Full wwPDB EM Validation Report

Jul 25, 2022 – 06:01 pm BST

PDB ID	:	7QUR
EMDB ID	:	EMD-14152
Title	:	SARS-CoV-2 Spike with ethylbenzamide-tri-iodo Siallyllactose, C3 symmetry
Authors	:	Naismith, J.H.; Yang, Y.; Liu, J.W.
Deposited on	:	2022-01-18
Resolution	:	2.27 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:

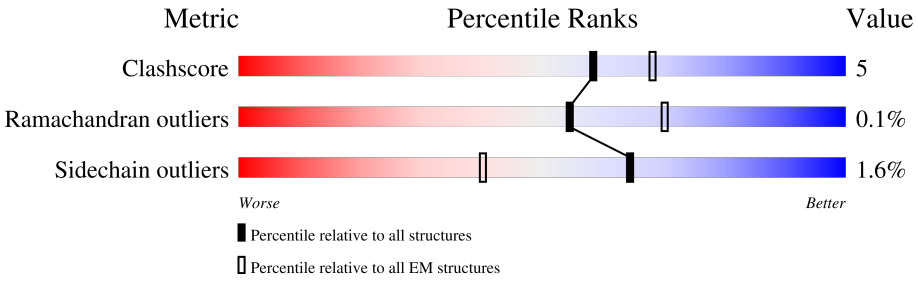
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.27 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	1259	75% 12% 13%
1	B	1259	75% 12% 13%
1	C	1259	76% 11% 13%
2	D	2	100%
2	E	2	100%
2	F	2	50% 100%
2	H	2	100%
2	I	2	100%

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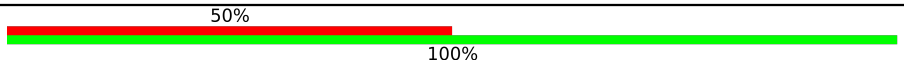
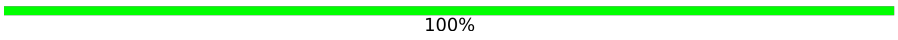
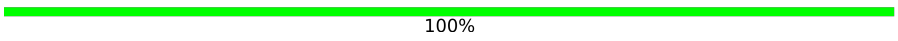
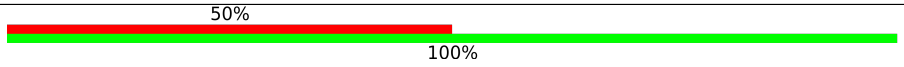
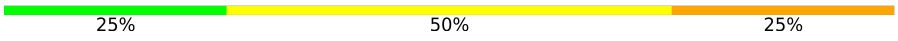
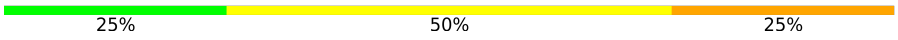
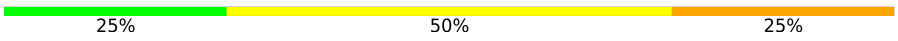
Mol	Chain	Length	Quality of chain
2	J	2	
2	L	2	
2	M	2	
2	N	2	
3	G	4	
3	K	4	
3	O	4	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 27174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1101	Total	C	N	O	S	2	0
			8611	5490	1440	1641	40		
1	B	1101	Total	C	N	O	S	2	0
			8611	5490	1440	1641	40		
1	C	1101	Total	C	N	O	S	2	0
			8611	5490	1440	1641	40		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	685	ALA	ARG	conflict	UNP P0DTC2
A	1214	SER	-	linker	UNP P0DTC2
A	1215	GLY	-	linker	UNP P0DTC2
A	1216	ARG	-	linker	UNP P0DTC2
A	1217	LEU	-	linker	UNP P0DTC2
A	1218	VAL	-	linker	UNP P0DTC2
A	1219	PRO	-	linker	UNP P0DTC2
A	1220	ARG	-	linker	UNP P0DTC2
A	1221	GLY	-	linker	UNP P0DTC2
A	1222	SER	-	linker	UNP P0DTC2
A	1223	PRO	-	linker	UNP P0DTC2
A	1224	GLY	-	linker	UNP P0DTC2
A	1225	SER	-	linker	UNP P0DTC2
A	1247	LEU	PHE	engineered mutation	UNP P10104
A	1253	GLY	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	HIS	-	expression tag	UNP P10104
A	1259	HIS	-	expression tag	UNP P10104
B	685	ALA	ARG	conflict	UNP P0DTC2
B	1214	SER	-	linker	UNP P0DTC2
B	1215	GLY	-	linker	UNP P0DTC2

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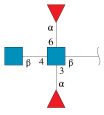
Chain	Residue	Modelled	Actual	Comment	Reference
B	1216	ARG	-	linker	UNP P0DTC2
B	1217	LEU	-	linker	UNP P0DTC2
B	1218	VAL	-	linker	UNP P0DTC2
B	1219	PRO	-	linker	UNP P0DTC2
B	1220	ARG	-	linker	UNP P0DTC2
B	1221	GLY	-	linker	UNP P0DTC2
B	1222	SER	-	linker	UNP P0DTC2
B	1223	PRO	-	linker	UNP P0DTC2
B	1224	GLY	-	linker	UNP P0DTC2
B	1225	SER	-	linker	UNP P0DTC2
B	1247	LEU	PHE	engineered mutation	UNP P10104
B	1253	GLY	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	HIS	-	expression tag	UNP P10104
B	1259	HIS	-	expression tag	UNP P10104
C	685	ALA	ARG	conflict	UNP P0DTC2
C	1214	SER	-	linker	UNP P0DTC2
C	1215	GLY	-	linker	UNP P0DTC2
C	1216	ARG	-	linker	UNP P0DTC2
C	1217	LEU	-	linker	UNP P0DTC2
C	1218	VAL	-	linker	UNP P0DTC2
C	1219	PRO	-	linker	UNP P0DTC2
C	1220	ARG	-	linker	UNP P0DTC2
C	1221	GLY	-	linker	UNP P0DTC2
C	1222	SER	-	linker	UNP P0DTC2
C	1223	PRO	-	linker	UNP P0DTC2
C	1224	GLY	-	linker	UNP P0DTC2
C	1225	SER	-	linker	UNP P0DTC2
C	1247	LEU	PHE	engineered mutation	UNP P10104
C	1253	GLY	-	expression tag	UNP P10104
C	1254	HIS	-	expression tag	UNP P10104
C	1255	HIS	-	expression tag	UNP P10104
C	1256	HIS	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	HIS	-	expression tag	UNP P10104
C	1259	HIS	-	expression tag	UNP P10104

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

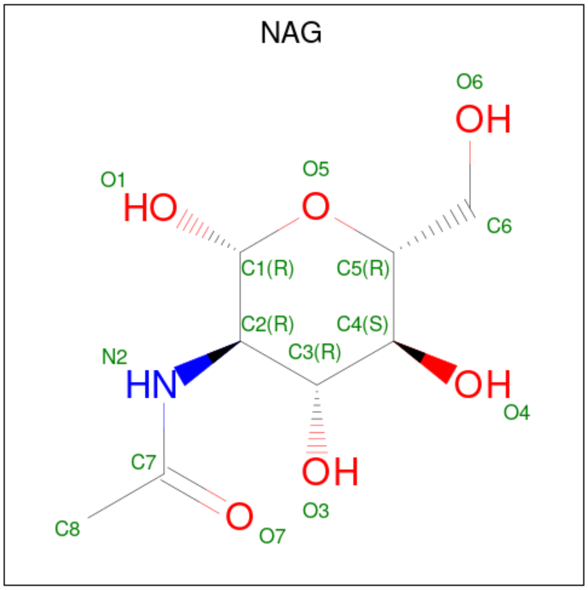
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	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		

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	4	Total	C	N	O	0	0
			48	28	2	18		
3	K	4	Total	C	N	O	0	0
			48	28	2	18		
3	O	4	Total	C	N	O	0	0
			48	28	2	18		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	A	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0

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Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	B	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0
4	C	1	Total C N O 168 96 12 60	0

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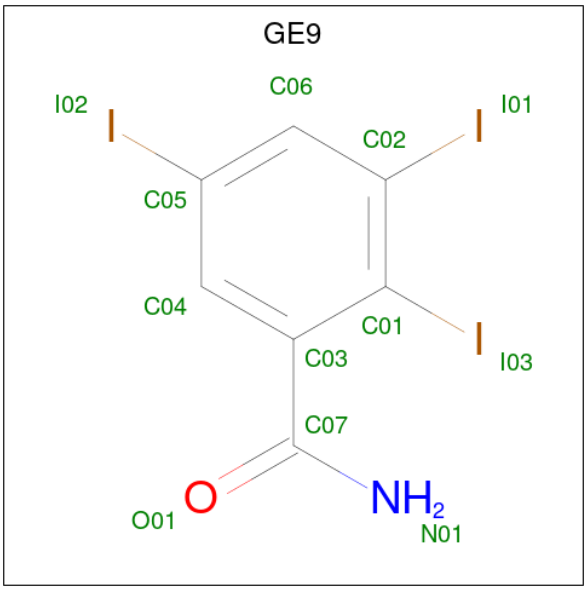
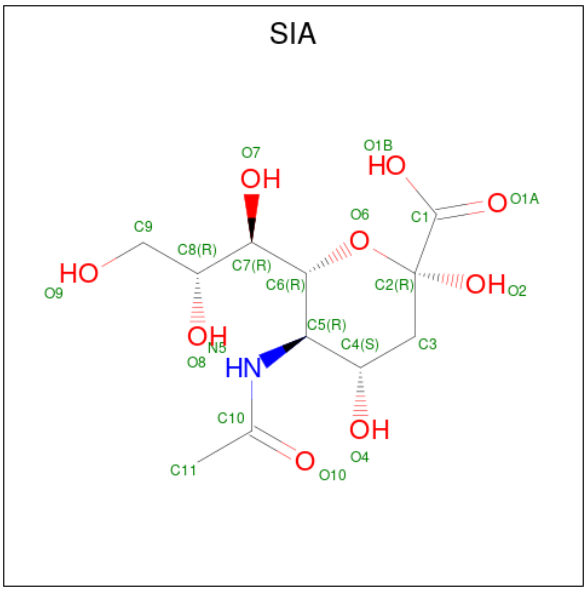
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			168	96	12	60	

- Molecule 5 is 2,3,5-tris(iodanyl)benzamide (three-letter code: GE9) (formula: $C_7H_4I_3NO$) (labeled as "Ligand of Interest" by depositor).



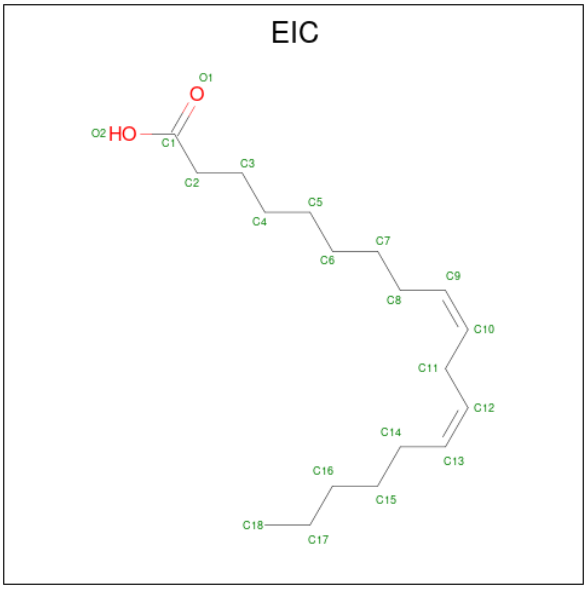
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	I	N	O	0
			12	7	3	1	1	
5	B	1	Total	C	I	N	O	0
			12	7	3	1	1	
5	C	1	Total	C	I	N	O	0
			12	7	3	1	1	

- Molecule 6 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			21	11	1	9	
6	B	1	Total	C	N	O	0
			21	11	1	9	
6	C	1	Total	C	N	O	0
			21	11	1	9	

- Molecule 7 is LINOLEIC ACID (three-letter code: EIC) (formula: $C_{18}H_{32}O_2$).



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

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

- Molecule 8 is water.

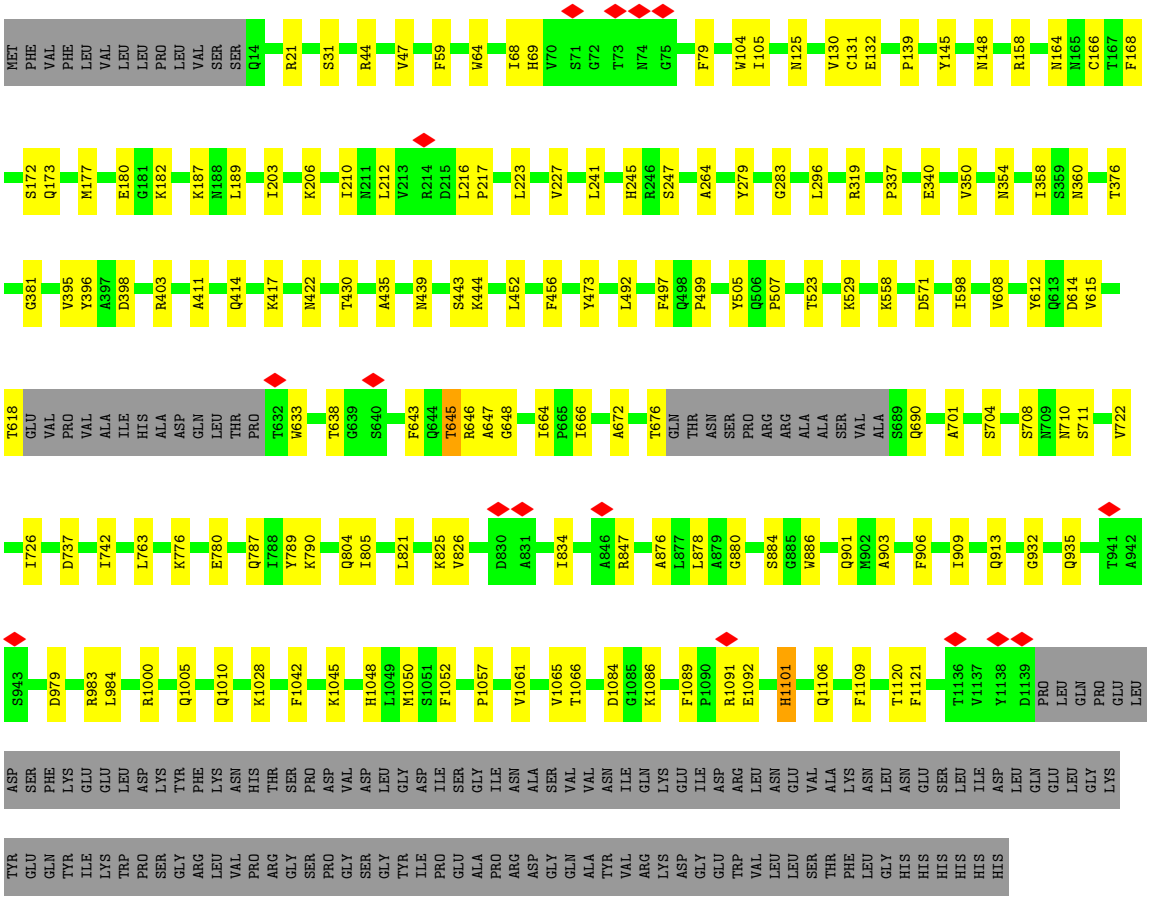
Mol	Chain	Residues	Atoms	AltConf
8	A	93	Total O 93 93	0
8	B	93	Total O 93 93	0
8	C	96	Total O 96 96	0

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.

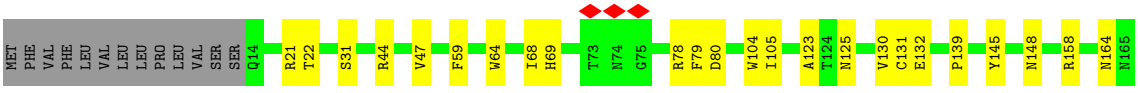
• Molecule 1: Spike glycoprotein,Fibritin

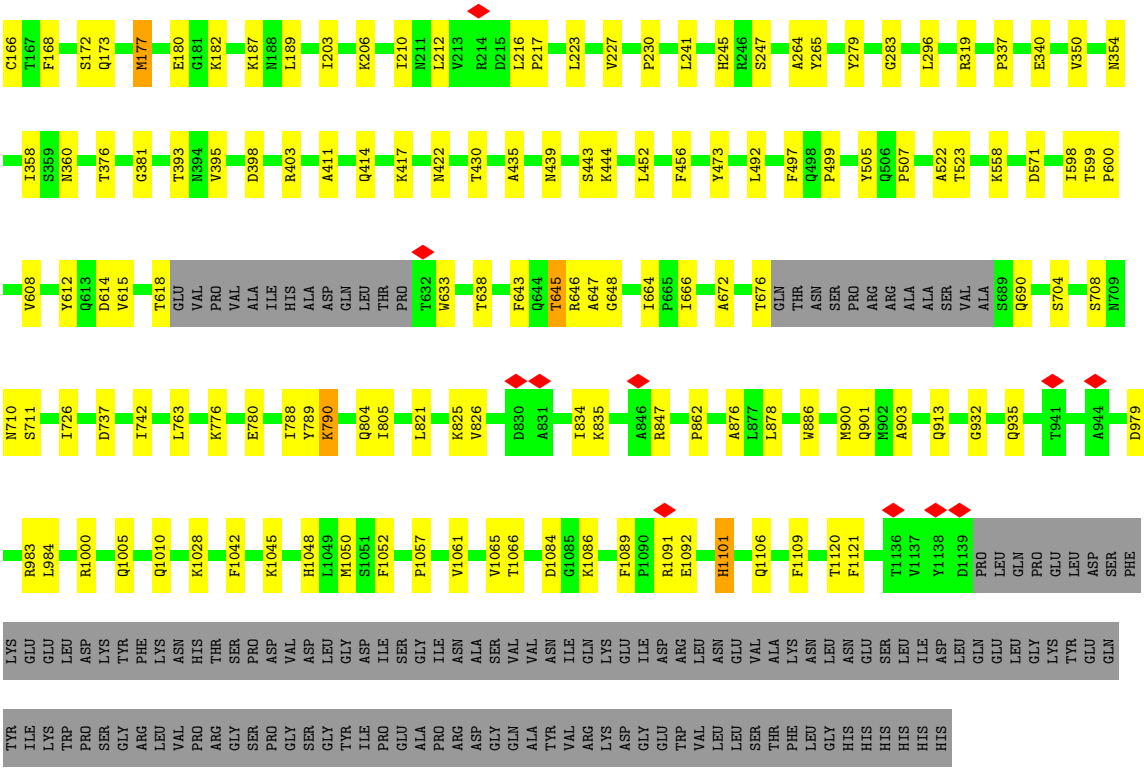
Chain A:



• Molecule 1: Spike glycoprotein,Fibritin

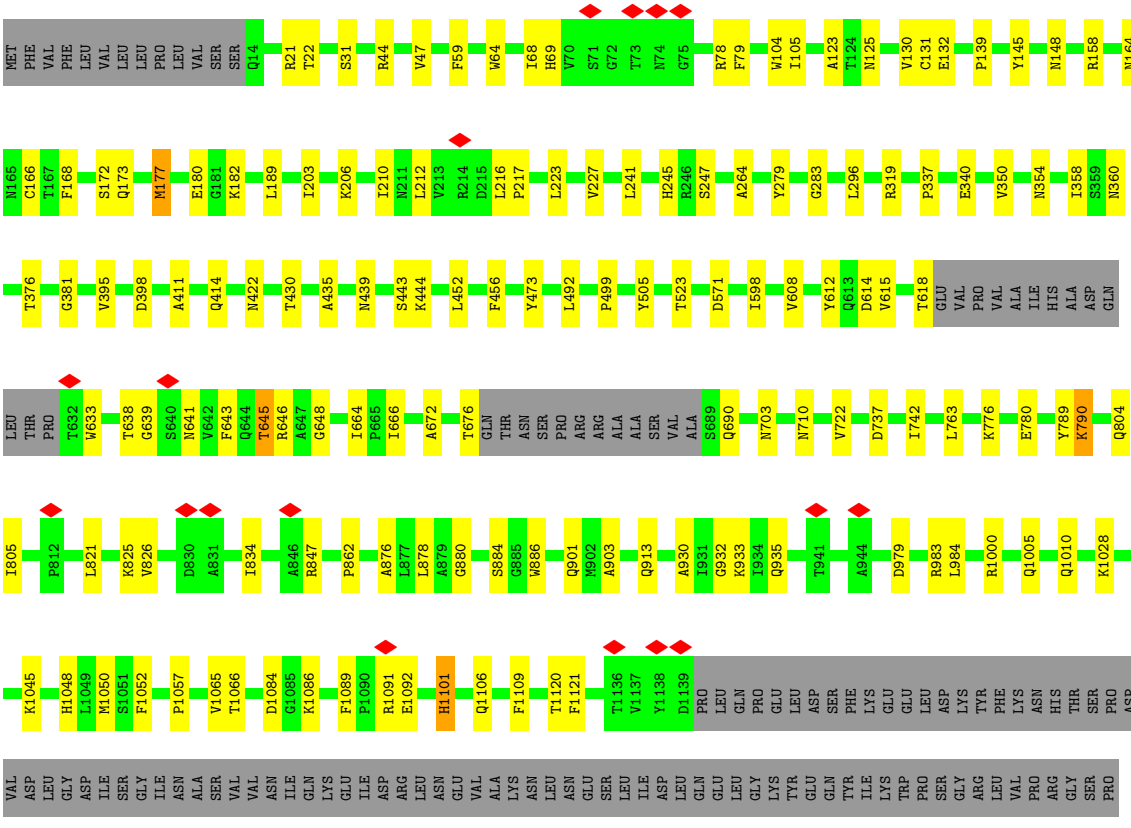
Chain B:





