122.90
3	B	1305	NAG	C2-N2-C7	-2.23	119.73	122.90
3	C	1305	NAG	C2-N2-C7	-2.23	119.73	122.90
3	A	1310	NAG	C2-N2-C7	-2.22	119.75	122.90
3	B	1308	NAG	C2-N2-C7	-2.20	119.77	122.90
3	A	1305	NAG	C2-N2-C7	-2.19	119.78	122.90
3	B	1310	NAG	C2-N2-C7	-2.19	119.78	122.90
3	C	1308	NAG	C2-N2-C7	-2.18	119.80	122.90
3	A	1308	NAG	C2-N2-C7	-2.17	119.82	122.90
3	A	1312	NAG	C8-C7-N2	2.14	119.73	116.10
3	C	1312	NAG	C8-C7-N2	2.14	119.72	116.10
3	B	1312	NAG	C8-C7-N2	2.12	119.69	116.10
3	A	1306	NAG	C1-O5-C5	-2.10	109.35	112.19
3	C	1306	NAG	C1-O5-C5	-2.09	109.37	112.19
3	B	1306	NAG	C1-O5-C5	-2.08	109.38	112.19
3	C	1305	NAG	C6-C5-C4	-2.07	108.15	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1305	NAG	C6-C5-C4	-2.04	108.23	113.00
3	A	1305	NAG	C6-C5-C4	-2.03	108.24	113.00
5	C	1313	BLR	CAA-CBA-CGA	-2.01	108.12	113.76
5	B	1313	BLR	CAA-CBA-CGA	-2.01	108.13	113.76
5	A	1313	BLR	CAA-CBA-CGA	-2.00	108.14	113.76
5	C	1313	BLR	CMB-C2B-C1B	-2.00	121.66	124.17
3	B	1307	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1313	BLR	C3D-C4D-CHA-C1A
5	A	1313	BLR	NA-C4A-CHB-C1B
5	A	1313	BLR	C3A-C4A-CHB-C1B
5	A	1313	BLR	C2B-C3B-CAB-CBB
5	A	1313	BLR	C2C-C3C-CAC-CBC
5	A	1313	BLR	ND-C1D-CHD-C4C
5	A	1313	BLR	C2D-C1D-CHD-C4C
5	A	1313	BLR	C4D-C3D-CAD-CBD
5	A	1313	BLR	C3D-CAD-CBD-CGD
5	B	1313	BLR	C3D-C4D-CHA-C1A
5	B	1313	BLR	NA-C4A-CHB-C1B
5	B	1313	BLR	C3A-C4A-CHB-C1B
5	B	1313	BLR	C2B-C3B-CAB-CBB
5	B	1313	BLR	C2C-C3C-CAC-CBC
5	B	1313	BLR	ND-C1D-CHD-C4C
5	B	1313	BLR	C2D-C1D-CHD-C4C
5	B	1313	BLR	C4D-C3D-CAD-CBD
5	B	1313	BLR	C3D-CAD-CBD-CGD
5	C	1313	BLR	C3D-C4D-CHA-C1A
5	C	1313	BLR	NA-C4A-CHB-C1B
5	C	1313	BLR	C3A-C4A-CHB-C1B
5	C	1313	BLR	C2B-C3B-CAB-CBB
5	C	1313	BLR	C2C-C3C-CAC-CBC
5	C	1313	BLR	ND-C1D-CHD-C4C
5	C	1313	BLR	C2D-C1D-CHD-C4C
5	C	1313	BLR	C4D-C3D-CAD-CBD
5	C	1313	BLR	C3D-CAD-CBD-CGD
3	A	1306	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1306	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	A	1312	NAG	O5-C5-C6-O6
3	B	1312	NAG	O5-C5-C6-O6
3	C	1312	NAG	O5-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1302	NAG	C1-C2-N2-C7
3	B	1302	NAG	C1-C2-N2-C7
3	C	1302	NAG	C1-C2-N2-C7
3	A	1307	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	A	1311	NAG	C4-C5-C6-O6
3	B	1311	NAG	C4-C5-C6-O6
3	C	1311	NAG	C4-C5-C6-O6
3	A	1312	NAG	C4-C5-C6-O6
3	B	1312	NAG	C4-C5-C6-O6
3	C	1312	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1309	EIC	C5-C6-C7-C8
4	B	1309	EIC	C5-C6-C7-C8
4	C	1309	EIC	C5-C6-C7-C8
4	A	1309	EIC	C13-C14-C15-C16
4	B	1309	EIC	C13-C14-C15-C16
4	C	1309	EIC	C13-C14-C15-C16
5	A	1313	BLR	C4B-C3B-CAB-CBB
5	B	1313	BLR	C4B-C3B-CAB-CBB
5	C	1313	BLR	C4B-C3B-CAB-CBB
5	A	1313	BLR	C4C-C3C-CAC-CBC
5	B	1313	BLR	C4C-C3C-CAC-CBC
5	C	1313	BLR	C4C-C3C-CAC-CBC
4	A	1309	EIC	C15-C16-C17-C18
4	B	1309	EIC	C15-C16-C17-C18
4	C	1309	EIC	C15-C16-C17-C18
4	B	1309	EIC	C2-C3-C4-C5
4	A	1309	EIC	C2-C3-C4-C5
4	C	1309	EIC	C2-C3-C4-C5
3	A	1312	NAG	C1-C2-N2-C7
3	B	1312	NAG	C1-C2-N2-C7
3	C	1312	NAG	C1-C2-N2-C7
5	A	1313	BLR	C2D-C3D-CAD-CBD
5	B	1313	BLR	C2D-C3D-CAD-CBD
5	C	1313	BLR	C2D-C3D-CAD-CBD
4	A	1309	EIC	C14-C15-C16-C17
4	C	1309	EIC	C14-C15-C16-C17
4	B	1309	EIC	C14-C15-C16-C17
3	A	1302	NAG	C3-C2-N2-C7
3	B	1302	NAG	C3-C2-N2-C7
3	C	1302	NAG	C3-C2-N2-C7
3	B	1302	NAG	C4-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
4	A	1309	EIC	C12-C13-C14-C15
4	B	1309	EIC	C12-C13-C14-C15
4	C	1309	EIC	C12-C13-C14-C15
5	B	1313	BLR	CAD-CBD-CGD-O1D
5	C	1313	BLR	CAD-CBD-CGD-O1D
5	A	1313	BLR	CAD-CBD-CGD-O1D
5	A	1313	BLR	CAD-CBD-CGD-O2D
5	B	1313	BLR	CAD-CBD-CGD-O2D
5	C	1313	BLR	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
4	A	1309	EIC	O1-C1-C2-C3
4	A	1309	EIC	O2-C1-C2-C3
4	C	1309	EIC	O2-C1-C2-C3
4	B	1309	EIC	O1-C1-C2-C3
4	B	1309	EIC	O2-C1-C2-C3
4	C	1309	EIC	O1-C1-C2-C3
3	A	1312	NAG	C3-C2-N2-C7
3	B	1312	NAG	C3-C2-N2-C7
3	C	1312	NAG	C3-C2-N2-C7
5	A	1313	BLR	C2A-C1A-CHA-C4D
5	B	1313	BLR	C2A-C1A-CHA-C4D
5	C	1313	BLR	C2A-C1A-CHA-C4D

There are no ring outliers.