• Molecule 1: Spike glycoprotein,Fibritin

Chain C:



GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY HIS HIS HIS HIS HIS HIS

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

Chain D: 100%

NAG1 NAG2

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

Chain E: 100%

NAG1 NAG2

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

Chain F: 50% 100%

NAG1 NAG2

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

Chain H: 100%

NAG1 NAG2

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

Chain I: 100%

NAG1 NAG2

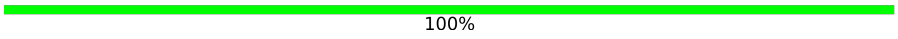
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 50% 100%

NAG1 NAG2

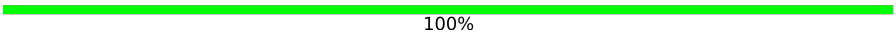
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



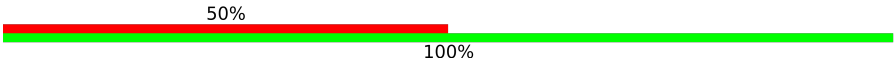
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



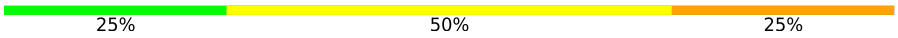
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



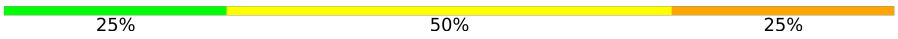
• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



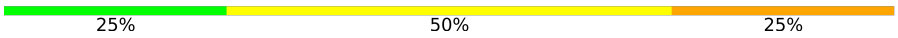
• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	312018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.214	Depositor
Minimum map value	-3.297	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.135	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	308.32, 308.32, 308.32	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EIC, GE9, NAG, SIA, FUC

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	0/8813	0.48	0/11992
1	B	0.26	0/8813	0.48	0/11992
1	C	0.25	0/8813	0.48	0/11992
All	All	0.26	0/26439	0.48	0/35976

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	615	VAL	Peptide
1	B	615	VAL	Peptide
1	C	615	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8611	0	8385	88	0
1	B	8611	0	8385	93	0
1	C	8611	0	8385	81	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	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	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
3	G	48	0	43	1	0
3	K	48	0	43	1	0
3	O	48	0	43	1	0
4	A	168	0	156	5	0
4	B	168	0	156	4	0
4	C	168	0	156	4	0
5	A	12	0	0	1	0
5	B	12	0	0	1	0
5	C	12	0	0	1	0
6	A	21	0	18	1	0
6	B	21	0	18	1	0
6	C	21	0	18	1	0
7	A	20	0	31	0	0
7	B	20	0	31	0	0
7	C	20	0	31	0	0
8	A	93	0	0	0	0
8	B	93	0	0	0	0
8	C	96	0	0	0	0
All	All	27174	0	26124	257	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 (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD22	1:A:217:PRO:HG2	1.71	0.72
1:C:189:LEU:HD22	1:C:217:PRO:HG2	1.71	0.72
1:B:189:LEU:HD22	1:B:217:PRO:HG2	1.71	0.71
1:A:614:ASP:HA	1:B:834:ILE:HG13	1.75	0.67
1:A:645:THR:OG1	1:A:646:ARG:O	2.15	0.65
1:A:319:ARG:NH2	1:B:737:ASP:OD2	2.30	0.65
1:C:645:THR:OG1	1:C:646:ARG:O	2.15	0.65
1:B:645:THR:OG1	1:B:646:ARG:O	2.15	0.64
1:C:903:ALA:HB1	1:C:913:GLN:HB2	1.80	0.64
1:B:903:ALA:HB1	1:B:913:GLN:HB2	1.80	0.63
1:A:903:ALA:HB1	1:A:913:GLN:HB2	1.80	0.63
1:B:763:LEU:HD21	1:B:1005:GLN:HG3	1.81	0.62
1:A:763:LEU:HD21	1:A:1005:GLN:HG3	1.81	0.62
1:B:614:ASP:HA	1:C:834:ILE:HG13	1.80	0.62
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.82	0.62
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.81	0.62
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.81	0.62
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.82	0.61
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.81	0.61
1:C:763:LEU:HD21	1:C:1005:GLN:HG3	1.81	0.61
1:A:647:ALA:HB2	1:B:862:PRO:HG3	1.83	0.61
1:B:139:PRO:HA	1:B:158:ARG:O	2.01	0.61
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.82	0.61
1:B:319:ARG:NH2	1:C:737:ASP:OD2	2.34	0.60
1:A:139:PRO:HA	1:A:158:ARG:O	2.01	0.60
1:C:139:PRO:HA	1:C:158:ARG:O	2.01	0.60
1:A:737:ASP:OD2	1:C:319:ARG:NH2	2.36	0.58
1:B:676:THR:OG1	1:B:690:GLN:OE1	2.20	0.58
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.32	0.58
1:A:834:ILE:HG13	1:C:614:ASP:HA	1.86	0.57
1:B:212:LEU:HD21	1:B:217:PRO:HG3	1.86	0.57
1:C:31:SER:O	1:C:59:PHE:HA	2.05	0.57
1:A:31:SER:O	1:A:59:PHE:HA	2.05	0.57
1:B:31:SER:O	1:B:59:PHE:HA	2.05	0.57
1:B:618:THR:HB	1:B:633:TRP:HE1	1.70	0.57
1:B:131:CYS:HB2	1:B:166:CYS:HA	1.87	0.56
1:C:676:THR:OG1	1:C:690:GLN:OE1	2.20	0.56
1:A:676:THR:OG1	1:A:690:GLN:OE1	2.20	0.56
1:C:131:CYS:HB2	1:C:166:CYS:HA	1.87	0.56
1:B:821:LEU:O	1:B:825:LYS:HG3	2.06	0.56
1:A:131:CYS:HB2	1:A:166:CYS:HA	1.87	0.56
1:A:212:LEU:HD21	1:A:217:PRO:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:LEU:O	1:A:825:LYS:HG3	2.06	0.56
1:A:618:THR:HB	1:A:633:TRP:HE1	1.70	0.56
1:C:212:LEU:HD21	1:C:217:PRO:HG3	1.86	0.56
1:C:618:THR:HB	1:C:633:TRP:HE1	1.70	0.56
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.32	0.55
1:C:821:LEU:O	1:C:825:LYS:HG3	2.06	0.55
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.32	0.55
1:A:456:PHE:HB3	1:A:473:TYR:CD2	2.42	0.54
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.90	0.54
1:B:456:PHE:HB3	1:B:473:TYR:CD2	2.43	0.54
1:A:704:SER:HB2	1:B:790:LYS:NZ	2.23	0.53
1:C:456:PHE:HB3	1:C:473:TYR:CD2	2.43	0.53
1:A:68:ILE:HD12	1:A:69:HIS:H	1.74	0.53
1:B:68:ILE:HD12	1:B:69:HIS:H	1.74	0.53
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.90	0.53
1:A:886:TRP:HZ3	1:A:901:GLN:HG3	1.75	0.52
1:B:886:TRP:HZ3	1:B:901:GLN:HG3	1.75	0.52
1:C:68:ILE:HD12	1:C:69:HIS:H	1.74	0.52
1:C:886:TRP:HZ3	1:C:901:GLN:HG3	1.75	0.52
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.90	0.52
1:C:1091:ARG:HB2	1:C:1121:PHE:HD1	1.75	0.52
1:B:173:GLN:HA	1:B:173:GLN:OE1	2.10	0.52
1:C:173:GLN:OE1	1:C:173:GLN:HA	2.10	0.51
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.93	0.51
1:A:31:SER:O	1:A:59:PHE:CA	2.59	0.51
1:A:1091:ARG:HB2	1:A:1121:PHE:HD1	1.75	0.51
1:C:350:VAL:HG22	1:C:422:ASN:HB3	1.93	0.51
1:A:173:GLN:OE1	1:A:173:GLN:HA	2.10	0.51
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.93	0.51
1:B:1091:ARG:HB2	1:B:1121:PHE:HD1	1.75	0.51
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.93	0.51
1:B:31:SER:O	1:B:59:PHE:CA	2.59	0.50
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.93	0.50
1:A:932:GLY:O	1:A:935:GLN:HB2	2.11	0.50
1:B:932:GLY:O	1:B:935:GLN:HB2	2.11	0.50
1:B:983:ARG:HG3	1:B:984:LEU:HG	1.94	0.50
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.93	0.50
1:C:932:GLY:O	1:C:935:GLN:HB2	2.11	0.50
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.93	0.50
1:A:983:ARG:HG3	1:A:984:LEU:HG	1.94	0.50
1:C:31:SER:O	1:C:59:PHE:CA	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:VAL:HG12	1:C:279:TYR:HB2	1.94	0.50
1:C:983:ARG:HG3	1:C:984:LEU:HG	1.94	0.50
1:B:47:VAL:HG12	1:B:279:TYR:HB2	1.94	0.50
1:A:47:VAL:HG12	1:A:279:TYR:HB2	1.94	0.50
1:A:787:GLN:HE21	1:C:703:ASN:CG	2.15	0.49
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.93	0.49
1:C:381:GLY:HA3	1:C:430:THR:HG23	1.94	0.49
1:B:358:ILE:HB	1:B:395:VAL:HB	1.94	0.49
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.93	0.49
1:C:643:PHE:CD2	1:C:645:THR:HG22	2.48	0.49
1:A:381:GLY:HA3	1:A:430:THR:HG23	1.94	0.49
1:A:643:PHE:CD2	1:A:645:THR:HG22	2.48	0.49
1:C:358:ILE:HB	1:C:395:VAL:HB	1.94	0.49
1:A:358:ILE:HB	1:A:395:VAL:HB	1.94	0.48
1:C:21:ARG:HH11	1:C:79:PHE:HB3	1.78	0.48
5:A:1313:GE9:I03	5:A:1313:GE9:O01	3.02	0.48
1:B:643:PHE:CD2	1:B:645:THR:HG22	2.48	0.48
5:C:1314:GE9:O01	5:C:1314:GE9:I03	3.02	0.48
1:B:245:HIS:HB3	6:B:1314:SIA:H113	1.96	0.48
1:A:21:ARG:HH11	1:A:79:PHE:HB3	1.78	0.48
1:B:381:GLY:HA3	1:B:430:THR:HG23	1.94	0.47
1:C:203:ILE:HB	1:C:227:VAL:HG12	1.96	0.47
1:B:337:PRO:HB2	1:B:340:GLU:HB2	1.95	0.47
1:C:337:PRO:HB2	1:C:340:GLU:HB2	1.95	0.47
1:A:337:PRO:HB2	1:A:340:GLU:HB2	1.95	0.47
1:B:21:ARG:HH11	1:B:79:PHE:HB3	1.78	0.47
1:A:203:ILE:HB	1:A:227:VAL:HG12	1.96	0.47
5:B:1313:GE9:I03	5:B:1313:GE9:O01	3.02	0.47
3:O:2:FUC:H3	3:O:3:NAG:HN2	1.80	0.47
1:A:206:LYS:HB2	1:A:223:LEU:HA	1.96	0.47
1:A:376:THR:HB	1:A:435:ALA:HB3	1.97	0.47
1:B:206:LYS:HB2	1:B:223:LEU:HA	1.96	0.47
3:G:2:FUC:H3	3:G:3:NAG:HN2	1.79	0.47
1:B:131:CYS:CB	1:B:166:CYS:HA	2.45	0.47
1:A:245:HIS:HB3	6:A:1314:SIA:H113	1.96	0.47
1:A:776:LYS:HE3	1:A:780:GLU:OE1	2.15	0.47
1:B:203:ILE:HB	1:B:227:VAL:HG12	1.96	0.47
1:A:131:CYS:CB	1:A:166:CYS:HA	2.45	0.46
3:K:2:FUC:H3	3:K:3:NAG:HN2	1.80	0.46
1:B:31:SER:O	1:B:59:PHE:N	2.48	0.46
1:B:148:ASN:HD21	4:B:1307:NAG:H82	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ILE:HG13	1:B:878[B]:LEU:HD21	1.98	0.46
1:C:245:HIS:HB3	6:C:1315:SIA:H113	1.96	0.46
1:C:878[A]:LEU:HD21	1:C:1052:PHE:HB3	1.97	0.46
4:C:1307:NAG:O7	4:C:1307:NAG:O3	2.30	0.46
1:C:206:LYS:HB2	1:C:223:LEU:HA	1.96	0.46
1:A:31:SER:O	1:A:59:PHE:N	2.48	0.46
1:B:354:ASN:O	1:B:398:ASP:HA	2.16	0.46
1:B:776:LYS:HE3	1:B:780:GLU:OE1	2.15	0.46
1:C:148:ASN:HD21	4:C:1308:NAG:H82	1.80	0.46
1:C:805:ILE:HG13	1:C:878[B]:LEU:HD21	1.98	0.46
1:C:296:LEU:HB2	1:C:608:VAL:HG11	1.98	0.46
1:A:354:ASN:O	1:A:398:ASP:HA	2.16	0.46
1:C:354:ASN:O	1:C:398:ASP:HA	2.16	0.46
1:C:776:LYS:HE3	1:C:780:GLU:OE1	2.15	0.46
1:A:452:LEU:HD23	1:A:492:LEU:HB3	1.98	0.46
1:C:31:SER:O	1:C:59:PHE:N	2.48	0.46
1:A:805:ILE:HG13	1:A:878[B]:LEU:HD21	1.98	0.46
1:A:886:TRP:CZ3	1:A:901:GLN:HG3	2.51	0.45
1:C:131:CYS:CB	1:C:166:CYS:HA	2.45	0.45
1:A:132:GLU:HB2	1:A:164:ASN:O	2.16	0.45
1:B:704:SER:HB2	1:C:790:LYS:NZ	2.32	0.45
1:C:452:LEU:HD23	1:C:492:LEU:HB3	1.98	0.45
1:B:132:GLU:HB2	1:B:164:ASN:O	2.16	0.45
1:C:132:GLU:HB2	1:C:164:ASN:O	2.16	0.45
1:C:886:TRP:CZ3	1:C:901:GLN:HG3	2.51	0.45
1:B:376:THR:HB	1:B:435:ALA:HB3	1.97	0.45
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.82	0.45
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.50	0.45
1:A:187:LYS:HA	1:A:187:LYS:HD3	1.78	0.45
1:B:296:LEU:HB2	1:B:608:VAL:HG11	1.98	0.45
1:A:148:ASN:HD21	4:A:1307:NAG:H82	1.80	0.45
1:A:878[A]:LEU:HD21	1:A:1052:PHE:HB3	1.99	0.45
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.50	0.45
1:C:376:THR:HB	1:C:435:ALA:HB3	1.97	0.45
1:C:105:ILE:HG23	1:C:241:LEU:HD11	2.00	0.45
1:C:1101:HIS:CE1	4:C:1311:NAG:H5	2.52	0.45
1:B:452:LEU:HD23	1:B:492:LEU:HB3	1.98	0.44
1:B:1101:HIS:CE1	4:B:1310:NAG:H5	2.52	0.44
1:A:1101:HIS:CE1	4:A:1310:NAG:H5	2.52	0.44
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.82	0.44
1:B:105:ILE:HG23	1:B:241:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LYS:HA	1:A:558:LYS:HD3	1.83	0.44
1:A:1086:LYS:HE3	1:A:1086:LYS:HB2	1.79	0.44
1:B:878[A]:LEU:HD21	1:B:1052:PHE:HB3	1.99	0.44
1:C:639:GLY:O	1:C:641:ASN:N	2.50	0.44
1:A:296:LEU:HB2	1:A:608:VAL:HG11	1.98	0.44
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.50	0.44
1:B:1089:PHE:O	1:B:1120:THR:HA	2.18	0.44
4:A:1306:NAG:O7	4:A:1306:NAG:O3	2.30	0.43
1:A:44:ARG:O	1:A:283:GLY:HA2	2.18	0.43
1:B:886:TRP:CZ3	1:B:901:GLN:HG3	2.51	0.43
1:A:105:ILE:HG23	1:A:241:LEU:HD11	1.99	0.43
4:B:1306:NAG:O7	4:B:1306:NAG:O3	2.30	0.43
1:C:710:ASN:HB3	4:C:1309:NAG:H82	2.01	0.43
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.82	0.43
1:C:880:GLY:O	1:C:884:SER:OG	2.28	0.43
1:A:1089:PHE:O	1:A:1120:THR:HA	2.19	0.43
1:B:80:ASP:O	1:B:265:TYR:OH	2.25	0.43
1:B:1089:PHE:HB2	1:B:1121:PHE:CE1	2.54	0.43
1:B:598:ILE:HG23	1:B:664:ILE:HG21	2.00	0.43
1:C:1089:PHE:HB2	1:C:1121:PHE:CE1	2.54	0.43
1:A:710:ASN:HB3	4:A:1308:NAG:H82	2.01	0.43
1:B:44:ARG:O	1:B:283:GLY:HA2	2.19	0.43
1:C:598:ILE:HG23	1:C:664:ILE:HG21	2.00	0.43
1:A:598:ILE:HG23	1:A:664:ILE:HG21	2.00	0.43
1:B:612:TYR:O	1:B:648:GLY:HA3	2.19	0.43
1:C:1089:PHE:O	1:C:1120:THR:HA	2.19	0.43
1:A:701:ALA:O	1:B:788:ILE:N	2.38	0.43
1:B:125:ASN:ND2	1:B:172:SER:O	2.48	0.43
1:B:180:GLU:HB3	1:B:182:LYS:HE3	2.01	0.43
1:B:647:ALA:HB2	1:C:862:PRO:HG3	2.00	0.43
1:C:612:TYR:O	1:C:648:GLY:HA3	2.19	0.43
1:A:880:GLY:O	1:A:884:SER:OG	2.29	0.42
1:B:1086:LYS:HB2	1:B:1086:LYS:HE3	1.79	0.42
1:C:44:ARG:O	1:C:283:GLY:HA2	2.19	0.42
1:A:612:TYR:O	1:A:648:GLY:HA3	2.19	0.42
1:A:1106:GLN:HG3	1:A:1109:PHE:O	2.20	0.42
1:C:1106:GLN:HG3	1:C:1109:PHE:O	2.20	0.42
1:A:125:ASN:ND2	1:A:172:SER:O	2.48	0.42
1:A:1089:PHE:HB2	1:A:1121:PHE:CE1	2.54	0.42
1:A:180:GLU:HB3	1:A:182:LYS:HE3	2.01	0.42
1:B:710:ASN:HB3	4:B:1308:NAG:H82	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ASN:H	1:C:523:THR:HG23	1.85	0.42
1:A:614:ASP:HB3	1:B:835:LYS:O	2.20	0.42
1:B:411:ALA:HB3	1:B:414:GLN:HG2	2.02	0.42
1:C:125:ASN:ND2	1:C:172:SER:O	2.48	0.42
1:C:145:TYR:HB3	1:C:247:SER:HB3	2.02	0.42
1:A:411:ALA:HB3	1:A:414:GLN:HG2	2.02	0.41
1:A:529:LYS:HD3	1:A:529:LYS:HA	1.80	0.41
4:A:1306:NAG:H82	1:B:834:ILE:HG21	2.01	0.41
1:B:1050:MET:HG2	1:B:1065:VAL:HB	2.02	0.41
1:A:360:ASN:H	1:A:523:THR:HG23	1.85	0.41
1:A:396:TYR:CE1	1:B:230:PRO:HG3	2.56	0.41
1:A:444:LYS:O	1:A:499:PRO:HD3	2.21	0.41
1:B:444:LYS:O	1:B:499:PRO:HD3	2.21	0.41
1:B:708:SER:HB3	1:B:711:SER:HB3	2.03	0.41
1:C:411:ALA:HB3	1:C:414:GLN:HG2	2.02	0.41
1:C:439:ASN:O	1:C:443:SER:HB2	2.20	0.41
1:A:439:ASN:O	1:A:443:SER:HB2	2.20	0.41
1:C:1086:LYS:HB2	1:C:1086:LYS:HE3	1.79	0.41
1:B:599:THR:HA	1:B:600:PRO:HD3	1.95	0.41
1:C:444:LYS:O	1:C:499:PRO:HD3	2.21	0.41
1:B:439:ASN:O	1:B:443:SER:HB2	2.20	0.41
1:C:180:GLU:HB3	1:C:182:LYS:HE3	2.01	0.41
1:A:1050:MET:HG2	1:A:1065:VAL:HB	2.02	0.41
1:B:558:LYS:HA	1:B:558:LYS:HD3	1.83	0.41
1:B:1106:GLN:HG3	1:B:1109:PHE:O	2.20	0.41
1:C:789:TYR:O	1:C:876:ALA:HA	2.21	0.41
1:C:930:ALA:HA	1:C:933:LYS:HE2	2.03	0.41
1:A:145:TYR:HB3	1:A:247:SER:HB3	2.02	0.41
1:A:708:SER:HB3	1:A:711:SER:HB3	2.03	0.41
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	2.03	0.41
1:B:497:PHE:CG	1:B:507:PRO:HG3	2.56	0.41
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	2.03	0.41
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	2.03	0.41
1:B:360:ASN:H	1:B:523:THR:HG23	1.85	0.41
1:C:22:THR:O	1:C:78:ARG:NH2	2.54	0.41
1:A:906:PHE:O	1:A:909:ILE:HG13	2.22	0.40
1:B:145:TYR:HB3	1:B:247:SER:HB3	2.02	0.40
1:B:900:MET:HE3	1:B:900:MET:HB3	1.96	0.40
1:A:497:PHE:CG	1:A:507:PRO:HG3	2.56	0.40
1:A:789:TYR:O	1:A:876:ALA:HA	2.21	0.40
1:B:123:ALA:HA	1:B:177:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LYS:HE2	1:B:417:LYS:HB3	1.81	0.40
1:B:789:TYR:O	1:B:876:ALA:HA	2.21	0.40
1:C:123:ALA:HA	1:C:177:MET:SD	2.62	0.40
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	2.03	0.40
1:C:1050:MET:HG2	1:C:1065:VAL:HB	2.02	0.40
1:B:22:THR:O	1:B:78:ARG:NH2	2.54	0.40
1:B:393:THR:HA	1:B:522:ALA:HA	2.04	0.40
1:B:403:ARG:HH21	1:B:417:LYS:NZ	2.20	0.40
1:A:403:ARG:HH21	1:A:417:LYS:NZ	2.20	0.40
1:B:187:LYS:HD3	1:B:187:LYS:HA	1.78	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	1097/1259 (87%)	1053 (96%)	43 (4%)	1 (0%)	51	63
1	B	1097/1259 (87%)	1054 (96%)	42 (4%)	1 (0%)	51	63
1	C	1097/1259 (87%)	1053 (96%)	43 (4%)	1 (0%)	51	63
All	All	3291/3777 (87%)	3160 (96%)	128 (4%)	3 (0%)	54	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ILE
1	B	210	ILE
1	C	210	ILE