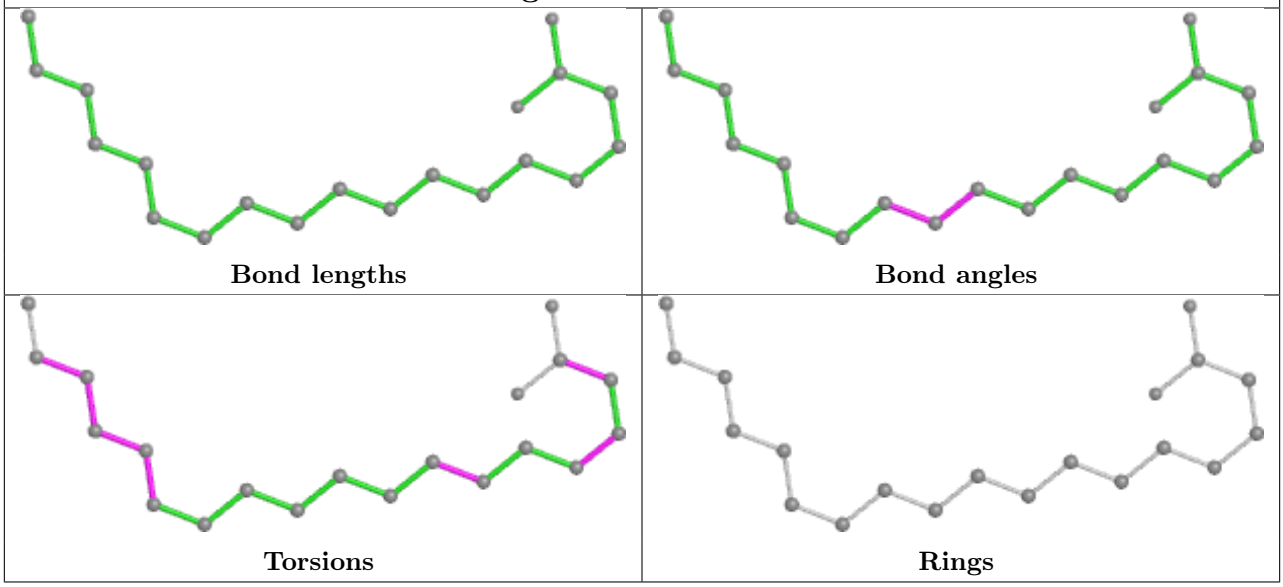
15 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1312	NAG	1	0
3	A	1305	NAG	1	0
3	C	1305	NAG	1	0
3	C	1311	NAG	1	0
3	B	1304	NAG	1	0
3	A	1304	NAG	1	0
3	C	1304	NAG	1	0
5	B	1313	BLR	16	0
3	B	1312	NAG	1	0
3	A	1312	NAG	1	0
5	C	1313	BLR	16	0
3	A	1311	NAG	1	0
3	B	1311	NAG	1	0
5	A	1313	BLR	17	0
3	B	1305	NAG	1	0

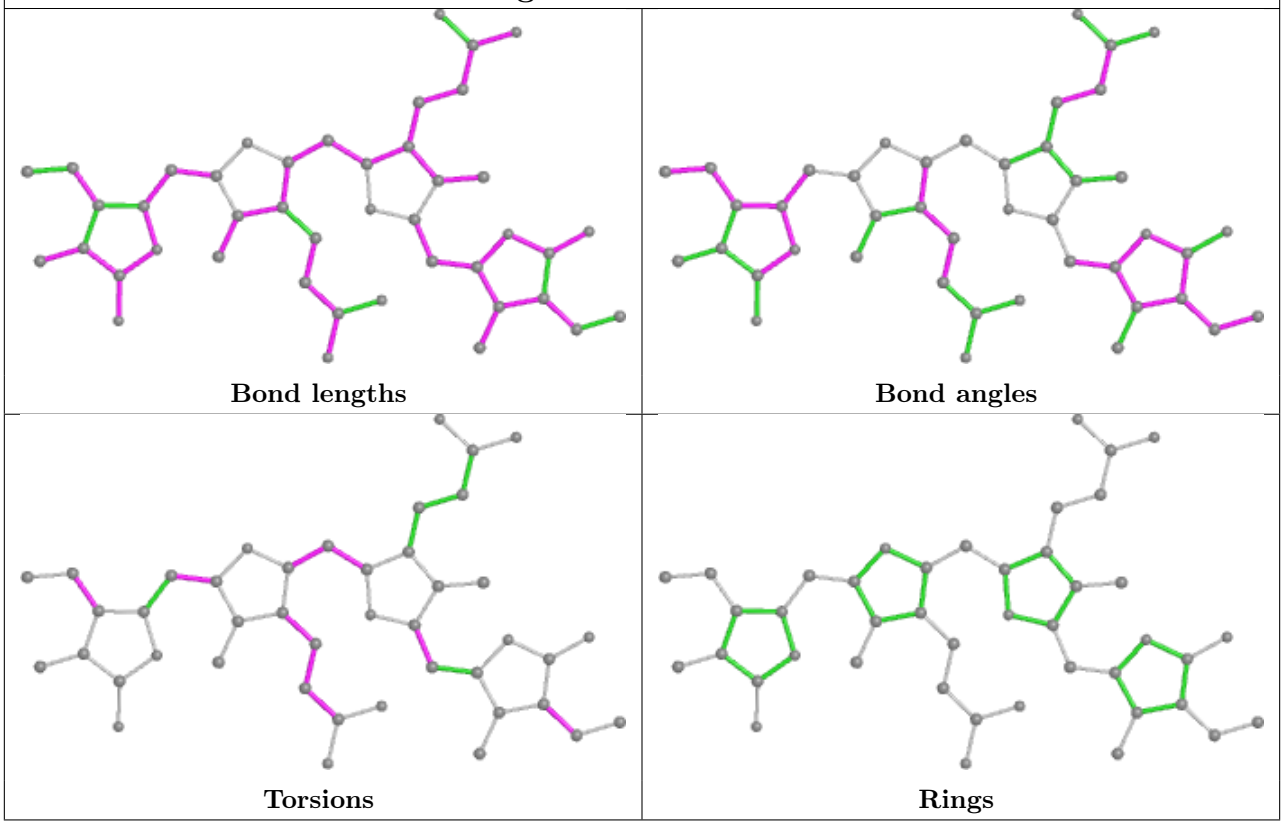
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