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	958/1095 (88%)	942 (98%)	16 (2%)	60	74
1	B	958/1095 (88%)	942 (98%)	16 (2%)	60	74
1	C	958/1095 (88%)	942 (98%)	16 (2%)	60	74
All	All	2874/3285 (88%)	2826 (98%)	48 (2%)	64	74

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	TRP
1	A	177	MET
1	A	505[A]	TYR
1	A	505[B]	TYR
1	A	571	ASP
1	A	638	THR
1	A	645	THR
1	A	790	LYS
1	A	804	GLN
1	A	847	ARG
1	A	979	ASP
1	A	1010	GLN
1	A	1045	LYS
1	A	1084	ASP
1	A	1092	GLU
1	A	1101	HIS
1	B	104	TRP
1	B	177	MET
1	B	505[A]	TYR
1	B	505[B]	TYR
1	B	571	ASP
1	B	638	THR
1	B	645	THR
1	B	790	LYS
1	B	804	GLN
1	B	847	ARG

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Mol	Chain	Res	Type
1	B	979	ASP
1	B	1010	GLN
1	B	1045	LYS
1	B	1084	ASP
1	B	1092	GLU
1	B	1101	HIS
1	C	104	TRP
1	C	177	MET
1	C	505[A]	TYR
1	C	505[B]	TYR
1	C	571	ASP
1	C	638	THR
1	C	645	THR
1	C	790	LYS
1	C	804	GLN
1	C	847	ARG
1	C	979	ASP
1	C	1010	GLN
1	C	1045	LYS
1	C	1084	ASP
1	C	1092	GLU
1	C	1101	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

30 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	D	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	E	1	2,1	14,14,15	0.22	0	17,19,21	0.55	0
2	NAG	E	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	F	1	2,1	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	G	1	3,1	14,14,15	0.68	1 (7%)	17,19,21	1.03	2 (11%)
3	FUC	G	2	3	10,10,11	0.93	1 (10%)	14,14,16	1.25	1 (7%)
3	NAG	G	3	3	14,14,15	0.21	0	17,19,21	0.47	0
3	FUC	G	4	3	10,10,11	0.61	0	14,14,16	0.84	0
2	NAG	H	1	2,1	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	H	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	I	1	2,1	14,14,15	0.22	0	17,19,21	0.55	0
2	NAG	I	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	J	1	2,1	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	J	2	2	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	K	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	1.03	2 (11%)
3	FUC	K	2	3	10,10,11	0.93	1 (10%)	14,14,16	1.25	1 (7%)
3	NAG	K	3	3	14,14,15	0.21	0	17,19,21	0.47	0
3	FUC	K	4	3	10,10,11	0.62	0	14,14,16	0.84	0
2	NAG	L	1	2,1	14,14,15	0.25	0	17,19,21	0.49	0
2	NAG	L	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	M	1	2,1	14,14,15	0.22	0	17,19,21	0.55	0
2	NAG	M	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	N	1	2,1	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	N	2	2	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	O	1	3,1	14,14,15	0.68	1 (7%)	17,19,21	1.03	2 (11%)
3	FUC	O	2	3	10,10,11	0.93	1 (10%)	14,14,16	1.25	1 (7%)
3	NAG	O	3	3	14,14,15	0.22	0	17,19,21	0.47	0
3	FUC	O	4	3	10,10,11	0.62	0	14,14,16	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	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	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	3/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
3	NAG	G	3	3	-	2/6/23/26	0/1/1/1
3	FUC	G	4	3	-	-	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	3/6/23/26	0/1/1/1
3	FUC	K	2	3	-	-	0/1/1/1
3	NAG	K	3	3	-	2/6/23/26	0/1/1/1
3	FUC	K	4	3	-	-	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	4/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	3/6/23/26	0/1/1/1
3	FUC	O	2	3	-	-	0/1/1/1
3	NAG	O	3	3	-	2/6/23/26	0/1/1/1
3	FUC	O	4	3	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	2	FUC	C1-C2	2.25	1.57	1.52
3	K	2	FUC	C1-C2	2.25	1.57	1.52
3	G	2	FUC	C1-C2	2.25	1.57	1.52
3	K	1	NAG	C1-C2	2.07	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	C1-C2	2.06	1.55	1.52
3	O	1	NAG	C1-C2	2.06	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	FUC	C1-O5-C5	3.03	119.65	112.78
3	K	2	FUC	C1-O5-C5	3.03	119.65	112.78
3	O	2	FUC	C1-O5-C5	3.03	119.64	112.78
3	O	1	NAG	C1-O5-C5	2.19	115.16	112.19
3	K	1	NAG	C1-O5-C5	2.19	115.16	112.19
3	G	1	NAG	C1-O5-C5	2.19	115.16	112.19
3	K	1	NAG	O4-C4-C3	2.01	114.99	110.35
3	O	1	NAG	O4-C4-C3	2.01	114.98	110.35
3	G	1	NAG	O4-C4-C3	2.00	114.98	110.35

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	3	NAG	C4-C5-C6-O6
3	K	3	NAG	C4-C5-C6-O6
3	O	3	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
3	G	3	NAG	O5-C5-C6-O6
3	K	3	NAG	O5-C5-C6-O6
3	O	3	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7
2	M	1	NAG	C3-C2-N2-C7
2	F	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3	NAG	1	0
3	O	3	NAG	1	0
3	K	2	FUC	1	0
3	O	2	FUC	1	0
3	G	2	FUC	1	0

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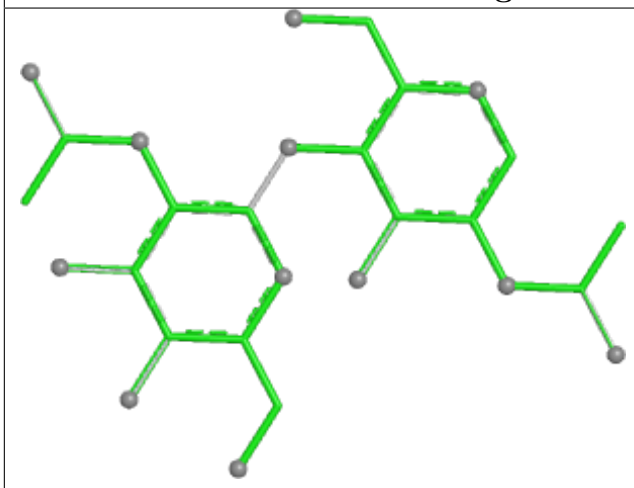
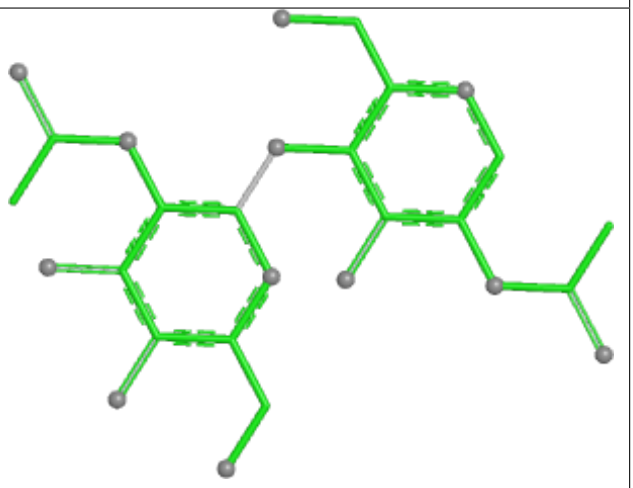
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	3	NAG	1	0