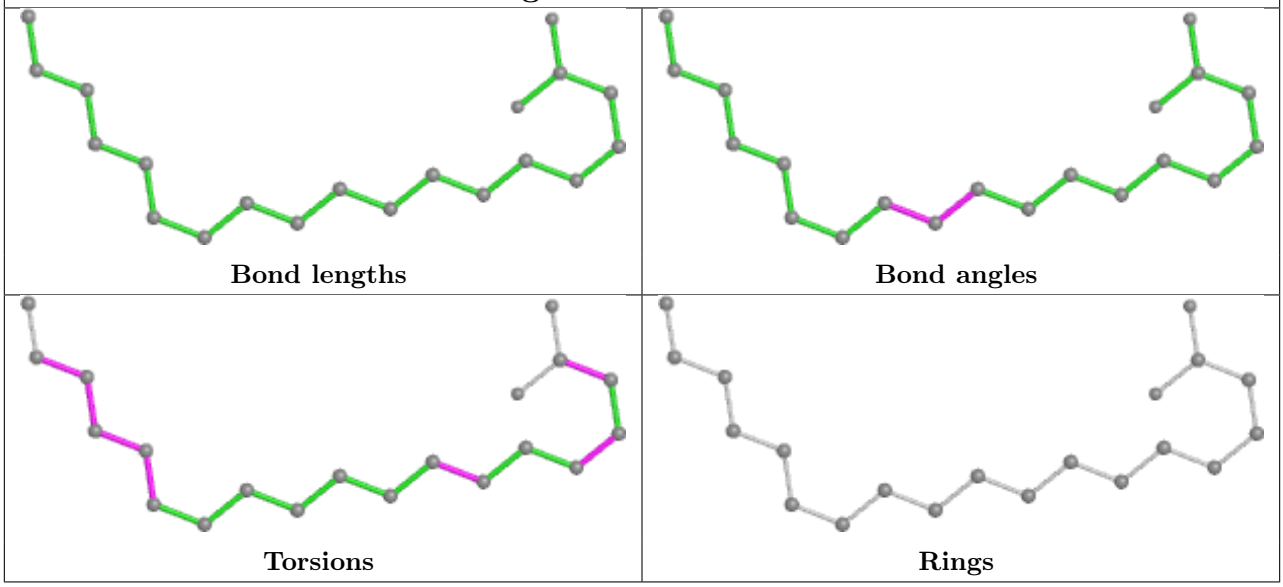
Ligand EIC A 1309



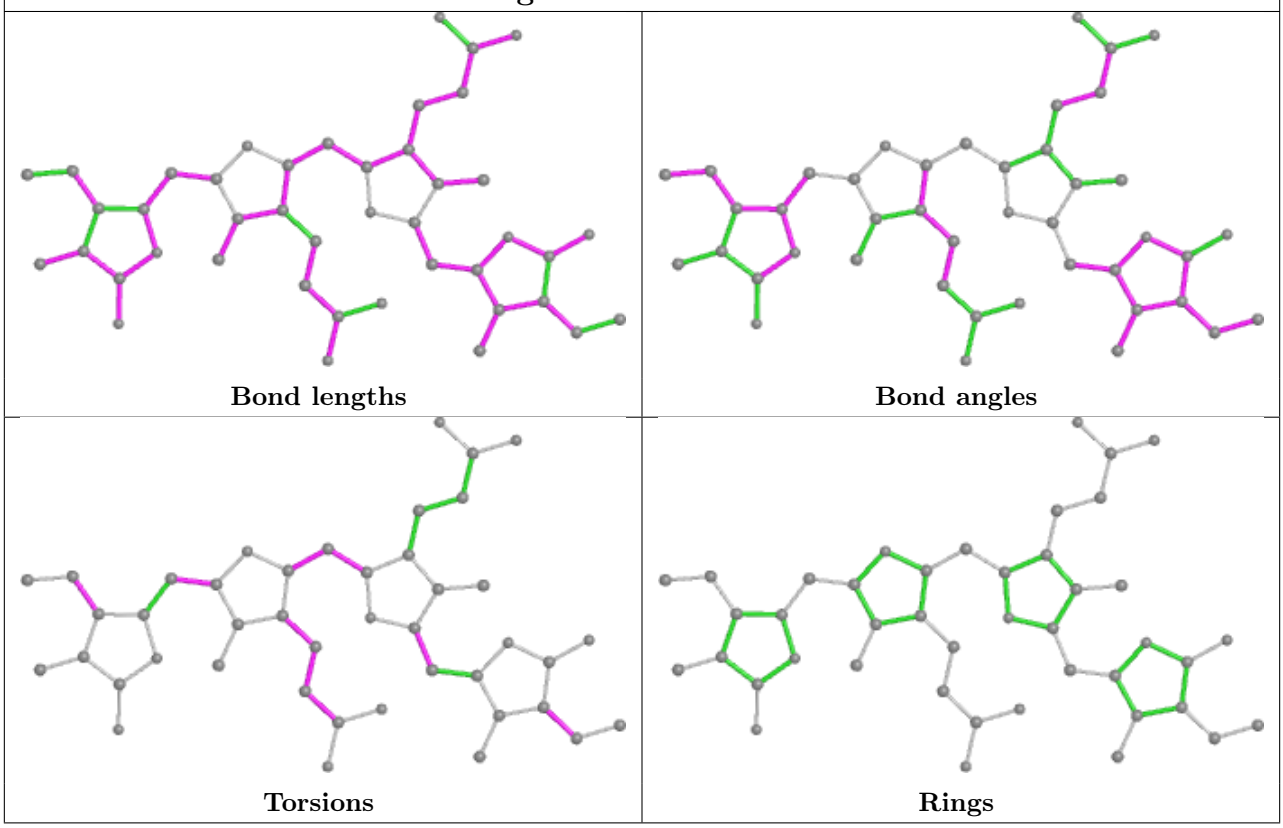
Ligand BLR B 1313



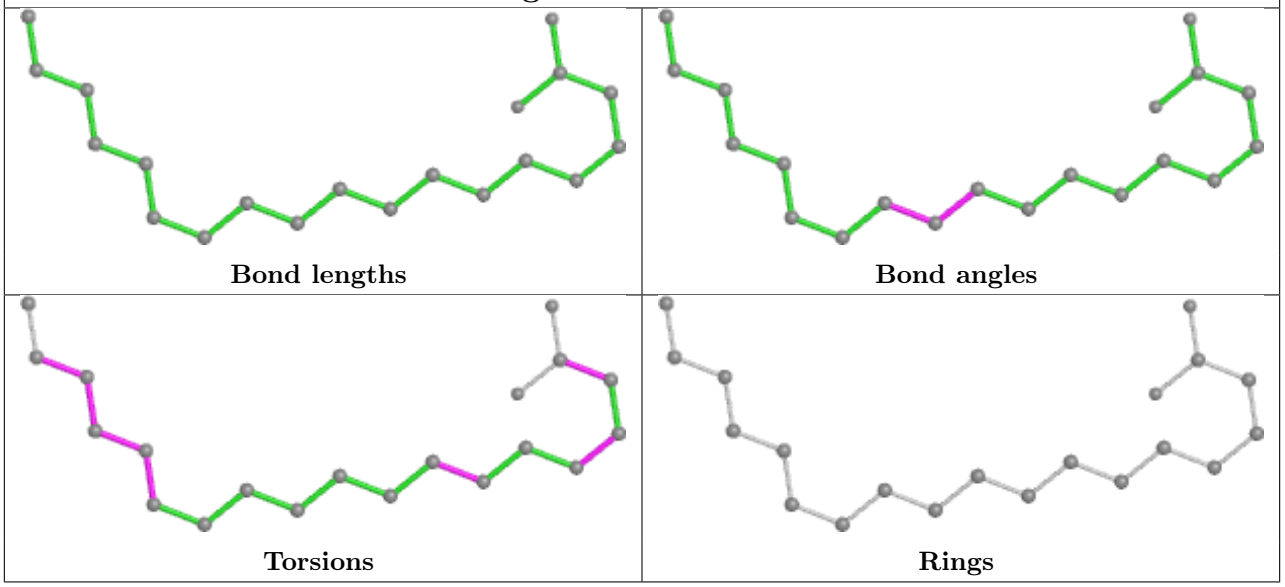
Ligand EIC C 1309



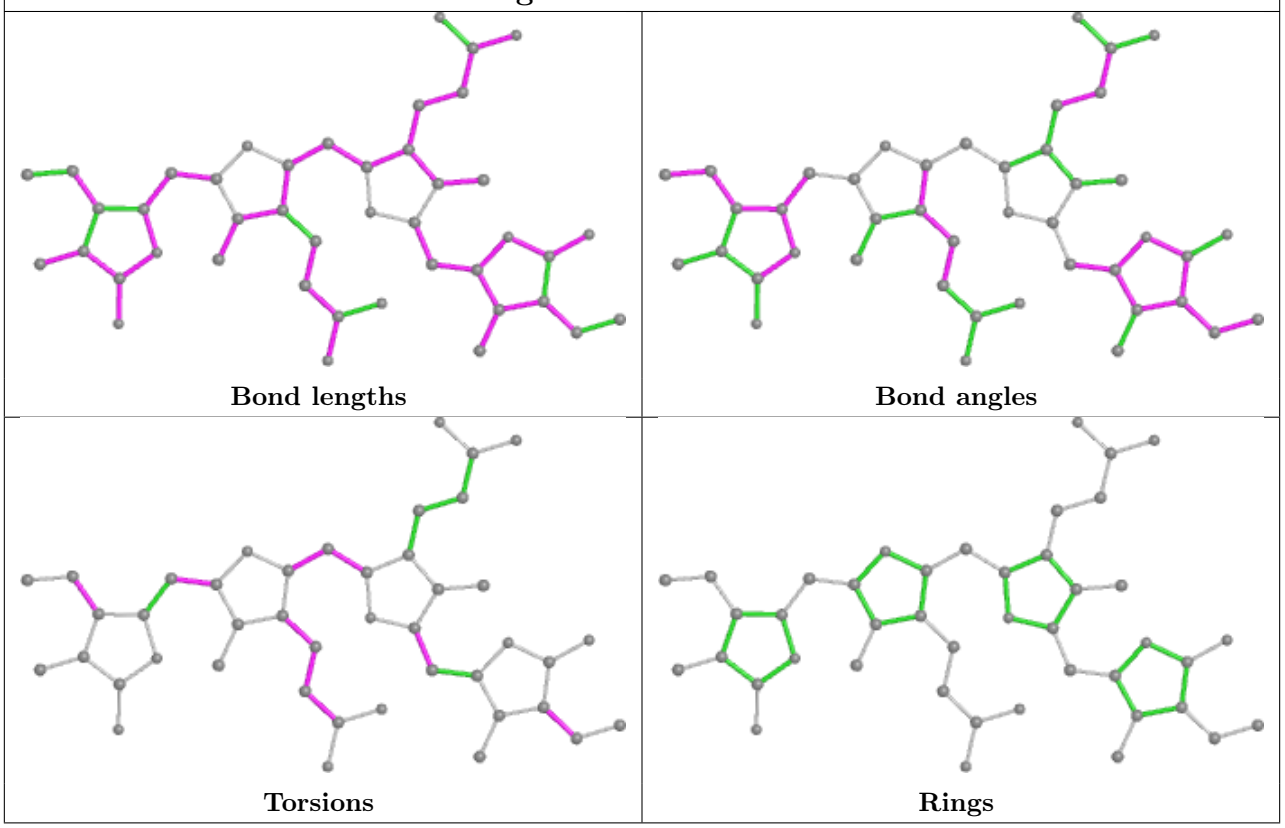
Ligand BLR C 1313



Ligand EIC B 1309



Ligand BLR A 1313



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

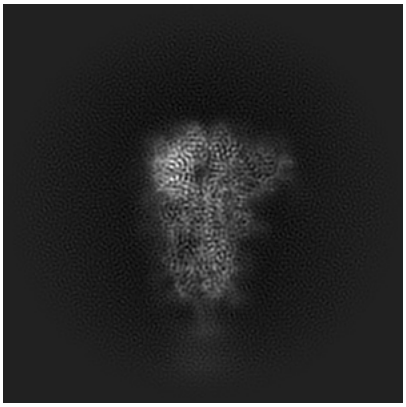
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32490. These allow visual inspection of the internal detail of the map and identification of artifacts.

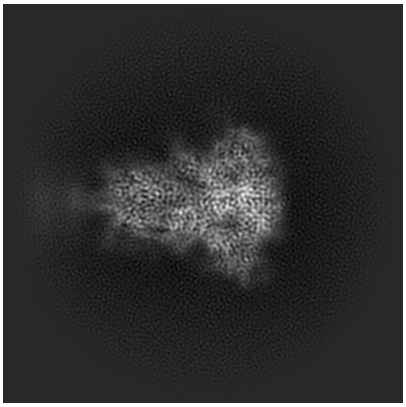
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

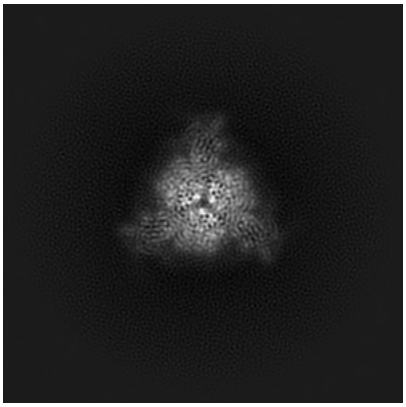
6.1.1 Primary map



X



Y

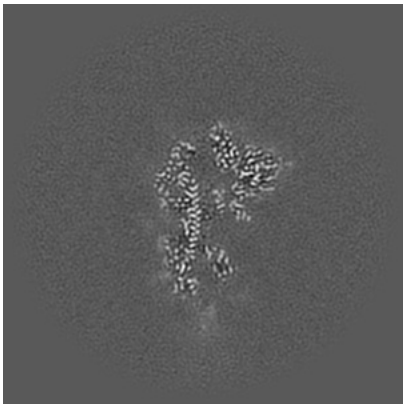


Z

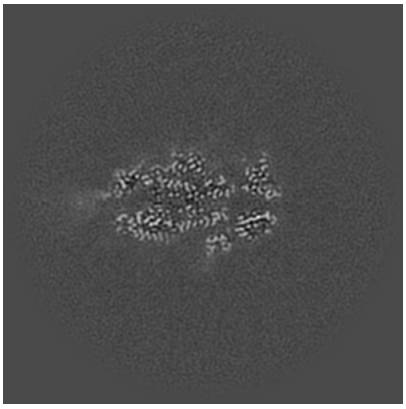
The images above show the map projected in three orthogonal directions.