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

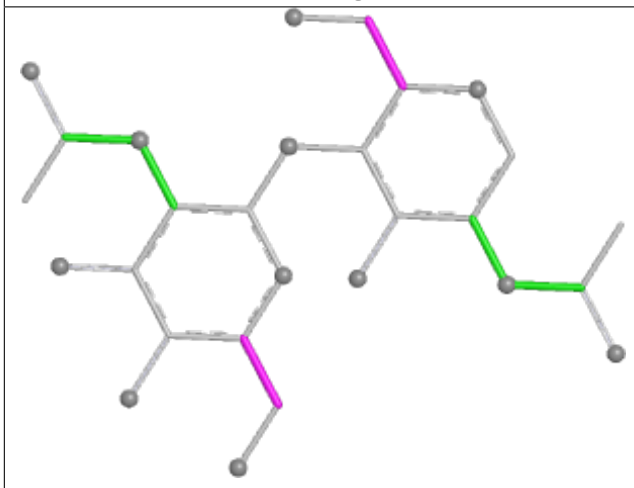
Oligosaccharide Chain D



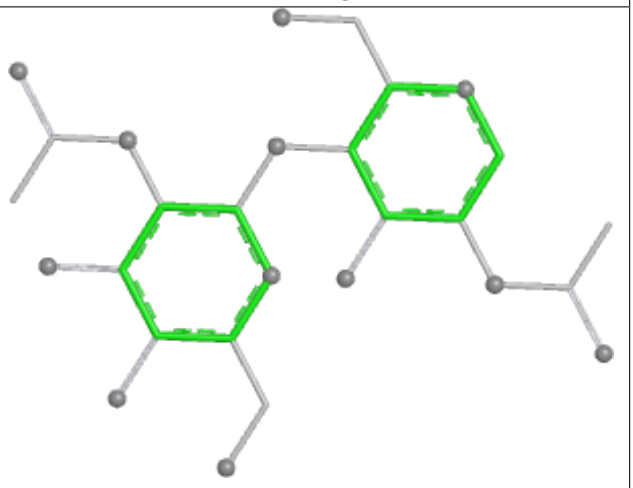
Bond lengths



Bond angles

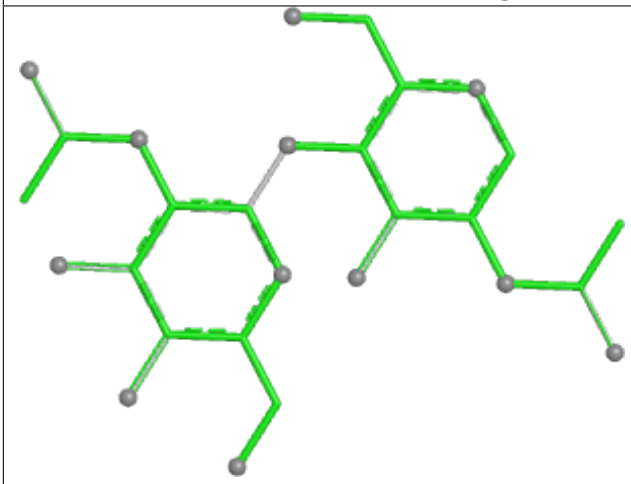


Torsions

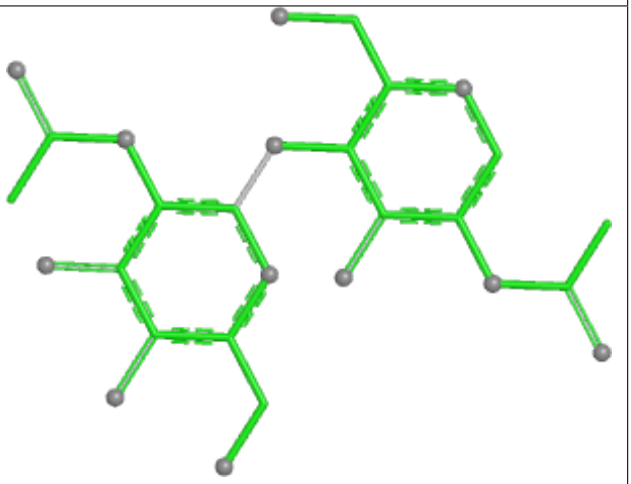


Rings

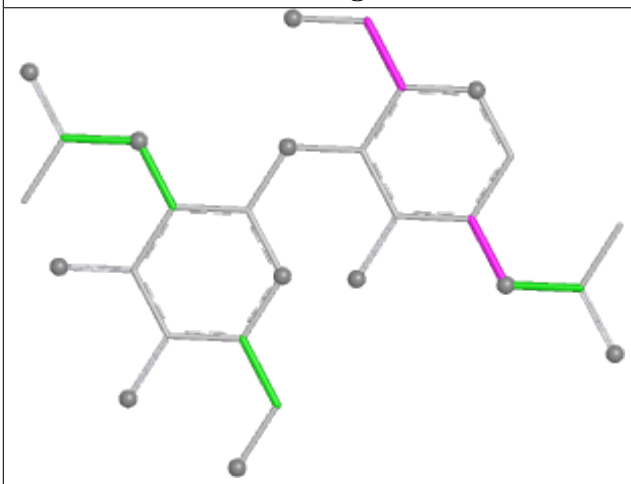
Oligosaccharide Chain E



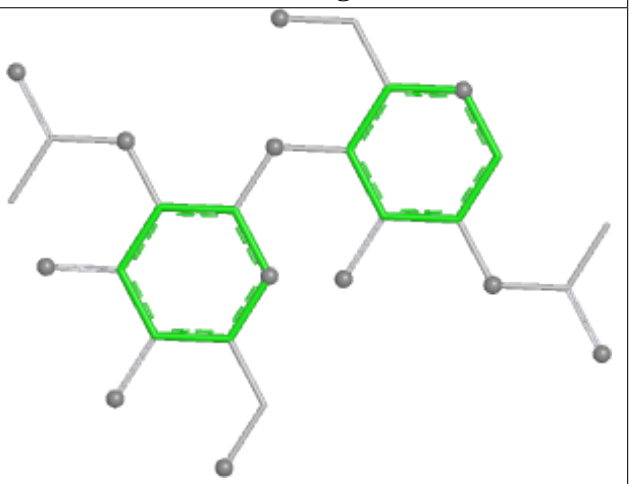
Bond lengths



Bond angles

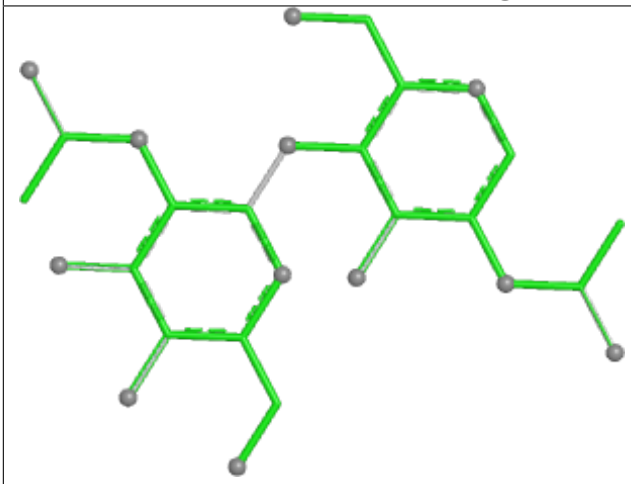


Torsions

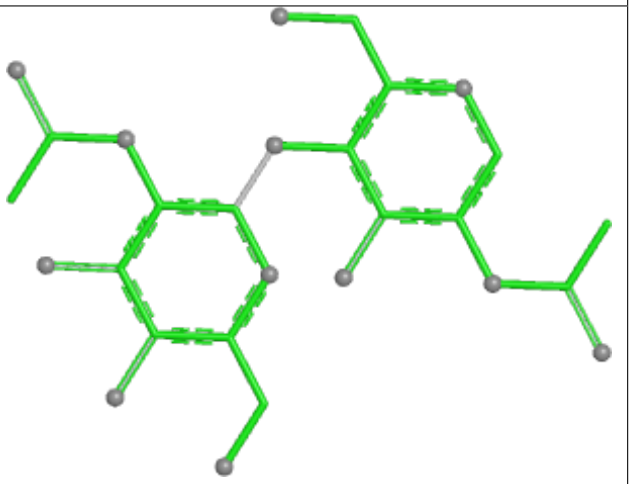


Rings

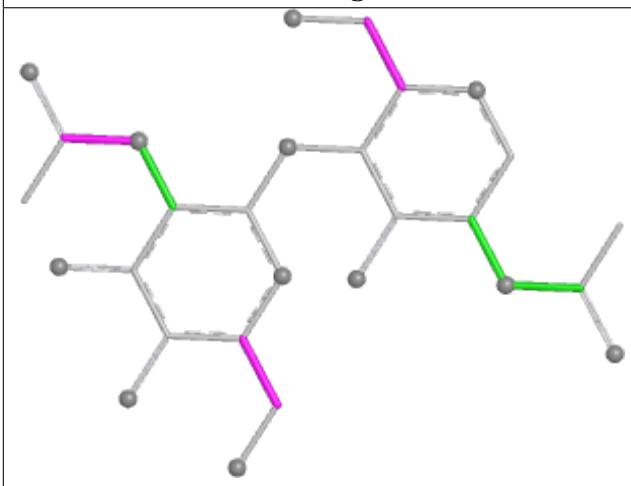
Oligosaccharide Chain F



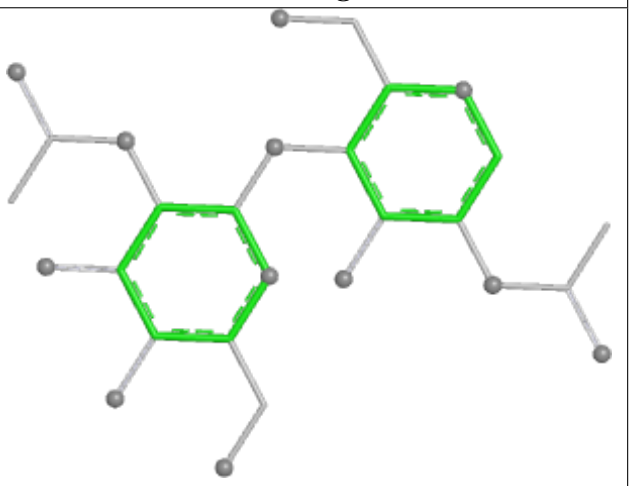
Bond lengths



Bond angles

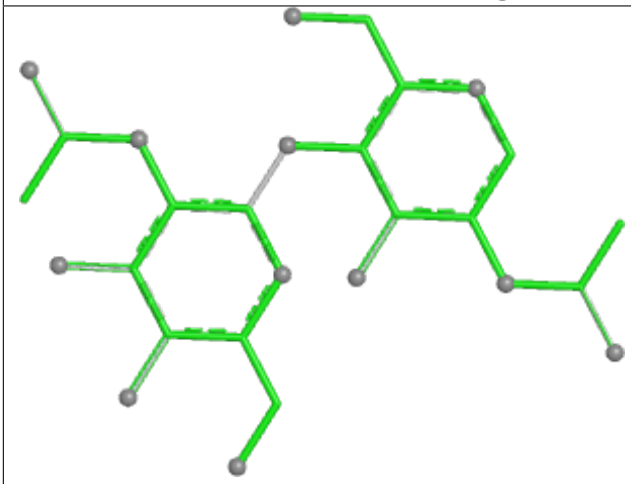


Torsions

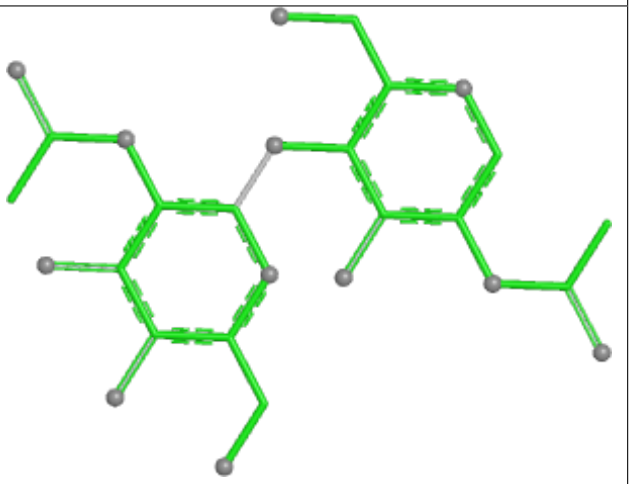


Rings

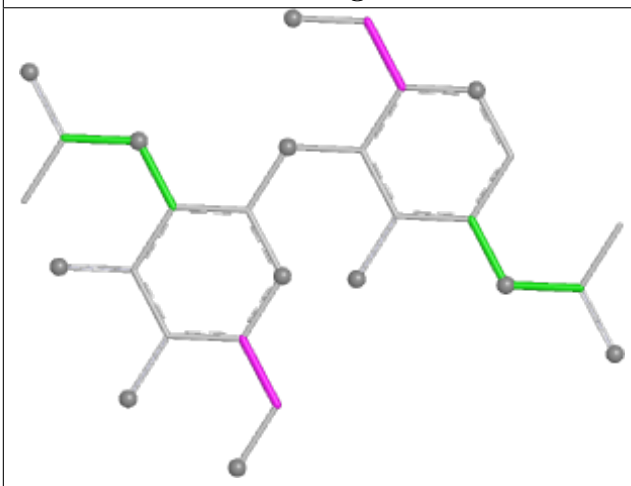
Oligosaccharide Chain H



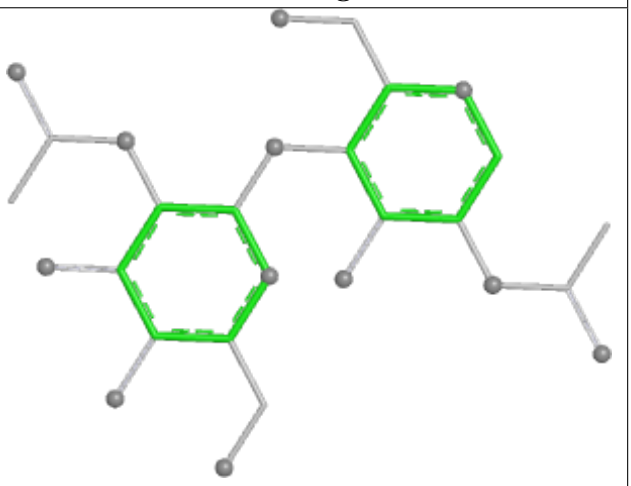
Bond lengths



Bond angles

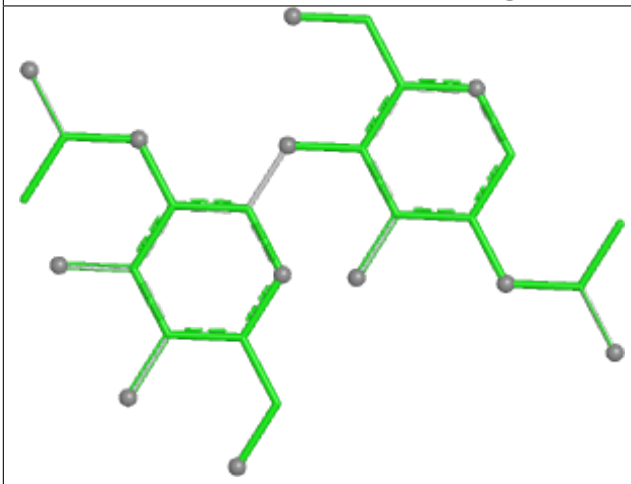


Torsions

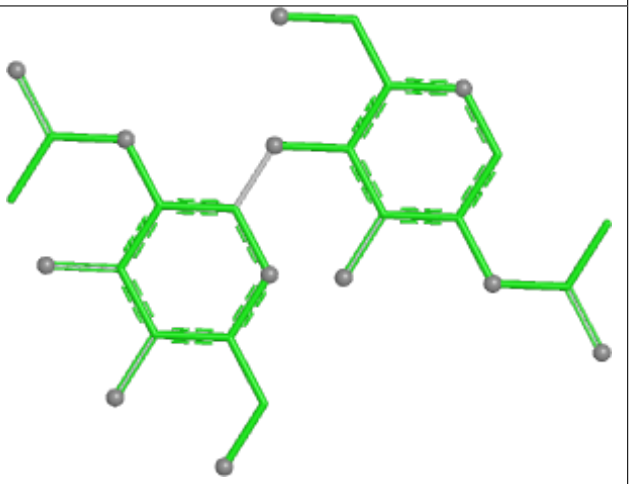


Rings

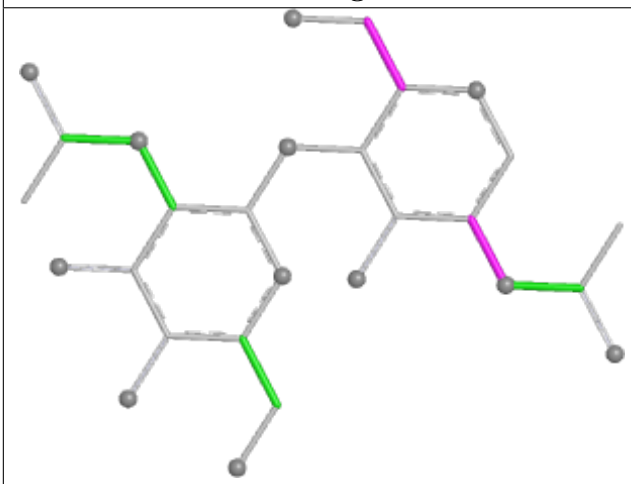
Oligosaccharide Chain I



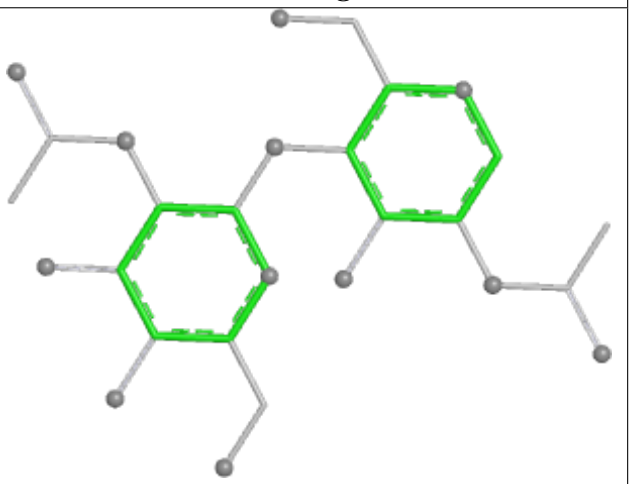
Bond lengths



Bond angles

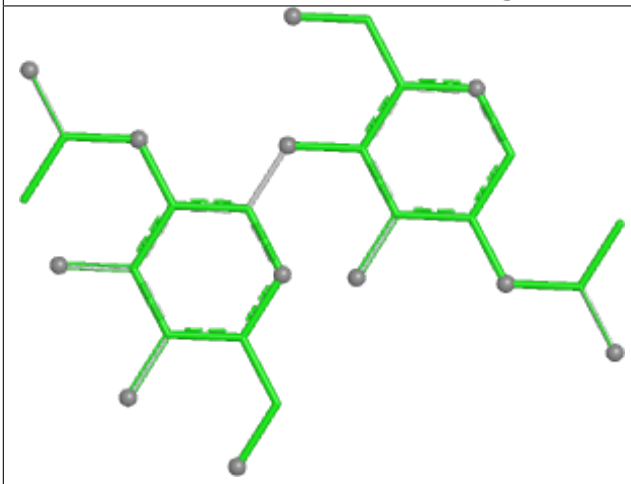


Torsions

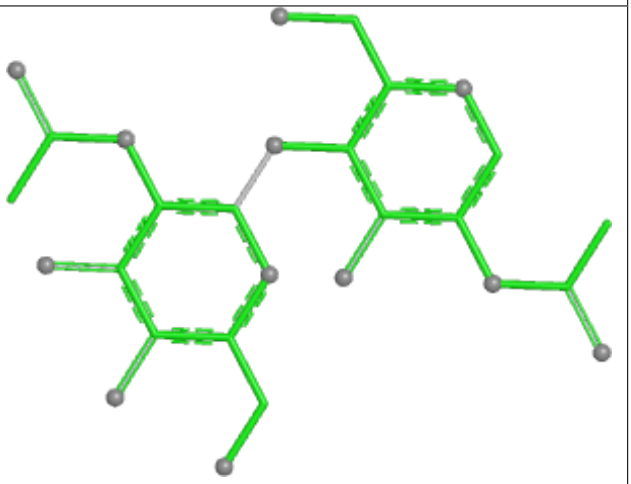


Rings

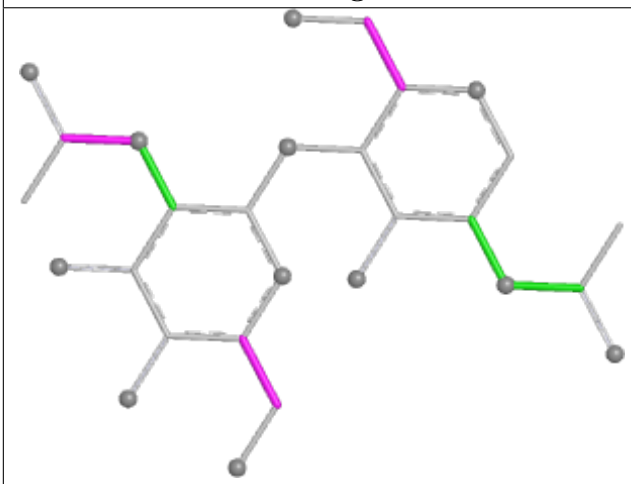
Oligosaccharide Chain J



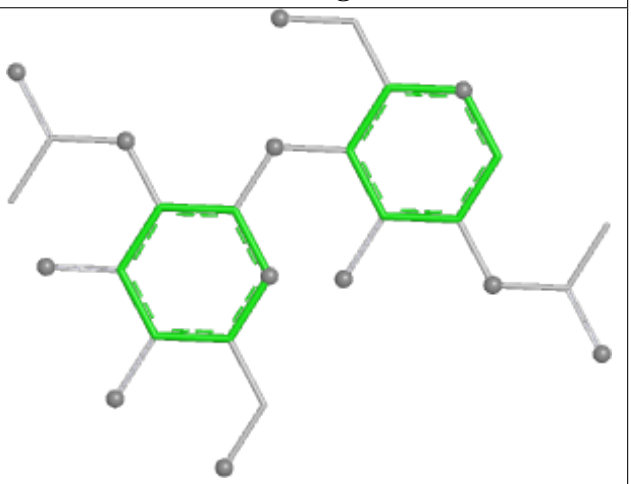
Bond lengths



Bond angles

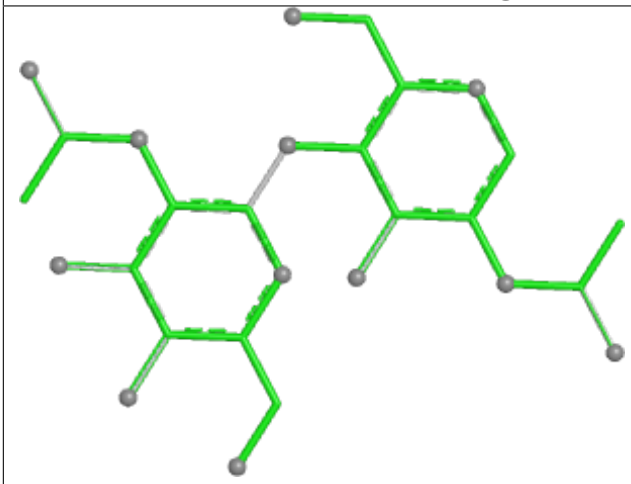


Torsions

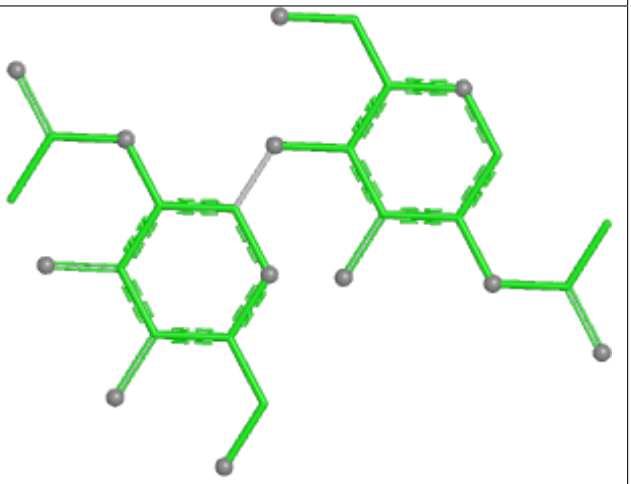


Rings

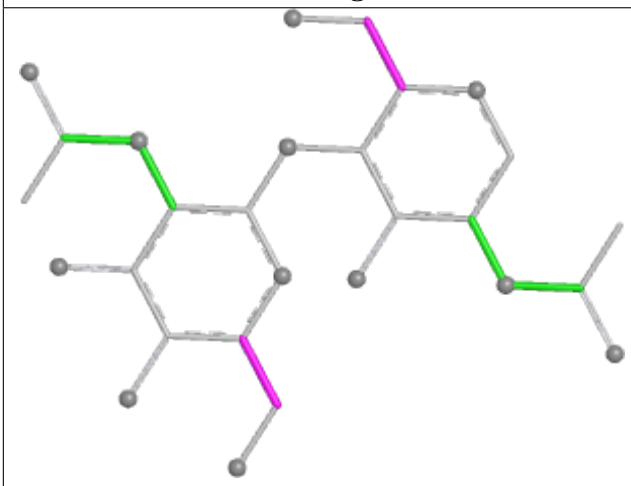
Oligosaccharide Chain L



Bond lengths



Bond angles



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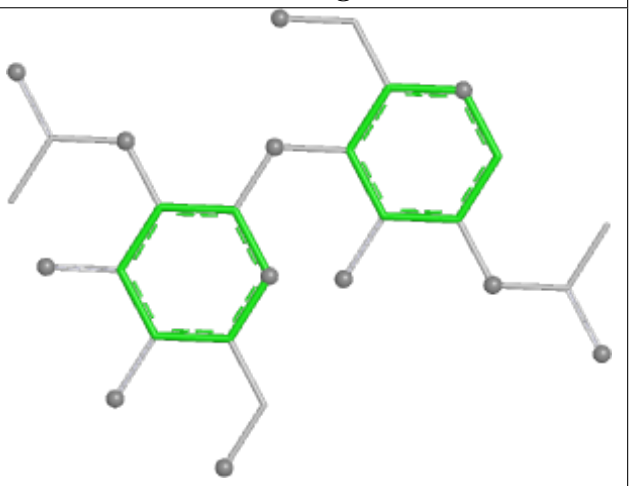
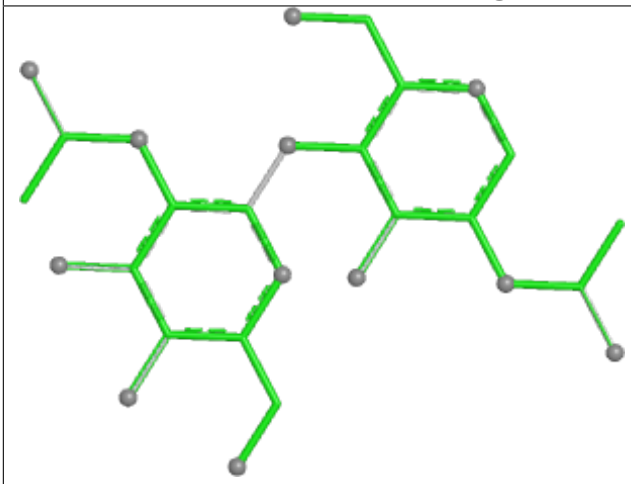
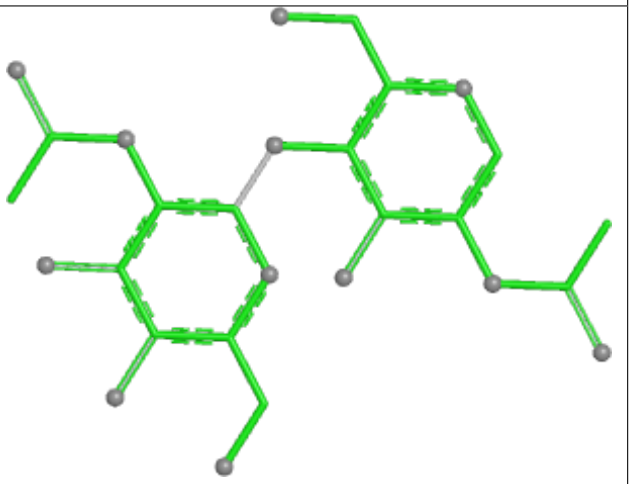