6.2 Central slices

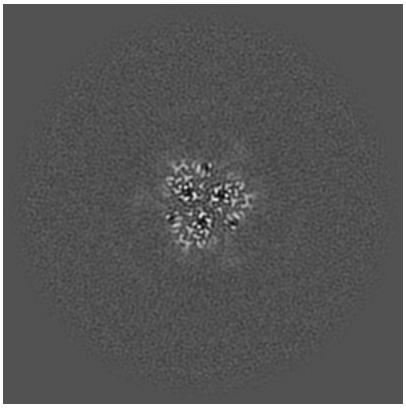
6.2.1 Primary map



X Index: 128



Y Index: 128

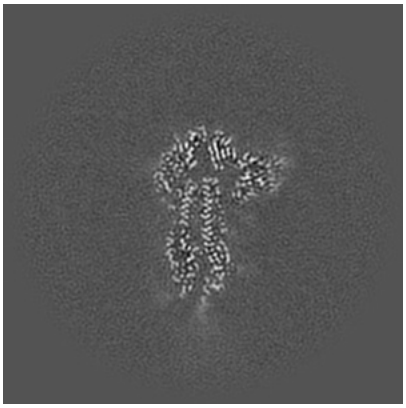


Z Index: 128

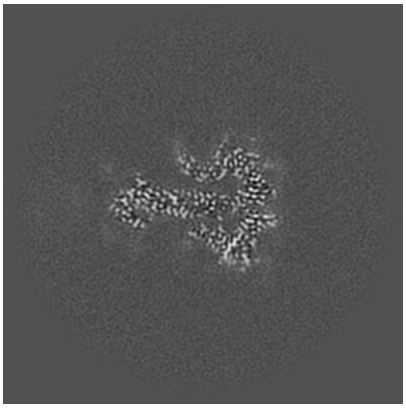
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

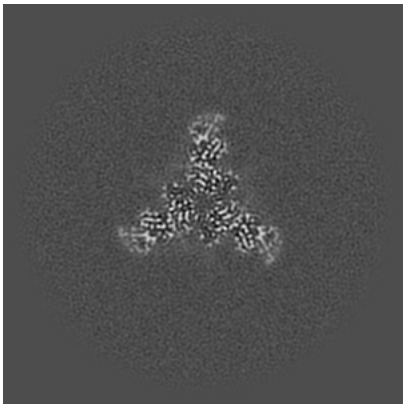
6.3.1 Primary map



X Index: 133



Y Index: 118



Z Index: 155

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

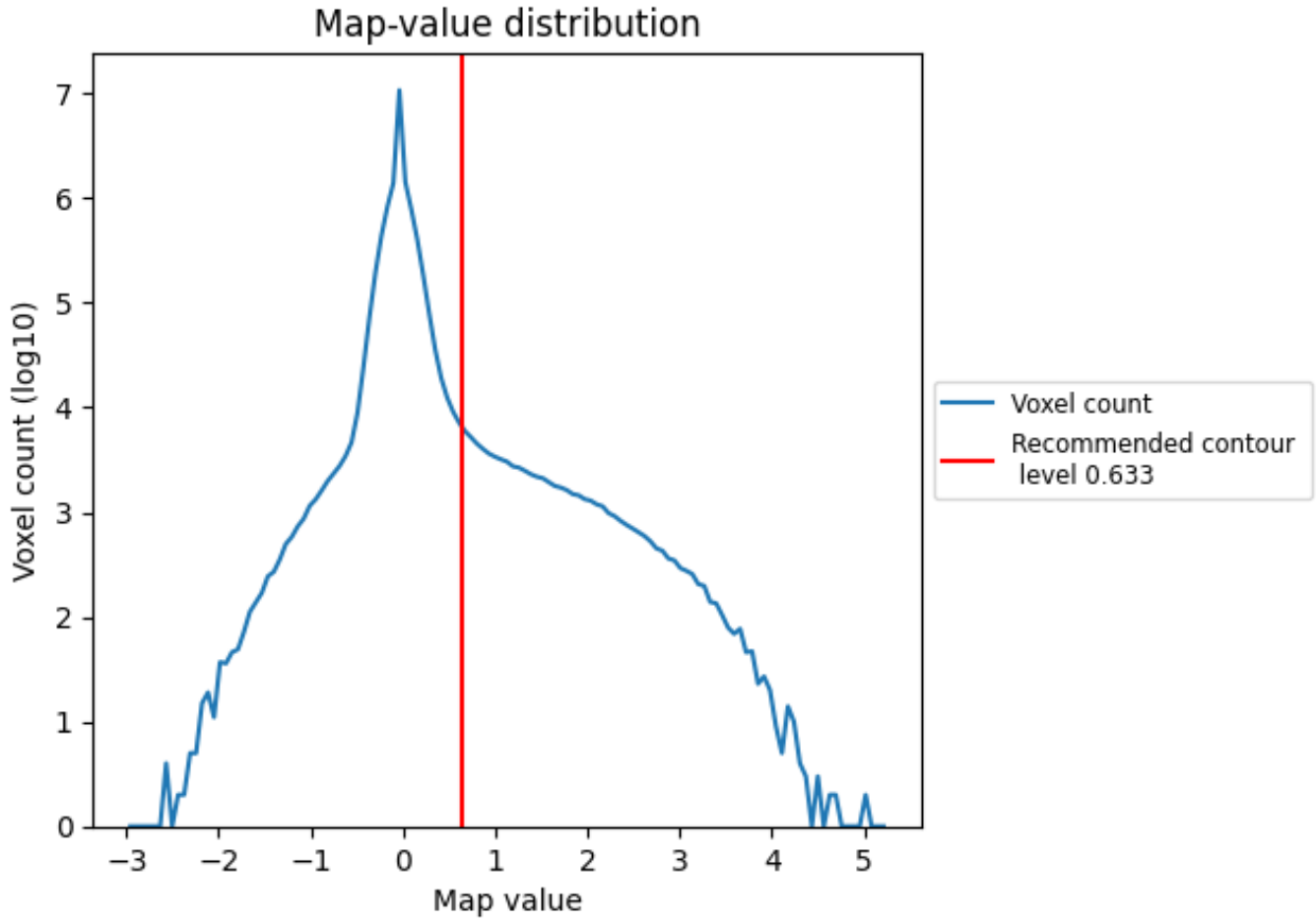
6.5 Mask visualisation (i)

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

7 Map analysis

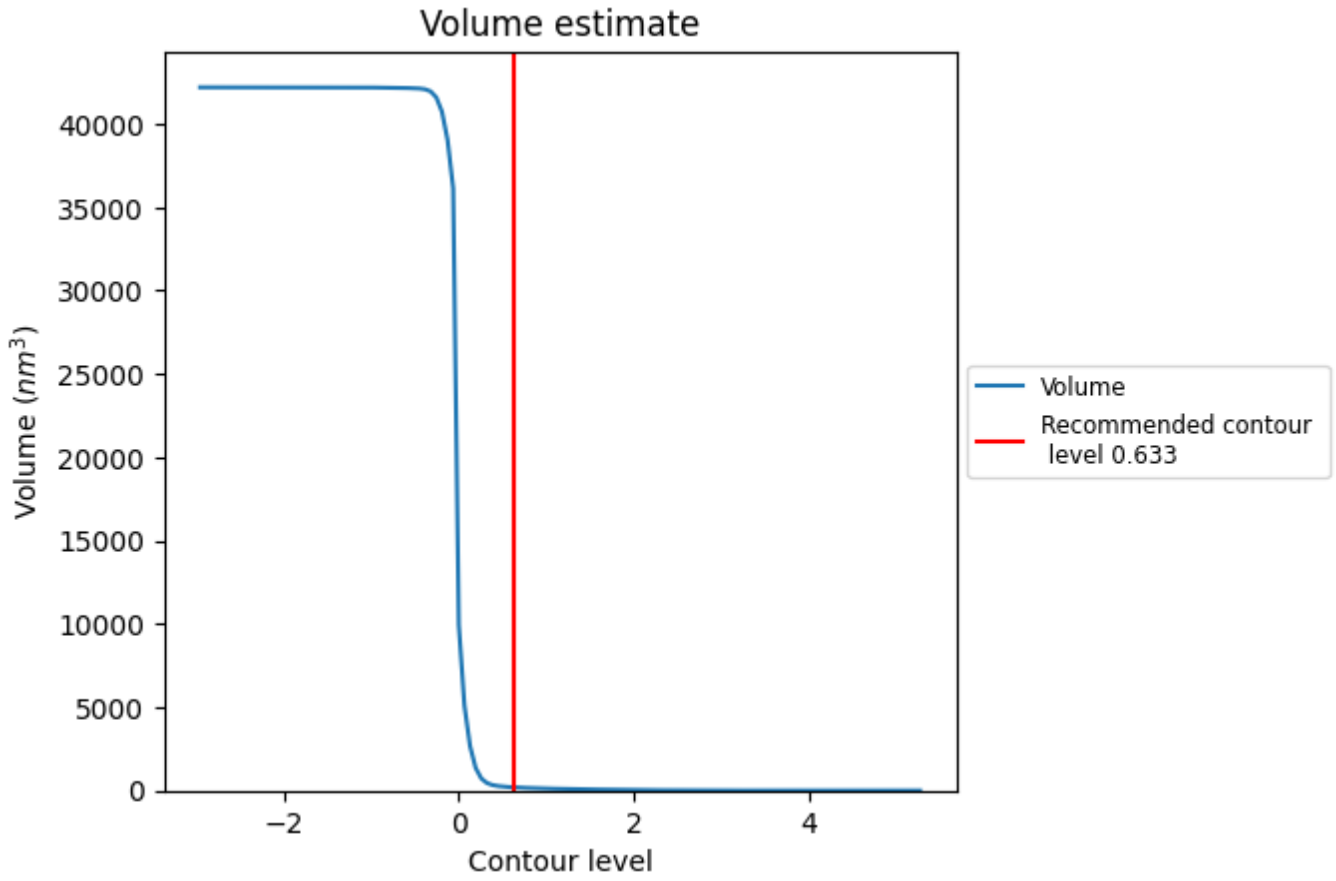
This section contains the results of statistical analysis of the map.

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.

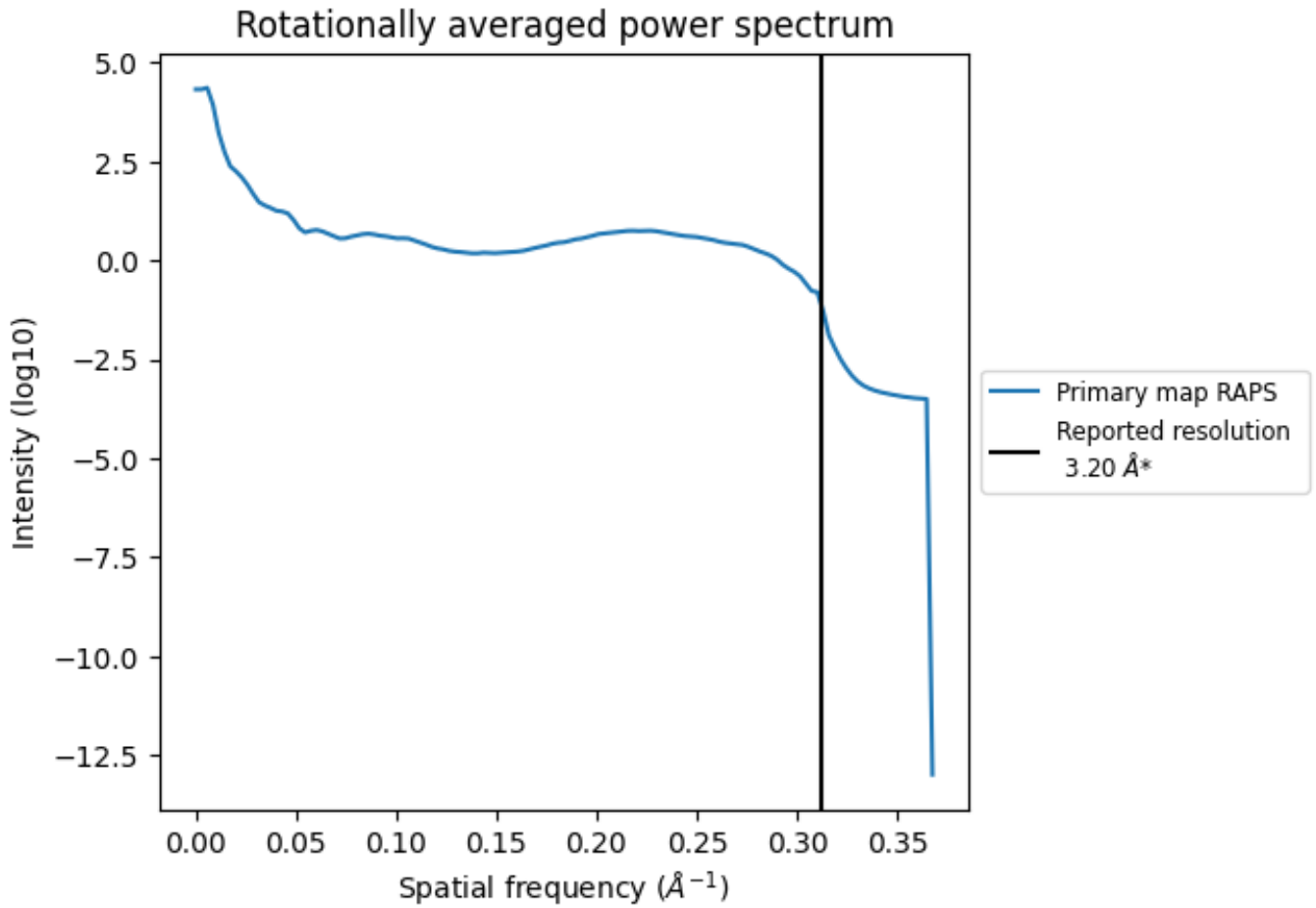
7.2 Volume estimate



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 174 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)