Rings

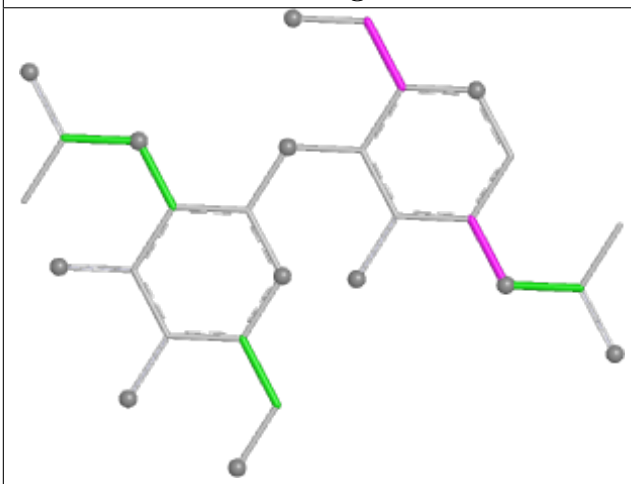
Oligosaccharide Chain M



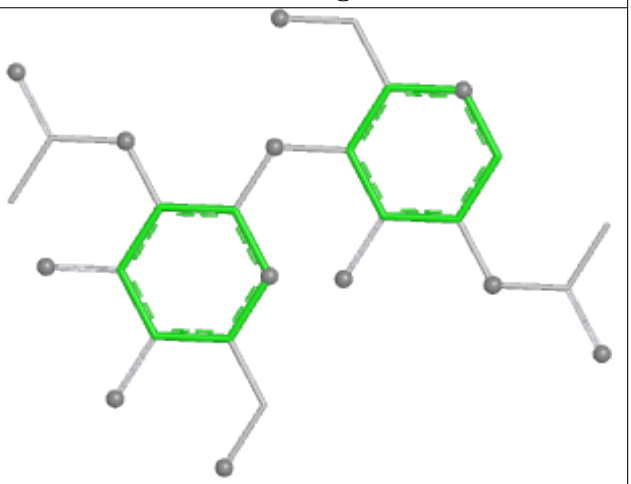
Bond lengths



Bond angles

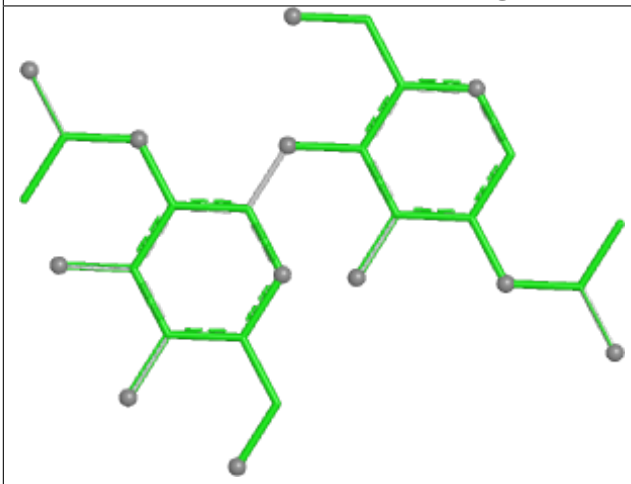


Torsions

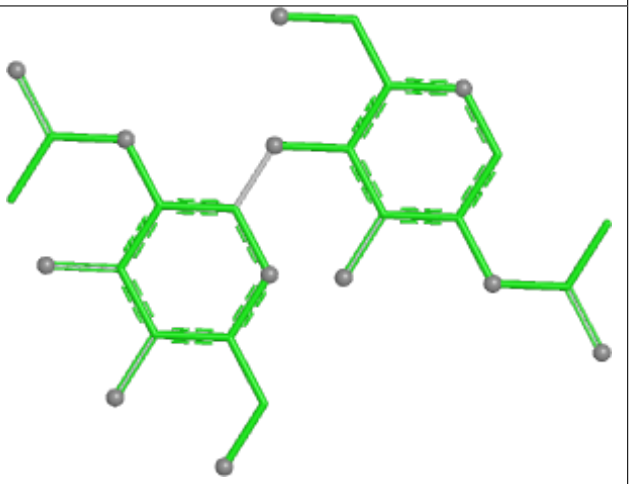


Rings

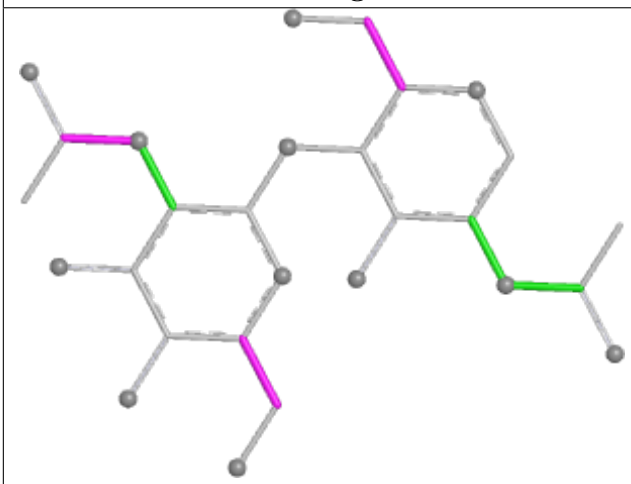
Oligosaccharide Chain N



Bond lengths



Bond angles



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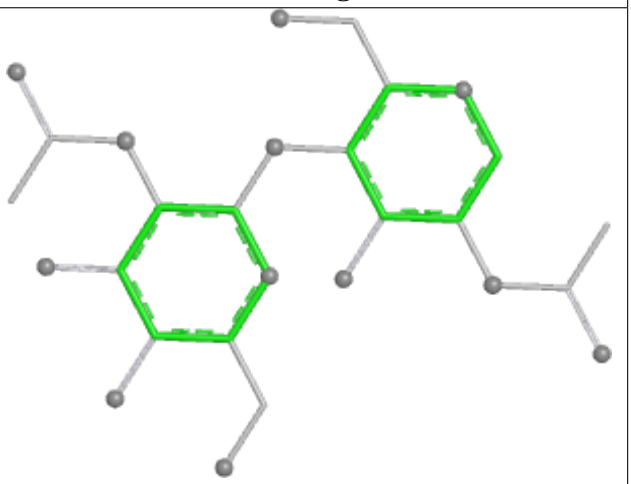
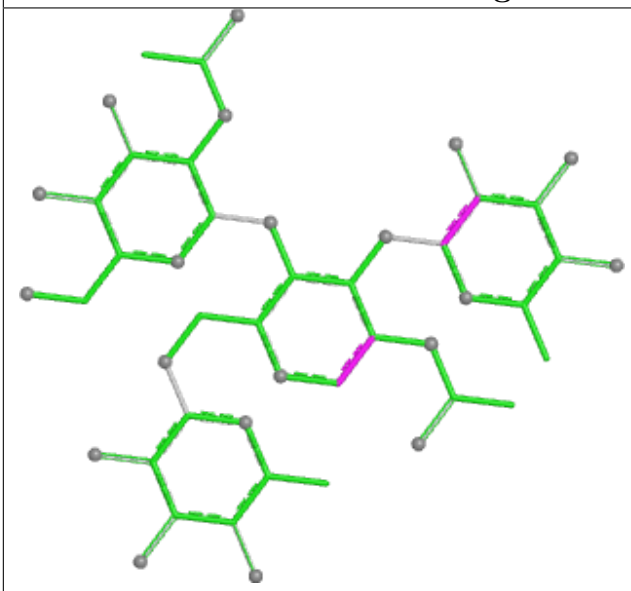
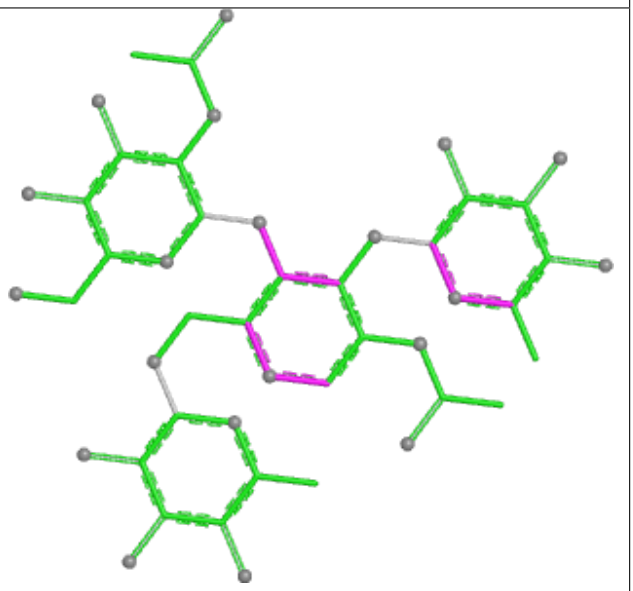


Rings

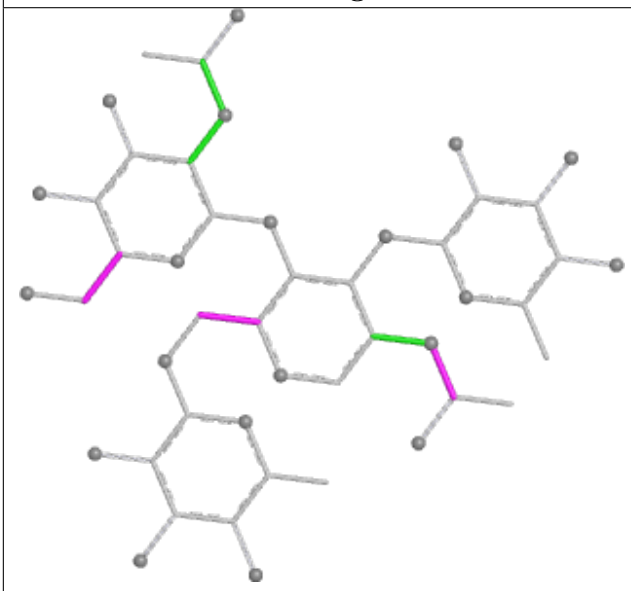
Oligosaccharide Chain G



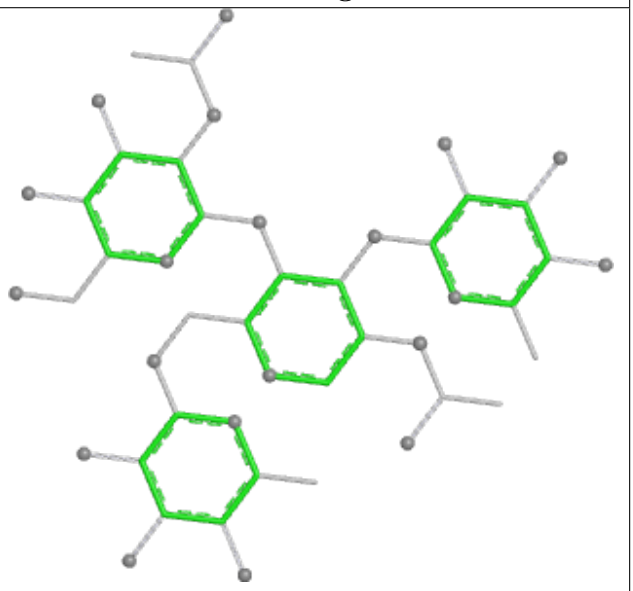
Bond lengths



Bond angles

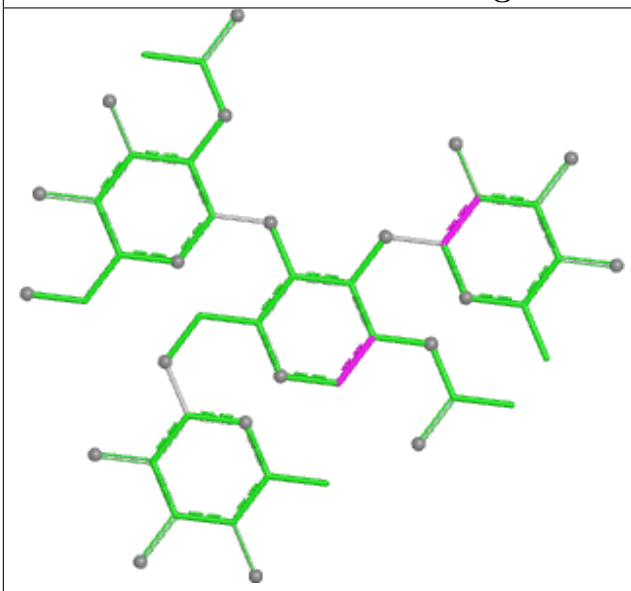


Torsions

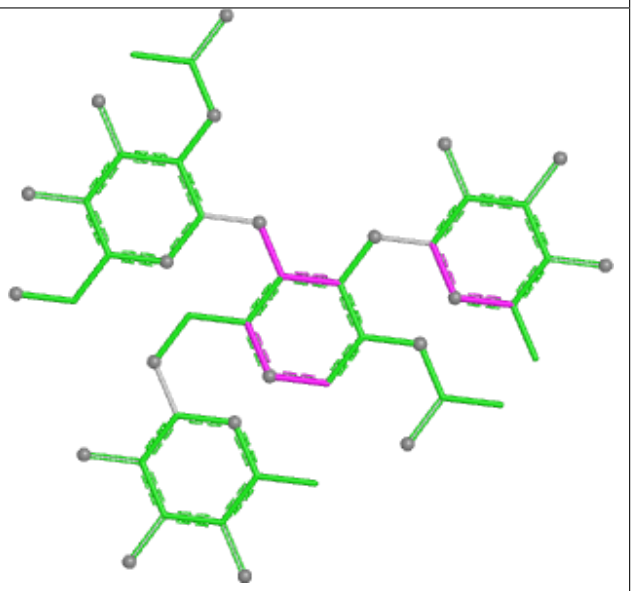


Rings

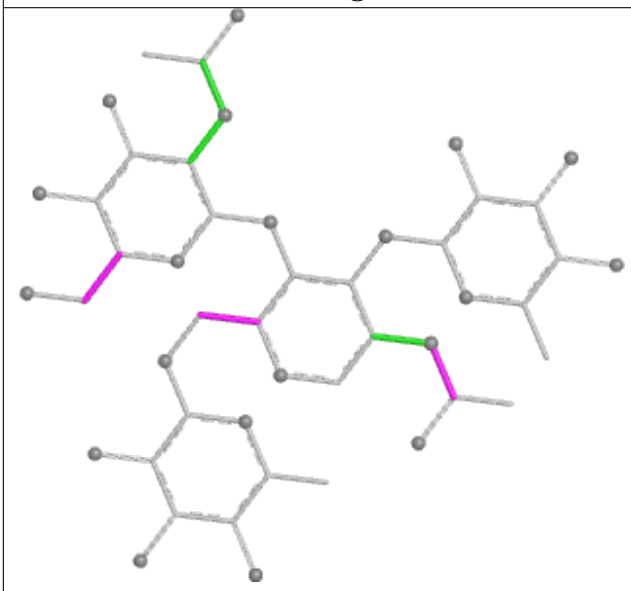
Oligosaccharide Chain K



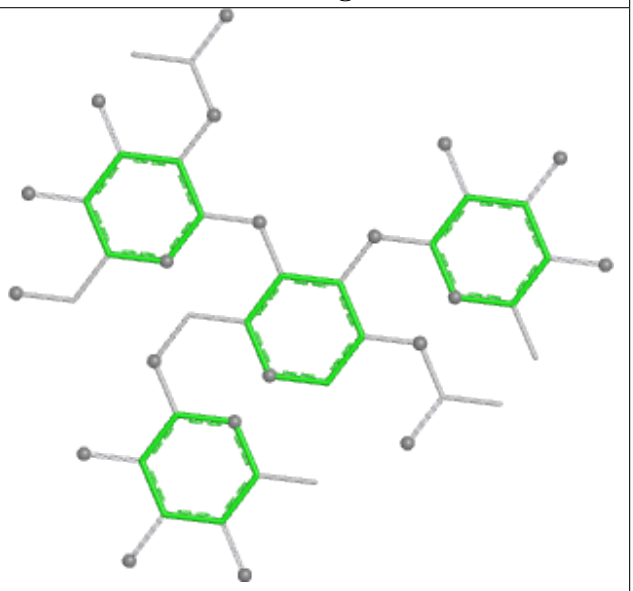
Bond lengths



Bond angles

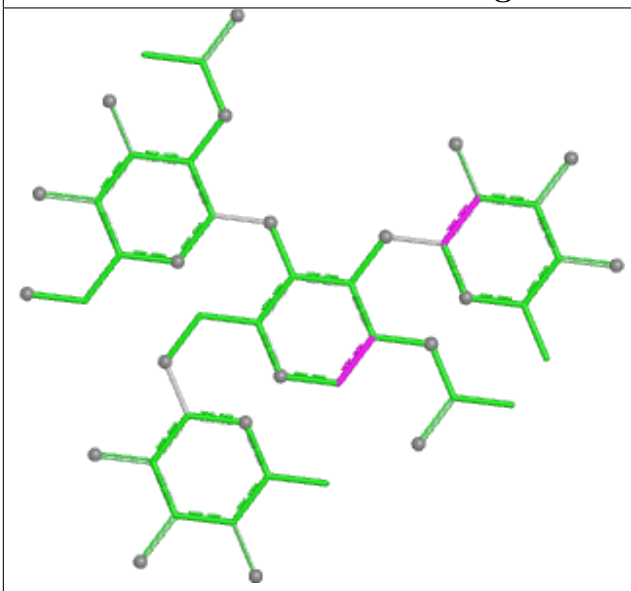


Torsions

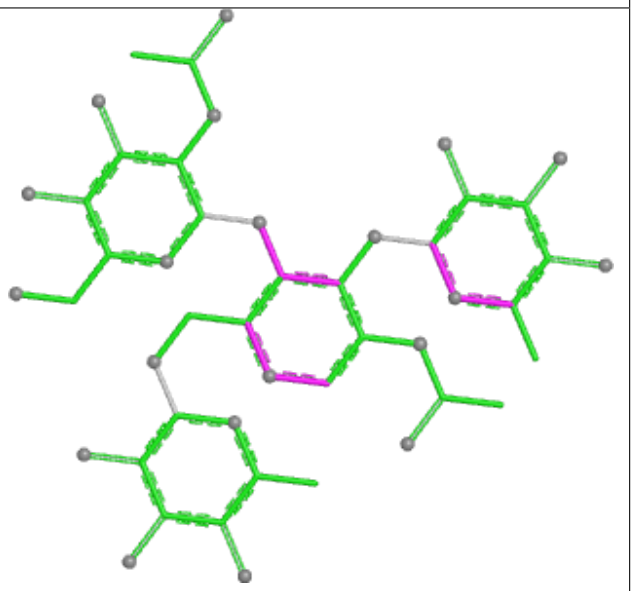


Rings

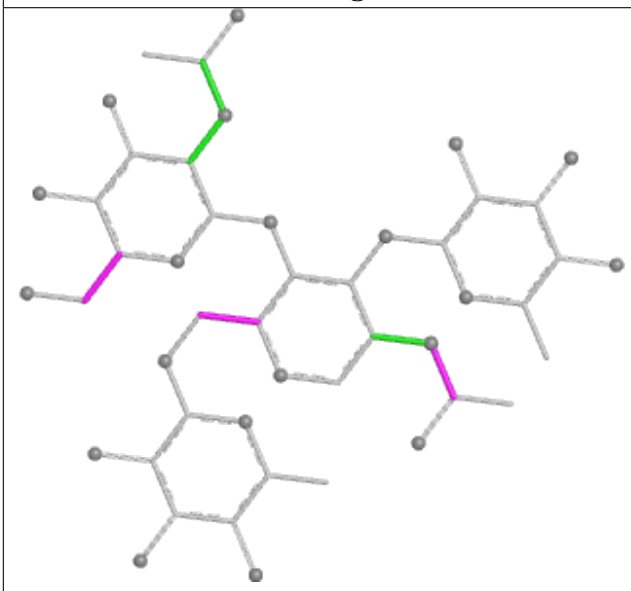
Oligosaccharide Chain O



Bond lengths



Bond angles



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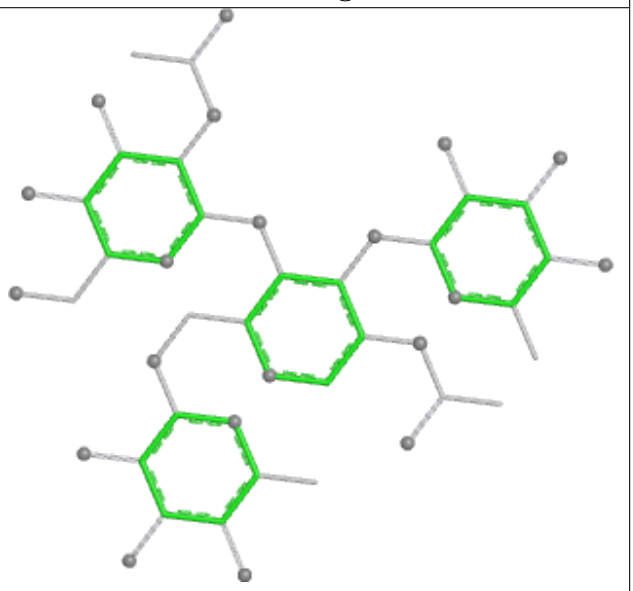

Rings

5.6 Ligand geometry (i)

45 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	A	1310	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	C	1310	1	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	C	1311	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	A	1311	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.33	0
4	NAG	B	1305	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	B	1302	1	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	A	1309	1	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.33	0
7	EIC	B	1315	-	19,19,19	0.93	0	19,19,19	1.10	1 (5%)
4	NAG	C	1303	1	14,14,15	0.27	0	17,19,21	0.46	0
5	GE9	C	1314	-	12,12,12	2.29	3 (25%)	15,17,17	1.95	3 (20%)
4	NAG	B	1306	1	14,14,15	0.68	1 (7%)	17,19,21	0.50	0
4	NAG	B	1312	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	A	1308	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	C	1308	1	14,14,15	0.38	0	17,19,21	0.62	1 (5%)
6	SIA	C	1315	-	21,21,21	3.30	12 (57%)	25,31,31	1.37	5 (20%)
4	NAG	A	1305	1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	A	1312	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.45	0
5	GE9	A	1313	-	12,12,12	2.29	3 (25%)	15,17,17	1.95	3 (20%)
4	NAG	C	1313	1	14,14,15	0.22	0	17,19,21	0.42	0
7	EIC	C	1301	-	19,19,19	0.93	0	19,19,19	1.10	1 (5%)
4	NAG	A	1306	1	14,14,15	0.68	1 (7%)	17,19,21	0.50	0
7	EIC	A	1315	-	19,19,19	0.93	0	19,19,19	1.10	1 (5%)
6	SIA	B	1314	-	21,21,21	3.31	12 (57%)	25,31,31	1.36	5 (20%)
4	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1309	1	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	B	1308	1	14,14,15	0.24	0	17,19,21	0.44	0
6	SIA	A	1314	-	21,21,21	3.30	12 (57%)	25,31,31	1.36	5 (20%)
4	NAG	B	1307	1	14,14,15	0.38	0	17,19,21	0.62	1 (5%)
4	NAG	C	1309	1	14,14,15	0.24	0	17,19,21	0.44	0
5	GE9	B	1313	-	12,12,12	2.29	3 (25%)	15,17,17	1.94	3 (20%)
4	NAG	B	1311	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	B	1310	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	C	1307	1	14,14,15	0.68	1 (7%)	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1307	1	14,14,15	0.38	0	17,19,21	0.62	1 (5%)
4	NAG	C	1312	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1305	1	14,14,15	0.21	0	17,19,21	0.33	0
4	NAG	A	1302	1	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
7	EIC	B	1315	-	-	4/17/17/17	-
4	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
5	GE9	C	1314	-	-	0/4/4/4	0/1/1/1
4	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
6	SIA	C	1315	-	-	4/20/38/38	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	GE9	A	1313	-	-	0/4/4/4	0/1/1/1
4	NAG	C	1313	1	-	1/6/23/26	0/1/1/1
7	EIC	C	1301	-	-	4/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
7	EIC	A	1315	-	-	4/17/17/17	-
6	SIA	B	1314	-	-	4/20/38/38	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
6	SIA	A	1314	-	-	4/20/38/38	0/1/1/1
4	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
5	GE9	B	1313	-	-	0/4/4/4	0/1/1/1
4	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1313	GE9	C07-N01	6.62	1.45	1.33
5	B	1313	GE9	C07-N01	6.62	1.45	1.33
5	C	1314	GE9	C07-N01	6.62	1.45	1.33
6	B	1314	SIA	O6-C6	6.03	1.53	1.44
6	A	1314	SIA	O6-C6	6.02	1.53	1.44
6	C	1315	SIA	O6-C6	6.02	1.53	1.44
6	A	1314	SIA	C7-C6	-5.65	1.45	1.53
6	B	1314	SIA	C7-C6	-5.65	1.45	1.53
6	C	1315	SIA	C7-C6	-5.65	1.45	1.53
6	B	1314	SIA	O6-C2	5.47	1.48	1.43
6	C	1315	SIA	O6-C2	5.46	1.48	1.43
6	A	1314	SIA	O6-C2	5.46	1.48	1.43
6	B	1314	SIA	C10-N5	4.98	1.51	1.34
6	C	1315	SIA	C10-N5	4.98	1.51	1.34
6	A	1314	SIA	C10-N5	4.97	1.51	1.34
6	B	1314	SIA	C3-C4	-4.71	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1314	SIA	C3-C4	-4.71	1.46	1.53
6	C	1315	SIA	C3-C4	-4.71	1.46	1.53
6	B	1314	SIA	C4-C5	-4.27	1.49	1.53
6	C	1315	SIA	C4-C5	-4.27	1.49	1.53
6	A	1314	SIA	C4-C5	-4.26	1.49	1.53
6	B	1314	SIA	O4-C4	4.00	1.51	1.43
6	A	1314	SIA	O4-C4	4.00	1.51	1.43
6	C	1315	SIA	O4-C4	4.00	1.51	1.43
6	B	1314	SIA	O10-C10	-3.28	1.15	1.23
6	C	1315	SIA	O10-C10	-3.28	1.15	1.23
6	A	1314	SIA	O10-C10	-3.28	1.15	1.23
6	B	1314	SIA	O1A-C1	3.26	1.32	1.22
6	C	1315	SIA	O1A-C1	3.26	1.32	1.22
6	A	1314	SIA	O1A-C1	3.26	1.32	1.22
5	B	1313	GE9	O01-C07	-2.92	1.18	1.24
5	A	1313	GE9	O01-C07	-2.92	1.18	1.24
5	C	1314	GE9	O01-C07	-2.92	1.18	1.24
6	B	1314	SIA	C5-N5	2.87	1.50	1.45
6	C	1315	SIA	C5-N5	2.87	1.50	1.45
6	A	1314	SIA	C5-N5	2.87	1.50	1.45
5	B	1313	GE9	C03-C07	2.78	1.53	1.50
5	C	1314	GE9	C03-C07	2.78	1.53	1.50
5	A	1313	GE9	C03-C07	2.77	1.53	1.50
6	A	1314	SIA	O2-C2	2.58	1.42	1.39
6	B	1314	SIA	O2-C2	2.58	1.42	1.39
6	C	1315	SIA	O2-C2	2.58	1.42	1.39
4	A	1306	NAG	O5-C1	-2.17	1.40	1.43
4	B	1306	NAG	O5-C1	-2.17	1.40	1.43
4	C	1307	NAG	O5-C1	-2.17	1.40	1.43
6	B	1314	SIA	C3-C2	-2.12	1.49	1.51
6	C	1315	SIA	C3-C2	-2.12	1.49	1.51
6	A	1314	SIA	C3-C2	-2.11	1.49	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1314	GE9	C02-C01-I03	-4.54	116.89	121.01
5	B	1313	GE9	C02-C01-I03	-4.54	116.89	121.01
5	A	1313	GE9	C02-C01-I03	-4.53	116.89	121.01
5	A	1313	GE9	C01-C02-I01	-3.50	119.62	122.96
5	B	1313	GE9	C01-C02-I01	-3.50	119.62	122.96
5	C	1314	GE9	C01-C02-I01	-3.49	119.63	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1301	EIC	C11-C10-C9	3.43	152.54	123.57
7	B	1315	EIC	C11-C10-C9	3.43	152.54	123.57
7	A	1315	EIC	C11-C10-C9	3.43	152.53	123.57
6	C	1315	SIA	O6-C6-C5	-2.94	106.91	109.78
6	B	1314	SIA	O6-C6-C5	-2.94	106.91	109.78
6	A	1314	SIA	O6-C6-C5	-2.94	106.91	109.78
5	A	1313	GE9	O01-C07-N01	-2.79	118.62	122.58
5	B	1313	GE9	O01-C07-N01	-2.79	118.62	122.58
5	C	1314	GE9	O01-C07-N01	-2.79	118.62	122.58
6	A	1314	SIA	O1A-C1-C2	-2.19	120.27	123.59
6	B	1314	SIA	O1A-C1-C2	-2.19	120.27	123.59
6	C	1315	SIA	O1A-C1-C2	-2.19	120.28	123.59
6	A	1314	SIA	C11-C10-N5	2.19	119.80	116.10
6	C	1315	SIA	C11-C10-N5	2.19	119.80	116.10
6	B	1314	SIA	C11-C10-N5	2.18	119.79	116.10
6	B	1314	SIA	C3-C2-C1	-2.16	108.98	113.00
6	C	1315	SIA	C3-C2-C1	-2.16	108.98	113.00
6	A	1314	SIA	C3-C2-C1	-2.16	108.98	113.00
4	B	1307	NAG	C1-O5-C5	2.13	115.08	112.19
4	C	1308	NAG	C1-O5-C5	2.13	115.08	112.19
4	A	1307	NAG	C1-O5-C5	2.13	115.08	112.19
6	B	1314	SIA	C8-C7-C6	-2.03	109.19	113.03
6	C	1315	SIA	C8-C7-C6	-2.03	109.19	113.03
6	A	1314	SIA	C8-C7-C6	-2.03	109.19	113.03

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1314	SIA	O6-C6-C7-O7
6	B	1314	SIA	O6-C6-C7-O7
6	C	1315	SIA	O6-C6-C7-O7
4	A	1307	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	A	1306	NAG	C1-C2-N2-C7
4	B	1306	NAG	C1-C2-N2-C7
4	C	1307	NAG	C1-C2-N2-C7
4	A	1302	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1306	NAG	C4-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	C	1311	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	A	1310	NAG	C4-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	C	1311	NAG	C4-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	C	1303	NAG	C8-C7-N2-C2
4	C	1303	NAG	O7-C7-N2-C2
4	A	1301	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1304	NAG	C4-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6
4	C	1313	NAG	O5-C5-C6-O6
4	A	1307	NAG	C1-C2-N2-C7
4	B	1307	NAG	C1-C2-N2-C7
4	C	1308	NAG	C1-C2-N2-C7
6	A	1314	SIA	O1A-C1-C2-O6
6	B	1314	SIA	O1A-C1-C2-O6
6	C	1315	SIA	O1A-C1-C2-O6
6	A	1314	SIA	O8-C8-C9-O9
6	B	1314	SIA	O8-C8-C9-O9
6	C	1315	SIA	O8-C8-C9-O9
4	A	1306	NAG	C3-C2-N2-C7
4	B	1306	NAG	C3-C2-N2-C7
4	C	1307	NAG	C3-C2-N2-C7
7	A	1315	EIC	O1-C1-C2-C3
7	B	1315	EIC	O1-C1-C2-C3
7	C	1301	EIC	O1-C1-C2-C3
7	A	1315	EIC	O2-C1-C2-C3
7	B	1315	EIC	O2-C1-C2-C3
7	C	1301	EIC	O2-C1-C2-C3
7	A	1315	EIC	C7-C8-C9-C10
7	B	1315	EIC	C7-C8-C9-C10
7	C	1301	EIC	C7-C8-C9-C10
4	A	1307	NAG	C3-C2-N2-C7
4	B	1307	NAG	C3-C2-N2-C7
4	C	1308	NAG	C3-C2-N2-C7
6	A	1314	SIA	C7-C8-C9-O9
6	B	1314	SIA	C7-C8-C9-O9
6	C	1315	SIA	C7-C8-C9-O9
7	A	1315	EIC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
7	B	1315	EIC	C12-C13-C14-C15
7	C	1301	EIC	C12-C13-C14-C15

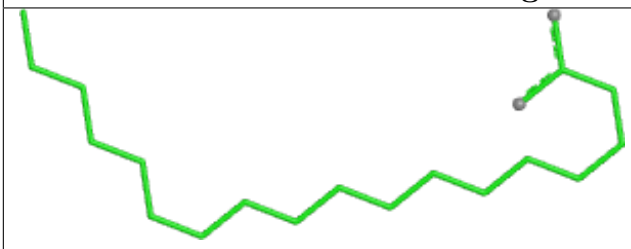
There are no ring outliers.

18 monomers are involved in 19 short contacts:

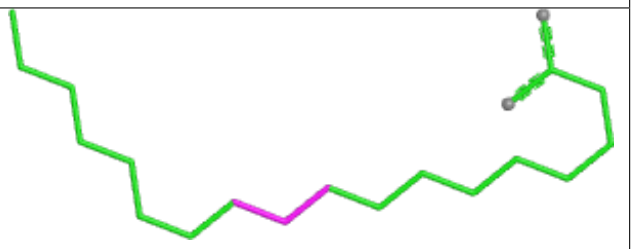
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1310	NAG	1	0
4	C	1311	NAG	1	0
5	C	1314	GE9	1	0
4	B	1306	NAG	1	0
4	A	1308	NAG	1	0
4	C	1308	NAG	1	0
6	C	1315	SIA	1	0
5	A	1313	GE9	1	0
4	A	1306	NAG	2	0
6	B	1314	SIA	1	0
4	B	1308	NAG	1	0
6	A	1314	SIA	1	0
4	B	1307	NAG	1	0
4	C	1309	NAG	1	0
5	B	1313	GE9	1	0
4	B	1310	NAG	1	0
4	C	1307	NAG	1	0
4	A	1307	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.