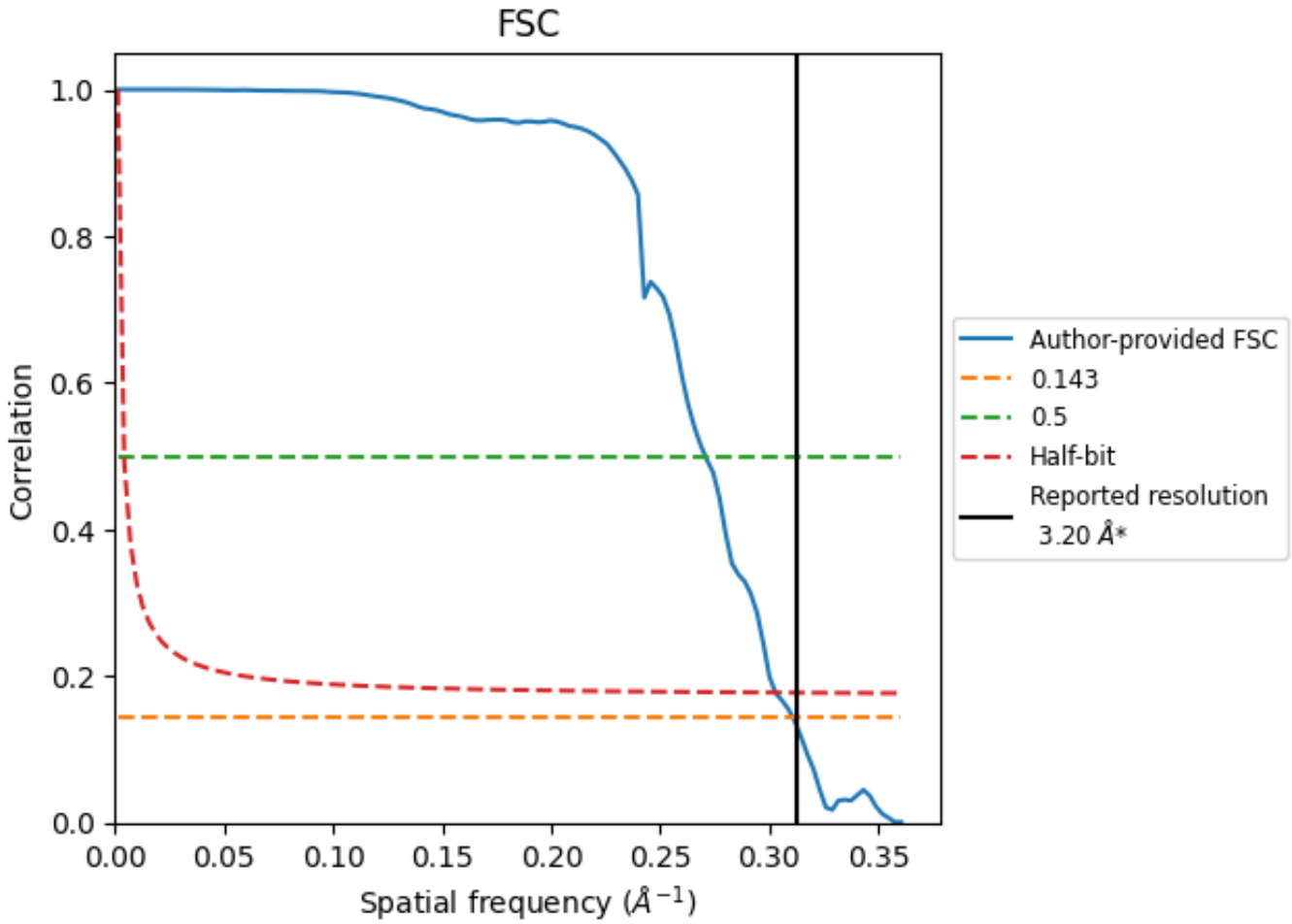


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

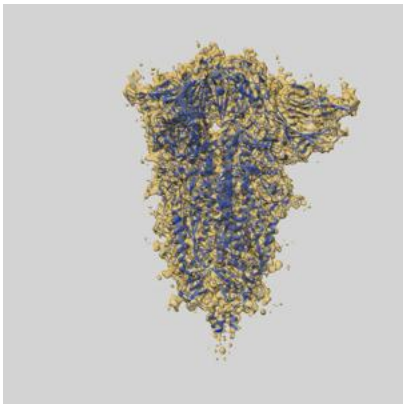
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.70	3.30
Unmasked-calculated*	-	-	-

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

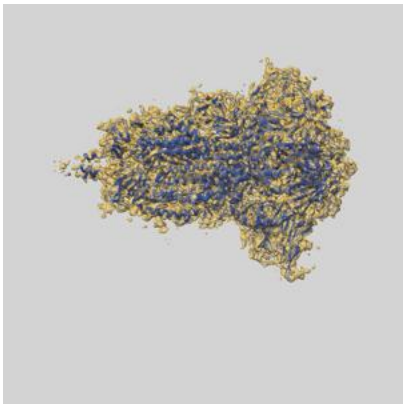
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32490 and PDB model 7WGV. Per-residue inclusion information can be found in section 3 on page 10.

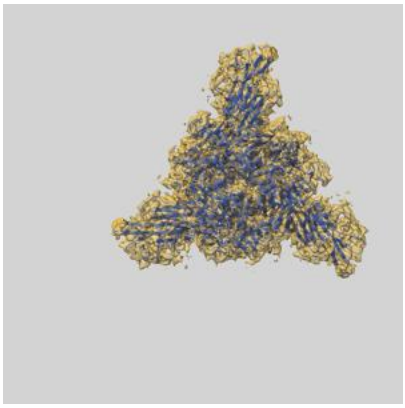
9.1 Map-model overlay



X



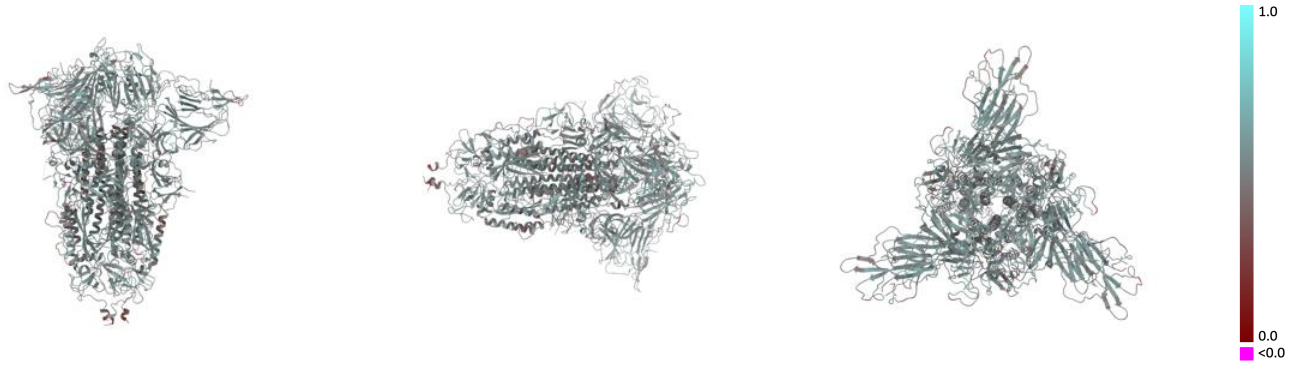
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.633 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.