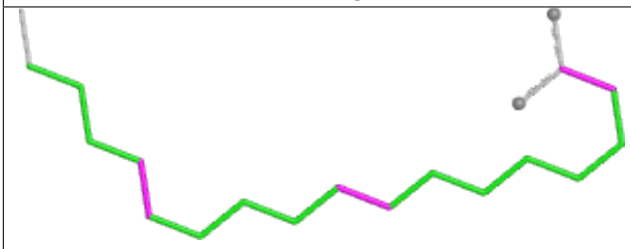
Ligand EIC B 1315



Bond lengths



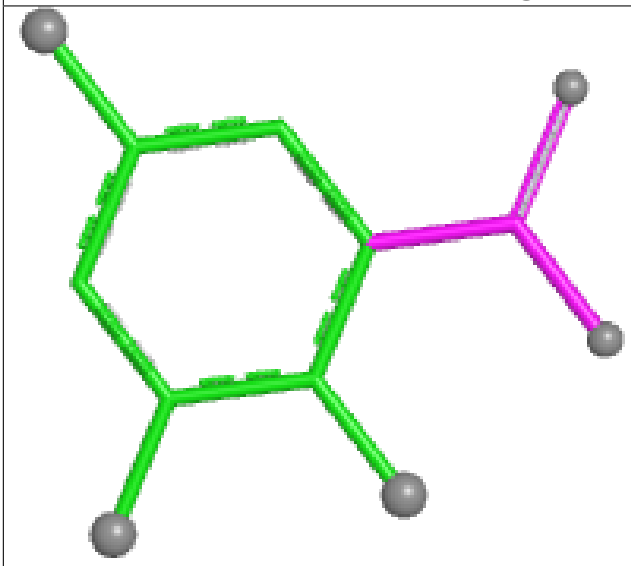
Bond angles



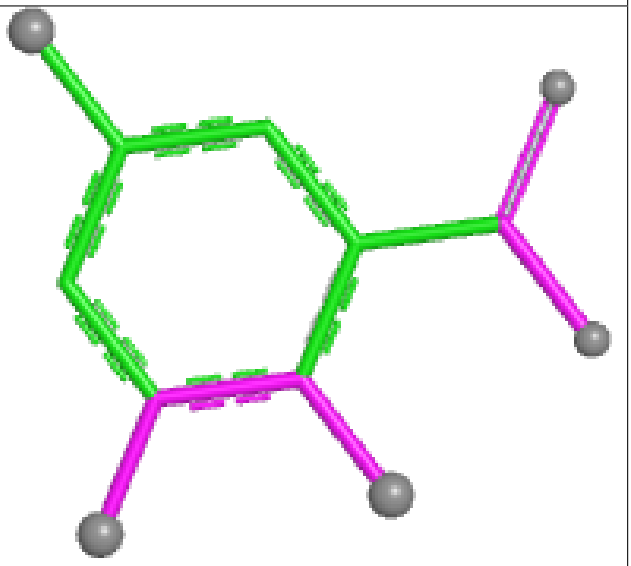
Torsions

Rings

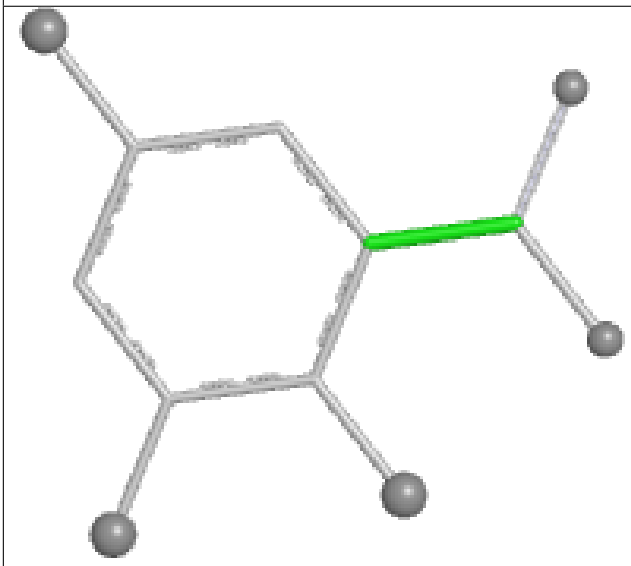
Ligand GE9 C 1314



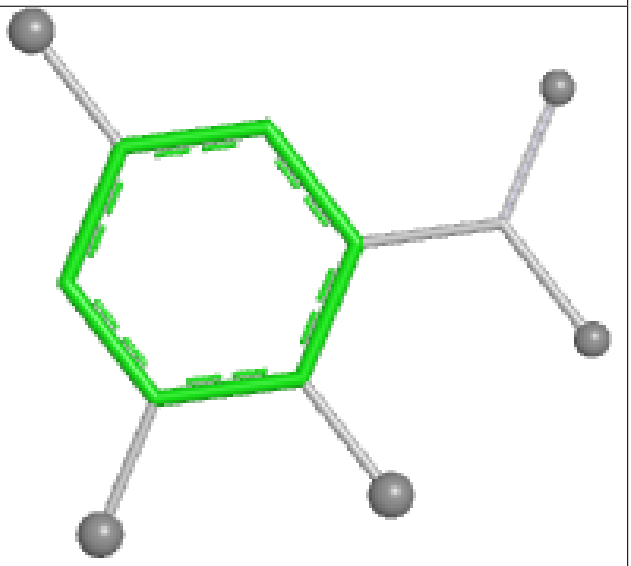
Bond lengths



Bond angles

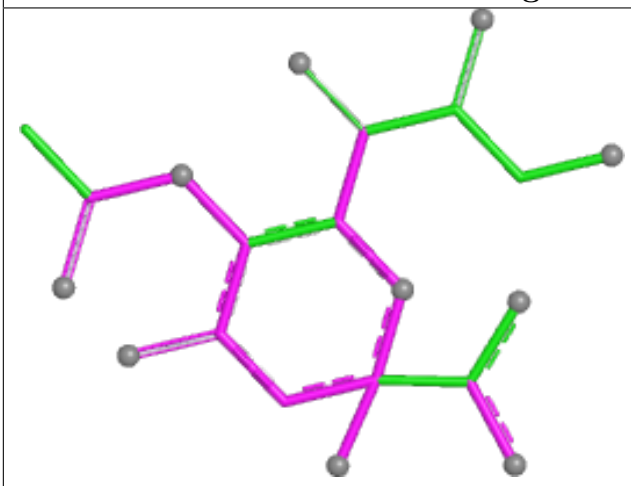


Torsions

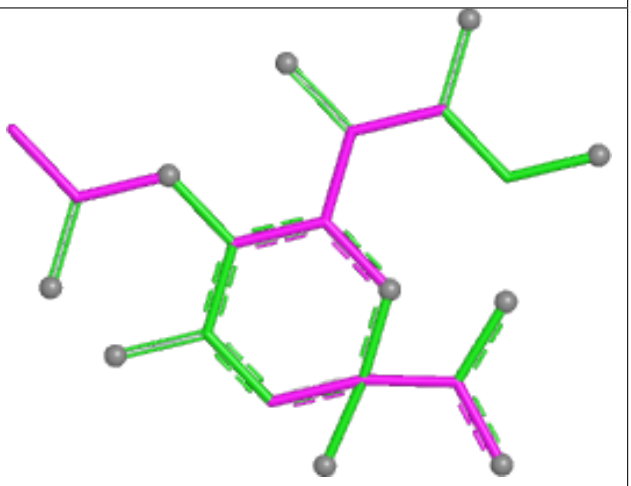


Rings

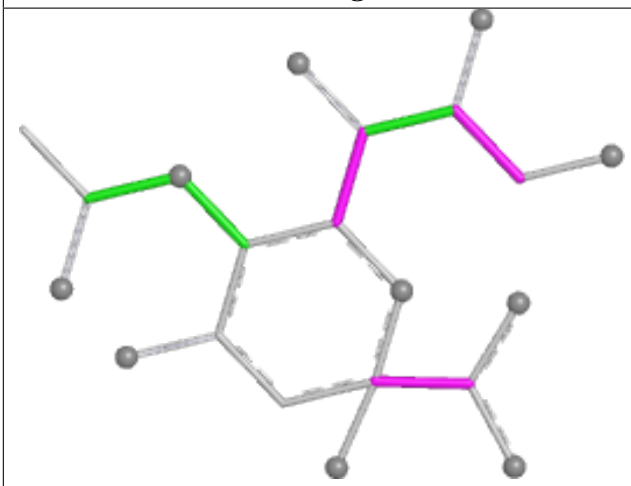
Ligand SIA C 1315



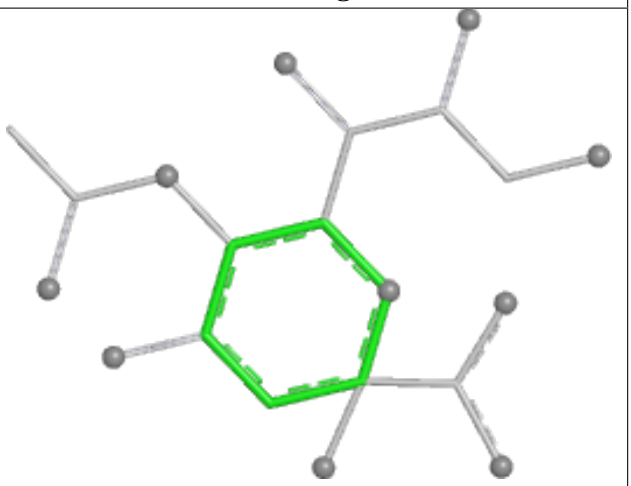
Bond lengths



Bond angles

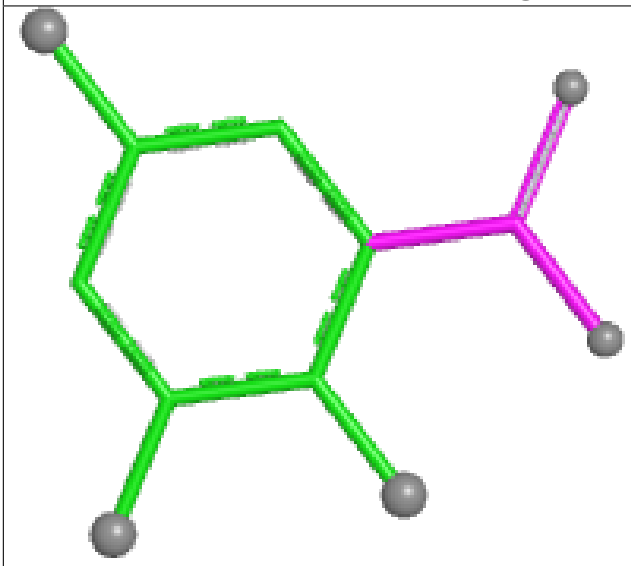


Torsions

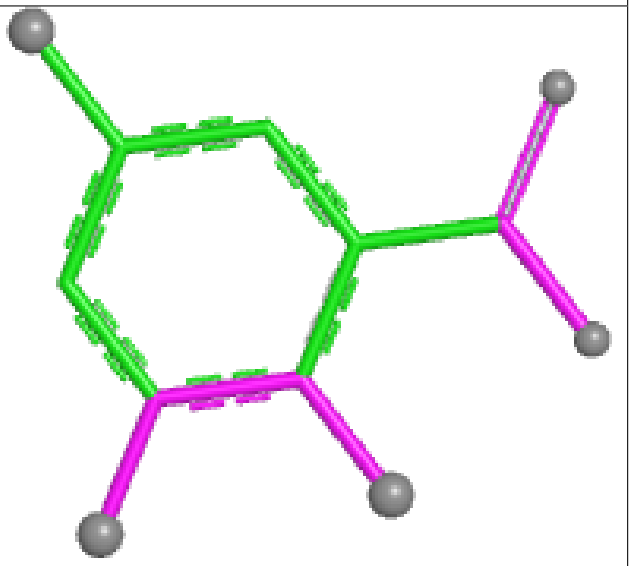


Rings

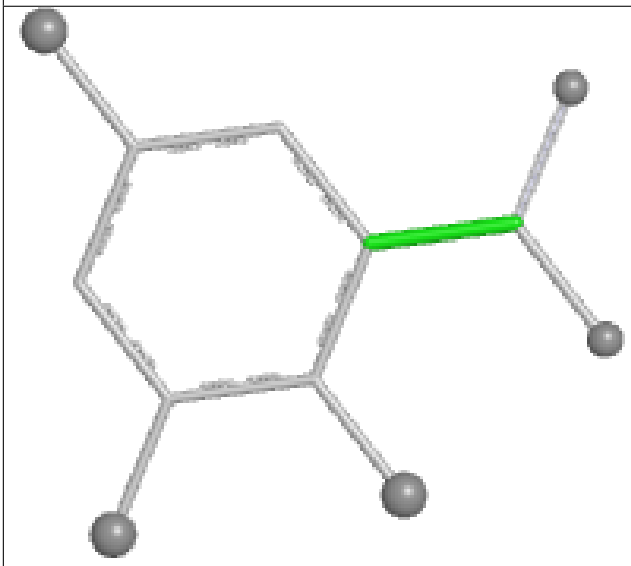
Ligand GE9 A 1313



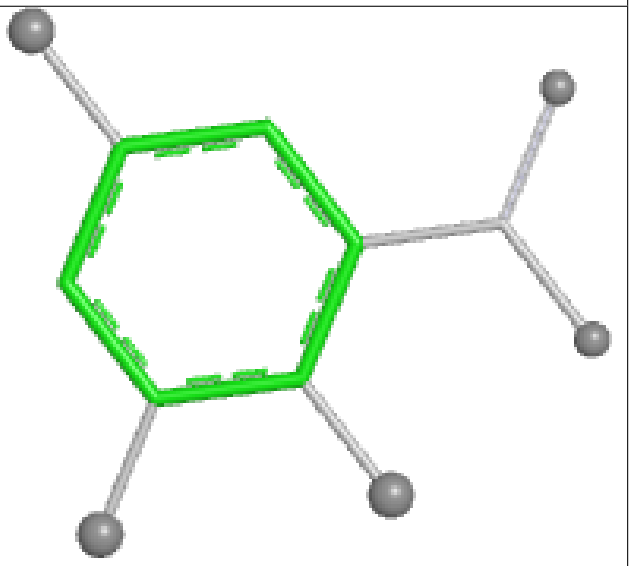
Bond lengths



Bond angles

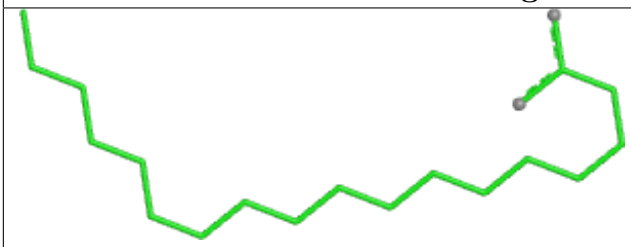


Torsions

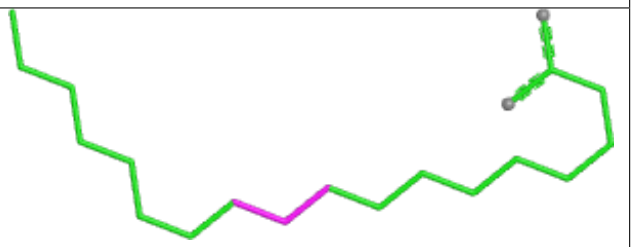


Rings

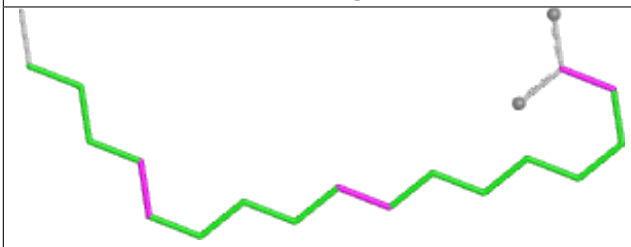
Ligand EIC C 1301



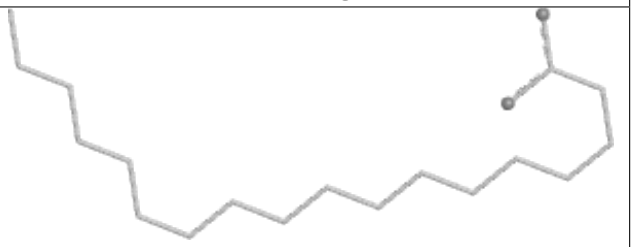
Bond lengths



Bond angles

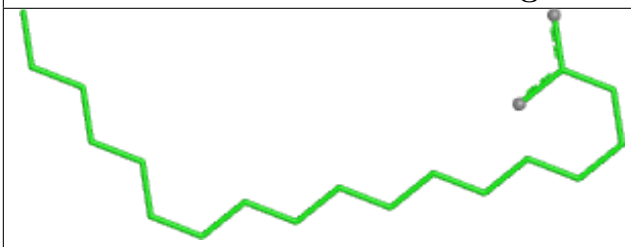


Torsions

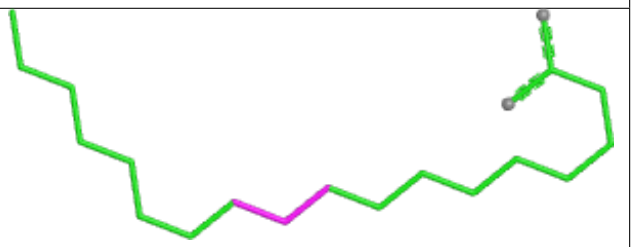


Rings

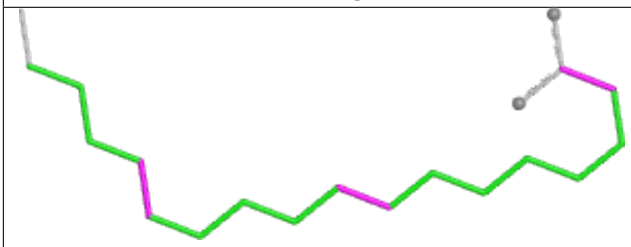
Ligand EIC A 1315



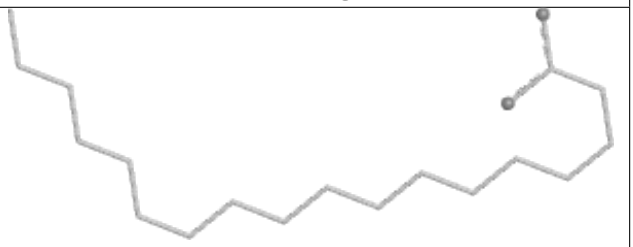
Bond lengths



Bond angles

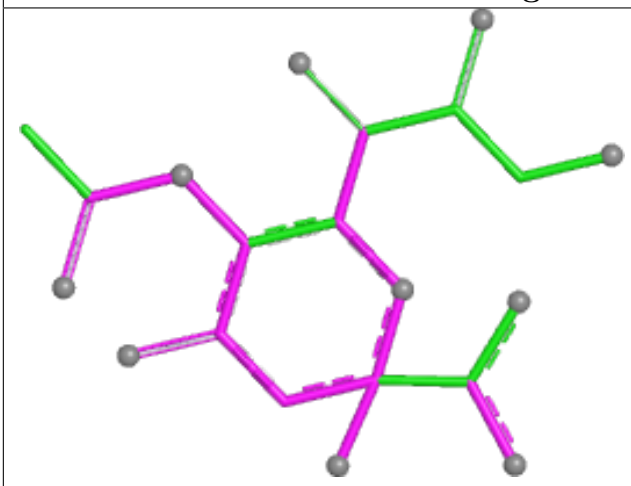


Torsions

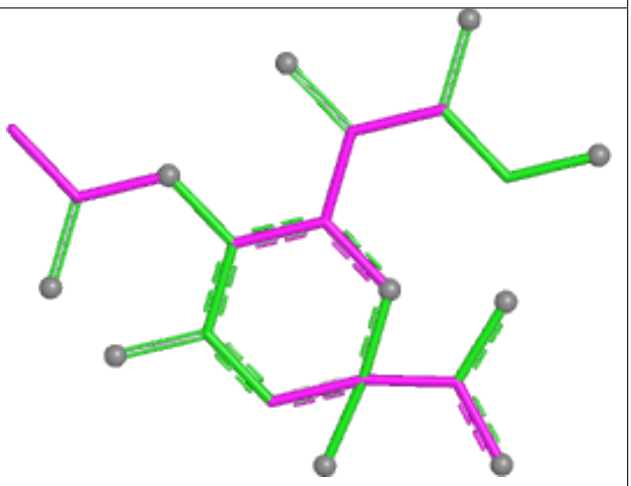


Rings

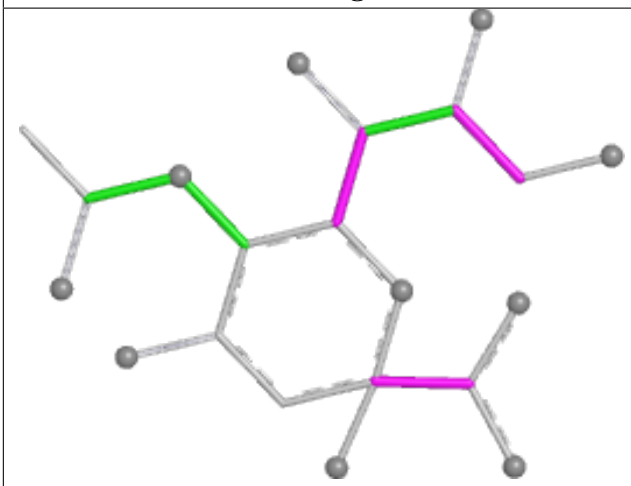
Ligand SIA B 1314



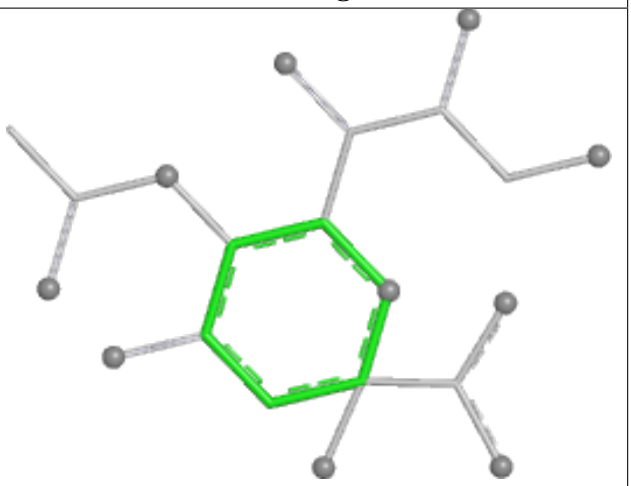
Bond lengths



Bond angles

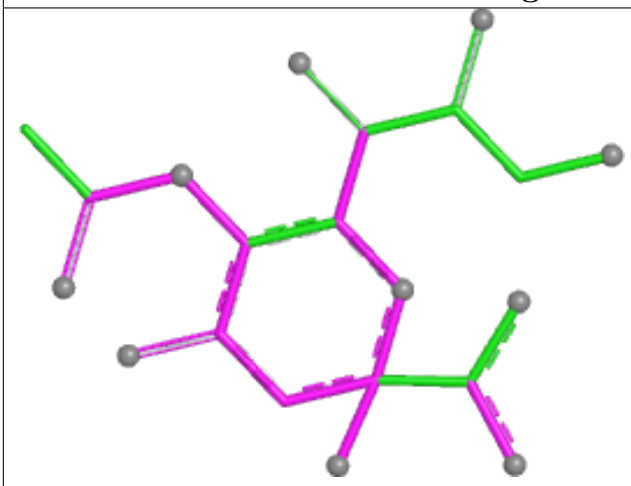


Torsions

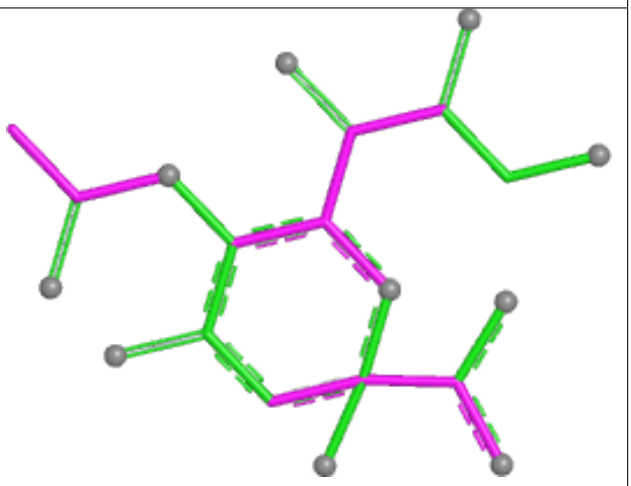


Rings

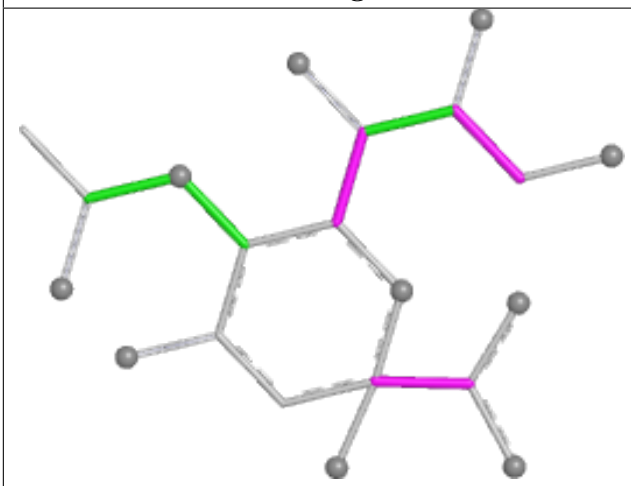
Ligand SIA A 1314



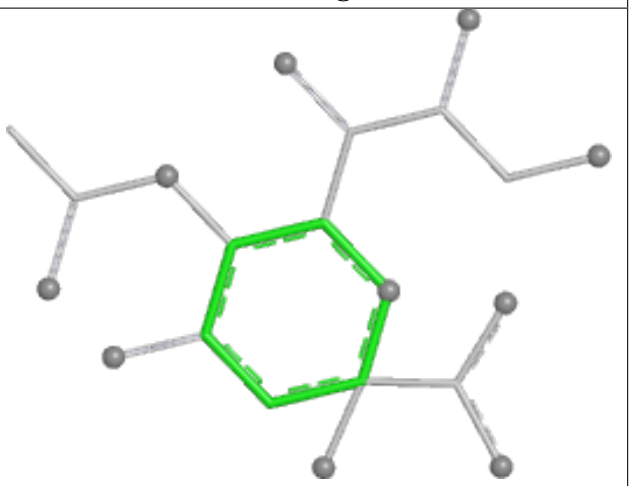
Bond lengths



Bond angles

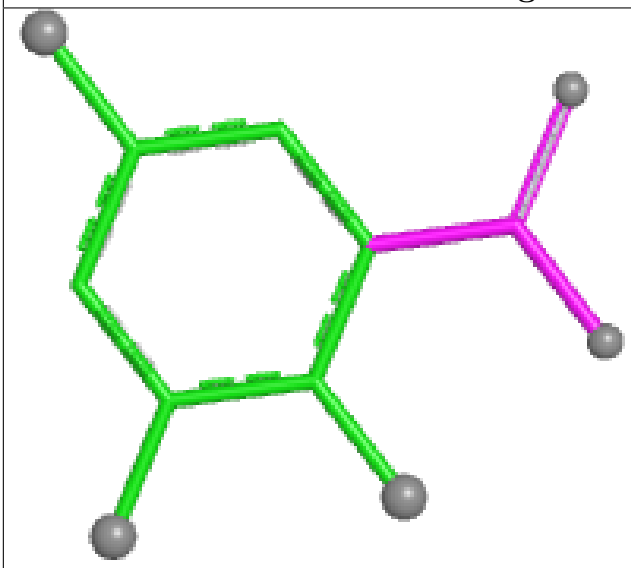


Torsions

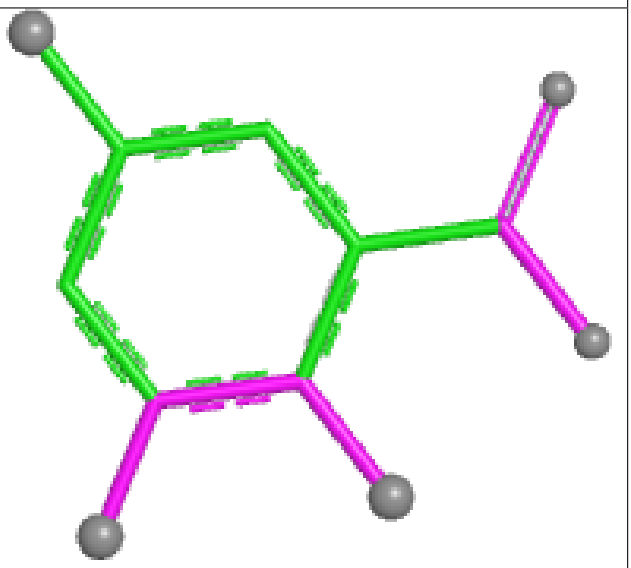


Rings

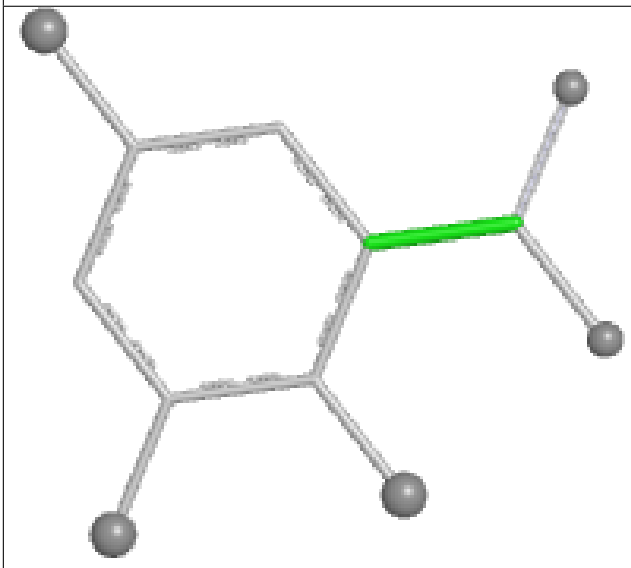
Ligand GE9 B 1313



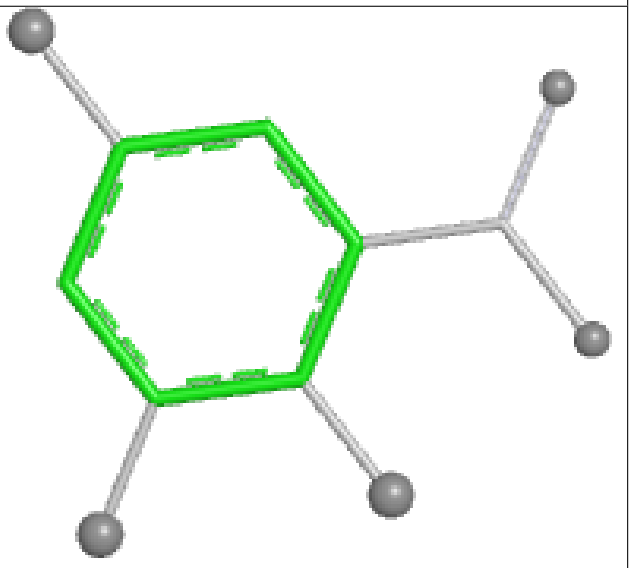
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

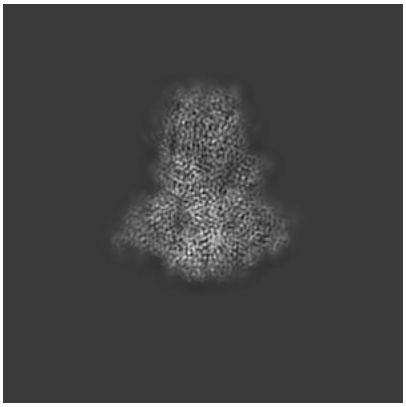
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14152. These allow visual inspection of the internal detail of the map and identification of artifacts.

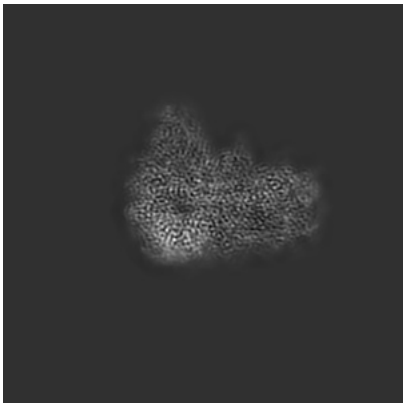
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

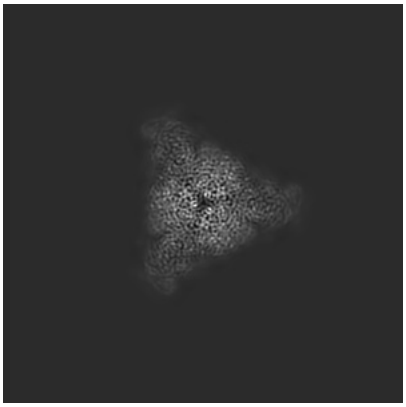
6.1.1 Primary map



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: 188

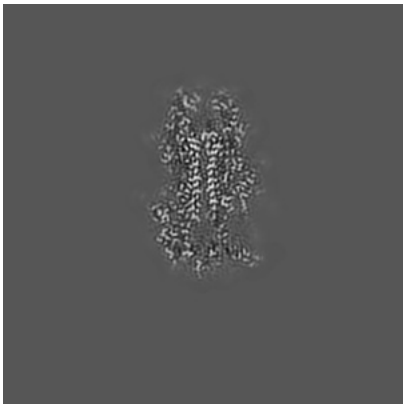
Y Index: 188

Z Index: 188

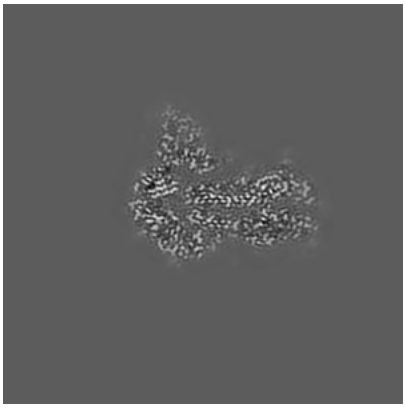
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 194



Y Index: 196

Z Index: 153

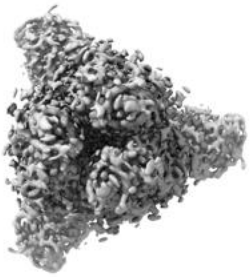
The images above show the largest variance slices of the map in three orthogonal directions.

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

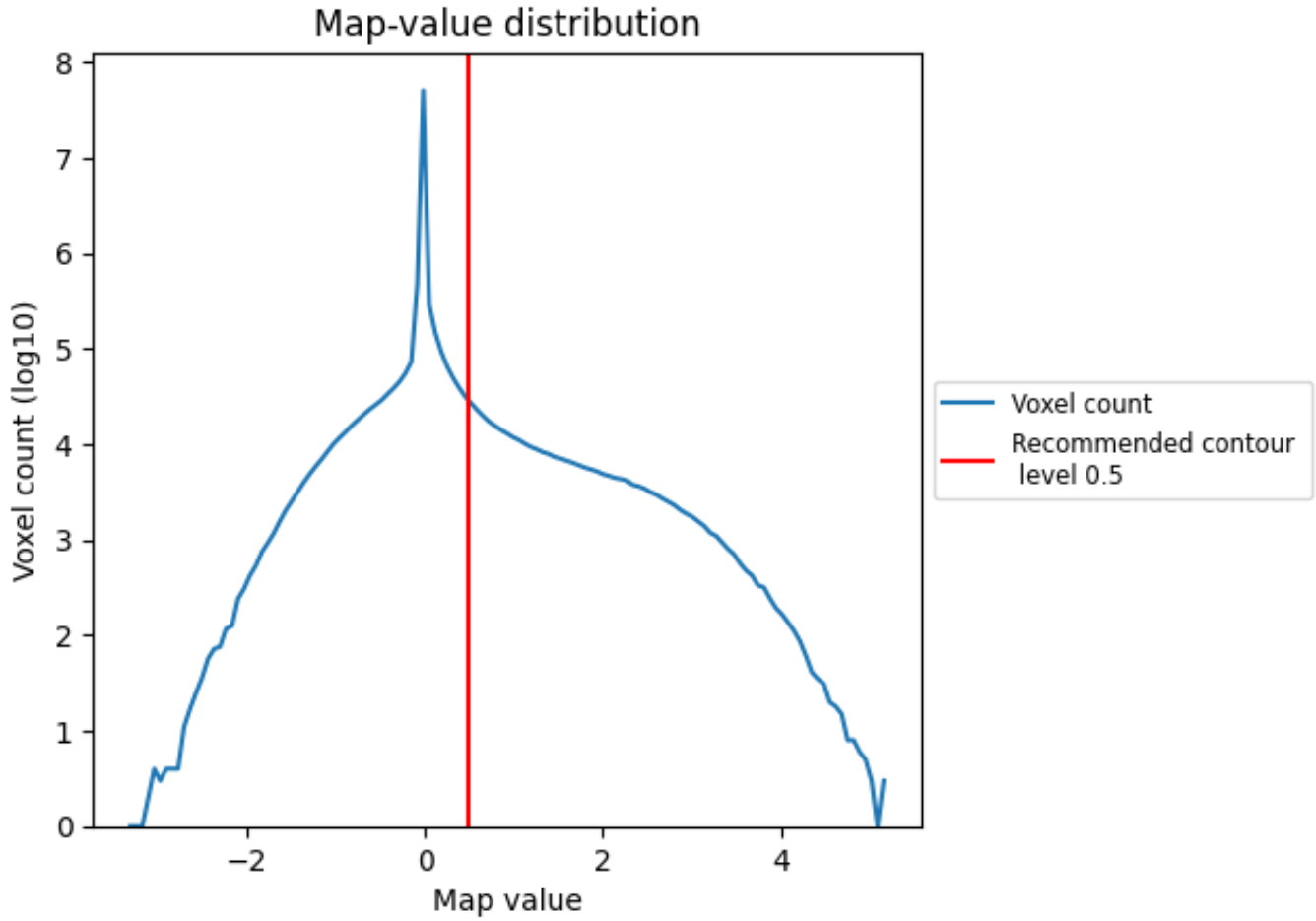
6.5 Mask visualisation (i)

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

7 Map analysis

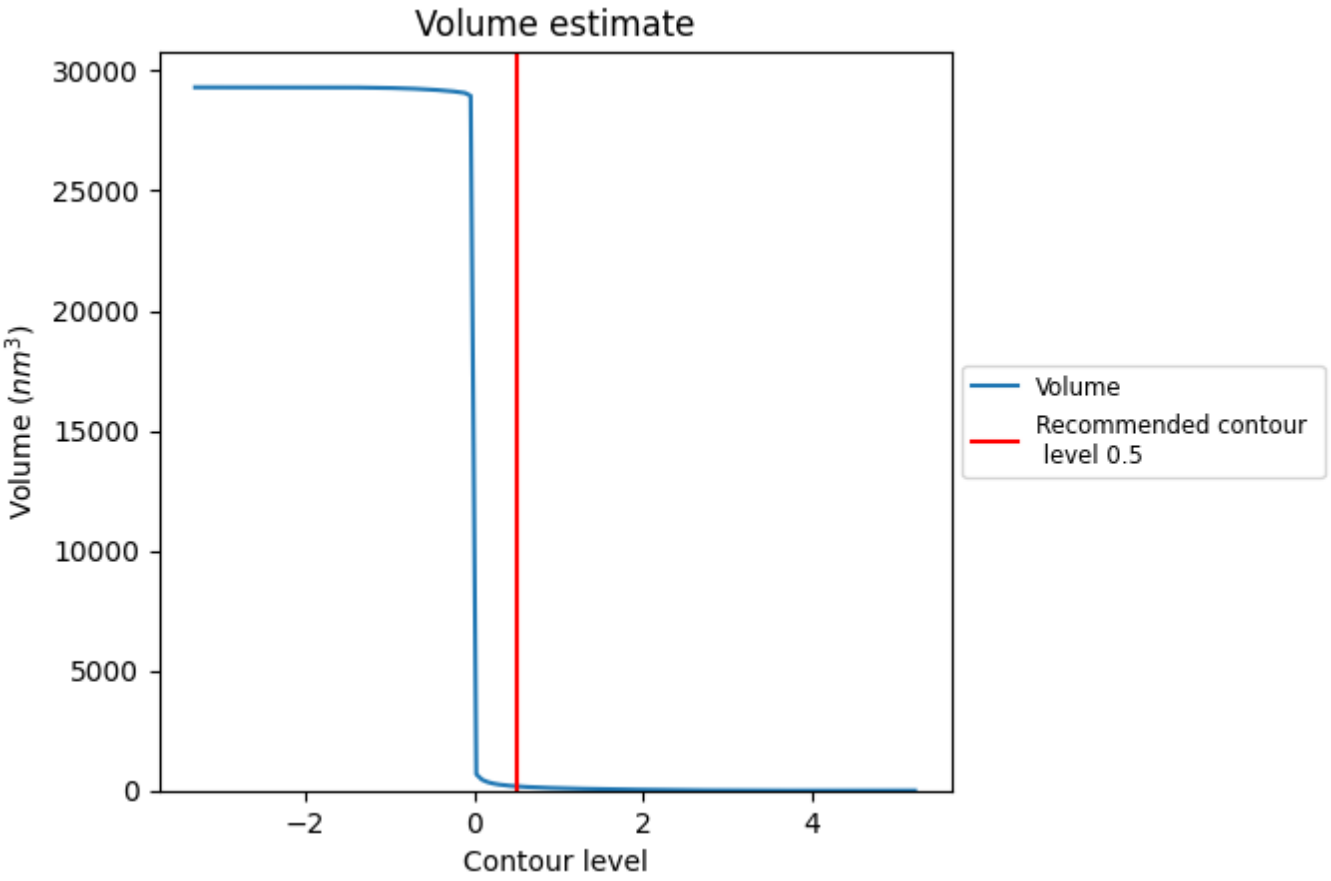
This section contains the results of statistical analysis of the map.

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.

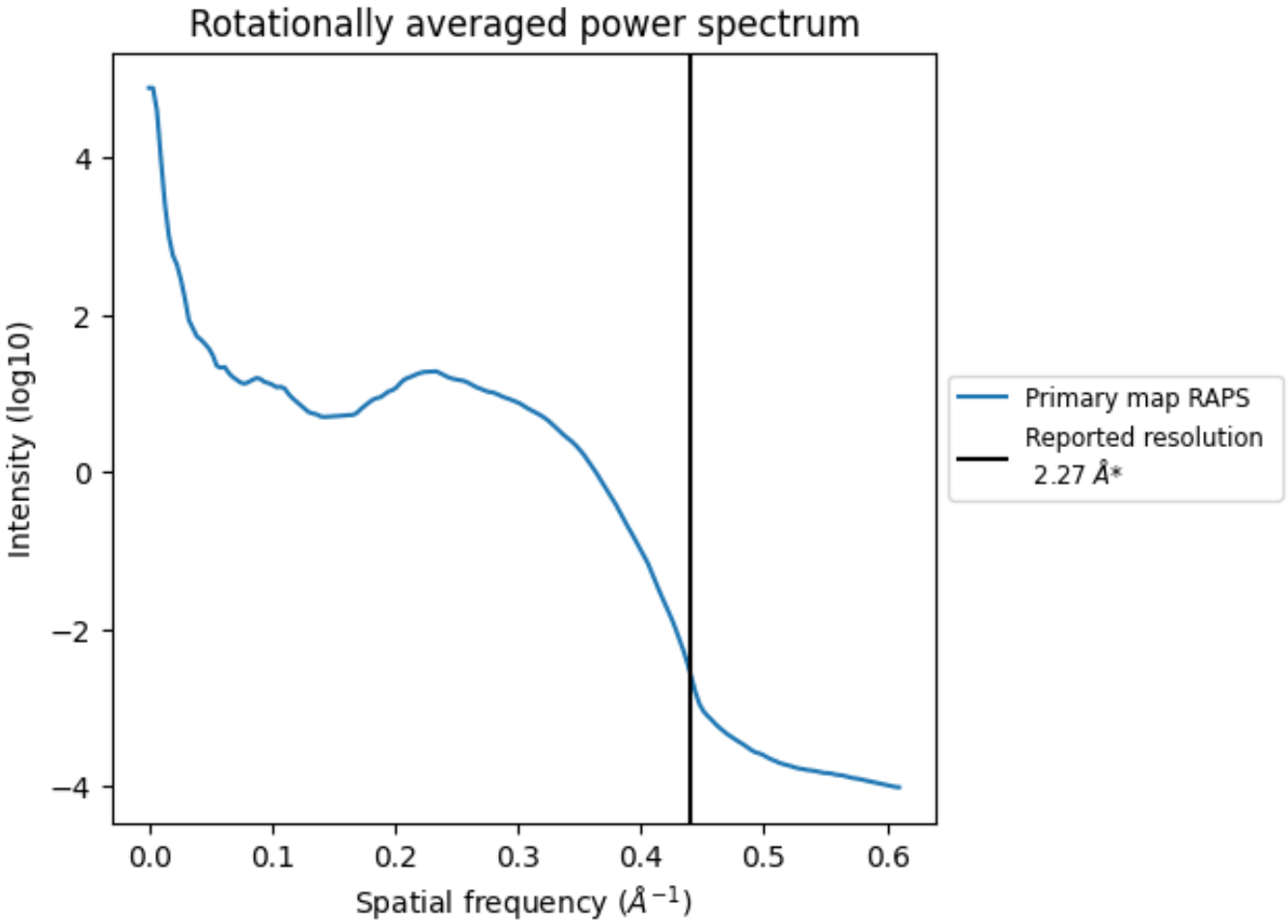
7.2 Volume estimate



The volume at the recommended contour level is 177 nm^3; this corresponds to an approximate mass of 160 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 0.441 Å^{-1}

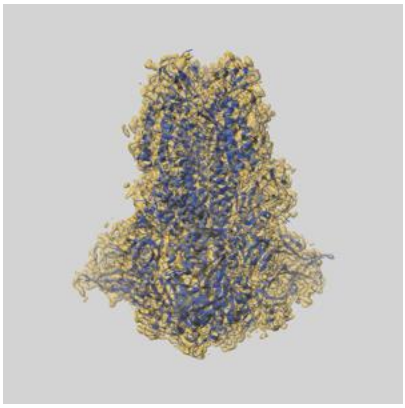
8 Fourier-Shell correlation

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

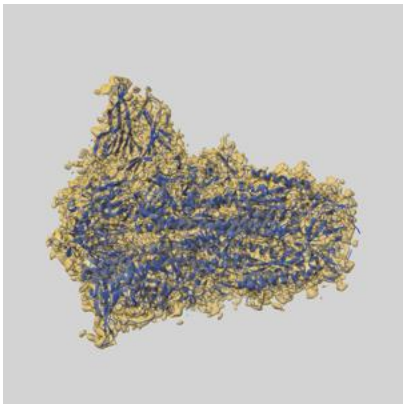
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14152 and PDB model 7QUR. Per-residue inclusion information can be found in section 3 on page 12.

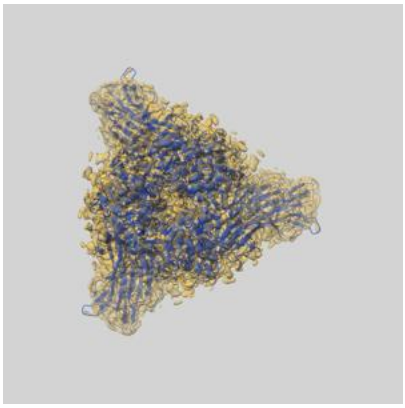
9.1 Map-model overlay



X



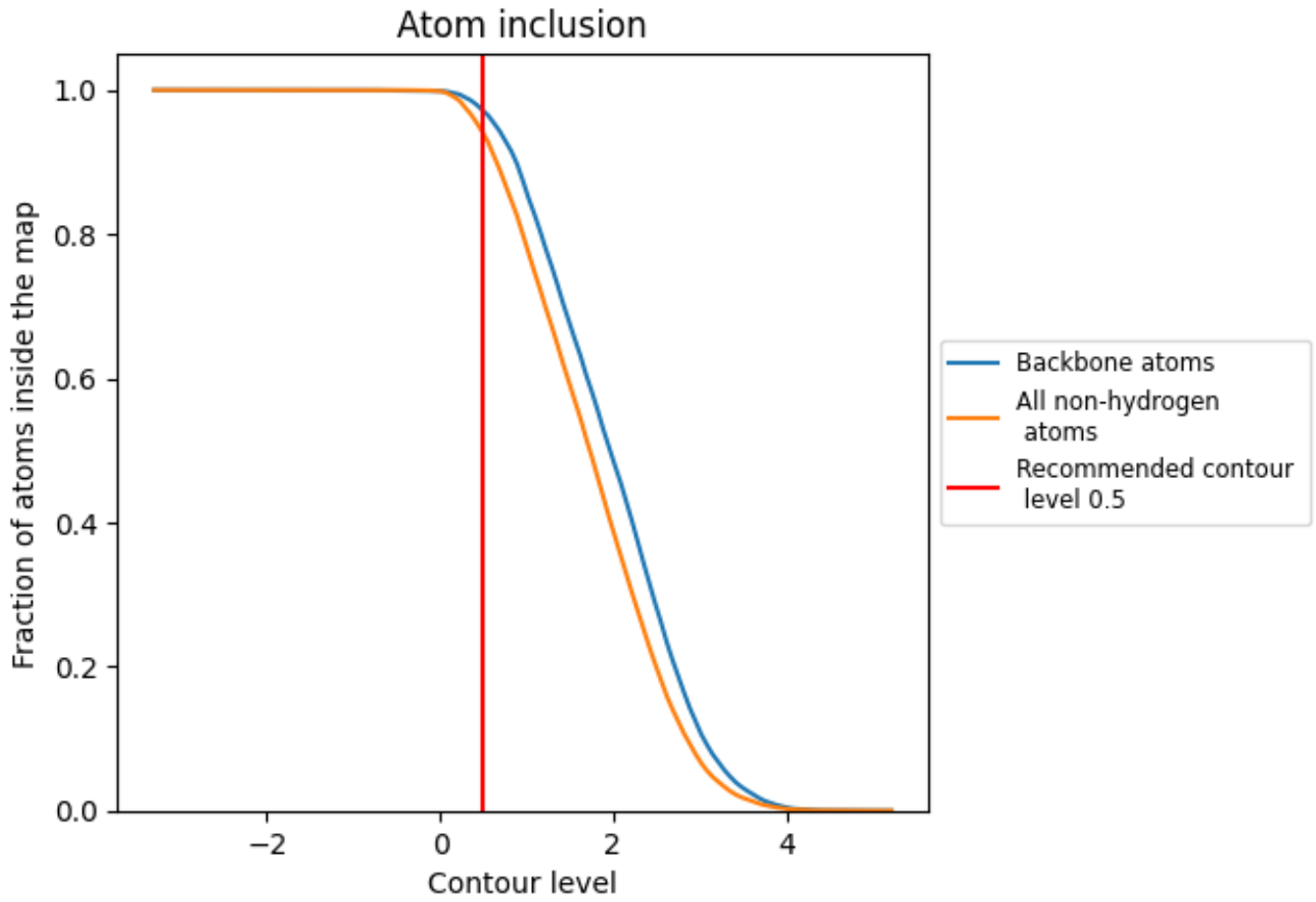
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.