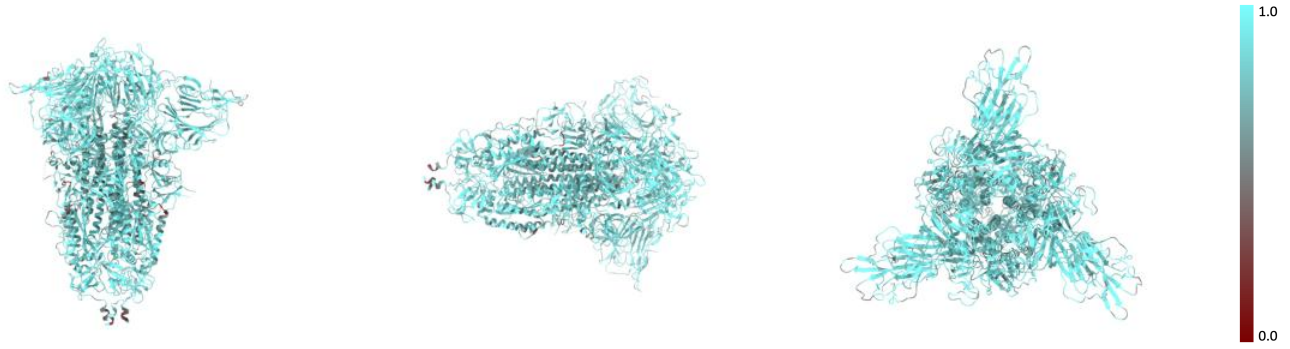
9.2 Q-score mapped to coordinate model (i)



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.

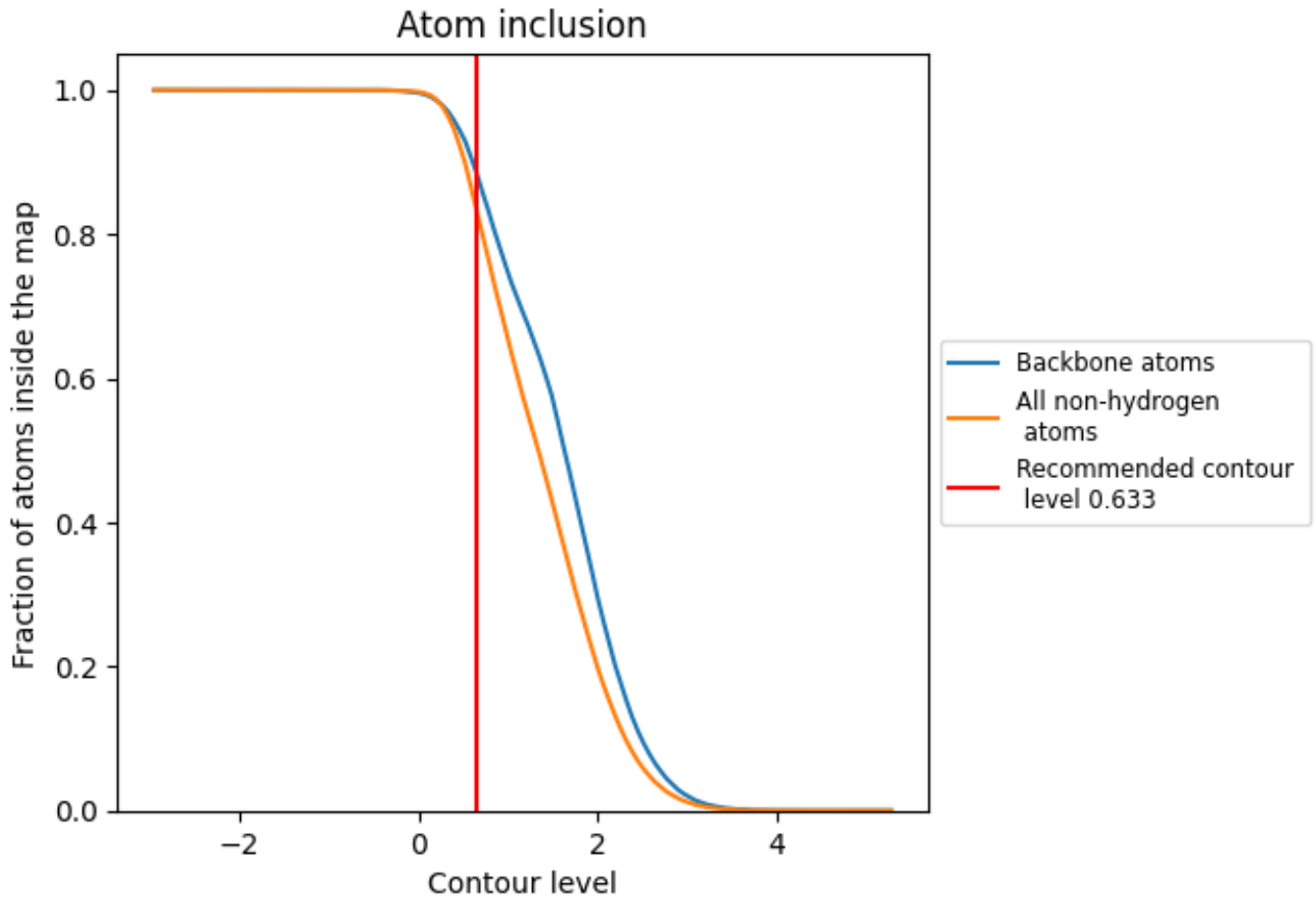
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.633).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.633) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.5130
A	0.8447	0.5150
B	0.8431	0.5130
C	0.8434	0.5140
D	0.6071	0.4190
E	0.5357	0.3770
F	0.4286	0.4300
G	0.7143	0.4820
H	0.7143	0.4450
I	0.6071	0.4140
J	0.5357	0.3770
K	0.4643	0.4220
L	0.7143	0.4810
M	0.7500	0.4580
N	0.6071	0.4160
O	0.5000	0.3610
P	0.5000	0.4490
Q	0.6786	0.4690
R	0.7500	0.4350